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Title: Using Computational Studies to Characterize Aqueous Metal Clusters: From Spectroscopy to Stability

Abstract approved: _____

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In this dissertation, the spectroscopic properties and thermodynamic stability of a class of materials known as metal oxo and hydroxo clusters are studied. In aqueous solutions, many metals can aggregate into discrete clusters of metals bridged by oxo or hydroxo ligands. These clusters are of particular interest to us for their use as precursors for metal oxide thin films. Understanding the stability of these clusters, along with distinguishing ways to uniquely identify particular clusters via spectroscopy, is vital to improving the quality of cluster precursors and the metal oxide thin film products.

Vibrational spectroscopy is an appealing technique for the identification of cluster species because of the relative ease to collect experimental IR and Raman spectra. However, uniquely identifying cluster vibrations is difficult due to the similarity of ligands types and vibrational modes between different clusters. Disclosed herein are two studies of vibrational spectroscopy applied to metal hydroxo clusters of Group 13 metals. These studies focus on one cluster structure in particular, the flat tridecamer, $M_{13}(OH)_{24}(H_2O)_{24}^{15+}$, where M= Al^{3+} or Ga^{3+}. The vibrations of the NO_3^- counterions used in these studies overlap with the frequencies associated with cluster vibration, which limits the uniqueness of the Raman and IR signals. Nonetheless, full assignment of peaks was made for solid state and solution phase flat tridecamers.

NMR spectroscopy is an appealing technique for the identification and characterization of cluster species because of the amount of structural information that

can be gleaned from NMR spectra. In one study, we used ^{1}H-NMR to characterize flat tridecamers with a mixture of gallium and indium. Computations struggle to predict NMR spectra because these spectra reflect average structures over time, and static computations rely on single structures and are especially sensitive to small deviations in atom positions. In this study, we computed the ^{1}H-NMR signals for the flat tridecamers $Ga_{13-x}In_x(OH)_{24}(H_2O)_{24}^{15+}$, and fully assigned the experimental proton signals to each proton coordination environment that is possible for these clusters.

Quantum mechanical computations can also be used to understand the stability of different cluster species relative to each other. In this dissertation, the stability of Al, Ga, and Hf clusters is explored. Hf tetramer clusters, $Hf_4(OH)_8(H_2O)_{16}^{8+}$, were examined with peroxide substitution for a pair of hydroxide or water ligands. These calculations suggest that peroxide prefers to substitute for the terminal water ligands versus the bridging hydroxide ligands. This study also highlights the importance of accurate solvation models for computing the structures and stabilities of clusters in aqueous solutions.

For the Group 13 metals aluminum and gallium, the stability of different clusters can be computed based on the identity and binding modes of the different ligands. Using ligand identities to compute hydrolysis energies can reproduce quantum mechanical computations of cluster stability with extremely high accuracy. However, these calculations do not include the cluster counterions, which can affect the stability of high-charge clusters. For a full determination of cluster speciation in solution, counterions are required for accurate speciation across all possible species. The speciation and structural conformations of Al clusters was studied with Cl^-, NO_3^-, HSO_4^-, and ClO_4^- counterions.

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Using Computational Studies to Characterize Aqueous Metal Clusters: From Spectroscopy to Stability

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I understand that my dissertation will become part of the permanent collection of Oregon State University libraries. My signature below authorizes release of my dissertation to any reader upon request.

Lindsay A. Wills, Author

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CONTRIBUTION OF AUTHORS

Chapter 2. Milton Jackson, Matthew Carnes, and Lawrence Scatena conducted the synthesis and collected the experimental spectra for this project. I-Ya Chang assisted in the IR computations and preparation of the manuscript. Darren Johnson, Paul Cheong, Milton Jacob, and Matthew Carnes also assisted in the preparation of this manuscript.

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Chapter 7. Cory Perkins contributed the experimental results used for verification of the computations. Paul Cheong assisted with the computations and preparation of the manuscript.

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Dedicated to my
loving parents,
dear friends and
devoted teachers
in my life.

Chapter 1. Introduction

The behavior of metal cations in water has been studied extensively for decades.[1] In water, metal cations can aggregate to form large oligomers know as clusters or precipitate from solution to form different minerals.[2] In aqueous systems, clusters of metal ions are usually connected by oxo or hydroxo ligands and capped by oxo or aquo ligands, depending on the identity of the metal. Originally of interest to geochemists, metal cation behavior was studied in water to better understand the species present in natural water systems. More recently, aqueous metal clusters have gathered interests from materials chemists for the application of clusters as precursors for high quality metal oxide thin films.[3-6] In biology and medicine, metal clusters have been suggested to have a role in neurodegenerative disorders such as Alzheimer's and Parkinson's. [7-11] The numerous applications of cluster chemistry make understanding the formation and stability of clusters in solution of potential widespread interest.

1.1 Hydrolysis of Metal Ions

The formation of metal clusters in solution occurs through a process called hydrolysis. The clusters formed through hydrolysis fall generally into one of two categories: polyoxometalates or metal hydroxo clusters. Polyoxometalates are metal clusters ligated and capped with oxo ligands, have a negative overall charge, and hence positively charged counterions. Polyoxometalates are typically formed from high charge transition metals such as vanadium and molybdenum. Metal hydroxo clusters, on the other hand, are ligated by hydroxo ligands and capped with water ligands. These clusters generally have a positive overall charge and negatively charged counterions. Metal hydroxo clusters typically form from lower charge metals, such as the Group 13 metals aluminum and gallium. Metal hydroxo clusters of aluminum, gallium, and (to a lesser degree) hafnium will be the focus of the studies herein.

At low pH in aqueous solutions, most metals coordinate with the water solvent to form an octahedrally-coordinated monomer, $M(H_2O)_6^{x+}$, where the charge is determined by the charge of the metal. Several units of the metal monomer linking together to form a larger cluster species with multiple metal ions linked together define hydrolysis reactions. These reactions also form a significant amount of water and hydronium as side-products. For +3 charge metal, like Al or Ga, a general hydrolysis reaction can be written as,

$$x\,M(H_2O)_6^{3+} \rightleftharpoons M_xO_w(OH)_y(H_2O)_z^{(3x-2w-y)+} + (6x-3w-2y-z)H_2O + (2w+y)H_3O^+$$

To determine the dominant cluster species in solution under specific pH conditions and concentration of M^+ ions, the equilibria of all possible clusters must be considered. Typically, the dominant cluster can be determined by plotting a speciation diagram based on the equilibrium constants for the hydrolysis of different cluster species.

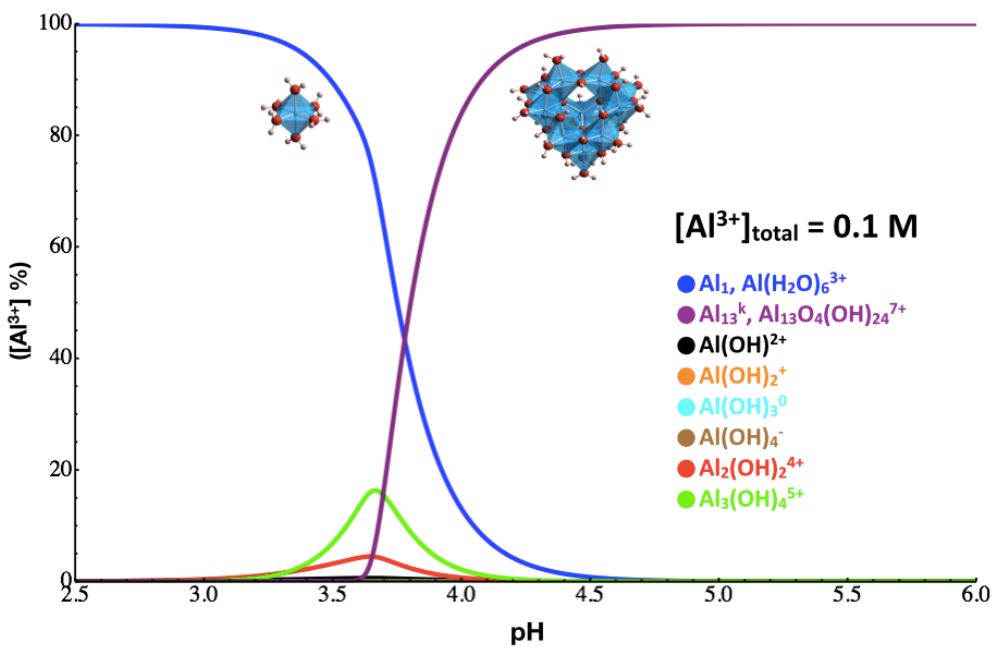

Figure 1.1. Speciation diagram for aqueous Al3+. Equilibium constants are based on potentiometric measurements of cluster stability and degree of hydrolysis.[1]

1.2 Computational Studies

With the increase in computing power and improvements in theoretical methods over the last several decades, quantum mechanical computations have demonstrated their potential to inform and predict. When used properly, computations can prove to be powerful, assisting in the understanding of the structural properties, thermodynamic stabilities, vibrational spectra, dynamics, and electronic properties of nanoscale clusters and particles.

1.2.1 Vibrational Spectroscopy

Vibrational spectroscopy is a common technique for characterizing nanoscale clusters and appealing for analyzing nanoscale materials due to the relative ease with which these spectra can be collected.[12] For most nanoscale clusters, the assignment of signals, and ultimately the elucidation of exactly what species are present in solution is difficult, if not impossible, without computations. Computations can be used to identify signature peaks for specific functional groups, allowing for identification of species with unique functional groups in subsequent experiments.

In practice, IR and Raman are straightforward to compute.[13] Computing these modes is a relatively simple process when a few factors are kept under consideration. First, the structure of a species needs to be properly optimized to the ground state before computing its vibrational modes. Poorly optimized structures or structures taken directly from crystals will yield nonsensical vibrational frequency values. Often, crystal structures cannot be used directly because the effect of the crystal lattice on the geometry is significant enough that one cannot always assume that the ground state geometry of the species remains constant from crystal to solution or gas phase.

Once the vibrational modes have been correctly computed, there are several steps required to produce a computed spectrum that is directly comparable to the experimental. Most crucially, peak broadening must be accounted for, as these effects are not treated at

all in normal mode analyses of commercially available computational software packages. We have resorted to numerical fitting methods to introduce peak broadening to produce computed vibrational spectra that are more easily compared to experiments with great success. Procedurally, each vibrational peak is fit to a Gaussian function. The computed frequency and intensity of each vibration are constant and scaled with concertedly. The widths of the vibrations are allowed to independently vary, within an accepted range of values, until the deviation between the computed and experimental spectra are minimized. It is important to limit the variation of width values; otherwise, the numerical solution found may be non-physical in nature**.** Vibrational widths may either become very narrow or wide if they are not limited, resulting in peaks that become too narrow and essentially disappear or become wide enough that they no longer represent a reasonable physical solution

This method has been used on a wide array of systems, from organic molecules to metal oxide and hydroxide clusters. This technique was applied to interpreting the IR and Raman signals of aqueous and solid samples of gallium and aluminum tridecameric hydroxide clusters, $[M_{13}(OH)_{24}(H_2O)_{24}](NO_3)_{15}$. This analysis procedure led to the full assignment of each spectrum and led to identification of each cluster's unique signals in both solid and aqueous samples. Unsurprisingly, this analysis worked better for solid samples than for aqueous solutions. The structure of these clusters is much better characterized in the solid state than in solution, including the understanding of protonation state and position of counterions. In solution, unlike the solid state, there also may be small amounts of other species present, as the cluster has the ability to fragment into smaller clusters and monomers in solution. This spectral fitting method has also been demonstrated for the α- and β-Keggin phosphomolybdate anions, where the authors studied the IR of the Keggin phosphomolybdate anion with the goal of determining the identity of the isomer of the anion by computing the IR of both the α- and β- isomers. The computed spectra for both of these anionic clusters were in reasonable agreement with the experimental IR spectrum, with each of the significant experimental peaks described

by an analogous computed vibrational mode. However, the computed spectra of the α- and β- isomers were too similar to allow for unique identification of isomers via IR.[14] This conclusion highlights the limits of using computations and vibrational spectroscopy to uniquely identify clusters.

1.2.2 Thermodynamic Stability

The thermodynamic stability of clusters is conceptually one of the easiest calculations to perform and interpret. The Gibbs free energy of each species is directly computed and provided as a scalar value in the results of most normal mode analyses. However, the challenge of thermodynamic stability is in knowing which method will yield accurate results with respect to experiments. In addition, it is often difficult to properly determine the appropriate environment including counterions and implicit or explicit solvent which significantly complicates matters. Often, the number of possibilities for the positions of counterions and solvent, as well as concerns for protonation states, makes the determination of the lowest energy structure extremely time-consuming.

There have been many studies examining the stability of nanoscale polyoxometalate clusters. The Keggin cluster family is a popular topic of study because this family of clusters has five different isomers based on the rotation of a trimeric group at the exterior of the cluster. Understanding the stability of these clusters is important for understanding the likelihood of synthesizing one isomer over another, especially if only one isomer is well-suited for a particular application. For the Keggin phosphotungstates, computations were able to reveal the stability of each of the five isomers.[15] When examining this stability trend, the authors found that the stability of each isomer was largely determined by how many unfavorable W-W contacts each isomer had, as each contact contributed approximately 8-9 kcal/mol in destabilization. A similar trend was computed for phosphomolybdate Keggin ions, though with a slightly lower destabilization energy per metal-metal contact.[16]

The geometries of ionic nanoscale species are strongly affected by solvation effects. This effect is particularly pronounced in aqueous solutions and particularly for species that are strong hydrogen bond donors or acceptors. In the case of metal hydroxo clusters, these clusters tend to optimize to geometries where intramolecular hydrogen bonding between water and hydroxo ligands are more significant than are expected in the aqueous solution, even with the use of implicit solvent models such as PCM and COSMO.[17,18] The formation of these intramolecular hydrogen bonds tends to lead to structures that exhibit significantly distorted bond angles. Explicit counterions and solvents can help to reduce these structural distortions; however, counterions alone may not be sufficient to fix these distortions. Minute changes can lead to large differences in the optimized structures, so it is important to understand all of the factors that could affect structure, including exact locations of protonations and counterions.

1.2.3 Dynamics

Molecular dynamics computations have the potential to solve a wide variety of problems. These can be divided into two general categories relating to the method of generating the Hamiltonian: molecular mechanics (MM) molecular dynamics (MMMD) or ab-initio molecular dyanmics (AIMD).. The MMMD approach is much less computationally demanding because the forces are computed using simple Newtonian forcefield models (ball and spring). Thus MMMD can be and has been applied to study extremely large systems (e.g. the giant polyoxometalate Mo_{132}**Error! Reference source not found.**), where quantum mechanical computations would be unable to yield results in a reasonable time frame.[19] Historically, these simulations have been useful in examining the diffusion of different species in solution and the interaction of these species with solvent molecules.[13] In addition, it has also been used to understand average coordination environments of metal ions, which can provide information about the mechanism of cluster formation.[20]

AIMD has the potential to inform scientists about a variety of solution behaviours not captured by MMMD (e.g. bond breaking, proton transfer, etc.). However AIMD has yet

to be used on a routine basis on nanoscale systems. One of the more appealing options is the use of mixed or hybrid quantum mechanical and molecular mechanical computations (QM/MM).[21] These types of computations are particularly appealing because they have the potential to provide the best of both worlds – accurate chemistry of the AIMD and the superior efficiency of the MMMD. This is appealing for looking at systems where the explicit solute-solvent interactions are of material interest to the chemistry.[22]

1.2.4 Electronic Properties

Electronic properties of materials are typically probed using density functional theory (DFT). Obtaining orbital energies, sizes, and shapes are trivial from static DFT. Optical gaps are often probed using the time-dependent variant (TD-DFT). Oprtical gaps can be obtained from many methods and basis sets with high accuracy; however, the accuracy of fundamental gaps requires more specific methods.[23]

The most practical applications of computing the electronic properties of nanomaterials are to determine the redox chemistry. This has been done extensively on a wide range of nanomaterials, from polyoxometalate clusters to nanoparticles.[24-27] Polyoxometalates and nanoparticles often make good oxidizing agents.[13,28] DFT can also be used to compute the HOMO-LUMO gaps of clusters and these can be used to estimate the relatively ability of multiple species to act as oxidizing agents.[23] The exact values for the HOMO-LUMO gaps cannot be used to determine the experimental redox potential without further information. Much like in experiments, the redox potential must always be described as relative to another reaction, in most cases, the standard hydrogen electrode. To reproduce these values computationally, the reaction of interest needs to be compared to the computed analog of the standard hydrogen electrode.[29] When properly computed, these calculations can be used to determine the relative oxidizing ability of many different agents and determine the one most suited for a particular application without ever having to enter a laboratory.

1.2.5 NMR

The NMR signals of nanoscale species can be and has been studied by computations, but these studies are limited by many of the same factors as the previous studies, particularly for solution NMR studies. These are incredibly sensitive to solvent, especially if the solvent being used for NMR is different than the solvent used for synthesis. The identity and specific interactions with counterions also significantly complicate matters. In addition, in structures optimized with full QM, equivalent atoms by cursory inspection of symmetry involving non-hydrogen atoms may not retain the symmetry after the geometry optimization is completed, depending on the formation of intramolecular hydrogen bonds and position of counterions. Depending on the proton exchange kinetics and conformational flexibilities, these high-symmetry structures may not be representative of the average structure seen on the NMR time-scale and hence yield inconsistent chemical shifts to experiments.

Despite these complicating factors, several studies have been reported, aimed at predicting the relative NMR shifts of various nuclei. The full proton assignment for the aqueous gallium and indium mixed metal tridecamers has been realized using computations. However, in this work and the study of ^{183}W NMR shifts of several POMs, the correct ordering of chemical shifts were obtained, but the quantitative values of the chemical shifts could not be reproduced.[30,31] In addition to these studies, computations have been used to compare theoretical shifts for similar size aqueous aluminium clusters.[32] However, experimental corroboration for these computed shifts has not been obtained. Computations have also assisted in understanding the solid state NMR of Group 13 tridecamers, also discussed previously. These studies have been useful in understanding the NMR of many inorganic nanoscale species; however, there is a large amount of work that remains to accurately reproduce quantitative chemical shifts of these species.

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Chapter 2. Identifying Nanoscale M_{13} Clusters in the Solid State and Aqueous Solution: Vibrational Spectroscopy and Theoretical Studies

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2.1 Abstract

Raman spectroscopy, infrared spectroscopy, and quantum mechanical computations were used to characterize and assign observed spectral features, highlight structural characteristics, and investigate the bonding environments of $[M_{13}(\mu_3\text{-OH})_6(\mu_2\text{-OH})_{18}(H_2O)_{24}](NO_3)_{15}$ (M = Al or Ga) nanoscale clusters in the solid phase and aqueous solution. Solid phase Raman spectroscopy was used to reveal that the metal-oxygen (M-O) symmetric stretch (breathing mode) for the Al_{13} cluster is observed at 478 cm^{-1}, while this same mode is seen at 464 cm^{-1} in the Ga_{13} cluster. The hydroxide bridges in each cluster are weakly Raman active, but show slightly stronger infrared activity. The breathing modes associated with the clusters in the solid state are not clearly visible in aqueous solution. This change in behavior in the solution phase may indicate a symmetry breaking of the cluster or exchange events between protons on the ligands and the protic solvent. Overall, each cluster has several unique vibrational modes in the low wavenumber region (< 1500 cm^{-1}) that are distinct from the parent nitrate salt and other polymeric species with similar structure, which allows for unambiguous identification of the cluster in solution and solid phases.

2.2 Introduction

In recent years, the semiconductor industry has increased research efforts toward developing greener and more cost effective methods of producing thin film devices.[1,2] Group 13 metal aquo-hydroxo clusters with the formula $[M_{13}(\mu_3\text{-OH})_6(\mu_2\text{-OH})_{18}(H_2O)_{24}](NO_3)_{15}$ (M = Al or Ga) offer great promise as precursor materials for a variety of applications associated with the fabrication of thin film devices from aqueous solutions.[3,4] However, there is limited knowledge about the growth mechanism, kinetics, solution dynamics, and film formation of these clusters in aqueous solution. To date, there are only a few reported studies on the solution speciation of such clusters.[5-7] A recent study revealed that the Ga_{13} cluster was visible via ^{1}H-NMR in 2 mmol d_6-DMSO.[7] However, since solution processed thin films are often fabricated in water and at higher concentrations, d_6-DMSO is not an ideal solvent to study for thin film

development.[8] As a first step to studying the speciation and solution dynamics in water, this study focuses on characterizing the vibrational modes of the metal clusters in the solid and aqueous solution phase using Raman and infrared spectroscopy, staple techniques which have found limited utility in the characterization of aqueous nanoscale clusters.[9]

The solution speciation and dynamics of these clusters during the spinning, curing, and annealing processes to produce films is of great interest to the material science community as they seek to fine tune the properties of metal oxide thin films. By identifying and characterizing these clusters in solution, we will be better equipped to monitor the evolution of monomeric Al and Ga species to solution intermediates, then to clusters, and eventually, to the production of thin films. By using computations to assign peaks, we have been able to differentiate between monomeric Al and Ga species and the more complex nanoscale Al_{13} and Ga_{13} clusters in the solid and solution states. This initial study adds to the arsenal of characterization techniques available for studying such aqueous clusters and shows that Raman spectroscopy in particular is an effective reporter of cluster species in solid and solution phases. These studies will provide a baseline for future investigations into understanding cluster formation mechanisms and dynamics/speciation in solution.

2.3 Experimental

2.3.1 Materials and Sample Preparation

FT-IR grade KBr (Aldrich 99.9%) was used in pellet preparation for infrared analysis. $Ga(NO_3)_3 \cdot xH_2O$ (Aldrich 99.9%) and $Al(NO_3)_3 \cdot 9H_2O$ (STREM 98+%) were used without further purification as references in both the solid state and aqueous solution.[7] The Al_{13} cluster was synthesized as previously reported via a zinc reduction method and crystallographically confirmed prior to spectral analysis using single crystal XRD.[10] Herein we show that the Zn reduction method can also be extended to forming the Ga_{13} cluster as well.

Zn reduction method for the synthesis of $Ga_{13}(\mu_3\text{-}OH)_6(\mu_2\text{-}OH)_{18}(H_2O)_{24}(NO_3)_{15}$. 2.55 g of $Ga(NO_3)_3 \bullet xH_2O$ was dissolved in 10 mL of 18.2 MΩ H_2O. Zinc powder was then added into the solution in a 2:1 molar ratio of Ga:Zn and the solution was stirred until the zinc was fully dissolved. The solution was then filtered and the filtrate was evaporated until crystals formed. The crystals were then washed with isopropyl alcohol to selectively remove excess $Zn(NO_3)_2$, $Ga(NO_3)_3$ and yielded ~57% of the final product. DOSY NMR spectra and single crystal XRD matched previous reports. In addition, Raman and IR spectra from a previous synthetic preparation were also identical. Stock solutions of the purified samples were prepared using ultrapure 18.2 MΩ H_2O and exhibited no appreciable changes over the duration of the experiment.

2.3.2 Raman and Infrared Instrumentation

Raman spectra were collected using an Alpha 300S SNOM confocal Raman microscope in a 180° backscattering configuration. A continuous wave pump laser delivered 45 mW of power with an excitation wavelength of 532 nm. A 0.3 m spectrometer equipped with 1800 grooves/mm grating was used to detect stokes Raman scattering and provided a resolution of 1 cm^{-1}. The spectra from each sample were averaged over 2000 accumulations at 0.5 s integration time per scan. The 520.5 cm^{-1} peak of Si was used as an internal standard.

Infrared spectra for both clusters were acquired with a Nicolet 6700 FTIR spectrometer using a KBr pellet. Spectra spanning the range of 400-4000 cm^{-1} were obtained with 64 scans at a resolution of 2 cm^{-1}. Multiple spectra of different sample batches were collected with each technique to ensure reproducibility of the results.

2.3.3 Computational Methods

All geometry optimizations and absolute energies were computed at the HF/6-31G(d,p) level of theory with the PCM-UFF continuum solvation model for water in Gaussian09.[11]

The fundamental frequencies of the nitrate ion vibrations were obtained from literature.[12] To identify the individual vibrational modes, a Least Squares Fitted Computed (LSFC) spectrum was created from the computed frequencies, as reported earlier.[13] The juxtaposition of the LSFC spectrum to the experimental spectrum enables the association of all the peaks with specific vibrational normal modes.

2.4 $Al_{13}(\mu\text{-}OH)_6(\mu\text{-}OH)_{18}(H_2O)_{24}]^{15+}$: Results and Discussion

2.4.1 Raman Spectroscopy: Solid Phase

Several weak modes in the Raman spectrum (Figure 2.1) of Al_{13} from 200-2000 cm^{-1} were observed that correspond to the Al-O vibrational modes in the core and shells of the clusters and are summarized in greater detail in the supplemental information (see supplemental Table S6). The peak at 478 cm^{-1} is attributed to the M-O symmetric stretch of the cluster. Quantum mechanical computations reveal several weak modes between 700-1200 cm^{-1} for the μ-OH hydroxyl bridges of the cluster, including a weak shoulder at ~1100 cm^{-1}. Though this region is expected for Al-(OH)-Al bridging vibrations, the peaks for the hydroxyl bridges are difficult to distinguish experimentally due to overlap with the NO_3^- vibrations.[14-16] The expected vibrational modes at 721 cm^{-1}, 1048 cm^{-1}, 1352 cm^{-1} and 1411 cm^{-1} are in good agreement with previous related reports.[14-16] The cluster also exhibited modes at 1641 cm^{-1}, 3277 cm^{-1}, and 3470 cm^{-1} which are attributed to the out-of-plane O-H water bending (OH_2•••NO_3^-), coordinated O-H stretching (Al-ηH_2O), and O-H stretch of disordered (non-coordinated) waters respectively.[17]

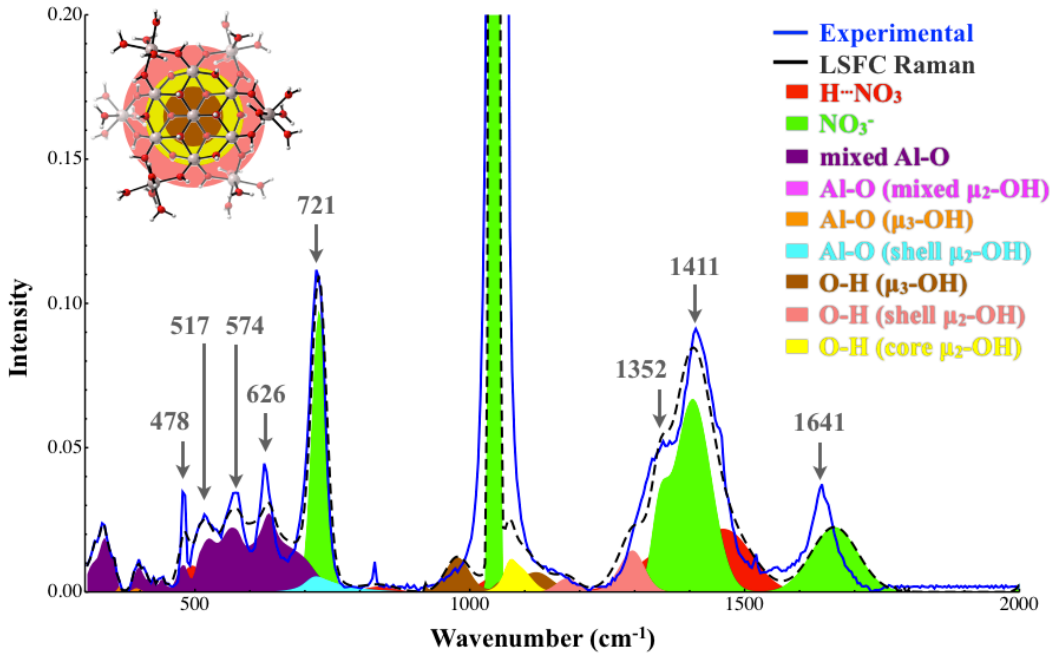

Figure 2.1. Al_{13} Raman spectrum from 200-2000 cm^{-1}. The symmetric stretch of the cluster is highlighted at 478 cm^{-1}. The RMSD for this LSFC Raman spectrum is 0.52 %.

In comparing the spectra of the Al_{13} cluster to that of $Al(NO_3)_3{\bullet}6H_2O$, we discovered that the spectra exhibit some contrasting features. $Al(NO_3)_3{\bullet}6H_2O$ in the solid state contains a single Al-O stretching vibration at 525 cm^{-1} that corresponds to the O_h $Al(H_2O)_6^{3+}$ ion and three weaker modes below 300 cm^{-1} that are indicative of an aluminum nitrato species.[18] The weak shoulder at ~1100 cm^{-1} in the Al_{13} spectrum is associated with the hydroxide bridges of the cluster and are not present in $Al(NO_3)_3{\bullet}9H_2O$. There are no significant frequency differences in the NO_3^- ion in the Al_{13} and $Al(NO_3)_3{\bullet}9H_2O$ spectra, with the exception of a split peak at 1058 cm^{-1}.[17] This suggests that the nitrates in the cluster are not integral to the overall structure and only coordinate to the cluster via hydrogen bonding, consistent with the crystal structure.

The Al_{13} cluster, Boehmite (η-AlO(OH)) and Gibbsite ($Al(OH)_3$), share analogous octahedral metal coordination geometries and bridging hydroxides in their crystal structures. In spite of their structural similarities, the Raman spectrum of Al_{13} remains

qualitatively different.[19,20] The Raman spectrum of Boehmite is highlighted by a strong Al-O stretching vibration at 360 cm^{-1}, an Al-(OH)-Al deformation at 1071 cm^{-1}, and two weaker O-H modes spanning from 2900-3100 cm^{-1}.[21-22] Gibbsite exhibits 12 Al-O modes from 200-500 cm^{-1}, 15 Al-(OH)-Al modes from 500-1100 cm^{-1}, and four intense and distinct O-H modes from 3300-3600 cm^{-1}.[18,19] While some of the reported modes are similar to those found in the cluster, in the region from 400-600 cm^{-1} the Al_{13} cluster exhibits vibrational modes that are distinct from both minerals.

2.4.2 Infrared Spectroscopy: Solid Phase

IR spectroscopic studies were performed on solid state samples of the Al_{13} cluster to elucidate information regarding the relationship between vibrational and structural properties (Figure 2.2). The O-H bending mode observed at 1660 cm^{-1} is also associated with the exterior waters (η-H_2O) of the Al_{13} cluster that hydrogen bond with the nitrate ions and are consistent with the water deformation mode at 1637 cm^{-1} observed in the Raman spectrum (see Section 2.1). The modes observed at ~1400 cm^{-1} and 825 cm^{-1} are indicative of the asymmetric and symmetric stretching vibrations of the nitrate ions.[17] Three medium intense Al-O vibrations of the exterior shell vibrations are detected at 500 cm^{-1}, 620 cm^{-1}, and 750 cm^{-1}. Smaller weak modes of the bridging hydroxides are observed at 850 cm^{-1}, 1000 cm^{-1}, and 1200 cm^{-1}, as reported for aluminum-containing minerals.[14-16] A strong, broad O-H absorption band also occurs at 3300 cm^{-1} that represents the water features of the cluster (not pictured in Figure 2.2, see supplemental Figures A1.3 and A1.6).

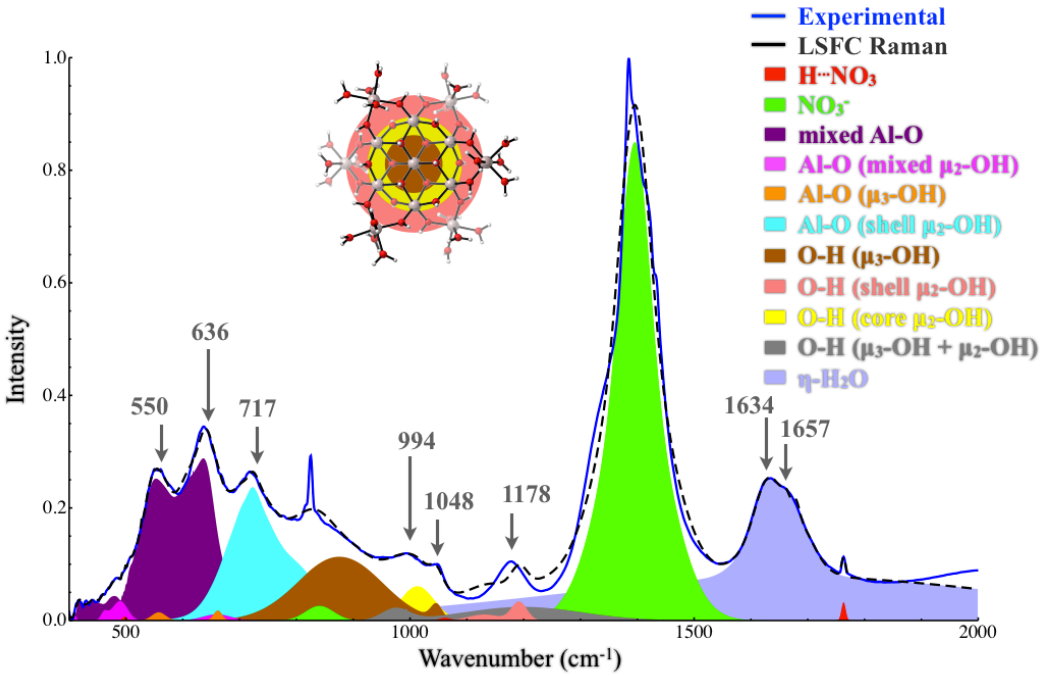

Figure 2.2. Experimental IR spectra of solid Al_{13} cluster from 400-1800 cm^{-1} displaying computational peak analysis. The RMSD for this LSFC IR spectrum is 2.0 %. A m_3-OH ligand is a hydroxide group that bridges the center Al^{3+} with two adjacent core Al^{3+}; m_2-OH_{core} is a hydroxide group that connects two neighboring core Al^{3+}; m_2-OH_{shell} is a hydroxide group that links one core Al^{3+} and its closest shell Al^{3+}; and h-H_2O is a terminal water group on the shell Al^{3+}.

The infrared spectrum of the cluster is also different from the respective nitrate salt and mineral. The monomeric species only exhibits a broad Al-O stretch at 600 cm^{-1}, which corresponds to the O_h Al-O stretching vibration of $Al(H_2O)_6^{3+}$.[17] Previous studies on γ-AlO(OH) demonstrated several Al-O modes that have similar vibrational characteristics to the Al_{13} cluster.[14-16] However, in contrast to the cluster spectrum, reported values for γ-AlO(OH) highlight various Al-O deformation modes below 400 cm^{-1} as well as Al-O stretching modes at 464 cm^{-1}, 563 cm^{-1}, and 626 cm^{-1}. Despite the similarities it is apparent from the infrared results that the γ-AlO(OH) species forms a different bonding network than Al_{13}. In summary, solid phase Raman and IR spectroscopy have shown that the Al_{13} cluster exhibits unique vibrational features from its monomeric parent and related polymeric species and both could be used as a viable option for identifying this cluster in the solid state.

2.4.3 Raman Studies: Solution Phase

Upon dissolution in water, the spectrum of the Al_{13} cluster (Figure 2.2) reveals that the unique weak vibrational modes featured in the solid state are no longer distinguishable due to broadening of the vibrational modes into one large feature. The disappearance of these features may indicate a break in symmetry of the cluster, an extended, dynamic hydrogen bonding network with the solvent, or cluster dissociation. The observed Al-O modes are weak and broad, spanning from ~450-675 cm^{-1}. The weak shoulder associated with the hydroxyl bridge at 1100 cm^{-1} is also not observed in the solution spectrum. The water features from 2800-3600 cm^{-1} seen in the solid state now resemble bulk water.[23] Upon further inspection, the solution phase Raman spectrum of the cluster is similar to that of aqueous $Al(NO_3)_3$. The only notable difference in the solution phase spectra arises from an increased broadness of the low frequency Al-O stretch associated with the cluster in relation to the narrower octahedral Al-O stretch at 525 cm^{-1} observed in $Al(NO_3)_3$.[17]

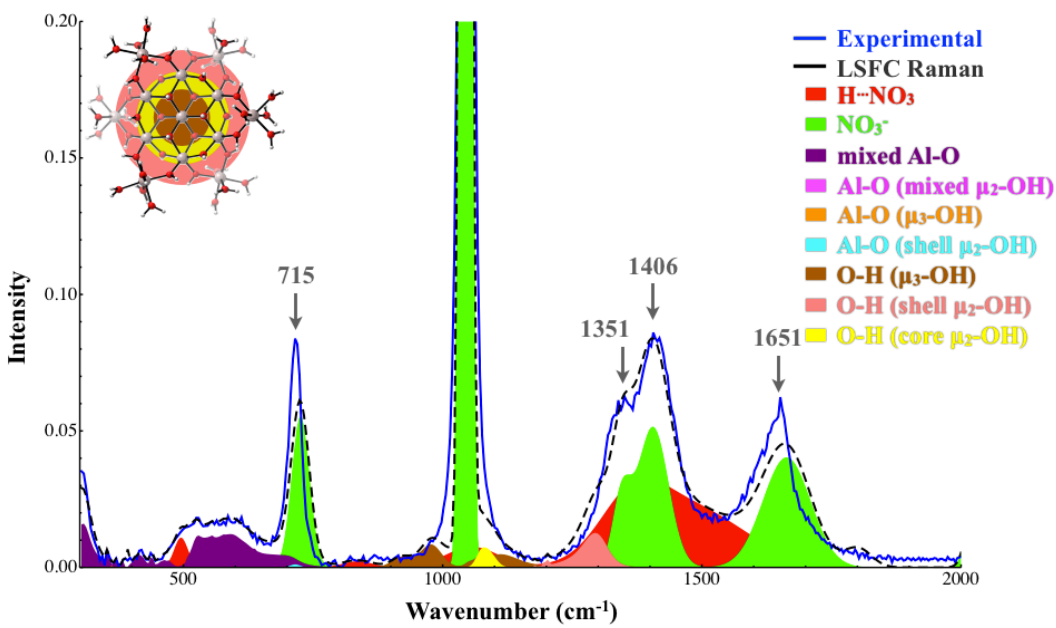

Figure 2.3. Overlay of simulated (black) and experimental (gray) Raman spectra of Al_{13} in 1M solution at 25 °C. All of the weak modes seen in the solid phase have merged into one broad feature ranging from 450-675 cm^{-1}. The RMSD for this LSFC Raman spectrum is 0.59 %.

The broadness of this peak may result from equilibrium exchange dynamics between the cluster and the solvent that give rise to partial dissociation in solution over time. However, aging the sample shows that this feature remains consistently broad for at least a month. Since the peak does not become narrower with aging to resemble $Al(H_2O)_6^{3+}$, we suspect that the cluster is still present in solution over extended periods of time, consistent with solution DOSY, DLS, SAXS and related studies on other similar clusters.[7,24] LSFC Raman spectra suggest that Al_{13} and $Al(H_2O)_6^{3+}$ coexist in aqueous solution because the experimental spectrum is best described by a combination of the Al_{13} and $Al(H_2O)_6^{3+}$ species, rather than either species individually. These studies reveal that solution phase Raman spectroscopy provides a complementary technique to determine the full, complex solution speciation of these and related clusters.[25]

2.5 $[Ga_{13}(\mu_3\text{-OH})_6(\mu_2\text{-OH})_{18}(H_2O)_{24}]^{15+}$: Results and Discussion

2.5.1 Raman Spectra Analysis: Solid Phase

Raman spectroscopy was also able to provide insight on the vibrational features of the Ga_{13} cluster. A band that appears at 464 cm^{-1} can be attributed to the Ga-O symmetric stretch, or breathing mode, associated with the cluster (Figure 2.4). Two weaker, but distinct bands of moderate intensity at 525 cm^{-1} and 556 cm^{-1} arise from the bending vibrations of the exterior shell of the cluster (See Table S7). Calculations suggest that the bands at 1000 cm^{-1} and 1100 cm^{-1} can be assigned to the μ_2-OH and μ_3-OH hydroxyl bridges. However, these bands overlap with the symmetric NO_3^- at 1048 cm^{-1} in the same manner as observed in the Al_{13} cluster. The modes at 720 cm^{-1} and the doublet feature at 1357 cm^{-1} and 1411 cm^{-1} are attributed to the asymmetric nitrate frequencies which are also present in the Al_{13} cluster (see above). Two broad water peaks appear in the traditional O-H stretching region at 3250 cm^{-1} and 3425 cm^{-1}. The 3250 cm^{-1} feature can be attributed to tetrahedrally coordinated water molecules with relatively strong hydrogen bonding interactions much like that of H_2O in ice, while the 3425 cm^{-1} feature can be assigned to water molecules with hydrogen bonding interactions similar to that of bulk water.[26] A narrow shoulder at 3533 cm^{-1}in the O-H stretching region is also observed and

likely due to strongly hydrogen bonded hydroxyl groups incorporated in the crystal lattice of the cluster.[17,26]

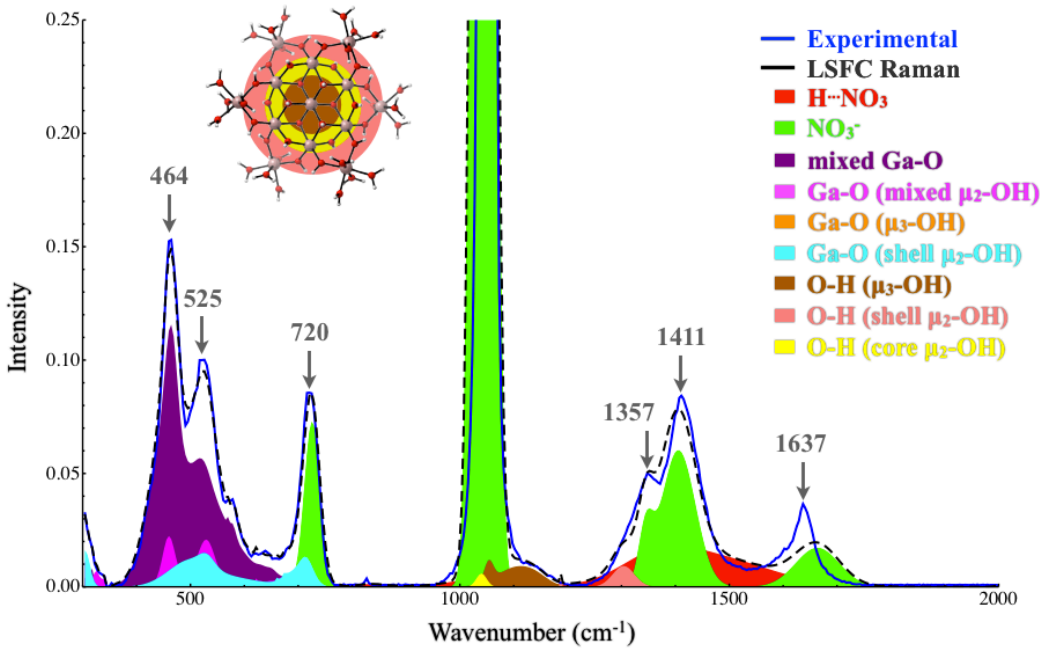

Figure 2.4. Simulated and experimental Raman spectra from 200-2000 cm^{-1} of crystalline Ga_{13} at 25 °C. The feature shown at 464 cm^{-1} arises from the primary breathing mode of the cluster. The RMSD for this LSFC Raman spectrum is 0.40 %.

Ga_{13}, like Al_{13}, shares similar and contrasting features with $Ga(NO_3)_3 \cdot xH_2O$. The observed breathing mode of the Ga_{13} cluster at 464 cm^{-1} is significantly lower in energy than the breathing mode of the $Ga(H_2O)_6^{3+}$ species at 525 cm^{-1}.[27,28] This observed energy difference can be attributed to elongation of the bonds in the cluster due to the influence of the extra gallium atoms that make up the cluster. Interestingly, the mode observed at 525 cm^{-1} in the cluster is in the same position as $Ga(H_2O)_6^{3+}$. The similarity most likely arises from the shell of the cluster oscillating in a nearly identical way to the monomer species. The Raman spectrum for $Ga(NO_3)_3 \cdot xH_2O$ also contains no evidence for bridging hydroxides that are observed in the cluster. Related Raman studies on synthetic nanorods of GaO(OH) identify several strong low energy Ga-O stretching modes around 300 cm^{-1} that are not observed in the Ga_{13} cluster.[29] Additionally, a signature at 605 cm^{-1} in the

spectrum of the GaO(OH) species represents a Ga-O stretch of tetrahedral coordination, which is predictably absent in the cluster.[25,26] Since the Ga-O bonds in the Ga_{13} cluster spectrum are of pseudo-octahedral coordination, this confirms this distinct coordination geometry of the Ga_{13} cluster.

2.5.2 Infrared Results: Solid Phase

To complement the results gathered by Raman, IR spectroscopy was also performed on the Ga_{13} cluster in the solid state. Congruent to what was observed by Raman, a broad water absorption that is associated with bulk water occurs at 3359 cm^{-1} (see Supporting Information Figure A2.3). The mode at 1620 cm^{-1} in the IR spectrum of Ga_{13} (Figure 2.5) is also consistent with the same water out of plane bending mode observed in the Al_{13} IR spectrum (Figure 2.2) and in the Raman spectra of both clusters (Figures 2.1 and 2.4), suggesting that the water in Ga_{13} is interacting with nitrate as previously described for the Al_{13} cluster. The peaks at 824 cm^{-1} and ~1381 cm^{-1} are indicative of the asymmetric and symmetric stretching vibrations of the nitrate ion. The bending and stretching vibrational modes of Ga-O in the exterior shell vibrations are detected at 560 cm^{-1}, 620 cm^{-1}, and 687 cm^{-1}.

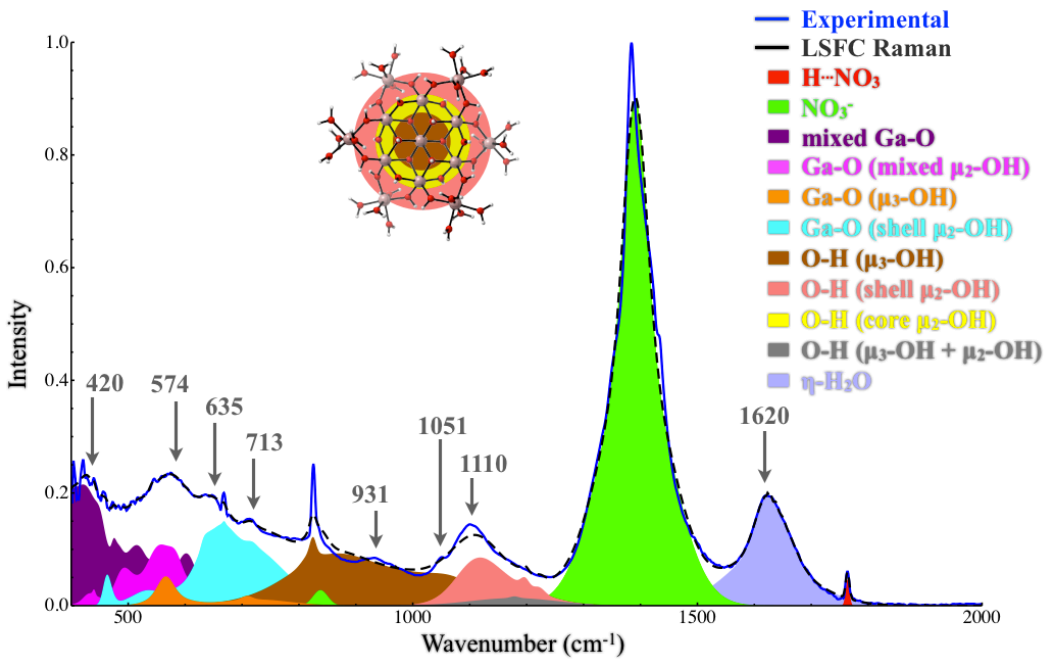

Figure 2.5. Experimental and simulated IR spectra of Ga_{13} in the solid phase from 400-2000 cm^{-1} with computational peak analysis shown. The RMSD for this LSFC IR spectrum is 1.7%.

Similar to $Al(NO_3)_3$, $Ga(NO_3)_3$ only contains one weak Ga-O IR signal at 560 cm^{-1}, while none of the modes for the hydroxide bridges are present. Smaller weak modes of the μ_x-OH (x = 2 or 3) bridges are observed at 906 cm^{-1} and 1102 cm^{-1}. As shown with the Al_{13} cluster, vibrational spectroscopy and computational analysis have given us insight into the vibrational characteristics of the cluster that show Ga_{13} is structurally unique when compared to the parent monomeric gallium nitrate and several oligomeric/polymeric species. However, because of the low intensity of the IR signals for the Ga-O stretch in the Ga_{13} cluster, it may not be the most ideal tool to identify this cluster. In spite of this, it is clear that with the use of vibrational spectroscopy and quantum mechanical calculations, we can characterize the Ga_{13} cluster and distinguish it from similar species in solution and the solid state.

2.5.3 Raman Spectra Analysis: Solution Phase

Upon dissolution, the peaks observed in the solid state decrease and appear as a broad Ga-O stretching vibration centered at 507 cm^{-1} and a shoulder at 450 cm^{-1} (Figure 2.5). This broadening phenomenon is very similar to what was observed for the Al_{13}. With increasing dilution, the overall relative intensity of the peaks at 507 cm^{-1} decrease linearly, however, the peak shape remains the same, suggesting the dominant species in solution does not change with serial dilution. In comparison to the Ga-O stretch of $Ga(H_2O)_6^{3+}$*(aq.)* at 525 cm^{-1}, the Ga-O stretch of the cluster at 507 cm^{-1} still vibrates at a slightly lower energy, suggesting that Ga_{13} is still present in aqueous solution. This is supported by a previous report showing that the cluster has a size of 5.6 ± 1.8 angstroms in aqueous solution via Small Angle X-ray scattering.[7] As observed with Al_{13}, this feature does not change over the period of a month, suggesting potential long term stability of this species in solution.

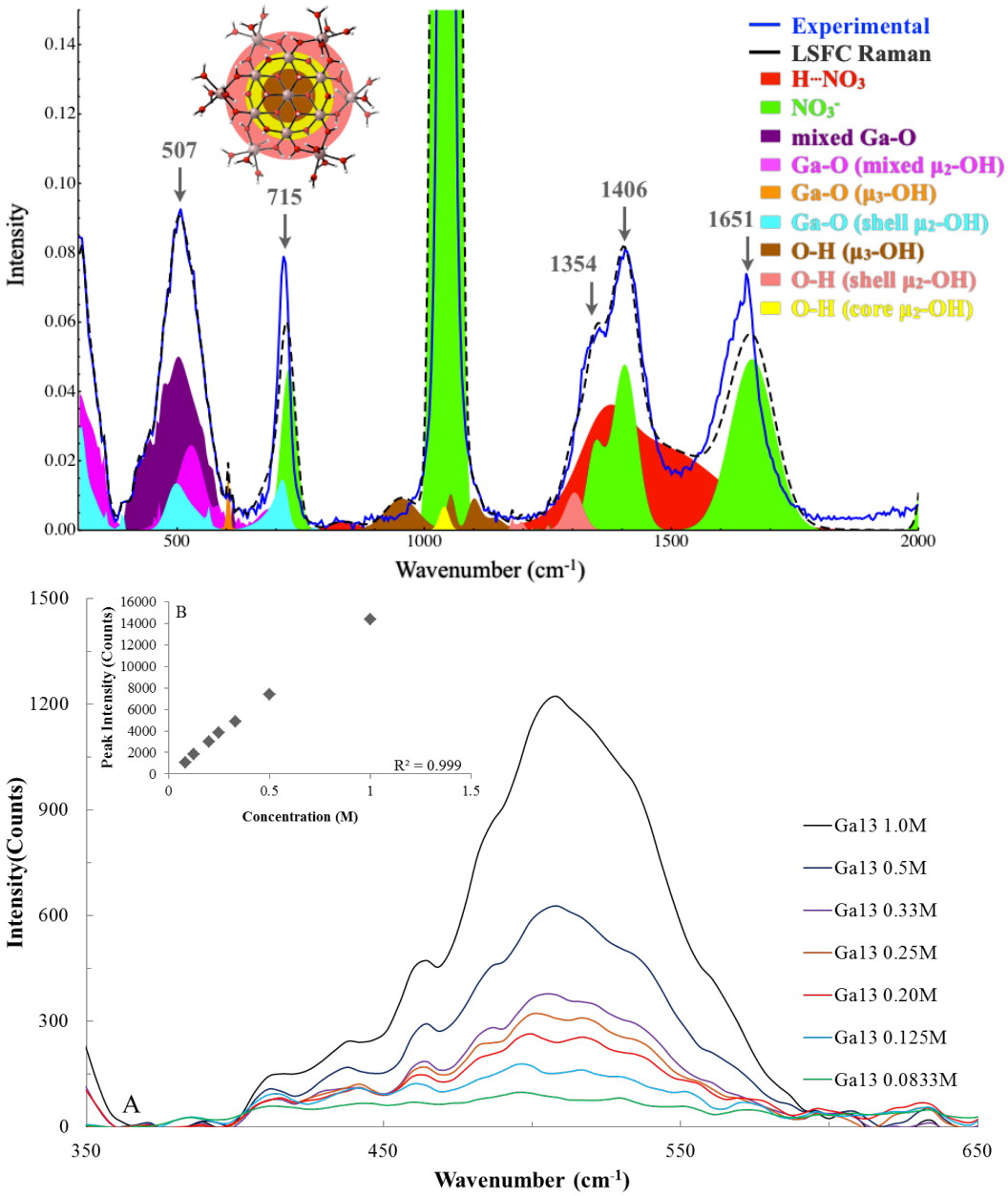

Figure 2.6. Simulated (top) and experimental (bottom) Raman spectra of the Ga_{13} cluster in solution phase from 350-650 cm^{-1}. The RMSD for this LSFC Raman spectrum is 0.57 %. The Ga-O modes coalesce into a broad feature at 502 cm^{-1}. Upon dilution, only the peak intensity changes with dilution suggesting that the species remains persistent in solution (bottom insert). A plot of the intensity of the peak at 502 cm^{-1} versus concentration shows a linear decrease with dilution. In spite of the limitations observed with IR, it is clear that with the use of vibrational spectroscopy, particularly Raman in

conjunction with quantum mechanical calculations, we can characterize and identify the Ga_{13} cluster and distinguish it from similar species in solution and the solid state.

2.6 Al_{13} vs Ga_{13}: Discussion

Under the assumption that the outer coordinated waters are treated as point particles, the $M_{13}(\mu\text{-OH})_6(\mu\text{-OH})_{18}(H_2O)_{24}^{15+}$ clusters have D_{3d} symmetry. Prior to analysis, we presumed that the clusters would have similar spectra based on the structure and the similar spectroscopic features of their parent nitrate salts.[8,13,14] However, Raman and infrared spectroscopy reveal that the Ga_{13} and Al_{13} clusters have distinct vibrational spectra, allowing for definitive characterization and monitoring of cluster species in solution and the solid phase. In the Raman spectra, the observed ν_1 breathing mode for the Al_{13} cluster is observed at 478 cm^{-1}, while this same mode occurs at 464 cm^{-1} for the Ga_{13} cluster. This phenomenon is also readily apparent in the IR spectra that reveal that the core and shell hydroxide bridges vibrate at 1110 cm^{-1} for Ga_{13} versus 1178 cm^{-1} for Al_{13}.

In a direct comparison of the Raman spectra of each cluster from 300-600 cm^{-1}, the relative intensities of the M-O vibrations in the Ga_{13} cluster spectra are far more intense in the solid state than Al_{13}. In addition, the Al-O bonds in Al_{13} cluster give stronger infrared absorptions as well as more discrete peaks in relation to Ga_{13}. The origins of this phenomenon are complex and could arise from several different factors. One possibility is due to the phenomenon of d-block contraction, Gallium (1.81χ) is more electronegative (Pauling's scale) than Aluminum (1.61χ) and the dipole moment (μ) experienced by any specified M-O bond would be greater for Al, which results in greater IR activity. The opposite effect is shown to be true for Ga_{13} in that it is more susceptible to being distorted by an applied electric field (more polarizable), favoring Raman activity. In the solution phase, both polymeric species lose features that are prominent in the crystalline phase resulting in one broad feature because of the additional degrees of vibrational freedom. With dilution, it appears that the Ga_{13} cluster remains present in solution over a wide variety of concentrations and it remains persistent in solution over extended periods of

time. However, dilution studies of the Al_{13} cluster were inconclusive due to the weak signal shown in the Raman spectrum.

2.7 Conclusions

Raman and infrared spectroscopy, as well as quantum mechanical calculations have been used to characterize Al_{13} and Ga_{13} clusters in the solid and solution phases. Our findings show that these clusters exhibit unique vibrational characteristics that differ from the parent monohydrate salts as well as natural and synthetic minerals that have comparable bonding arrangements. We have also shown that even though these clusters are analogous to each other, they have very different vibrational characteristics from each other and their parent nitrate salt starting materials. The Al_{13} cluster exhibited several Al-O modes in both Raman and IR spectra, but showed more prominent IR activity. The Ga_{13} cluster had more intense Ga-O Raman signals, but was not as resolved in the IR spectrum. In solution, both clusters experienced an apparent break in symmetry and many of the peaks observed in the solid phase are no longer observable. The M-O mode for each cluster remains constant over an extended period of time, suggesting that both clusters remain the predominant species in solution. In summary, this report reveals that both Al_{13} and Ga_{13} can be identified in the solid state and aqueous solution by vibrational spectroscopy and shows that these clusters are present in H_2O over a long time period, suggesting that vibrational spectroscopy is an effective complementary technique to more "modern" approaches aimed at probing nanoscale structure in solution.[23]

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Chapter 3. Electrolytic Synthesis of Aqueous Aluminum Nanoclusters and In Situ Characterization by Femtosecond Raman Spectroscopy and Computations

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3.1 Abstract

The selective synthesis and in situ characterization of aqueous Al containing clusters is a long-standing challenge. We report a newly developed integrated platform that combines (i) a selective, atom economical, step-economical, scalable synthesis of Al-containing nanoclusters in water via precision electrolysis with strict pH control, and (ii) an improved femtosecond stimulated Raman spectroscopic method covering a broad spectral range of ca. 350^{-1},400 cm^{-1} with high sensitivity, aided by ab initio computations, to elucidate Al aqueous cluster structures and formation mechanisms in real time. Using this platform, a unique view of flat $[Al_{13}(\mu_3\text{-}OH)_6(\mu_2\text{-}OH)_{18}(H_2O)_{24}](NO_3)_{15}$ nanocluster formation is observed in water, in which three distinct reaction stages are identified. The initial stage involves the formation of an $[Al_7(\mu_3\text{-}OH)_6(\mu_2\text{-}OH)_6(H_2O)_{12}]^{9+}$cluster core as an important intermediate toward the flat Al_{13} aqueous cluster.

3.2 Introduction

The importance of Al (aluminum) in the biosphere and to human civilization is enormous. The scale of mining and production of Al compounds is second only to that of Fe (iron). Our lives are influenced by its use in electronics, cooking and eating utensils, and food packaging, and as structural materials in the construction, automotive, and aircraft industries.[1,2] Its deposition and migration as a mineral ore are controlled by its aqueous chemistry and speciation. Millions of tons of Al compounds are used worldwide each year for water treatment, and it is found in all drinking water.[3] The behavior of Al in water plays significant roles in soil chemistry and plant growth, for example, governing Al bioavailability, toxicity, and its overall impact in aquatic ecosystems.[4-6] Meanwhile, aqueous Al clusters are gaining importance as solution precursors for the large-area deposition of Al_2O_3 coatings with broad technological applications.[7,8]

Despite more than a century of study, the complete portrait of aqueous Al chemistry remains unclear.[9,10] Studies of aqueous Al chemistry are notoriously difficult because of the variety and complexity of the species that can be formed, encompassing monomeric,

oligomeric, and polymeric hydroxides; colloidal solutions and gels; and precipitates. Synthesis is complicated by the fact that the counter-ions and the method and rate of pH change all have dramatic effects on product formation.[11–19] Few methods exist for the in situ determination and assignment of molecular-level structures. For instance, ^{27}Al NMR can only identify certain Al aqueous species.[15] Furthermore, unlike organic compounds, systematic spectroscopic signatures of metal hydroxide clusters are less accessible, making interpretation of experimental spectra challenging. We hereby report a combined synthesis, experiment, and theory platform for the study of aqueous metal clusters. Electrolysis is exploited to control the solution pH and counter-ion content precisely during cluster synthesis without using chemical reagents. The evolution of solution species is followed in situ by an improved femtosecond stimulated Raman (FSR) technique that can detect weak signals associated with structure-defining vibrational modes.[20–22] The resulting pH dependent Raman spectra are interpreted by juxtaposition to quantum mechanically computed vibrational modes to assign specific molecular structures. Through this integrated approach, we have discovered a speciation behavior for Al in water that has not previously been observed. We focus here on the synthesis and formation pathway of the flat $[Al_{13}(\mu_3\text{-}OH)_6(\mu_2\text{-}OH)_{18}(H_2O)_{24}]^{15+}$ cluster (Al_{13}) that is practically important for its use as a "green" solution precursor for the large-scale/large-area preparation of Al_2O_3 thin films and nanoparticles that have broad utility in electronics, catalysis, and corrosion prevention.[7,8,23–27]

3.3 Materials and Methods

3.3.1 Electrochemical Synthesis

The 1.0-M $Al(NO_3)_3$ (aq) starting solution was made with $Al(NO_3)_3{\cdot}9H_2O$ (American Chemical Society grade; Baker Analyzed Reagent) and ultrapure water (ρ = 18.2 MΩ·cm). Constant current bulk electrolysis was carried out using an EG&G 263A potentiostat in two-electrode mode with the reference electrode input lead connected to the counterelectrode. A custom-built, two-compartment cell comprising a 15-mL cathode, a 50-mL anode, and a standard medium porosity glass frit (Chemglass) to separate the

two compartments was used. The solution volumes in the cathode and anode were 10 mL and 30 mL, respectively. Pt (platinum) wire coils were used for both electrodes. To minimize local pH gradients in the cathode compartment where the cluster is synthesized, the cathode solution was stirred rapidly during electrolysis and a large-surface area (23 cm^2) Pt wire coil was used as the working electrode. The current was set to 75 mA during the experiment, which required ca. 4 V across the working and counterelectrodes due to the kinetic overpotentials associated with the hydrogen and oxygen evolution reactions, as well as the series resistance of the two-compartment cell. The charge Q was determined by Q = I·t. No significant temperature changes were observed during the prolonged electrolysis reaction, consistent with the low-power dissipation (75 mA Å~ ~4 V = 0.3 W). The pH of the cathode compartment solution was monitored in real time using an ion-sensitive field-effect transistor pH probe. Upon reaching the desired pH, the cathode solution was directed into a flow cell for the in situ FSR spectroscopic measurements.

3.3.2 Improved FSR Spectroscopy

The FSR spectroscopic setup consists of a modelocked Ti:sapphire oscillator (Mantis-5) and regenerative amplifier (Legend Elite-USP-1K-HE; Coherent), which provides 35-fs, 800-nm pulses with ~4.1 mJ per pulse energy at a repetition rate of 1 kHz. The fundamental beam of ~1.6 mJ per pulse energy is dispersed by a reflective grating (1,200 grooves per millimeter, 750-nm blaze) and passed through a 90-μm wide slit to generate the Raman pump of ~10-cm−1 bandwidth and ~3.5-ps pulse duration. The Raman probe represents an advancement of conventional methods, which originates from CFWM sideband signals generated by crossing two laser pulses [the 800-nm beam (~35 fs, 3 μJ per pulse) and the IR component of the supercontinuum white light generated in a 2-mm thick sapphire plate followed by prism compression (~45 fs, 100 nJ per pulse)] in a 0.1-mm thick β-barium borate crystal (type I, θ = 27.8°).[22, 34] The incident beam diameters on the crystal are ~0.2 mm, and the crossing angle is ~6°. One of the CFWM signals with an ~900-nm center wavelength is selected as the Raman probe, corresponding to the Stokes

frequency range from ca. 100–3,000 cm−1 and a pulse duration of ~30 fs. The Raman pump and probe beams are then focused onto the 1-mm path length sample flow cell by an off-axis parabola (to avoid pulse chirp). Only the transmitted probe beam carrying the stimulated Raman signal enters the spectrograph to be dispersed by a 600-groovesper-millimeter grating (1,000-nm blaze) and imaged onto a CCD camera (PIXIS 100F; Princeton Instruments), which consists of a 1,340 Å~ 100-pixel array and is synchronized with the laser repetition. Each sample spectrum is averaged from 180,000 Raman spectra within ~6 min, and the 1.0-M$Al(NO_3)_3$ precursor solution spectrum is collected in exactly the same manner right before each pH-specific sample solution measurement as the standard for NO_3^- mode intensity normalization and generation of the differential FSR spectra (Fig. 3.2). Both the spectral dips and peaks in the differential spectra are multi-Gaussian least-squares fitted across the wide spectral range, and the integrated peak areas are plotted vs. pH to capture the real-time evolution of the broad signal intensity during electrolysis.[21]

3.3.3 Computations

The geometries and spectra of the Al clusters of interest were computed using HF/6-31G(d,p) with the IEFPCM-UFF continuum solvation model for water at the electronic ground state.[36–39] The least-squares fitting procedure is described below.

i) Each computed Raman vibrational mode was mathematically described with a Gaussian function using the computed Raman vibrational frequency and intensity. A frequency parameter (F) was used to modulate the frequencies of all species, amplitude parameters (A) for the amplitude of each species, and width parameters (W) for the width of each Gaussian .The sum of all Gaussian curves constitutes the LSFC Raman spectrum.

ii) The parameters (F, Ai, and Wij) were then iterated to minimize the rmsd between the trial LSFC Raman spectrum and the experimental spectrum. The vibrational

modes of all eliminated peaks were checked and verified manually for chemical relevance.

iii) The individual Gaussians in the final LSFC Raman spectra can then be identified according to the functional groups and partitioned as shown in Fig. 3.

3.4 Results and Discussion

Although the flat cluster $[Al_{13}(\mu_3\text{-}OH)_6(\mu_2\text{-}OH)_{18}(H_2O)_{24}]^{15+}$ is commonly considered a minor component in Al speciation that does not appear in published predominance (i.e., Pourbaix) diagrams, it can now be synthesized in large quantities.[28–32] Here, we demonstrate complete atom economy and step economy in the selective synthesis of the Al_{13} cluster using an electrochemical method to increase the pH of a 1.0-M $Al(NO_3)_3$ (aq) solution smoothly.

The predominant Al species in a 1.0-M $Al(NO_3)_3$ (aq) solution is the monomeric hexa-aqua ion $Al(H_2O)_6^{3+}$ (aq).[33] As the pH of the solution increases, condensation of the monomeric ion occurs, leading to the formation of polynuclear Al hydroxide clusters. To prevent the steep pH gradients commonly associated with base titrations, the pH change is achieved by proton reduction in a two-compartment electrochemical cell (Fig. 1). In the cathode compartment, protons are reduced to hydrogen gas, increasing the pH. In the anode compartment, water oxidation results in a decrease in pH. The reaction rate is controlled by adjusting the electrical current through the cell. A porous glass frit eliminates convective mixing between the two compartments. Because the NO_3^- and $Al(H_2O)_6^{3+}$ are present in large concentrations (i.e., ~3.0 and 1.0 M, respectively) relative to H^+ in the pH range explored, the bulk of the charge-balancing ionic current across the frit is carried by NO_3^- migration into the anode compartment and $Al(H_2O)_6^{3+}$ migration into the cathode compartment. The pH of the cathode compartment is plotted against total charge passed in Fig. 1. In this study, we primarily focus on the highlighted range of pH

= 2.70–3.18, because it covers the crucial steps for initial formation of Al hydroxide nanoclusters.

The Keggin Al13 hydroxide cluster is the most commonly observed polynuclear species in pH-based speciation studies.[18,19] The Keggin structure is characterized by a core, tetrahedral AlO_4 unit surrounded by 12 AlO_6 octahedra. A solution ^{27}Al NMR spectrum of the final cathode solution (pH = 3.18) indicates only a minor presence of Al atoms in a tetrahedral site associated with the Keggin Al_{13} structure. Consistent with this observation, we find that all crystals obtained from cathode solutions in the pH range of 2.60–3.10 exhibit unit cell parameters equivalent to that of the flat Al_{13} cluster $[Al_{13}(\mu_3\text{-}OH)_6(\mu_2\text{-}OH)_{18}(H_2O)_{24}]^{15+}$. This cluster contains only distorted octahedral AlO_6 groups, lacking the tetrahedral AlO_4 core of the Keggin cluster. The ease of isolating the flat cluster points to the efficacy of the electrolysis method for selective synthesis through precision pH control.[32] The electrolysis method is also especially well suited for in situ analysis because of the lack of any additional reagents.

To monitor the formation of the flat Al_{13} cluster as a function of pH, the cathode solution is studied in situ by nonresonant (800 nm) FSR spectroscopy with a newly developed Raman probe pulse.[21] The probe pulse is selected from one of the cascaded four-wave mixing (CFWM) signals generated by crossing two femtosecond near-IR laser pulses in one thin transparent medium, providing good spatial separation between self-compressed multicolor sideband lasers and the fundamental beams for ultrabroad spectral coverage.[22,34] This unique approach enables the measurement of stimulated Raman signals to frequencies as low as 350 cm^{-1}, significantly extending established low-frequency detection limits, ca. 600–800 cm^{-1}, of conventional probe-light generation in FSR spectroscopy. To capture subtle spectral changes and correct for the effects of laser fluctuations, the spectrum of a control 1.0-M $Al(NO_3)_3$ (aq) solution was acquired before measuring each pH-specific sample.

The resulting differential FSR spectra (i.e., the differences between sample and control measurements) across the pH range of 1.9–3.18 are shown in Fig. 2. In these spectra, negative peaks represent species being consumed, whereas positive peaks represent new species emerging at the cathode. Three pronounced negative peaks appear at 525 (Al-O stretching of $[Al(H_2O)_6]^{3+}$), 718, and 1,048 cm^{-1} (NO_3^- vibrations).[33] Positive peaks, associated with polynuclear Al clusters, are centered at 386, 585, 675, 777, 937, 1,151, and 1,275 cm^{-1}. Although these Raman peaks are weak, mainly due to high symmetry and small polarizabilities of the Al nanoclusters, their signal-to-noise ratios are statistically significant. The peak located near 1,006 cm^{-1} can be resolved by least-squares peak fitting with multiple Gaussians. Because it partially overlaps with the intense negative peak at 1,048 cm^{-1}, there is considerable uncertainty in assigning a precise position in the differential spectrum; hence, it has not been used in the ensuing analyses.

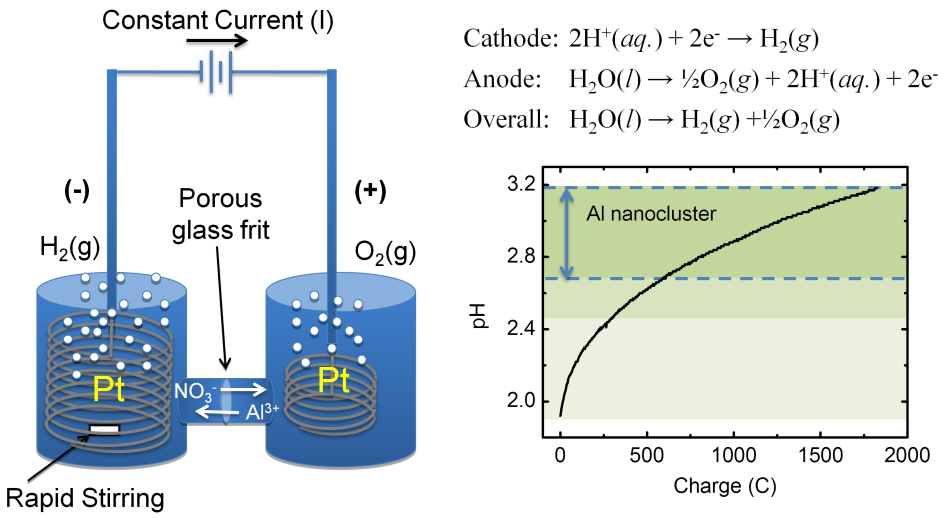

Figure 3.1. (Left) Cell for $Al(NO_3)_3$ (aq) electrolysis. (Right) Balanced reactions under acidic conditions are shown in the upper part of the graph. Cathode solution pH vs. total charge passed through the system is shown in the lower part of the graph; the region of Al nanocluster formation is highlighted.

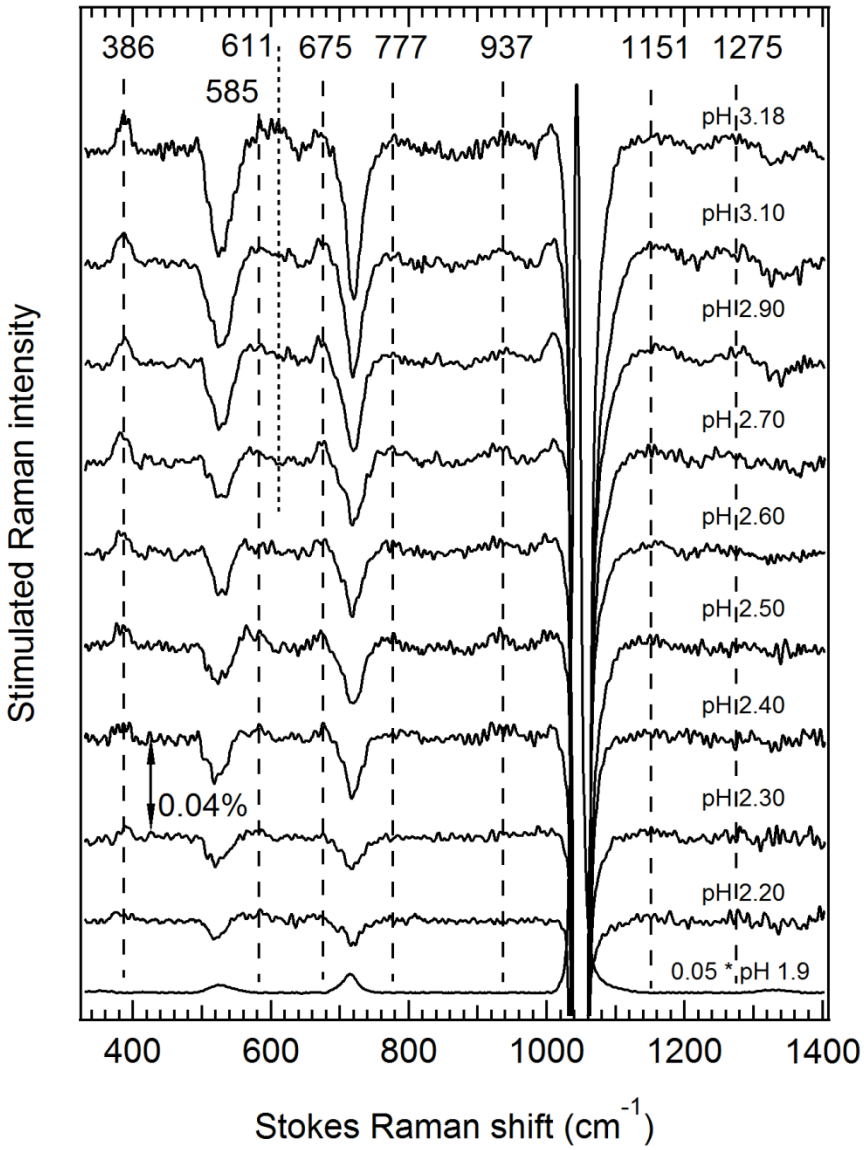

Figure 3.2. Differential FSR spectra of the cathode solution as pH increases from 1.90 to 3.18. The vertical double-headed arrow indicates a stimulated Raman gain of 0.04%. The FSR spectrum of the precursor solution (pH = 1.9) is scaled by a factor of 0.05 and plotted at the bottom for comparison. The nascent Raman peaks during reaction are marked by dashed lines.

To identify the individual Raman vibrational modes that constitute each of the peaks in the differential FSR spectrum in Fig. 2, least-squares fitted computed (LSFC) Raman spectra were created from the Raman frequencies and intensities of model nanocluster species computed by the Hartree-Fock (HF) method with 6-31G(d,p) basis set.[35-37] All the

computations were undertaken with the integral-equation formalism polarizable continuum model (IEFPCM) for aqueous solution and universal force field (UFF) van der Waals radii.[38,39] Results for pH = 3.18 are summarized in Fig. 3. The region from 900–1,300 cm^{-1} exhibits resolved hydroxo group vibrations that collectively define fingerprints for the clusters. We classify these vibrations into three types: μ_3-OH, μ_2-OH_{core}, and μ_2-OH_{shell}, where the subscripts of μ denote the number of Al atoms bound to each hydroxo group. $[Al_7(\mu_3\text{-}OH)_6(\mu_2\text{-}OH)_6(H_2O)_{12}]^{9+}$ (Al_7) represents the planar core of the flat Al_{13}: It contains a central Al atom that is bridged to six next nearest-neighbor Al atoms by μ_3-OH groups (red circle in Fig. 3.3E). These groups give rise to signals near 937 and 1,006 cm^{-1}. The outer six Al atoms are also connected to each other by μ_2-OH core bridges (yellow circle in Fig. 3.3E), producing bands near 1,075 and 1,151 cm^{-1}. The flat Al_{13} exhibits the Al_7 core with six additional Al atoms appended via μ_2-OH_{shell} linkages. These groups (blue circle in Fig. 3.3C), produce signals near 1,190 and 1,275 cm^{-1}. Mixed bands, comprising both μ_3-OH and μ_2-OH vibrations, are also observed for the Al_{13} cluster near 1,075 and 1,270 cm^{-1}. The structural form of these hydroxo groups is replicated in Al_{7+1} (Fig. 3.3D), where one additional Al atom is appended to the Al_7 core.

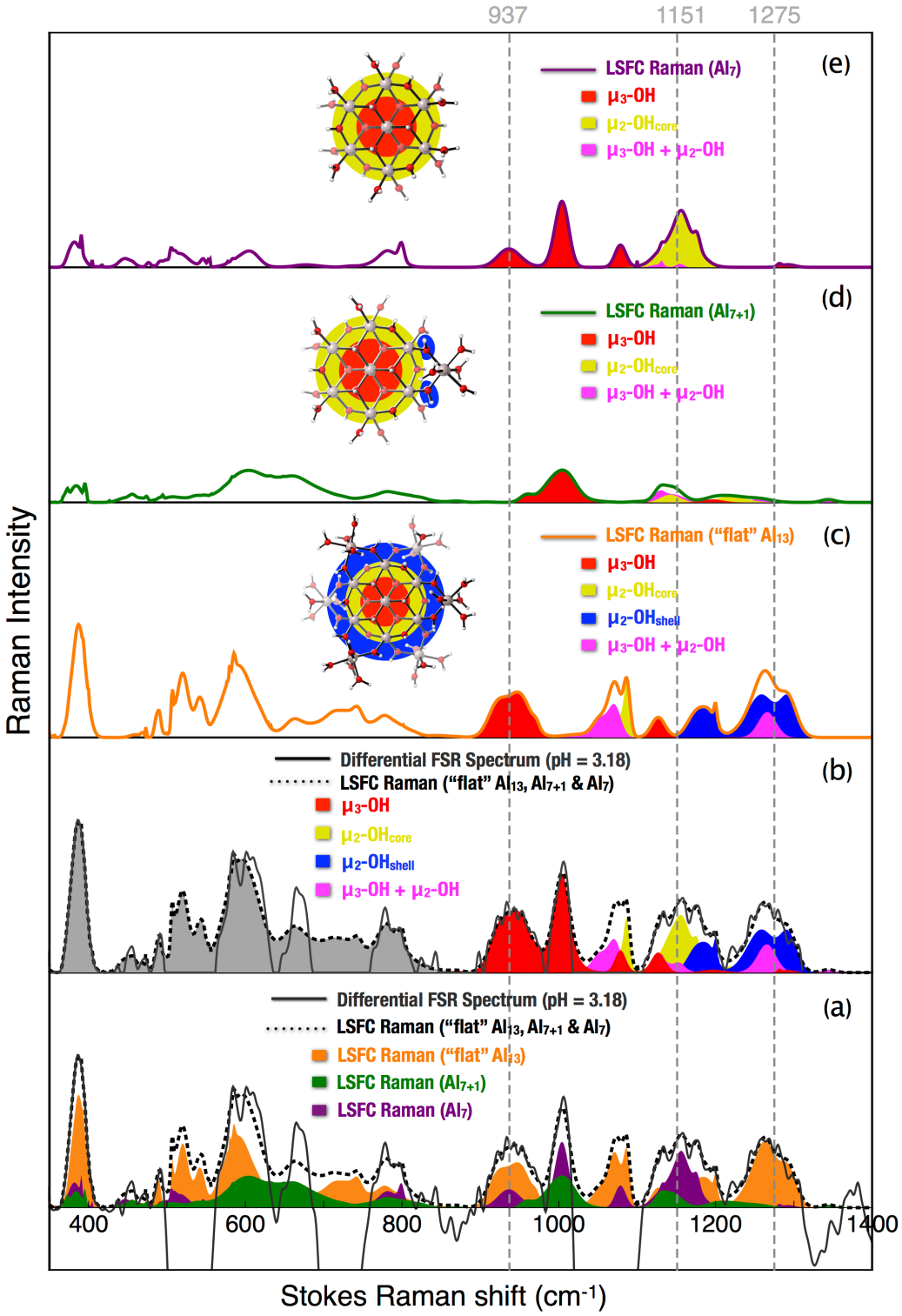

Figure 3.3. Differential FSR spectra (pH = 3.18) from each cluster (A) and each hydroxyl ligand (B) and LSFC spectra of flat Al_{13} (C, orange), Al_{7+1} (D, green), and Al_7 (E, violet).

Deconvolution of the total LSFC spectrum (Fig. 3.3A) reveals that the solution contains the flat Al_{13} cluster as well as the Al_7 species (see Fig. 3.3 A, C, and E). The peaks near 1,000 and 1,151 cm^{-1} provide strong evidence for the existence of Al_7; the peak at 1,151 cm^{-1} is uniquely associated with the μ_2-OH_{core} in Al_7 (Fig. 3.3E). In addition, the Al_{7+1} species $[Al_8(\mu_3\text{-}OH)_6(\mu_2\text{-}OH)_8(H_2O)_{14}]^{10+}$ can be added to the spectrum without negatively affecting the fit, suggesting it likely exists in the solution. The total computed spectrum, incorporating the aforementioned three clusters, correlates well to the differential FSR spectrum over the entire frequency range of 350–1,400 cm^{-1} (Fig. 3.3 A and B). Computations also reveal that Al-O vibrations dominate in the region from 350–900 cm^{-1}. The rise in the positive signal at ~386 cm−1 is thus a strong and unique indication of Al cluster formation with increasing pH.

To follow the assembly pathway of the Al aqueous clusters, the integrated areas of the 525, 718, and 1,048-cm^{-1} negative peaks and of the 937, 1,151, and 1,275-cm^{-1} positive peaks in Fig. 3.2 have been normalized and plotted against solution pH in Fig. 3.4. Three reaction stages are revealed. In stage I (pH = 2.20–2.45), both the NO_3^- and $[Al(H_2O)_6]^{3+}$ concentrations decrease in the cathode solution. The decreasing $[Al(H_2O)_6]^{3+}$ concentration is directly correlated to the formation of Al clusters (increasing 937 and 1,151 cm^{-1} signals) and the concomitant decrease of the NO_3^- concentration (718 and 1,048 cm^{-1}); NO_3^- migrates from the cathode to the anode compartment to maintain the charge balance. As noted above, the 1,151-cm^{-1} peak is uniquely associated with the μ_2-OH_{core} in Al_7 (Fig. 3.3). Because no significant intensity is detected in the spectral region around 1,275 cm^{-1} corresponding to the μ_2-OH_{shell} of flat Al_{13}, we associate this initial reaction stage with the formation of the Al_7 core structure.

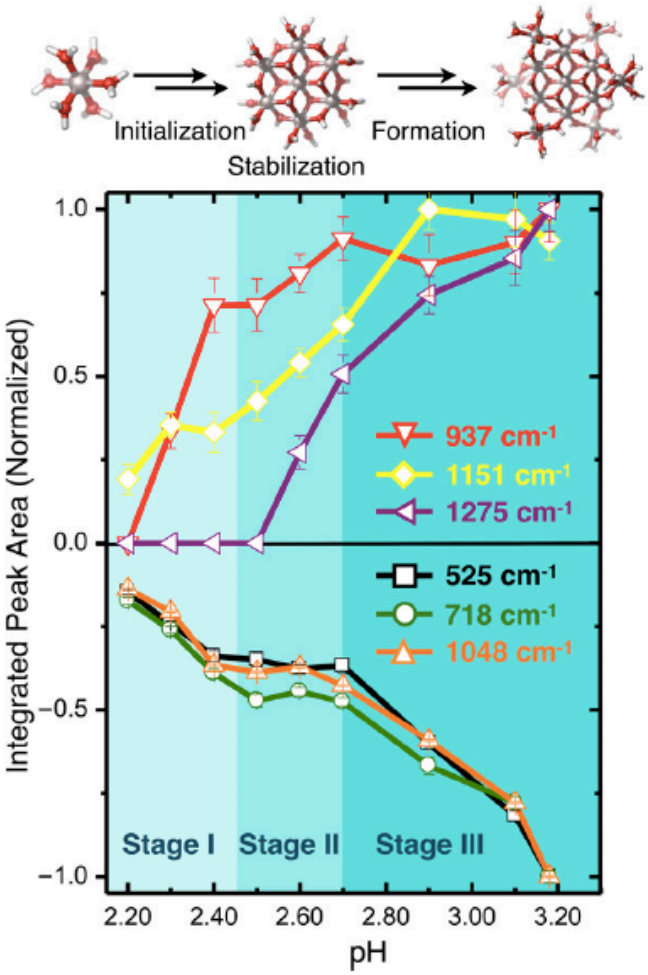

Figure 3.4. Differential FSR signal intensity vs. pH for 1.0-M $Al(NO_3)_3$ (aq) solution in reaction. Peak assignments for the Al clusters are 937 cm^{-1} (μ_3-OH), 1,151 cm^{-1} (μ_2-OH_{core}), and 1,275 cm^{-1} (μ_2-OH_{shell} and μ_3-OH + μ_2-OH). The signal at 525 cm^{-1} corresponds to Al-O vibrations in $Al(H_2O)_6^{3+}$, and the signals at 718 cm^{-1} and 1,048 cm^{-1} are associated with NO_3^-. The error bar represents 1 SD from the individual mode intensity average of multiple independent measurements on the Al speciation in water. (Upper) Proposed three-stage reaction pathways to form the flat Al_{13} via an Al_7 intermediate are delineated.

In stage II (pH = 2.45–2.70), the Al_7 cluster continues to dominate, but the appearance and growth of the 1,275-cm^{-1} signal uniquely indicate the formation of the Al_{13} cluster. There is little change in the NO_3^- and $[Al(H_2O)_6]^{3+}$ concentrations across this region, suggesting a predominance of hydrolysis, stabilization, and condensation of Al species in response to the pH change. The continuously rising 1,151-cm^{-1} signal in concert with the

1,275-cm^{-1} peak is a clear indication that Al_7 and Al_{13} concentrations are increasing. Intermediate species, such as Al_{7+1}, may also be forming, but assignments here are less certain. Moreover, the Al_{7+1} structure is probably only one of a set of sequential species Al_{7+n} (n = 1–5) contributing to initial formation of flat Al_{13}.

In stage III (pH = 2.70–3.18), the increasing 1,275-cm^{-1} signal is consistent with a continuing shift of equilibria favoring flat Al_{13}. The 937- and 1,151-cm^{-1} signals are associated with both Al_7 and Al_{13}, and no significant changes are expected as the equilibrium shifts; hence, the plateau in these spectral signatures is explained. This stage also covers the pH range where crystals of flat Al_{13} nitrate can most readily be harvested from the cathode solution. Both the NO_3^- and $[Al(H_2O)_6]^{3+}$ signals decrease to a larger extent than that in stage I, representing further nitrate migration from the cathode as the reaction progresses toward building larger Al nanoclusters.

3.5 Conclusion

The combined techniques described herein are a powerful toolset for the synthesis and analysis of aqueous metal clusters. The single reagent electrolytic synthesis provides precise control of product selectivity and scalability. The smoothly varying pH eliminates the sharp gradients that may lead to nucleation of the tetrahedral AlO_4 species at low apparent pH values, while also enabling the in situ study, isolation, and crystallization of flat Al_{13} in a clean and efficient way. The femtosecond spectroscopic approach provides an effective means to establish both chemical identity and detailed molecular structure for a metal species in water, corroborated by systematic computations for structural-mode assignment. We have demonstrated the power of this integrated approach by providing a vivid view of aqueous Al chemistry in action, which extends the highly cited Al predominance diagrams by quantifying and elucidating a unique three-stage formation pathway for the important flat Al_{13} cluster via an Al_7 intermediate. The proposed condensation pathway, involving only octahedrally coordinated Al, is also consistent with

the existence and structures of the common minerals gibbsite and boehmite, which contain Al only in distorted octahedral coordination environments.

Taken together, this report provides unique insights and tools concerning the nature of the equilibria and intermediates contributing to the complex condensation and speciation chemistries of Al, while raising questions about behavior outside the pH range studied here. The methods open a new chapter in the study of Al, a biologically and technologically important element, and also provide a general approach for establishing the molecular structures of species in other aqueous metal systems.

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Chapter 4. Solution Structural Characterization of an Array of Nanoscale Aqueous Inorganic $Ga_{13-x}In_x$ ($0 \leq x \leq 6$) Clusters by ^{1}H-NMR and QM Computations

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4.1 Abstract

NMR spectroscopy is the go-to technique for determining the solution structures of organic, organometallic, and even macromolecular species. However, structure determination of nanoscale aqueous inorganic clusters by NMR spectroscopy remains an unexplored territory. The few hydroxo-bridged inorganic species well characterized by ^{1}H Nuclear Magnetic Resonance spectroscopy (^{1}H-NMR) do not provide enough information for signal assignment and prediction of new samples. ^{1}H-NMR and quantum mechanical (QM) computations were used to characterize the NMR spectra of the entire array of inorganic flat-$\mathbf{Ga_{13-x}In_x}$ ($0 \leq x \leq 6$) nanoscale clusters in solution. A brief review of the known signals for μ_2-OH and μ_3-OH bridges gives expected ranges for certain types of protons, but does not give enough information for exact peak assignment. Integration values and NOESY data were used to assign the peaks of several cluster species with simple ^{1}H-NMR spectra. Computations agree with these hydroxide signal assignments and allow for assignment of the complex spectra arising from the remaining cluster species. This work shows that ^{1}H-NMR spectroscopy provides a variety of information about the solution behavior of inorganic species previously thought to be inaccessible by NMR due to fast ligand and/or proton exchange in wet solvents.

4.2 Introduction

Proton Nuclear Magnetic Resonance spectroscopy (^{1}H-NMR) is an important tool heavily utilized by chemists and biochemists since its discovery in 1945.[1] Unfortunately, it is often not often a viable technique for characterizing purely inorganic clusters due to the fast exchange of protons and/or ligands in aqueous coordination clusters dissolved in wet/polar solvents. The reliable trends and generalizations in ^{1}H-NMR shifts tabulated for numerous carbon-containing molecules do not translate to this purely inorganic world. The focus of this manuscript is to correlate the ^{1}H-NMR spectral shifts of nanoscale aqueous clusters dissolved in wet solvents to their hydroxo ligands to substantiate cluster characterization and speciation in solution. The ^{1}H-NMR spectrum of $[Ga_{13}(\mu_3\text{-OH})_6(\mu_2\text{-OH})_{18}(H_2O)_{24}]\text{-}(NO_3)_{15}$ (Ga_{13}) in wet d_6-DMSO is known.[2] Due to the spectral

complexity, no peaks were assigned to specific hydroxo and aquo protons in the structure at that time. Further analysis coupled with computations of the complete series of $[Ga_{13-x}In_x(\mu_3\text{-}OH)_6(\mu_2\text{-}OH)_{18}(H_2O)_{24}]\text{-}(NO_3)_{15}$ clusters ($1 \leq x \leq 6$: $Ga_{12}In_1$, $Ga_{11}In_2$, $Ga_{10}In_3$, Ga_9In_4, Ga_8In_5, Ga_7In_6) provides trends and clarity, allowing partial ^{1}H signal assignment and complete assignment of all hydroxo bridges in the "mother clusters" (i.e., clusters entirely capped with water molecules that potentially undergo exchange with coordinating solvents, Figure 4.1).

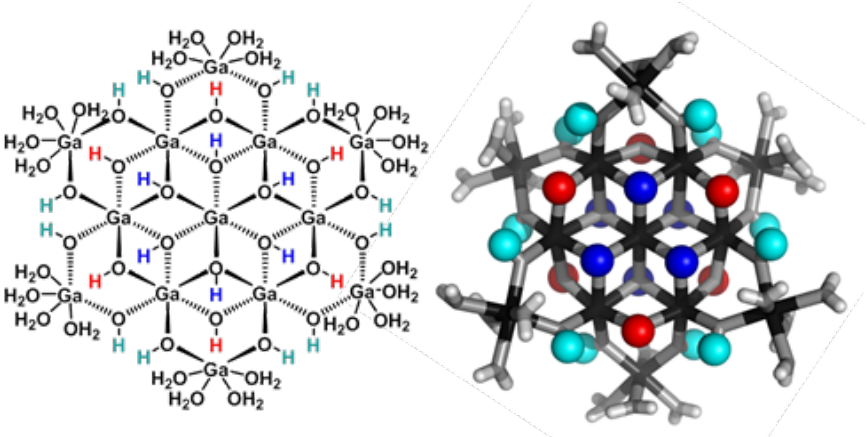


Figure 4.1. Structure of $Ga_{13-x}In_x$ ($0 \leq x \leq 6$, pictured x=0) mother clusters. Left: Full bonding scheme for clusters including atom identity. Right: Top view of 3 dimensional structure depicting 3 types of hydroxide bridges. The μ_3-OH are blue, internal μ_2-OH are red, and external μ_2-OH are cyan.

^{1}H-NMR spectroscopy is the first characterization technique used in modern organic, organometallic, and coordination chemistry, yet such data are only sporadically reported for aqueous inorganic clusters. We have found that under the right conditions such clusters often exhibit rich ^{1}H-NMR spectra that enable characterization by 2D NMR techniques as well.[2] A bottleneck in determining solution structure by NMR spectroscopy has been the lack of tabulated data for such clusters and predictive methods for peak assignment. For instance, there is no known way for predicting where M-H_2O or M-(μ_2-OH)-M ^{1}H-NMR signals should resonate like there is for organic compounds. In this manuscript we provide a literature survey of ^{1}H-NMR spectroscopic resonances reported for known hydroxo- and aquo-coordinated metal complexes. To the best of our

knowledge, such data have not been aggregated in one location. We then use this information and complementary quantum mechanical (QM) computations to provide the complete solution structure and peak assignment for a series of clusters.

The $\mathbf{Ga_{13-x}In_x}$ clusters in this work are completely inorganic. Clusters of this type are often more difficult to isolate and challenging to characterize[13] than organic ligand-supported versions, because the ligands lower the cluster charge and can increase stability.[14] However, the lack of organic ligands makes these species attractive candidates as precursors (inks) for metal oxide films, as the lack of organic additives that must be "burned" off during film formation/condensation leads to fewer defects and increases density of thin films. These clusters also serve as excellent inks/precursors due to their high solubility in aqueous and alcoholic solutions, which eliminates toxic solvents often used in thin film production. Minimizing the organic ligands for such applications has produced superior precursors,[13] but the lack of spectroscopic handles has limited the complete understanding of the solution behavior of these species.

Previously, single crystal X-ray diffraction (XRD) and elemental analysis were the techniques used to differentiate the seven known flat-$\mathbf{Ga_{13-x}In_x}$ clusters.[15] These techniques suggest that multiple cluster species might co-crystallize during isolation (for example, $\mathbf{Ga_{10.2}In_{2.8}}$ has been isolated, which could be an 80/20 mixture of $\mathbf{Ga_{10}In_3}$ and $\mathbf{Ga_{11}In_2}$ or some other such combination). $\mathbf{Ga_{13}}$ has been recently characterized in solution using NMR, Small Angle X-ray Scattering (SAXS), and Raman.[2,16] Although single crystal XRD can provide excellent solid-state data, it cannot answer pressing current questions. Does $\mathbf{Ga_{10}In_3}$ even exist or are all of the mixed clusters simply various ratios of $\mathbf{Ga_{13}}$ and $\mathbf{Ga_7In_6}$? Do all of the possible isomers in the $\mathbf{Ga_9In_4}$-$\mathbf{Ga_{11}In_2}$ clusters (Figure 4.1) co-crystallize or are certain ones thermodynamically favored? Is there a way to determine the ratio of isomers present in a sample? Using ^{1}H-NMR, we have established a quick technique for characterizing samples that could address these

questions and will accelerate the synthesis and identification of cluster species in solution.

4.2.1 ^{1}H-NMR Spectra of Hydroxo/Aquo Bridged Coordination Compounds

Only a limited number of reports of completely inorganic, hydroxo bridged species have been studied via ^{1}H-NMR spectroscopy. However, the moderate chemical shift library of hydroxo protons identified in ligand-supported metal complexes and coordinated water allows for some comparison. The typical chemical shifts of coordinated water ligands are generally downfield (Table 4.1). Typically hexaaquo species have proton signals in the range of 8.3 to 11.3 ppm, while water ligands on metal oligomers tend to appear slightly upfield between 6.3 and 10 ppm.

Table 4.1. ^{1}H-NMR Data for Water Ligands Bound to Metal Atoms.

Metal	Type of Complex	Chem. Shift (ppm)	NMR Conditions	Ref.
Al^{III}	Hexaaquo	10.2	d_6-Acetone; 400 MHz	3
Ga^{III}	Hexaaquo	8.3	d_6-Acetone;-50°C; 500 Hz	4
Rh^{III}	Hexaaquo	9.0—9.2	d_6-Acetone; -83°C; 400 MHz	5
Sn^{IV}	Hexaaquo	10.1—11.3	d_6-Acetone;-100°C; 60 MHz	6
Al^{III}	Oligomer (Al_{13}-Keggin)	7.5	d_6-Acetone; -30°C; 400 MHz	7
Al^{III}	Oligomer (Al_{13}-Keggin)	6.3	d_3-Acetonitrile; 400 MHz	7
Al^{III}	Oligomer (Al_{13}-Keggin)	8.0	H_2O/d_6-Acetone (2.5:1); -20.6 to -5.2°C; 500 MHz	8
Al^{III}	Oligomers	7—10	d_6-Acetone; 400 MHz	3
Al^{III}	Oligomers	8—9.5	-	5,7
Rh^{III}	Oligomers	8.4, 8.7	d_6-Acetone; -83°C; 400 MHz	5

Table 4.2. ^{1}H-NMR Data for μ_2-OH Bridges Linking Trivalent Octahedral Metals in Homo-Metallic Complexes.

Metal	**Molecular Geometry of MX**	**μ2-OH Chem. Shift (ppm)**	**NMR Conditions**	**Ref.**
Al^{III}	Octahedral (Al_{13}-Keggin)	3.8, 3.9	*d*6-Acetone; -30°C; 400 MHz	7
Al^{III}	Octahedral (Al_{13}-Keggin)	2.8, 3.0	*d*3-Acetonitrile; 400 MHz	7
Al^{III}	Octahedral (Al_{13}-Keggin)	3.8, 4.5	H2O/*d*6-Acetone (2.5:1); -20.6 to -5.2°C; 500 MHz	8
Al^{III}	Octahedral (Al_{13}-Keggin)	3.8	H2O/*d*6-DMSO (2:1); 3.7 to 95.2°C; 500 MHz	8
Al^{III}	Octahedral	4.8	-	5
Ga^{III}	Octahedral	2.03	*d*6-DMSO; 400 MHz	9
Ga^{III}	Octahedral	4.2	*d*3-Acetonitrile/D2O; 250 MHz	10
IrI^{II}	Distorted Octahedral	1.6	*d*-Chloroform; 25°C; 270 MHz	11
Rh^{III}	Octahedral (Di/Trimer)	3.7, 4.3	*d*6-Acetone; -83°C; 400 MHz	5
W^{III}	Octahedral	2.05	*d*-Chloroform; 19 and 55°C; 400 MHz	12

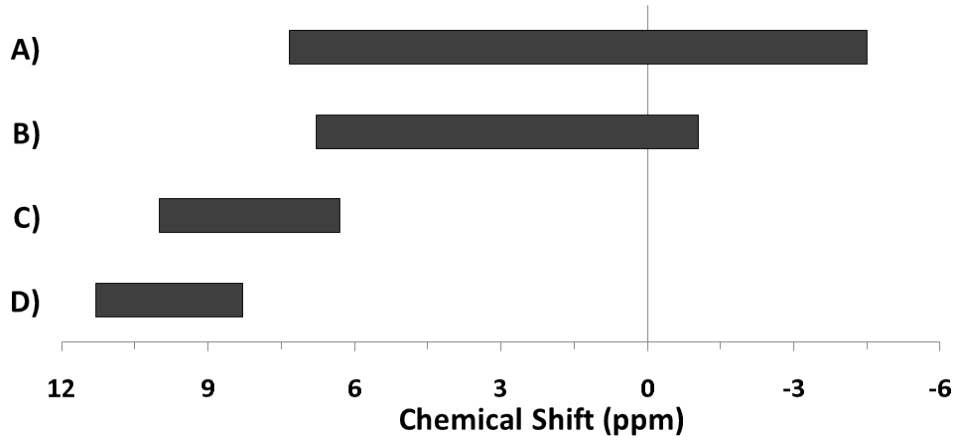


Figure 4.2. General ^{1}H-NMR signal regions for bridging hydroxides and aquo ligands in all metal complexes surveyed. A) μ_2-OH bridges (-4.5—7 ppm); B) μ_3-OH bridges (-1.05—6.79 ppm); C) aquo ligands in multimetallic complexes (6.3—10 ppm); D) hexaquo metal complexes (8.3—11.3 ppm).

Little is known about the potential trends for these hydroxide bridges in inorganic species, although it appears that the metal atom and its coordination number are main contributors to the chemical shift of these hydroxo protons. The collected chemical shifts have been tabulated and discussed for the readers benefit. (Tables 2-5) For diamagnetic complexes, μ_2-OH protons fall between -4.5 and 7 ppm; while μ_3-OH proton signals occur from -1.05 to 6.79 ppm (Figure 4.2). The observation of these ^{1}H-NMR signals at lower chemical shifts than that of the hexaaquo species and the free hydroxide ions is caused by the increased electron density around the proton in the bridge.[5] These are fairly large regions that are not distinguishable from one another, but can be differentiated from water ligands. By looking more closely at specific metals, coordination environments, and groups on the periodic table, refined assignments of chemical shift regions and apparent trends emerge.

Octahedral M(III) ions (M=Al, Ga, Ir, Rh, and W), the most relevant for this work, tend to produce signals for μ_2-OH protons that range from 1.5—5.0 ppm, although this does

not hold true for Co(III).[17–21] Geometries, chemical shift data, and available NMR conditions for these metal complexes are shown in Table 2. The majority of this data was referenced to TMS or residual protic peaks described in the primary papers. Solvent and temperature do not appear to significantly affect the chemical shifts.[12]

The top section of Table 3 indicates some metal complexes with different oxidation states and/or non-octahedral geometries exhibit resonance for hydroxide bridges similar to the ranges observed for "trivalent octahedral" metal complexes. In addition to experimental data, computational data is occasionally found for bridging hydroxides. For instance, computed ^{1}H-NMR shifts during the oligomerization of Be(II) species mirrors the experimental measurement of 4.3 ppm.[22,23] Like the trivalent octahedral complexes listed above, certain metals have distinct areas within the bigger region were the ^{1}H-NMR signals of μ_2-OH bridges appear. The data presented in the bottom section of Table 3 reveals these ranges. As previously mentioned, octahedral Co(III) complexes differ from the other trivalent octahedral complexes with signals appearing between -4.5 and 0.5 ppm.[17–21] Mixed valence Os(0/II) compounds tend to have bridges in the -2.8 to -0.44 ppm range.[24,25] Square planar Pd(II) and Pt(II) complexes have μ_2-OH bridges that range from -3 to 2 ppm.[26–34] Sn has the largest range producing signals anywhere from 1.63 to 7.33 ppm.[35–39] Yttrium hydroxo bridges tend to have chemical shift values downfield ranging from 5.2 to 6.4 ppm.[40] Zn(II) bridges fall into the -1.15 to 4.16 range.[41–43] The proton signal for the only example of a Cd-(μ_2-OH)-Cd bridge appeared at -2.43 ppm.[42] The typical ranges of these metal hydroxo bridges have been plotted in Figure 4.3 to allow for easy comparison.

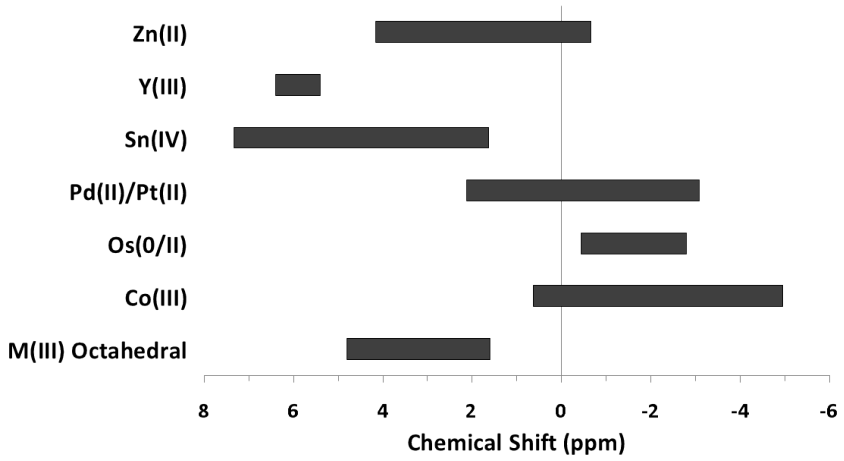


Figure 4.3. General ^{1}H-NMR signal regions for homometallic μ_2-OH bridges in a variety of metal complexes.

Data from the literature for heterometallic complexes was also analysed because the present work focuses on heterometallic Ga/In clusters as well. Not all of the heterometallic complexes in Table 4 feature bridging hydroxides between two different metal atoms, but for completeness they were included.

The hydroxo bridges in trivalent Group 13 octahedral metal complexes are the most relevant for this report. Akitt and colleagues suggests a range of 3 to 6 ppm for Al^{3+} μ_2-OH bridges.[3] However, the data listed above suggests these resonances should fall within the 2.0 to 4.8 ppm region. The heterometallic octahedral Ga-(μ_2-OH)-M (M $\neq$ Ga) bridges have very similar chemical shifts to the homometallic hydroxo bridges listed in Table 2. This indicates that Ga-(μ_2-OH)-Ga bridges may not easily be distinguished from

Ga-(μ_2-OH)-In bridges. Figure 4.4 illustrates the regions where μ_2-OH bridges and capping water ligands on the **$Ga_{13-x}In_x$** clusters most likely will resonate.

Table 4.3. ^{1}H NMR Data for μ_2-OH Bridges in Homo-Metallic Complexes

Metal	**Molecular Geometry of M^{X+}**	**μ_2-OH Chem. Shift (ppm)**	**NMR Conditions**	**Ref.**
Be^{II}	Tetrahedral	4.3	-55°C; 220 MHz	22
Mg^{II}	Trigonal Bipyramidal	3.99	d_8-THF; 25°C; 300 MHz	44
Mo^{II}	Square Pyramidal‡	2.44	-	45
Mo^{II}	Pentagonal Bipyramidal	1.24	d_2-Dichloromethane; -78°C; 400 MHz	46
Ru^{II}	Five coordinate†	3.00, 2.94	d_6-Acetone; 60 & 220 MHz	47
Sn^{IV}	Trigonal Bipyramidal	2.61, 3.85, 2.3	*d*-Chloroform; 360 & 400 MHz	36–38
W^{II}	Pentagonal Bipyramidal	1.7	d_2-Dichloromethane; -78°C; 400 MHz	46
Zn^{II}	Trigonal bipyramidal	4.16	d_3-Acetonitrile; 270 MHz	41
Zn^{II}	Octahedral	2.08	d_6-DMSO	43
Zr^{IV}	Pentagonal Bipyramidal	3.8	d_8-THF; 200MHz	48
Zr^{IV}	Octahedral‡	1.39 – 1.57Ł	d_6-DMSO; 400MHz	49
Cd^{II}	Trigonal Bipyramidal	-2.43	d_3-Acetonitrile; 20°C; 400 MHz	42
Co^{III}	Octahedral	-2	d_6-DMSO	17
Co^{III}	Octahedral	0.63	d_3-Acetonitrile; 250 MHz	18
Co^{III}	Octahedral	-4.18	d_6-DMSO	19
Co^{III}	Octahedral	-0.15, -2.56, -4.95	d_6-DMSO; 20°C; 300 MHz	21
Co^{III}	Octahedral	-1.195, 1.397	d_6-DMSO; 25°C;	20

			600 MHz	
Co^{III}	Octahedral	-0.702, -0.670	D_2O; 4°C; 600 MHz	20
Ga^{III}	Tetrahedral	0.14	d_6-Benzene; 300 MHz	50
In^{I}	Square Pyramidal	0.93	d_6-Benzene; 400 MHz	51
$Os^{0/II}$	Six/Seven coordinate†	-2.8	d_2-Dichloromethane; 400 MHz	24
$Os^{0/II}$	Octahedral	-1.98 – -0.44Ł	*d*-Chloroform; 200 MHz	25
Pd^{II}	Square Planar	-1.58, -1.66, -2.96, -3.09	-	26
Pd^{II}	Square Planar	-2.84, -1.53, -1.67	*d*-Chloroform; 200 MHz	27
Pd^{II}	Square Planar	-1.01, -1.17, -1.25	d_6-Acetone; 200 and 300 MHz	28
Pd^{II}	Square Planar	-0.9, -1.0	*d*-Chloroform; -3 and 27°C; 600 MHz	29
Pd^{II}	Square Planar	-0.85	*d*-Chloroform; 200 MHz	30
Pt^{II}	Square Planar	-0.14	d_2-Dichloromethane; 200 MHz	31
Pt^{II}	Square Planar	-2.04, -1.22, -1.03, -0.56	*d*-Chloroform; 25°C; 80 MHz	32
Pt^{II}	Square Planar	1.9, -0.8, -0.46	*d*-Chloroform; 80 and 200 MHz	34
Pt^{II}	Square Planar	2.0, -0.9, -0.45	d_2-Dichloromethane; 80 and 200 MHz	34
Pt^{II}	Square Planar	2.12	*d*-Chloroform; 300 MHz	33
Sn^{IV}	Octahedral	7.33	d_6-DMSO; 300 MHz	39
Sn^{IV}	Octahedral	7.02	d_2-Dichloromethane; 300 MHz	39
Y^{III}	Eight coordinate†	6.4, 5.45	d_3-Acetonitrile; 300 MHz	40
Y^{III}	Dodecahedral‡	5.4	d_3-Acetonitrile; 300	40

			MHz	
Y^{III}	Bicapped Trig. Prismatic	5.23, 5.35	d_3-Acetonitrile; 300 MHz	40
Y^{III}	Square Antiprismatic‡	6.2	d_2-Dichloromethane; 300 MHz	40
Zn^{II}	Trigonal Bipyramidal‡	-1.15, -0.66	d_3-Acetonitrile; 20°C; 300 & 400 MHz	42

Table 4.4. ^{1}H NMR Data for μ_2-OH Bridges in Hetero-Metallic Complexes.

Metals	**Molecular Geometry of M^{X+}**	**μ_2-OH Chem. Shift (ppm)**	**NMR Conditions**	**Ref.**
Fe^{0} / \ Ru^{I}-(OH)-Ru^{I}	Octahedral	-2.16, -1.78, -1.75	*d*-Chloroform	52
Fe^{II} / \ Sn^{II}-(OH)-Sn^{II}	Tetrahedral	1.7	d_6-Benzene; 27°C; 300 and 500 MHz	35
Co^{III} / \ Sn^{II}-(OH)-Sn^{II}	Tetrahedral	1.63	d_6-Benzene; 27°C; 300 and 500 MHz	35
Ga^{III}-(OH)-Ca^{II}	Octahedral (Ga)	4.73	*d*-Chloroform; 25°C; 500 MHz	53
Ga^{III}-(OH)-Sr^{II}	Octahedral (Ga)	4.49	*d*-Chloroform; 25°C; 500 MHz	53

Table 4.5. ^{1}H NMR Data for μ_3-OH Bridges Linking Homometallic Atoms

Metal	Molecular Geometry of M^{X+}	μ_3-OH Chem. Shift (ppm)	NMR Conditions	Ref
Ca^{II}	Octahedral	1.32, 2.77, 4.57	d_6-Benzene; 25°C; 300 MHz	44
Rh^{I}	Six coordinate†	-1.05	d_4-Methanol; 300 MHz	54
Rh^{I}	Six coordinate†	-0.61, -0.48, -0.02	d_2-Dichloromethane; 300 MHz	54
Sn^{IV}	Trigonal Bipyramidal	3.219, 3.221	*d*-Chloroform; 500 MHz	55
Th^{IV}	Square Pyramidal‡	5.97, 6.16, 6.79	d_6-DMSO; 500 MHz	56
Y^{III}	Dodecahedral£	2.93, 3.1	d_3-Acetonitrile; 300 MHz	57
Y^{III}	Dodecahedral	6.05	d_3-Acetonitrile	58

Zn^{II}	Trig. Bipyramidal/Octahedral	5.4	*d*-Chloroform; 25°C; 300 MHz	59

One trend that stood out in the general data was that hydroxide bridges shift downfield with increased coordination number of the metal. This trend is visible with metals such as Sn, Ga, and Zr (Figure 4.5). These were the only metals that had data from several independent sources allowing reasonable conclusions to be made. This trend holds true for all of Group 13, not just gallium (Figure 4.6). Tetrahedral gallium has a Ga-(μ_2-OH)-Ga bridge at 0.14 ppm,[50] Square Pyramidal gallium and indium have peaks in the 1 to 1.5 ppm range,[51,60] and as stated above octahedral aluminium and gallium produce signals between 2 and 5 ppm.

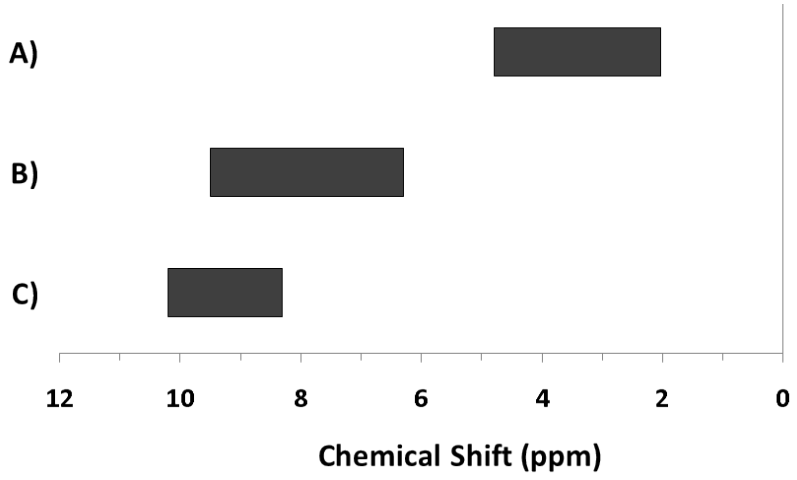


Figure 4.4. General ^{1}H-NMR signal regions for hydroxo bridges and aquo ligands on Group 13 Metals. A) μ_2-OH ligands; B) aquo ligands in multimetallic complexes; C) hexaaquo metal complexes.

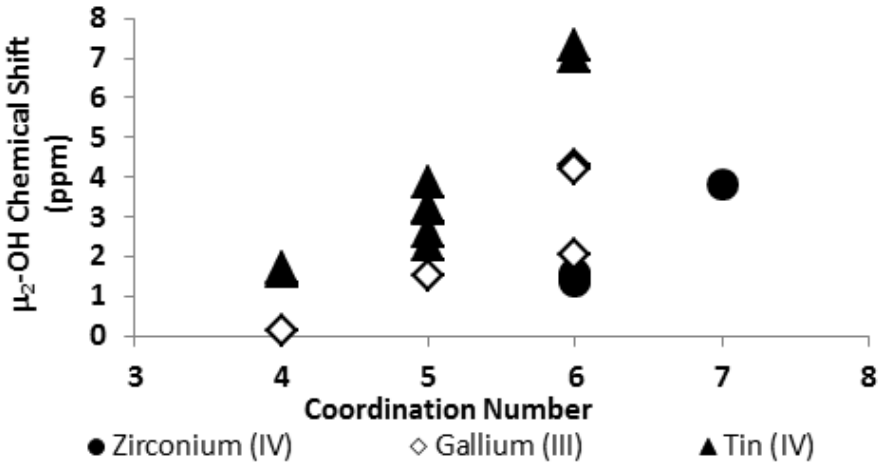


Figure 4.5. As the coordination number of a cation increases, the ^{1}H-NMR signals shift downfield (Tables 2 and 3).

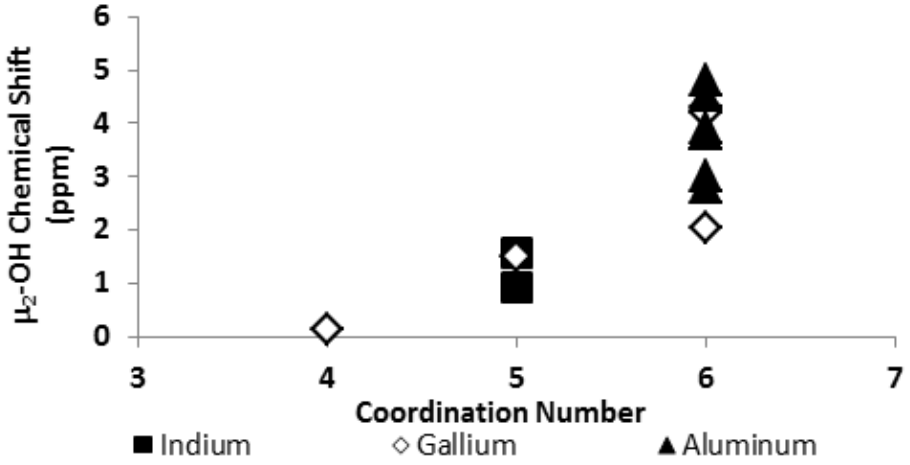


Figure 4.6. As the coordination number in Group 13 increases, the ^{1}H-NMR signals shift downfield (Tables 2 and 3).

^{1}H-NMR data reported for μ_3-OH protons are even scarcer. As previously stated, these signals appear from -1.05 to 6.79 ppm. The proton chemical shifts in these complexes are listed in Table 5. No examples of Group 13 metals with μ_3-OH ligands were found. The most relevant is the trivalent yttrium complex with a proton signal at 6.05 ppm.[58] Related hydroxide ligands in Th(IV) and Zn(II) compounds also resonate in this region.[56,59] Unfortunately, there are not enough examples of μ_3-OH protons to suggest any trends or regions for specific metals or coordination geometries.

This brief literature survey will not only help the structural study and assignments presented herein, but we hope this serves as a useful resource for others seeking to assign aquo and bridging hydroxo ligands in inorganic clusters and related compounds. This survey highlights some of the challenges in interpreting even the most basic NMR signals. For example, when two distinct μ_2-OH signals arise in the same ^{1}H-NMR spectrum, it can be difficult to tell them apart. Two examples of this from above are the Al-(μ_2-OH)-Al bridges of Elders and colleagues' Keggin cluster,[7] and the hexanuclear yttrium species by Hubert-Pfalzgraf and coworkers.[57]

These data can also help with identifying possibly missioned signals. For instance, in $[Al(\mu\text{-}OH)(hbo)_2]_2$ (hbo: 2-(2'-hydroxphenyl)-2-benzoxazole)) a peak at 11.47 ppm observed in $CDCl_3$ is proposed to be the bridging hydroxo ligands.[61] Is it possible that this is really a small amount of an aquo-Al(III) complex or some other aquo ligand-containing species? The data reported herein and our literature survey suggest that resonances this far downfield are typically due to aquo ligands; however, there are very few examples of NMR data reported for such species in $CDCl_3$, so much remains to be learned. Similarly, are the peaks assigned to aquo ligands in the spectra of Al(III) and Ga(III) porphyrins containing Ga-(μ_2-OH)-Ga and In-(μ_2-OH)-In bridges at 1.5 and 1.56 ppm, respectively, actually the hydroxide bridges?[60] Hopefully, these tabulated data can be helpful for the future assignment of μ_2-OH and μ_3-OH bridges in related compounds and help begin to develop a reliable database of such peak assignments.

4.3 Experimental

Chemicals were purchased from Sigma-Aldrich, TCI America, and STREM, and were used as received without further purification. The $Ga_{13-x}In_x$ clusters were synthesized using previously published methods.[13,15,62] ^{1}H-NMR experiments were conducted at 25°C in 5 mm tubes on a 500 MHz Varian spectrometer. Data were collected using Varian Software, referenced to TMS, and processed using MestReNova. The DOSY experiments were performed using the gradient stimulated echo with spin-lock and convection compensation (DgsteSL_cc) pulse sequences. All Varian software standard default settings were kept for DOSY unless otherwise stated. The diffusion delay was increased to 200 ms, the number of increments was increased to 20, and the highest gradient value was set to 25,000. The alternate gradient sign on odd scans and lock gating during gradient portions were also selected. All Varian software standard default settings were kept for NOESY unless otherwise stated. The NOESY experiment was performed after setting the 90° pulse-width to 13.0 ms, dscale increment to 700 ms, and the t1 increment to 256. To acquire quality resolution, 16 scans were performed.

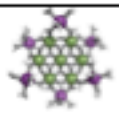
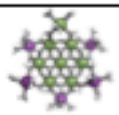
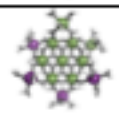
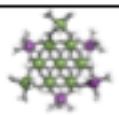
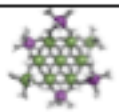
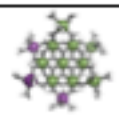
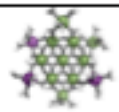
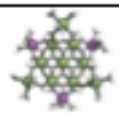
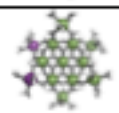
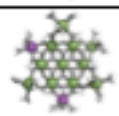
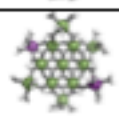
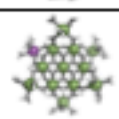
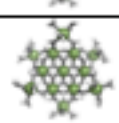
Quantum mechanical computations were used to predict the chemical shifts of each hydroxo proton in the clusters. The geometries of all of the clusters were obtained from the crystal structures, including the counterions. The NMR chemical shifts were computed using gauge-independent atomic orbital (GIAO) method in B3LYP/def2-SVP level of theory in the gas-phase, all as implemented in Gaussian03.[63] Since the position of the counterions was not perfectly symmetric, we computed the chemical shifts for multiple counterion positions for each cluster structure, in order to eliminate the effects of static, individual counterion positions on the proton shifts. For example, for Ga_8In_5, with one external gallium, we computed the chemical shifts of 6 geometries of this cluster, one for each position the gallium could occupy relative to the counterion positions. Each computed shifts of each type of proton were averaged across clusters of the same geometry discounting counterions, and the shifts were scaled using constant factors for each type.[16]

This particular method and procedure were chosen because exclusion of the counterions yielded incorrect ordering of the external and internal μ_2-OH protons, regardless of geometry of the protons at any level of theory attempted by our hands. Initially, we fully optimized the entire cluster species, including the proton positions. However, the resulting structures deviated largely from the known symmetry of these structures as determined by NMR, yielding wildly varying values for the chemical shifts of identical proton types. In addition, it is important to note that the theoretical predictions of the proton spectra appeared uncannily consistent with experimental spectra, even with accounting for all peaks. However, upon deeper examination of the experimental spectra of the clusters, we have discovered that the internal and external m2-OH signals were switched (See Appendix 3). Therefore, these were not used, and crystallographically determined positions were used instead. Bond lengths for the oxygen hydrogen bonds determined from crystallography may often be 0.2-0.3 Å short; however, we found that experimentally consistent and useful computed shift values could still be obtained in comparison to experiments, in contrast to results from DFT geometry optimizations.

4.4 Results and Discussion

The mixed $Ga_{13-x}In_x$ clusters each yield a unique ^{1}H-NMR spectrum after one day in d6-DMSO solution (Figure 4.7).[64] The clusters were crystallographically resolved prior to ^{1}H-NMR analysis to determine the stoichiometric ratio of the metal atoms. Diffusion Ordered Spectroscopy (DOSY) was used to verify the presence and integrity of clusters in solution. The hydrodynamic radius of each heterometallic cluster matches that of Ga_{13} (Figure 4.8), which was previously characterized using complementary techniques.[2,65] The combination of consistent hydrodynamic radii and the absence of any other proton signals (other than solvent) suggest that the spectra of the clusters consist of bridging hydroxide and/or capping water ligand signals. The distinct combinations of resonances observed in each spectrum confirm that the heterometallic clusters exist as distinct species.

Table 4.6. The symmetry and expected proton signal ratios for each type of hydroxide.

Cluster	Structure	Point Group	Expected Signals		
			6 μ_3-OH	6 μ_2-OH$_{int}$	12 μ_2-OH$_{ext}$
Ga_7In_6		D_{3d}	6 $H^{\mu_3}_{InInIn}$ (A)	6 $H^{\mu_2 int}_{InInIn}$ (G)	12 $H^{\mu_2 ext}_{InIn}$ (M)
Ga_8In_5		C_{3v}	3 $H^{\mu_3}_{InInIn}$ (A) 2 $H^{\mu_3}_{InInGa}$ (B) 1 $H^{\mu_3}_{InGaIn}$ (D)	3 $H^{\mu_2 int}_{InInIn}$ (G) 2 $H^{\mu_2 int}_{InInGa}$ (H) 1 $H^{\mu_2 int}_{InGaIn}$ (J)	8 $H^{\mu_2 ext}_{InIn}$ (M) 2 $H^{\mu_2 ext}_{InGa}$ (N) 2 $H^{\mu_2 ext}_{GaIn}$ (O)
Ga_9In_4		C_{3v}	2 $H^{\mu_3}_{InInIn}$ (A) 2 $H^{\mu_3}_{InInGa}$ (B) 2 $H^{\mu_3}_{GaGaIn}$ (E)	2 $H^{\mu_2 int}_{InInIn}$ (G) 2 $H^{\mu_2 int}_{InInGa}$ (H) 2 $H^{\mu_2 int}_{GaGaIn}$ (K)	6 $H^{\mu_2 ext}_{InIn}$ (M) 2 $H^{\mu_2 ext}_{InGa}$ (N) 2 $H^{\mu_2 ext}_{GaIn}$ (O) 2 $H^{\mu_2 ext}_{GaGa}$ (P)
		C_{3v}	1 $H^{\mu_3}_{InInIn}$ (A) 2 $H^{\mu_3}_{InInGa}$ (B) 1 $H^{\mu_3}_{GaInGa}$ (C) 2 $H^{\mu_3}_{InGaIn}$ (D)	1 $H^{\mu_2 int}_{InInIn}$ (G) 2 $H^{\mu_2 int}_{InInGa}$ (H) 1 $H^{\mu_2 int}_{GaInGa}$ (I) 2 $H^{\mu_2 int}_{InGaIn}$ (J)	4 $H^{\mu_2 ext}_{InIn}$ (M) 4 $H^{\mu_2 ext}_{InGa}$ (N) 4 $H^{\mu_2 ext}_{GaIn}$ (O)
		C_{3v}	4 $H^{\mu_3}_{InInGa}$ (B) 2 $H^{\mu_3}_{InGaIn}$ (D)	4 $H^{\mu_2 int}_{InInGa}$ (H) 2 $H^{\mu_2 int}_{InGaIn}$ (J)	4 $H^{\mu_2 ext}_{InIn}$ (M) 4 $H^{\mu_2 ext}_{InGa}$ (N) 4 $H^{\mu_2 ext}_{GaIn}$ (O)
$Ga_{10}In_3$		C_{3v}	1 $H^{\mu_3}_{InInIn}$ (A) 2 $H^{\mu_3}_{InInGa}$ (B) 2 $H^{\mu_3}_{GaGaIn}$ (E) 1 $H^{\mu_3}_{GaGaGa}$ (F)	2 $H^{\mu_2 int}_{InInIn}$ (G) 2 $H^{\mu_2 int}_{InInGa}$ (H) 2 $H^{\mu_2 int}_{GaGaIn}$ (K) 3 $H^{\mu_2 int}_{GaGaGa}$ (L)	4 $H^{\mu_2 ext}_{InIn}$ (M) 2 $H^{\mu_2 ext}_{InGa}$ (N) 2 $H^{\mu_2 ext}_{GaIn}$ (O) 4 $H^{\mu_2 ext}_{GaGa}$ (P)
		C_1	2 $H^{\mu_3}_{InInGa}$ (B) 1 $H^{\mu_3}_{GaInGa}$ (C) 1 $H^{\mu_3}_{InGaIn}$ (D) 2 $H^{\mu_3}_{GaGaIn}$ (E)	2 $H^{\mu_2 int}_{InInGa}$ (H) 1 $H^{\mu_2 int}_{GaInGa}$ (I) 2 $H^{\mu_2 int}_{InGaIn}$ (J) 2 $H^{\mu_2 int}_{GaGaIn}$ (K)	2 $H^{\mu_2 ext}_{InIn}$ (M) 4 $H^{\mu_2 ext}_{InGa}$ (N) 4 $H^{\mu_2 ext}_{GaIn}$ (O) 2 $H^{\mu_2 ext}_{GaGa}$ (P)
		C_{3v}	3 $H^{\mu_3}_{GaInGa}$ (C) 3 $H^{\mu_3}_{InGaIn}$ (D)	3 $H^{\mu_2 int}_{GaInGa}$ (I) 3 $H^{\mu_2 int}_{InGaIn}$ (J)	6 $H^{\mu_2 ext}_{InGa}$ (N) 6 $H^{\mu_2 ext}_{GaIn}$ (O)
$Ga_{11}In_2$		C_{3v}	2 $H^{\mu_3}_{InInGa}$ (B) 2 $H^{\mu_3}_{GaGaIn}$ (E) 2 $H^{\mu_3}_{GaGaGa}$ (F)	2 $H^{\mu_2 int}_{InInGa}$ (H) 2 $H^{\mu_2 int}_{GaGaIn}$ (K) 2 $H^{\mu_2 int}_{GaGaGa}$ (L)	2 $H^{\mu_2 ext}_{InIn}$ (M) 2 $H^{\mu_2 ext}_{InGa}$ (N) 2 $H^{\mu_2 ext}_{GaIn}$ (O) 6 $H^{\mu_2 ext}_{GaGa}$ (P)
		C_{3v}	2 $H^{\mu_3}_{GaInGa}$ (C) 1 $H^{\mu_3}_{InGaIn}$ (D) 2 $H^{\mu_3}_{GaGaIn}$ (E) 1 $H^{\mu_3}_{GaGaGa}$ (F)	2 $H^{\mu_2 int}_{GaInGa}$ (I) 1 $H^{\mu_2 int}_{InGaIn}$ (J) 2 $H^{\mu_2 int}_{GaGaIn}$ (K) 1 $H^{\mu_2 int}_{GaGaGa}$ (L)	4 $H^{\mu_2 ext}_{InGa}$ (N) 4 $H^{\mu_2 ext}_{GaIn}$ (O) 4 $H^{\mu_2 ext}_{GaGa}$ (P)
		C_{3v}	2 $H^{\mu_3}_{GaInGa}$ (C) 4 $H^{\mu_3}_{GaGaIn}$ (E)	2 $H^{\mu_2 int}_{GaInGa}$ (I) 4 $H^{\mu_2 int}_{GaGaIn}$ (K)	4 $H^{\mu_2 ext}_{InGa}$ (N) 4 $H^{\mu_2 ext}_{GaIn}$ (O) 4 $H^{\mu_2 ext}_{GaGa}$ (P)
$Ga_{12}In_1$		C_{3v}	1 $H^{\mu_3}_{GaInGa}$ (C) 2 $H^{\mu_3}_{GaGaIn}$ (E) 3 $H^{\mu_3}_{GaGaGa}$ (F)	1 $H^{\mu_2 int}_{GaInGa}$ (I) 2 $H^{\mu_2 int}_{GaGaIn}$ (K) 3 $H^{\mu_2 int}_{GaGaGa}$ (L)	2 $H^{\mu_2 ext}_{InGa}$ (N) 2 $H^{\mu_2 ext}_{GaIn}$ (O) 8 $H^{\mu_2 ext}_{GaGa}$ (P)
Ga_{13}		D_{3d}	6 $H^{\mu_3}_{GaGaGa}$ (F)	6 $H^{\mu_2 int}_{GaGaGa}$ (L)	12 $H^{\mu_2 ext}_{GaGa}$ (P)

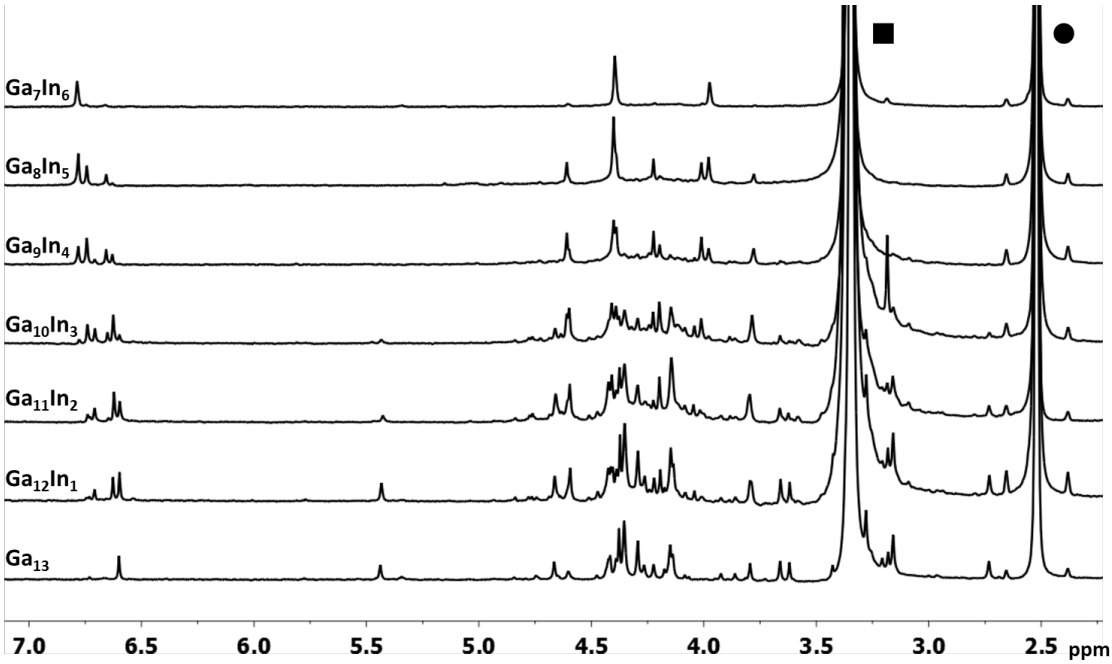


Figure 4.7. ^{1}H-NMR spectra of 2 mM clusters in d_6-DMSO one day after dissolution. H_2O peak (■) and DMSO peak (●).

Understanding the symmetry of these $Ga_{13-x}In_x$ clusters is essential for analyzing and assigning the proton shifts from NMR. The symmetry of each cluster dictates the number of expected signals that the cluster will have from the hydroxyl protons and aquo ligands. For example, the Ga_7In_6 and Ga_{13} clusters have identical symmetry, and therefore should only ideally yield three total signals from hydroxyl protons. Table 6 lists the symmetry of all $Ga_{13-x}In_x$ clusters studied herein.

Water ligands coordinated to multimetallic Group 13 complexes are known to produce signals from 7—10 ppm.[3] The $Ga_{13-x}In_x$ clusters contain signals between 2.5—7 ppm, which falls into the range expected for μ_2-OH and μ_3-OH bridges. The spectrum of Ga_7In_6 is much simpler than that of the Ga_{13} cluster.[2] We suspect this is due to the fact that the 1st order rate constant of water exchange for In(III) is 100x faster than for Ga(III) ($4x10^4$ s^{-1} and $4x10^2$ s^{-1}, respectively).[66] The lack of peaks in the 7—10 ppm region indicates that the exchange rate of the outer water ligands is too fast to observe on the NMR time scale.[2] The rapid aquo ligand exchange of the In(III) ions allows us to observe

only the protons associated with the central 7-atom Ga(III) core of Ga_7In_6 leading to 3 signals (μ_3-OH, μ_2-OH_{ext}, and μ_2-OH_{int}) are observable. This aquo ligand exchange process happens much slower with gallium; therefore, the symmetry within the core of Ga_{13} is not retained and results in a complex spectrum containing more proton signals.

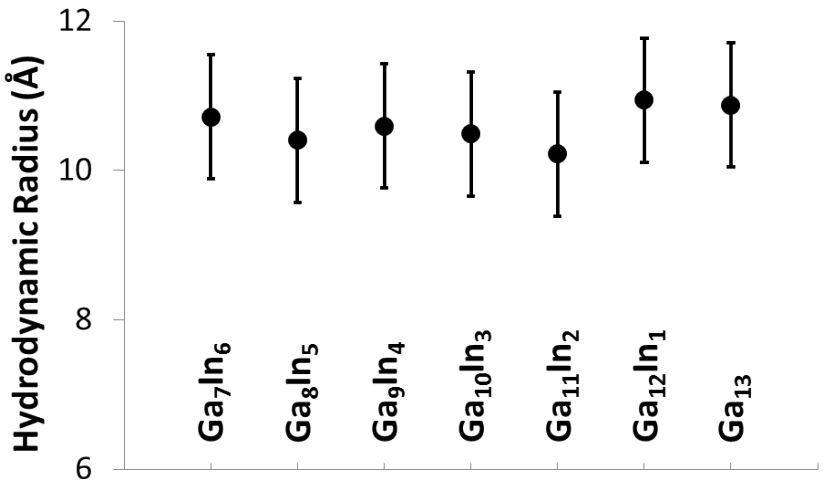


Figure 4.8. Hydrodynamic radii and standard deviation of the clusters measured via DOSY.

4.4.1 Ga_7In_6 Peak Assignments: Establishing a Basis for Comparison

Ga_7In_6 is a great test case to understand the more complicated clusters where gallium occupies one or more of the peripheral metal sites. The simplicity of the experimental data and the high symmetry of this cluster makes this cluster ideal for the purpose of assigning regions of the spectrum to particular types of protons, which in turn may be used to assign shifts for the other clusters. This assignment was in turn used to determine an appropriate computational method for predicting the proton shifts of the remaining clusters. The computations resulted in subtle differences in the positions of the signals from different types of hydroxo bridges in the clusters, in particular, the μ_2-OH region, which shows strong overlap of the two types of signals (Figure 4.7). The μ_3-OH proton signals are observed between 6.5–7.0 ppm. The remaining μ_2-OH_{int} and μ_2-OH_{ext} proton signals are found between 3.5–5.0 ppm.

Ga_7In_6 ^{1}H-NMR spectra reveal 3 signals, which can be assigned to the three types of bridging hydroxides (Figure 4.9). These three signals integrate to a 1:2:1 ratio, matching the number of protons on specific hydroxide bridges within the 7-atom cluster core (μ_3-OH:μ_2-OH$_{ext}$:μ_2-OH$_{int}$ ratio = 6:12:6) (Figure 4.1, Table 4.6). This suggests that the peak at 4.4 ppm corresponds to the μ_2-OH$_{ext,}$ which bridge between the 7-atom gallium core and the exterior indiums ions. Other examples of mixed metal Ga-(μ_2-OH)-M bridges corroborate this assignment (Ga-(μ_2-OH)-Ca and Ga-(μ_2-OH)-Sr; 4.73 ppm and 4.49 ppm respectively).[53] As stated above, the signal furthest downfield (~6.8 ppm) corresponds to the protons of the μ_3-OH, similar to the chemical shift of the μ_3-OH bridge in the octahedral Y^{3+} complex.[58] The final peak at 4.0 ppm represents the μ_2-OH$_{int}$ protons. This assignment is in agreement with M-(μ_2-OH)-M bridges reported for other Group 13 complexes.[5,7–10]

Due to the simplicity of Ga_7In_6, the spectra and analysis for this cluster make a good basis for determining a suitable theoretical method for computational elucidation of the μ_2-OH signals. Most importantly, computations performed without explicit counterions in the structure predict the exact opposite ordering of the internal and external μ_2-OH signals. This was so, regardless of the theoretical methods (HF, B3LYP), basis sets (6-31G*/LANL2DZ, def2-SVP,[69] def2-TZVP,[69] def2-QZVP,[69] etc.), or solvation methods (gas, COSMO,[67] PCM,[68] and CPCM) employed. From our observations, improvements in levels of theory are unlikely to address the discrepancy. However, when counterions are included, correct ordering is obtained, namely that the μ_2-OH$_{ext}$ signals are downfield from the μ_2-OH$_{int}$ protons (Figure 4.9). These results indicate that the presence, location, and identity of the counterions is immensely important for determining even the qualitative assignments of ^{1}H-NMR chemical shifts of aqueous metal clusters. The ordering or the μ_2-OH$_{int\ and}$ μ_2-OH$_{ext}$ protons is more difficult to see for the remainder of the clusters due to significant overlap of μ_2-OH signals, and computations were diagnostic in discriminating these convoluted overlapping signals in all the clusters.

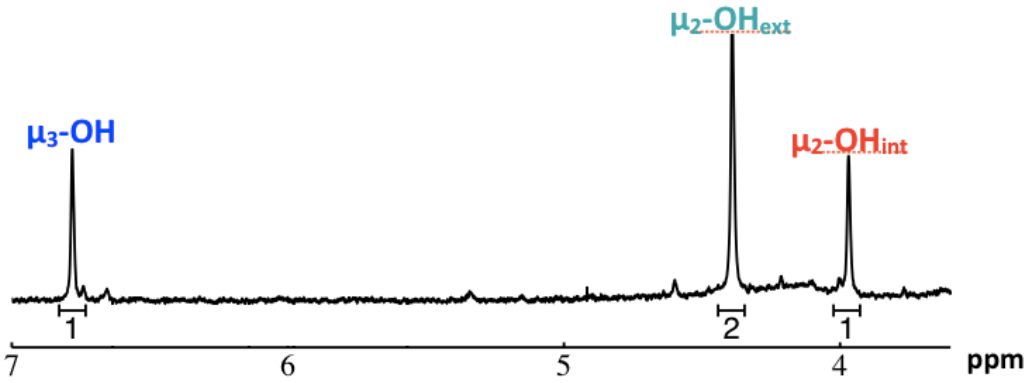


Figure 4.9. ^{1}H-NMR spectra of 2 mM Ga_7In_6 cluster in d_6-DMSO one day after dissolution: The visible signals correspond to the 3 types of bridging hydroxides.

4.4.2 Hydroxo Ligand Naming Convention

As gallium is substituted for indium in the exterior positions of the cluster, a greater number of proton types emerge (Figure 4.6). There are 16 unique types of protons in the clusters based on idealized symmetry: 6 μ_3-OH, 6 μ_2-OH_{int}, and 4 types of μ_2-OH_{ext} (Table 6). The environments of these protons were determined by the identity of the nearest external metal ion and its two nearest neighbors (i.e., Ga or In). For example, proton $H^{\mu_3}_{\mathrm{In}\mathbf{In}\mathrm{In}}$ is a μ_3-OH proton in a section of the cluster with an exterior indium ion directly outside (always indicated in bold) possessing two additional exterior indium atoms on either side (Figure 4.10). Proton $H^{\mu_{2\mathrm{int}}}_{\mathrm{In}\mathbf{In}\mathrm{In}}$ corresponds to the symmetry-equivalent μ_2-OH_{int} proton bridging the same metals as proton $H^{\mu_3}_{\mathrm{In}\mathbf{In}\mathrm{In}}$ (Figure 4.10) The μ_2-OH_{ext} protons are described in a similar manner. Proton $H^{\mu_{2\mathrm{ext}}}_{\mathbf{In}\mathrm{In}}$ corresponds to the μ_2-OH_{ext} proton connected to an indium ion (indicated in bold) and positioned facing towards a second indium. This naming system is comprehensively represented by Table 4.6.

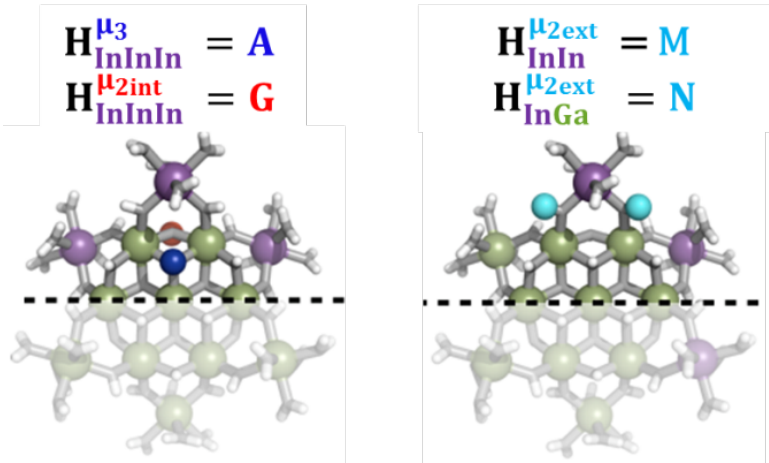


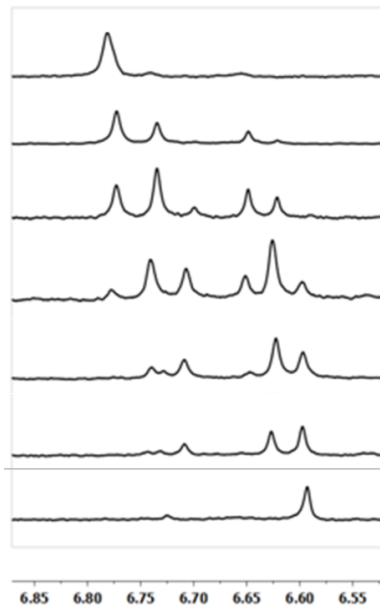
Figure 4.10. Naming system for protons in the $\mathbf{Ga_{13-x}In_x}$ clusters.

4.4.3 μ_3-OH Peak Assignments

The peak in the 6.55-6.85 ppm region of the Ga_7In_6 spectrum corresponds to the μ_3-OH protons. This region contains the simplest set of signals in all the mixed clusters. We suspect that this is because the μ_3-OH protons are the farthest away from, and therefore, the least affected by the bound DMSO. Each peak in this region for the 7 NMR spectra is corresponds to one of the 6 types of μ_3-OH protons (Table 7). Proximity to the indium ion causes downfield shifting in the proton signal. This is best shown in Ga_7In_6, which has one type of proton ($H^{\mu_3}_{InInIn}$), and exhibits the farthest downfield signal. Ga_{13} also has only one type of μ_3-OH proton ($H^{\mu_3}_{GaGaGa}$); however, the lack of indium atoms in the structure leads to the farthest upfield μ_3-OH signal. Ga_8In_5 and $Ga_{12}In_1$ each possess one isomer and 3 unique μ_3-OH proton types ($H^{\mu_3}_{InInIn}$, $H^{\mu_3}_{InInGa}$, $H^{\mu_3}_{InGaIn}$ and $H^{\mu_3}_{GaGaGa}$, $H^{\mu_3}_{GaGaIn}$, $H^{\mu_3}_{GaInGa}$, respectively) in 3:2:1 ratios. This is mirrored in the NMR spectra facilitating the assignment of each proton type to a peak (Table 7). Ga_9In_4, $Ga_{10}In_3$, and $Ga_{11}In_2$ are slightly more complicated because each has 3 possible isomers (Table 6), but each predicted μ_3-OH peak is observed. The $H^{\mu_3}_{InInIn}$ type protons are shifted farthest downfield, while the $H^{\mu_3}_{GaGaGa}$ type protons are shifted the farthest upfield, for an overall ranking from highest to lowest ppm of $H^{\mu_3}_{InInIn} > H^{\mu_3}_{InInGa} > H^{\mu_3}_{GaInGa} > H^{\mu_3}_{InGaIn} > H^{\mu_3}_{GaGaIn} > H^{\mu_3}_{GaGaGa}$ (Table 7). Computations support that these signals are produced by μ_3-OH protons and that the $H^{\mu_3}_{InInIn}$, $H^{\mu_3}_{InInGa}$, and $H^{\mu_3}_{GaInGa}$ protons should be more deshielded than the $H^{\mu_3}_{InGaIn}$, $H^{\mu_3}_{GaGaIn}$, and

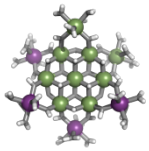
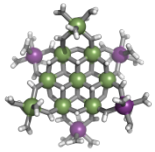
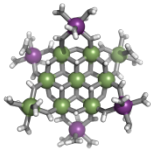
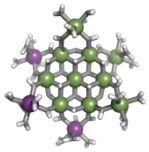
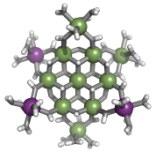
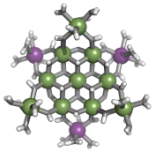
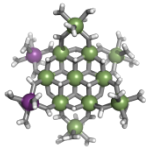
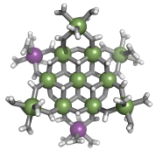
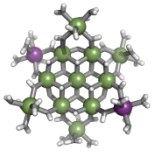
$H^{\mu_3}_{\mathbf{Ga}GaGa}$ protons. The calculations cannot corroborate or contradict the relative rankings within those two sets (Table 7).

Table 4.7. Unique μ_3-OH proton environments of each cluster and the corresponding ^{1}H-NMR fingerprint region. (*assuming 1:1:1 isomeric ratio)

Corresponding μ_3-OH NMR Spectra (ppm)	Cluster	Expected Proton Ratios (Observed Proton Ratios)						
		A	B	C	D	E	F	# of Isomers
	Ga_7In_6	6(6)	-	-	-	-	-	1
	Ga_8In_5	3(3)	2(2)	-	1(1)	-	-	1
	Ga_9In_4	3(4)	8(6)	1(1)	4(3)	2(2)	-	3*
	$Ga_{10}In_3$	1(1)	4(6)	4(3)	4(3)	4(6)	1(1)	3*
	$Ga_{11}In_2$	-	2(2)	4(3)	1(1)	8(6)	3(4)	3*
	$Ga_{12}In_1$	-	-	1(1)	-	2(2)	3(3)	1
	Ga_{13}	-	-	-	-	-	6(6)	1

In the case of clusters with multiple isomers, the peak integrations of the μ_3-OH protons in the NMRs can provide information about the ratio of each isomer present in the sample. The statistical probability of each isomer, along with the calculated % present in solution, is shown in Table 8. Similarities in the structures of Ga_9In_4 and $Ga_{11}In_2$ allow for comparisons.[70] The NMR data remarkably show a strong correlation to the statistical ratio of isomeric heterometallic clusters. This data indicates that no specific substitution pattern of indium in the outer shell of the clusters is kinetically favorable.

Table 4.8. The isomers of Ga_9In_4, $Ga_{10}In_3$, and $Ga_{11}In_2$ with relative μ_2-OH peak intensities predicted using the integration of μ_3-OH protons, ratio of isomers in solution based on probability, and experimental percentage of isomers present in solution calculated using the μ_3-OH proton integrations. Green: Gallium. Purple: Indium.

Protons	G	H	I	J	K	I	M	N	O	P
Integrations	4	6	1	3	2	-	12	8	8	2
Ga_9In_4 Isomers										
Experimental	40%				40%			20%		
Probability	40%				40%			20%		
Integrations	1	6	3	3	6	1	8	13	13	8
$Ga_{10}In_3$ Isomers										
Experimental	40%				50%			10%		
Probability	30%				60%			10%		
Integrations	-	2	3	1	6	4	2	8	8	12
$Ga_{11}In_2$ Isomers										
Experimental	-				-			-		
Probability	40%				40%			20%		

4.4.4 μ_2-OH Peak Assignments

The μ_2-OH regions of the NMR spectra are not as easily deconvoluted. Based on the Ga_7In_6 spectrum, the upfield peaks correspond to μ_2-OH bridges, but as more gallium atoms are introduced into the outermost shell and exchange between the coordinating water ligands and DMSO slows, symmetry is broken, and complexity increases. We now

propose to assign these peaks as well. As with the μ_3-OH protons, computations were used to establish the range in which the μ_2-OH protons should be found.

4.4.4.1 Ga_8In_5

After the Ga_7In_6 cluster, Ga_8In_5 is the next easiest to analyze because it only has one isomer. Using the information gained in the μ_3-OH assignment a similar analysis involving integrations of signals and protons signals can be assigned (Figure 4.11). The μ_2-OH_{int} are the same as their μ_3-OH counterparts existing in a 3:2:1 ratio ($H^{\mu_{2int}}_{\mathrm{In}\mathbf{In}\mathrm{In}}$: $H^{\mu_{2int}}_{\mathrm{In}\mathbf{In}\mathrm{Ga}}$: $H^{\mu_{2int}}_{\mathrm{In}\mathbf{Ga}\mathrm{In}}$). The μ_2-OH_{ext} appear in an 8:2:2 ratio ($H^{\mu_{2ext}}_{\mathbf{In}\mathrm{In}}$: $H^{\mu_{2ext}}_{\mathbf{In}\mathrm{Ga}}$: $H^{\mu_{2ext}}_{\mathbf{Ga}\mathrm{In}}$), making it difficult to differentiate between protons $H^{\mu_{2ext}}_{\mathbf{In}\mathrm{Ga}}$ and $H^{\mu_{2ext}}_{\mathbf{Ga}\mathrm{In}}$. However, Nuclear Overhauser Effect Spectroscopy (NOESY) correlates protons that are near each other through space. The μ_3-OH protons are 3.34 Å and 3.24 Å away from the neighboring μ_2-OH_{ext} bridges in the solid state. Since the μ_3-OH and μ_2-OH_{ext} bridges are significantly less than 5 Å,71 they exhibit strong through-space interactions allowing $H^{\mu_{2ext}}_{\mathbf{In}\mathrm{Ga}}$ and $H^{\mu_{2ext}}_{\mathbf{Ga}\mathrm{In}}$ to be assigned using NOESY (Figure 4.12).

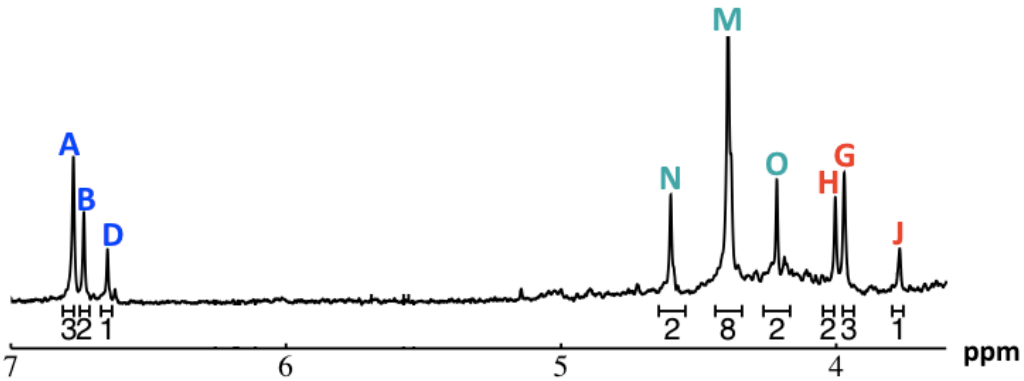


Figure 4.11. The ^{1}H-NMR of 2 mM $\mathbf{Ga_8In_5}$ in d_6-DMSO 1 day after dissolution with peak assignment. $H^{\mu_3}_{\mathrm{In}\mathbf{In}\mathrm{In}}$ (A), $H^{\mu_3}_{\mathrm{In}\mathbf{In}\mathrm{Ga}}$ (B), $H^{\mu_3}_{\mathrm{In}\mathbf{Ga}\mathrm{In}}$ (D), $H^{\mu_{2int}}_{\mathrm{In}\mathbf{In}\mathrm{In}}$ (G), $H^{\mu_{2int}}_{\mathrm{In}\mathbf{In}\mathrm{Ga}}$ (H), $H^{\mu_{2int}}_{\mathrm{In}\mathbf{Ga}\mathrm{In}}$ (J), $H^{\mu_{2ext}}_{\mathbf{In}\mathrm{In}}$ (M), $H^{\mu_{2ext}}_{\mathbf{In}\mathrm{Ga}}$ (N), $H^{\mu_{2ext}}_{\mathbf{Ga}\mathrm{In}}$ (O).

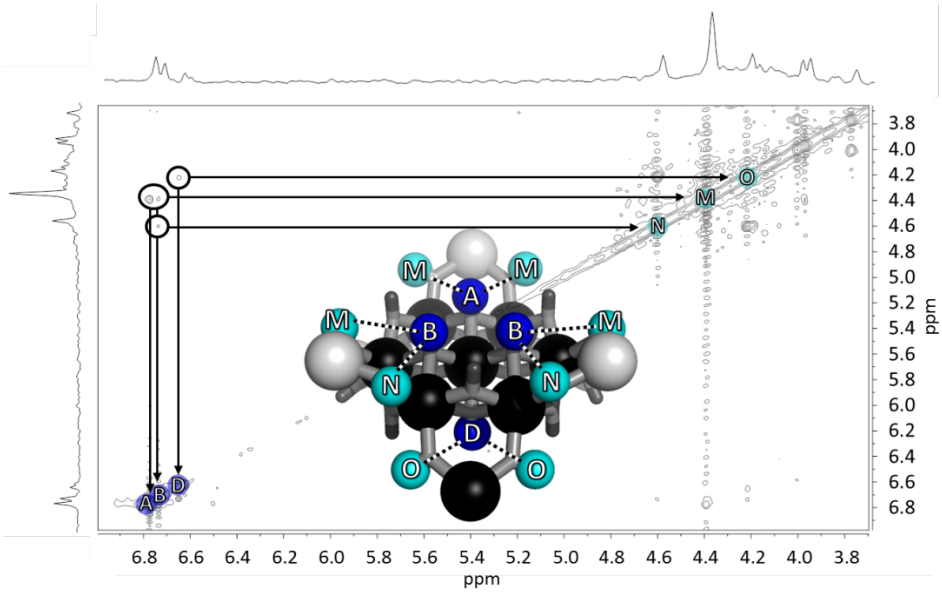


Figure 4.12. The NOESY of Ga_8In_5 indicating the proper peak assignment of the $H^{\mu_{2ext}}_{\mathbf{In}In}$ (M), $H^{\mu_{2ext}}_{\mathbf{In}Ga}$ (N), and $H^{\mu_{2ext}}_{\mathbf{Ga}In}$ (O) protons. Water ligands have been omitted from the structure for clarity. ● Gallium, ○ Indium, $H^{\mu_3}_{In\mathbf{In}In}$ (A), $H^{\mu_3}_{In\mathbf{In}Ga}$ (B), $H^{\mu_3}_{In\mathbf{Ga}In}$ (D).

The use of these experimental results allowed for additional verification of quantum mechanical methods. The assignments based on integration values and the NOESY spectra established a basis of comparison for determining the most accurate computational method. Using the average computed NMR shifts from the structures with counterions for each proton type, the computed results were compared to the experimentally determined proton shifts for several basis sets, mentioned previously. The def2-SVP basis set was found to provide the optimal combination of accuracy and computational time, as the computed proton rankings were an exact match with experimental results. Therefore, we know this computational method can be used to assign the protons in the more complicated spectra with a larger number of isomers and an increasing number of gallium centers.

4.4.4.2 Ga_9In_4

Ideally Ga_9In_4 has 5 types of μ_2-OH_{int} and all 4 types of μ_2-OH_{ext} bridges. As previously stated, this cluster has 3 isomers which exist in a 2:2:1 ratio. This means that the protons in Ga_9In_4 should integrate to the ratios shown in Table 9. Based on these integrations, peaks have been experimentally assigned to the Ga_9In_4 spectrum (Figure 4.13). Peaks $H^{\mu_{2int}}_{InInIn}$, $H^{\mu_{2int}}_{InInGa}$, and $H^{\mu_{2ext}}_{InGa}$ are the same as for Ga_8In_5. Proton $H^{\mu_{2int}}_{GaInGa}$ which integrates to 1 is too small to identify in the baseline noise between 3.7 and 4.8 ppm. The peak for proton $H^{\mu_{2int}}_{InGaIn}$ overlaps with $H^{\mu_{2int}}_{GaGaIn}$ giving an integration of 5 for the combined signal. There should still be a strong signal at 4.4 ppm from $H^{\mu_{2ext}}_{InIn}$ for Ga_9In_4; however, an integration of 14 suggests that proton $H^{\mu_{2ext}}_{GaGa}$ also appears at this chemical shift. Interestingly, the signal for proton $H^{\mu_{2ext}}_{GaIn}$ seems to have split into two peaks at ~4.2 ppm. This is most likely due to the slower exchange rate of the outer water ligands on gallium. Because $H^{\mu_{2ext}}_{GaIn}$ is bridging an outer gallium atom this may be the first sign of the complex spectrum we see for Ga_{13}. This may also explain the small shoulder/splitting of peak $H^{\mu_{2ext}}_{InGa}$ and $H^{\mu_{2ext}}_{InIn}$/$H^{\mu_{2ext}}_{GaGa}$.

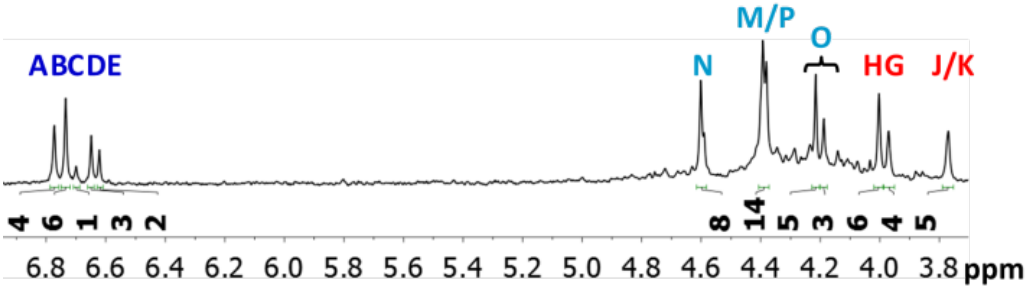


Figure 4.13. The ^{1}H-NMR of 2 mM Ga_9In_4 in d_6-DMSO 1 day after dissolution with experimental peak assignment. $H^{\mu_3}_{InInIn}$ (A), $H^{\mu_3}_{InInGa}$ (B), $H^{\mu_3}_{GaInGa}$ (C), $H^{\mu_3}_{InGaIn}$ (D), $H^{\mu_3}_{GaGaIn}$ (E), $H^{\mu_{2int}}_{InInIn}$ (G), $H^{\mu_{2int}}_{InInGa}$ (H), $H^{\mu_{2int}}_{InGaIn}$ (J), $H^{\mu_{2int}}_{GaGaIn}$ (K), $H^{\mu_{2ext}}_{InIn}$ (M), $H^{\mu_{2ext}}_{InGa}$ (N), $H^{\mu_{2ext}}_{GaIn}$ (O), $H^{\mu_{2ext}}_{GaGa}$ (P).

Computations are particularly useful for corroborating the assignments in the spectra of Ga_9In_4. Because many of the peaks overlap with others, the integrations are no longer solely reliable for making full assignments. Therefore, the relative values of the computed NMR shiftswere used alongside the known assignments from Ga_7In_6 and Ga_8In_5 for the most precise results. This allowed for the $H^{\mu_{2ext}}_{InIn}$ and $H^{\mu_{2ext}}_{GaGa}$ peaks to be distinguished, as well as the $H^{\mu_{2ext}}_{GaIn}$ and $H^{\mu_{2int}}_{GaInGa}$ peaks (Figure 4.14). For the $H^{\mu_{2ext}}_{InIn}$ and $H^{\mu_{2ext}}_{GaGa}$ peaks, computations showed that the $H^{\mu_{2ext}}_{InIn}$ peak should have a slightly downfield chemical shift compared to $H^{\mu_{2ext}}_{GaGa}$. Likewise, the computed shift for the $H^{\mu_{2int}}_{GaInGa}$was compared to the signals from the other internal and external μ_2-OH protons. This analysis showed that I should have the farthest downfield shift of the internal μ_2-OH protons, but should not be higher than any of the external μ_2-OH protons. After determining the identity of the peaks in the Ga_9In_4 spectrum, this method was used to further assign the peaks in the spectra of the clusters with increasing gallium content.

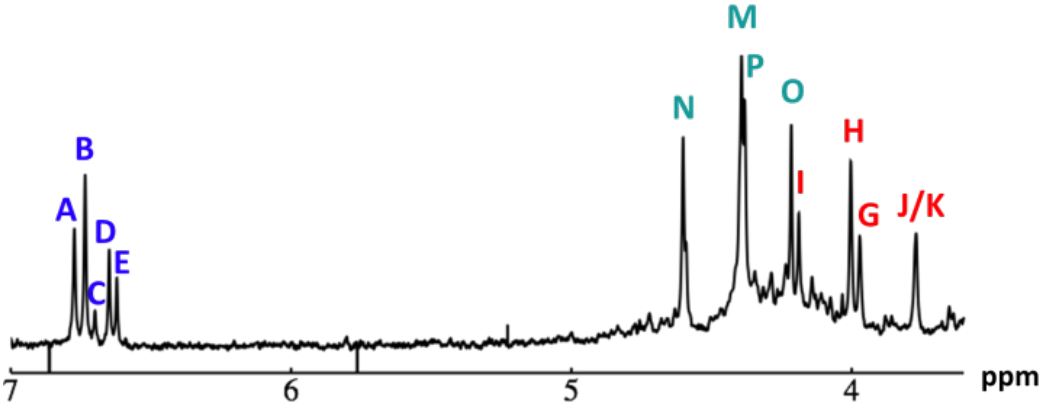


Figure 4.14. The ^{1}H-NMR of 2 mM Ga_9In_4 in d_6-DMSO 1 day after dissolution with computed peak assignment. $H^{\mu_3}_{\mathbf{In}\mathbf{In}In}$ (A), $H^{\mu_3}_{In\mathbf{In}Ga}$ (B), $H^{\mu_3}_{Ga\mathbf{In}Ga}$ (C), $H^{\mu_3}_{In\mathbf{Ga}In}$ (D), $H^{\mu_3}_{Ga\mathbf{Ga}In}$ (E), $H^{\mu_{2int}}_{In\mathbf{In}In}$ (G), $H^{\mu_{2int}}_{In\mathbf{In}Ga}$ (H), $H^{\mu_{2int}}_{Ga\mathbf{In}Ga}$ (I), $H^{\mu_{2int}}_{In\mathbf{Ga}In}$ (J), $H^{\mu_{2int}}_{Ga\mathbf{Ga}In}$ (K), $H^{\mu_{2ext}}_{\mathbf{In}In}$ (M), $H^{\mu_{2ext}}_{\mathbf{In}Ga}$ (N), $H^{\mu_{2ext}}_{\mathbf{Ga}In}$ (O), $H^{\mu_{2ext}}_{\mathbf{Ga}Ga}$ (P).

While these computations were successful in reproducing the relative ordering of proton signals, the present method is not sufficient to quantitatively reproduce the exact proton shifts. This is because this method does not rely on quantum

mechanically determined positions of the counterions with respect to the clusters. Quantitative predictions will necessitate a more rigorous method for determining the cluster–counterion complex. We suspect that the success of our method in being able to reproduce qualitative ordering of the proton peaks suggests that the counterions are loosely coordinated around the cluster and is dynamically equilibrating among the different sites in the NMR time scale. Work is continuing in this area to produce quantitative predictions from ab-initio molecular dynamics simulations with explicit counterions and solvents.

4.4.4.3 $Ga_{10}In_3$-Ga_{13}

Experimental data suggests that $Ga_{10}In_3$ also exists as three isomers but in a 3:6:1 ratio leading to the peak integrations listed in Table 8. Unfortunately, the complexity caused by the increasing number of exterior gallium atoms and the isomers does not allow these signals to be assigned experimentally. Similar issues arise for $Ga_{11}In_2$ to Ga_{13}. Given the complexity of the signals arising from the protons in these clusters, computations are particularly useful for peak assignment.

Computed shifts were used to assign the remaining types of protons for each of these clusters (Figure 4.16). Unfortunately, we are unable to compute the changes based on coordinated DMSO breaking the symmetry; therefore, only the peaks of the "mother cluster" (fully H_2O ligated) can be assigned in these spectra. Primarily, this involved computing the position of $H^{\mu_{2int}}_{\mathrm{Ga\mathbf{Ga}Ga}}$, which represents the protons in a section of the cluster with three external gallium ions next to each other. Computed results suggest that $H^{\mu_{2int}}_{\mathrm{Ga\mathbf{Ga}Ga}}$ should have the lowest shift of all of the internal μ_2-OH protons, which is the lowest ppm value for all of the computed signals.

The Ga_{13} mother cluster peaks ($H^{\mu_3}_{\mathrm{GaGaGa}}$, $H^{\mu_{2int}}_{\mathrm{GaGaGa}}$, and $H^{\mu_{2ext}}_{\mathrm{GaGa}}$) assigned via computations were thereafter confirmed experimentally. By plotting the ^{1}H-NMR spectra of Ga_{13}

dissolved in a variety of ratios of d_6-DMSO and d_7-DMF, it is clearly visible that only 3 peaks persist from 100% d_6-DMSO to 100% d_7-DMF (Figure 4.16). The other peaks visible in the spectra are caused by "daughter clusters" substituted with either DMSO or DMF ligands at the aquo sites; therefore, the only shared species must be the mother cluster.

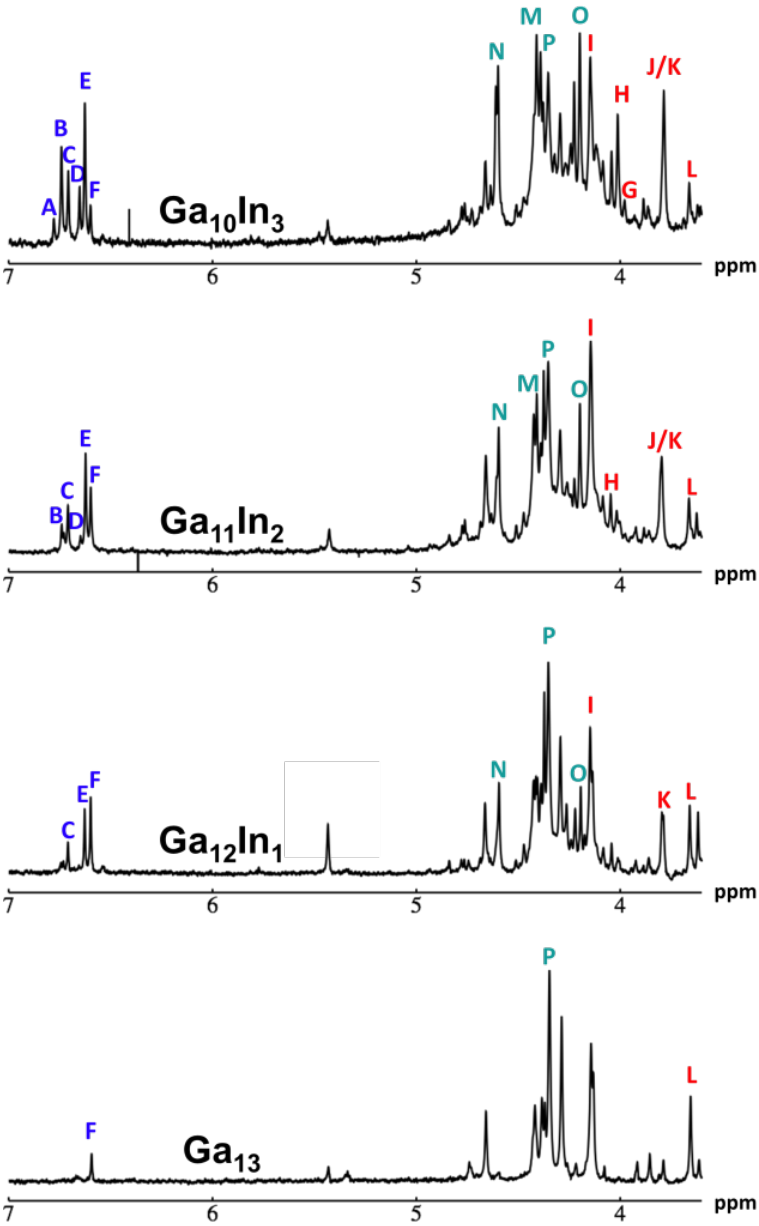


Figure 4.15. Computed results for μ_3-OH and μ_2-OH proton signals are shown overlaid with ^{1}H-NMR spectra of 2 mM $Ga_{10}In_3$, $Ga_{11}In_2$, $Ga_{12}In_1$, and Ga_{13} cluster in d_6-DMSO one day after dissolution $H^{\mu_3}_{\mathrm{In}\mathbf{In}\mathrm{In}}$ (A), $H^{\mu_3}_{\mathrm{In}\mathbf{In}\mathrm{Ga}}$ (B), $H^{\mu_3}_{\mathrm{Ga}\mathbf{In}\mathrm{Ga}}$ (C), $H^{\mu_3}_{\mathrm{In}\mathbf{Ga}\mathrm{In}}$ (D), $H^{\mu_3}_{\mathrm{Ga}\mathbf{Ga}\mathrm{In}}$ (E), $H^{\mu_3}_{\mathrm{Ga}\mathbf{Ga}\mathrm{Ga}}$ (F), $H^{\mu_{2\mathrm{int}}}_{\mathrm{In}\mathbf{In}\mathrm{In}}$ (G), $H^{\mu_{2\mathrm{int}}}_{\mathrm{In}\mathbf{In}\mathrm{Ga}}$ (H), $H^{\mu_{2\mathrm{int}}}_{\mathrm{Ga}\mathbf{In}\mathrm{Ga}}$ (I), $H^{\mu_{2\mathrm{int}}}_{\mathrm{In}\mathbf{Ga}\mathrm{In}}$ (J), $H^{\mu_{2\mathrm{int}}}_{\mathrm{Ga}\mathbf{Ga}\mathrm{In}}$ (K), $H^{\mu_{2\mathrm{int}}}_{\mathrm{Ga}\mathbf{Ga}\mathrm{Ga}}$ (L), $H^{\mu_{2\mathrm{ext}}}_{\mathbf{In}\mathrm{In}}$ (M), $H^{\mu_{2\mathrm{ext}}}_{\mathbf{In}\mathrm{Ga}}$ (N), $H^{\mu_{2\mathrm{ext}}}_{\mathbf{Ga}\mathrm{In}}$ (O), $H^{\mu_{2\mathrm{ext}}}_{\mathbf{Ga}\mathrm{Ga}}$ (P).

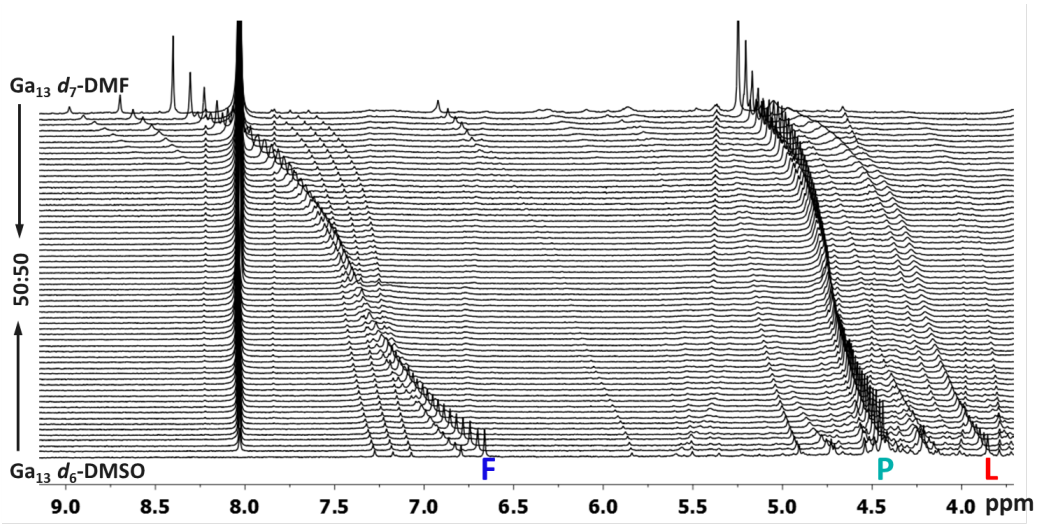


Figure 4.16. Stacked titration data indicating that only the $H^{\mu_3}_{\mathrm{Ga}\mathbf{Ga}\mathrm{Ga}}$(F), $H^{\mu_{2\mathrm{int}}}_{\mathrm{Ga}\mathbf{Ga}\mathrm{Ga}}$ (L), and $H^{\mu_{2\mathrm{ext}}}_{\mathbf{Ga}\mathrm{Ga}}$ (P) protons translate from the 100% d_6-DMSO to the 100% d_7-DMF spectrum. The triplet that persists in the 7.0 to 7.5 ppm region is attributed to ammonia in the sample.

4.5 Conclusion

This research has led to quick and cost effective differentiation and structural characterization of the $\mathbf{Ga_{13-x}In_x}$ clusters in solution via ^{1}H-NMR spectrscopy.[72] We have shown that each mixed $\mathbf{Ga_{13-x}In_x}$ cluster does independently exist in solution and that there are no kinetically or enthalpically favored isomers (i.e., only the expected statistical ratios of the various isomers were observed). These isomers exist in statistical ratios determined by probability of formation. In general, this study provides a complete method for experimentally and computationally predicting proton shifts for inorganic μ_3-OH and μ_2-OH signals in gallium and indium species, as well as, a literature review of hydroxide bridges for all diamagnetic metals available in the literature to the best of our knowledge. This knowledge will initiate the study of cluster dynamics in solution, allowing for better control and manipulation of precursor clusters. The solution behavior

of clusters condensing into films is a primary interest of this research; however, inorganic cluster species are not only relevant to the thin film and electronics markets. Many small clusters, including the $\mathbf{Ga_{13-x}In_{13}}$ clusters have structures much like fragment of minerals. The reverse process, bulk material breaking down into smaller components (i.e. minerals dissolving in acid rain) is a promising environment for locating dynamic clusters. It is possible that a plethora of clusters form naturally as minerals dissolve, but we have had no way of detecting these intermediate molecules. Geoscience may be greatly affected by the use of ^{1}H-NMR for the observation of inorganic –OH bridges. Al_{13} Keggin and calcium carbonate clusters have both been detected in nature.[73,74] It would be beneficial for the geoscience community to investigate water samples from streams, caves, hot springs, geysers, and ocean vents for the presence of these observable hydroxo bridges. ^{1}H-NMR research on completely inorganic systems is limited, but this study shows that it can lead to a variety of information previously thought to be inaccessible.

4.6 References

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Chapter 5. Group Additivity-Pourbaix Diagrams: First Universal Speciation Tool Including Thermodynamically Stable Pre-Nucleation Clusters in Aqueous Environments

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5.1 Abstract

Pourbaix diagrams map the equilibrium solid and solution phases in water, under varying conditions of pH and electrochemical potential. They are most often constructed based on the equilibria of solids with monomeric metal ions. However, the characterization of water-based corrosion, geochemical, environmental, and catalytic processes rely on accurate depiction of *all* stable phases. In many systems, solids dissolve in water to produce complex oxo-hydroxo polymetallic clusters, the identity of which can be difficult to probe experimentally. These clusters must be considered if Pourbaix diagrams are to realistically portray aqueous equilibria. Herein, we describe an expedient approach to compute Pourbaix diagrams with full consideration of cluster speciation. Comparisons with existing titration results from experiments yield excellent agreement. Applying this new GA-Pourbaix diagram to Group 13 elements, we arrive at a quantitative evaluation of cluster stability as a function of pH and concentration and present compelling evidence for *thermodynamically* stable aqueous clusters.

5.2 Introduction

Cluster formation in aqueous solutions have attracted renewed interest during the last decade.[1] Aqueous inorganic clusters are nanoscale molecular solvates composed of several metal ions linked via oxo and hydroxo ligands. They are crucial in a diverse range of chemical processes such as solution-deposition of device thin films,[2] biomineralization[3,4] and the natural cycling of minerals through soils, waters and biomass.[5] Aqueous clusters are also known to be causative agents of neurodegenerative disease and image enhancement additives.[6] In this work, we present two distinct computational procedures, which together provide an efficient route towards cluster stability evaluation and advocate the thermodynamic stability of clusters in aqueous solutions. Firstly, we reveal a group additivity (GA) method that can predict the Gibbs free energies of aqueous oxo/hydroxo metal clusters in excellent agreement with QM and experiments at a fraction of the cost. GA was developed by Benson in the 1950s to rapidly predict the thermodynamics of organic compounds.[24,25] No such analogous

method exists for pure aqueous inorganic compounds. We demonstrate the methodology on group 13 metal clusters which have drawn considerable attention recently due to their importance in catalytic microporous solids,[26] green aqueous precursors for large-area metal oxide thin films,[2] water treatment[18] as well as tumor diagnosis and possible treatment of malignancies.[27] Secondly, we use the resulting cluster free energies in the Pourbaix formalism of the Materials Project[28] developed by us.[29] The most important aspect of this formalism is that it uses a combination of computed solid states with experimentally obtained Gibbs free energies for the aqueous ions and water, which means that effects such as aqueous ion solvation are inherently accounted for. By combining the group additivity method with this formalism, we can for the first time build a foundation for evaluating the thermodynamic stability of clusters against the competing solid phases and monomeric aqueous ions.

Excitingly, *stable* aqueous cluster formation implicates an alternative nucleation process as compared to classical nucleation theory (CNT).[3,7–9] In this scenario, nucleation proceeds via aggregation of solvated pre-nucleation clusters, and not via a one-at-a-time attachment of monomeric species to a critical nucleus as assumed in CNT. The stability of aqueous clusters, in systems such as $CaCO_3$,[3,7,10,11] $NaClO_3$,[12] $AlPO_4$,[13] Ga,[14] Fe,[15] Fe oxyhydroxides,[16] Hf/Zr,[17] and Al [18] has been inferred from a variety of experimental visualization, speciation and spectroscopic observations. From the evidence, it is clear that these clusters i) form through a reversible process[3,19] whose speciation is governed by equilibria of molecular species in solution[3,12] and ii) are stable in solution for an extended time.[3,7,8] In spite of the accumulated knowledge indicating pre-nucleation cluster formation in solution, there are still many questions, e.g. as to the structures, the stability, the concentration ranges, counter-ion effects and the surrounding solvation structure of the pre-nucleation species as well as their role in the nucleation process. Theory can provide a means to elucidate some of these questions. For example, quantum mechanical (QM) studies of the structure, electronic and spectroscopic properties, absorption and reaction sites for clusters are well established[20,21]. Recently, molecular dynamics simulations have been used to unravel solute-solvent and ion-pairing

interactions as well as the dynamics of specific clusters.[20,22,23] However, despite these advances, no consistent framework for a quantitative measure of cluster stability across pH, pE, temperature, and concentrations has been offered, until now.

5.3 Methods

5.3.1 Quantum Mechanical Method for Group Additivity

The ground-state structures and Gibbs free energies are computed by HF/6-31G(d,p) with the IEFPCM-UFF continuum solvation model for water. The electronic energy was refined using the B3LYP/6-311+G(d) single point, and the solvation energy was recomputed using HF/6-311+G(d) with CPCM-UAKS for water.

5.3.2 Pourbaix Diagram Formalism

To integrate the group additivity free energies into the Persson Pourbaix formalism we express the clusters formation with respect to the monomeric aqueous ions:

$$m\mathrm{M}^{3+}_{(aq)} + n\mathrm{N}^{3+}_{(aq)} + (x+y+z)\mathrm{H_2O} \rightleftharpoons \mathrm{M}_m\mathrm{N}_n\mathrm{O}_x(\mathrm{OH})_y(\mathrm{H_2O})_z{}^{(3m+3n-2x-y)+} + (2x+y)\mathrm{H}^+ \quad (6)$$

The corresponding free energy of cluster hydrolysis is then obtained by:

$$\Delta g^{\circ}_{\mathrm{hydrolysis}} = \mu^{ref}_{\mathrm{M}_m\mathrm{N}_n\mathrm{O}_x(\mathrm{OH})_y(\mathrm{H_2O})_z{}^{(3m+3n-2x-y)+}} + 0 - m\cdot\mu^{ref}_{\mathrm{M}^{3+}_{(aq)}} - n\cdot\mu^{ref}_{\mathrm{N}^{3+}_{(aq)}} - (x+y+z)\cdot\mu^{ref}_{\mathrm{H_2O}} \quad (7)$$

where $\mu^{ref}_{\mathrm{M}_m\mathrm{N}_n\mathrm{O}_x(\mathrm{OH})_y(\mathrm{H_2O})_z{}^{(3m+3n-2x-y)+}}$, 0, $\mu^{ref}_{\mathrm{M}^{3+}_{(aq)}}$, $\mu^{ref}_{\mathrm{N}^{3+}_{(aq)}}$ and $\mu^{ref}_{\mathrm{H_2O}}$ are the chemical potentials of the cluster, protons, metal ions, and H_2O, respectively. All energies are provided at the standard state, and conform the consistent reference framework by Persson et al.[29] $\mu^{ref}_{\mathrm{M}^{3+}_{(aq)}}$, $\mu^{ref}_{\mathrm{N}^{3+}_{(aq)}}$ and $\mu^{ref}_{\mathrm{H_2O}}$ are known properties, while $\Delta g^{\circ}_{\mathrm{hydrolysis}}$ is calculated by the group additivity method presented here. Hence, $\mu^{ref}_{\mathrm{M}_m\mathrm{N}_n\mathrm{O}_x(\mathrm{OH})_y(\mathrm{H_2O})_z{}^{(3m+3n-2x-y)+}}$ is obtained from equation (7):

$$\mu^{ref}_{\mathrm{M}_m\mathrm{N}_n\mathrm{O}_x(\mathrm{OH})_y(\mathrm{H_2O})_z{}^{(3m+3n-2x-y)+}} = \Delta g^{\circ}_{\mathrm{hydrolysis}} + m \cdot \mu^{ref}_{\mathrm{M}^{3+}_{(aq)}} + n \cdot \mu^{ref}_{\mathrm{N}^{3+}_{(aq)}} + (x+y+z) \cdot \mu^{ref}_{\mathrm{H_2O}} \quad (8)$$

5.4 Results

To demonstrate our approach and study the thermodynamic stability of clusters in aqueous solutions, we consider group 13 metal clusters; in particular, the Al and Ga systems. In the case of Al, common monomeric species such as $[Al(H_2O)_6]^{3+}$, $[AlOH(H_2O)_5]^{2+}$, and $[Al(OH)_4]^{4-}$ as well as larger hydrolysis products can be identified by ^{27}Al-NMR as well as potentiometric studies.[30] Of the multimeric species, the dominant aluminum complex in aqueous systems is the large tridecamer $[Al_{13}O_4(OH)_{24}(H_2O)_{12}]^{7+}$, i.e. ε-Keggin ion, found across a broad pH range depending on aluminum ion concentration.

The aqueous behavior of Ga has significant similarities to Al. Like Al, Ga forms a few monomeric species, such as $[Ga(H_2O)_6]^{3+}$, $[GaOH(H_2O)_5]^{2+}$, and $[Ga(OH)_4]^{4-}$ under different concentration and pH conditions. Ga also forms larger hydrolysis products,[14] primarily in the form of the Ga_{13} Keggin cluster, though other hydrolysis products have also been synthesized.[31]

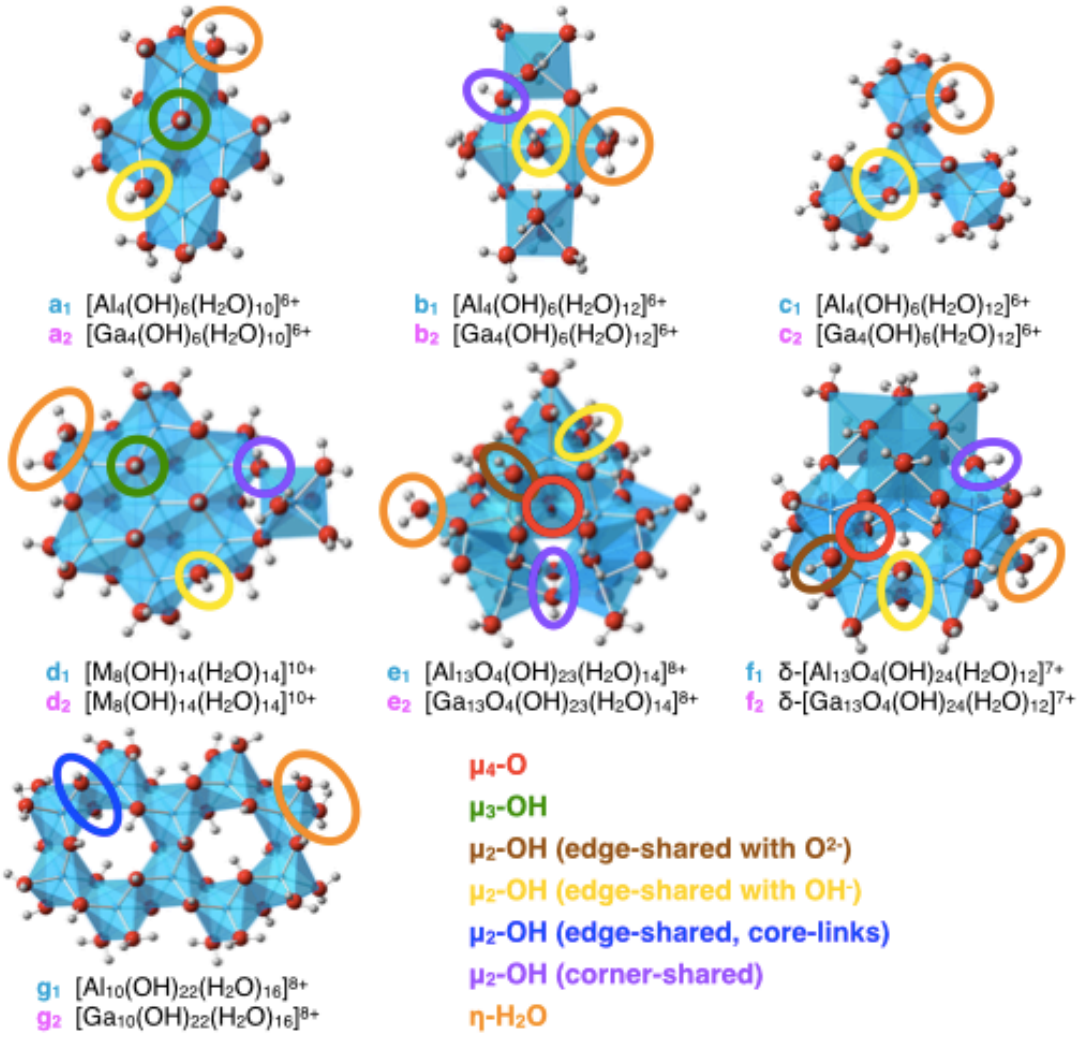

Figure 5.1. The seven metal aqueous oxo/hydroxo clusters used to compute the energies of the seven common ligands. The subscripts of μ denote the number of metal cations bound to each oxo/hydroxo ligand.

To efficiently obtain the energy of a generic cluster, we present a group additivity (GA) method that predicts the thermodynamic stabilities of aqueous group 13 metal hydroxide and oxide clusters, regardless of size or structure. The method quantitatively reproduces first-principles computations in predicting hydrolysis reaction energies and stabilities of both homometallic and heterometallic group 13 clusters with mean absolute error (MAE) of 3.0 kcal/mol. These calculations take seconds, a fraction of the cost of computing the QM values. In this method, the Gibbs free energy of any given aqueous metal

oxo/hydroxo cluster is expressed as the sum of the Gibbs free energies of the metal cations and the ligated oxo, hydroxo and aquo ligands. For instance, the absolute Gibbs free energy of Al dimer, $[Al_2(OH)_2(H_2O)_8]$ is:

$$G_{Al_2} = 2G_{Al^{3+}} + 2G_{\mu_2-OH} + 8G_{\eta-H_2O} \qquad (1)$$

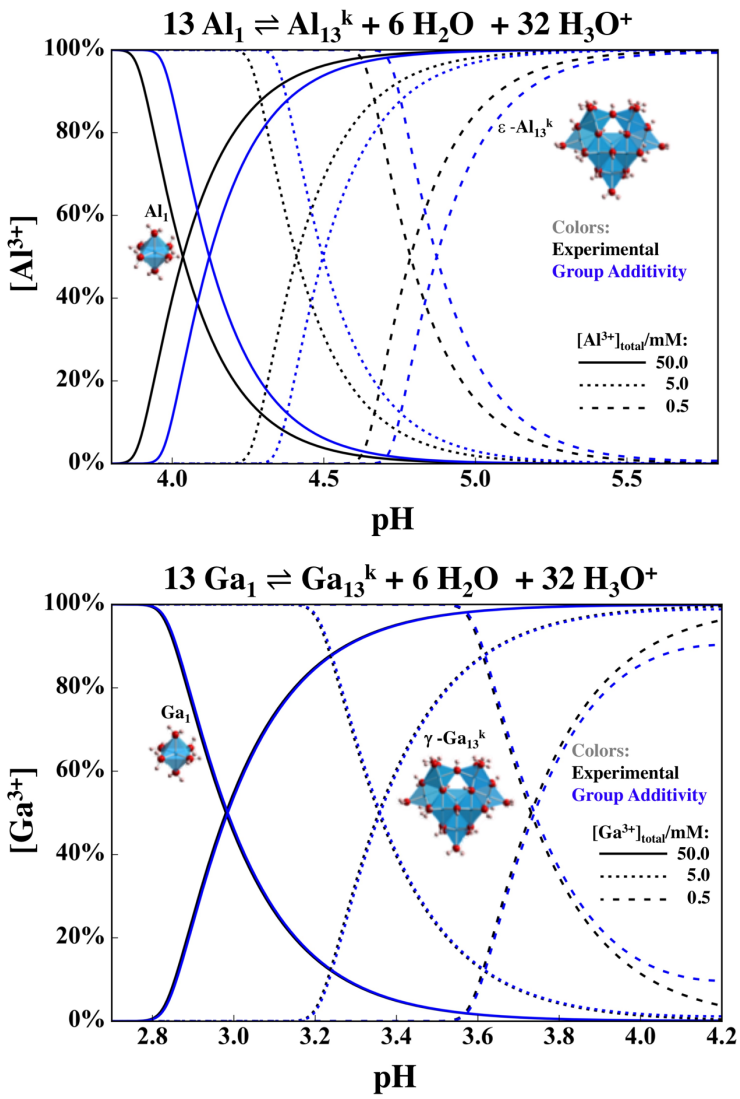

Figure 5.2. Speciation diagrams of aqueous aluminum (top) and gallium (bottom) clusters as a function of pH and concentrations with equilibrium constants from experiments, full quantum mechanics, and the group additivity method.

The general hydrolysis reaction can be written as the following equation, where {M, N} identify the group 13 metals and {m, n} denote the respective stoichiometries:

$$mM\left(H_2O\right)_6^{3+} + nN\left(H_2O\right)_6^{3+} \rightarrow M_mN_nO_x\left(OH\right)_y\left(H_2O\right)_z^{(3m+3n-2x-y)+} + (2x+y)H_3O^+ + (6m+6n-3x-2y-z)\ H_2O \quad (2)$$

Through inspection of group 13 clusters structures that have either been discovered or conjectured to exist and their QM computed energies,[5,32] we identify seven unique ligands that form the basis for replicating any structure (Figure 5.1). The Gibbs free energies of the seven basis cluster in Figure 5.1 can be written as a set of coupled linear equations with the ligand energies as unknown variables. Using first-principles computed free energies[33–35] for a set of clusters, the Gibbs free energies of the seven common ligands are fit.

The regression plots comparing the GA predicted and QM computed hydrolysis energies are shown in Figure 5.3. The linearity between the QM energy and GA predicted energy ($R^2 = 0.99$) shows that the GA method accurately reproduces the QM computed hydrolysis reaction energies of Al, Ga and Al/Ga aqueous oxo/hydroxo clusters. The methodology, the ligand energies and the validation are described in more detail in the Supporting Information (SI).

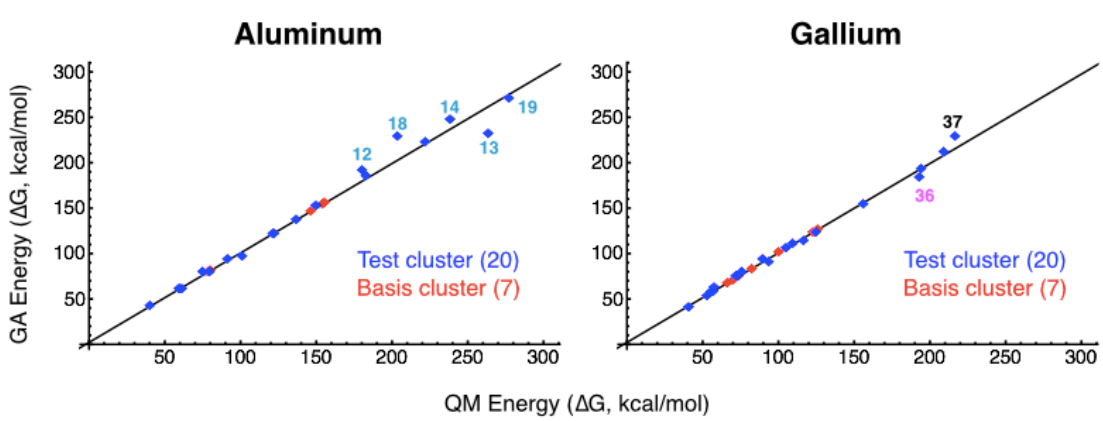

Figure 5.3. GA predicted versus QM computed hydrolysis energies for Al (left) and Ga (right). The slope of the linear regression line is near unity (0.98), the intercept is 2.10 and the R^2 value is 0.99. Clusters whose error are larger than 5 kcal/mol are labeled. Al clusters are in cyan, Ga in magenta, and heterometallic clusters in black.

To introduce the clusters to a rigorous thermodynamic framework which allows us to compare their stability with those of competing phases, e.g. solids and monomeric aqueous ions, we adopt the Pourbaix formalism, as implemented in the Materials Project.[28] The formation energies for the different species (experimental aqueous ions and first-principles computed solids) are imported through a common reference state scheme allowing for a grand canonical convex hull of stable aqueous and solid species as a function of pH and hydrogen potential. The Pourbaix diagram is constructed by projecting the convex hull to the E-pH plane. This formalism has been benchmarked[29] on almost all non-radioactive elements in the periodic table and reproduces or surpasses (due to its access to large amounts of computed solid polymorphs which have not been measured for their thermodynamic properties), the available experimental Pourbaix diagrams. Since launch in 2013, the Materials Project Pourbaix App has been used to successfully predict and interpret the stability of multiple materials and materials classes such as $Mn_2V_2O_7$,[36] $BiVO_4$,[37] $MnNiO_3$,[38] Cu vanadates,[37] 2D materials for photocatalyst applications,[39] and $CaCO_3$,[4] as a function of aqueous conditions. In this work we extend the framework by directly importing the cluster energies through equations similar to Eq (1). The resulting values for $\mu_{cluster}^{ref}$ are provided in SI. We note that the Materials Project database contains not only the known species in the available experimental Pourbaix diagrams consisting of monomeric aqueous ions and solid state phases, but also many metastable solids – against which the cluster Gibbs free energies are being evaluated, as a function of pH and potential.[28] To date, the Materials Project contains 106 unique Al-O_x-H_y, 41 Ga-O_x-H_y solid compounds and four Al as well as seven Ga monomeric aqueous ions. Furthermore, we emphasize that the aqueous species analyses do not include any counter-ion or salt effects in the aqueous solution.

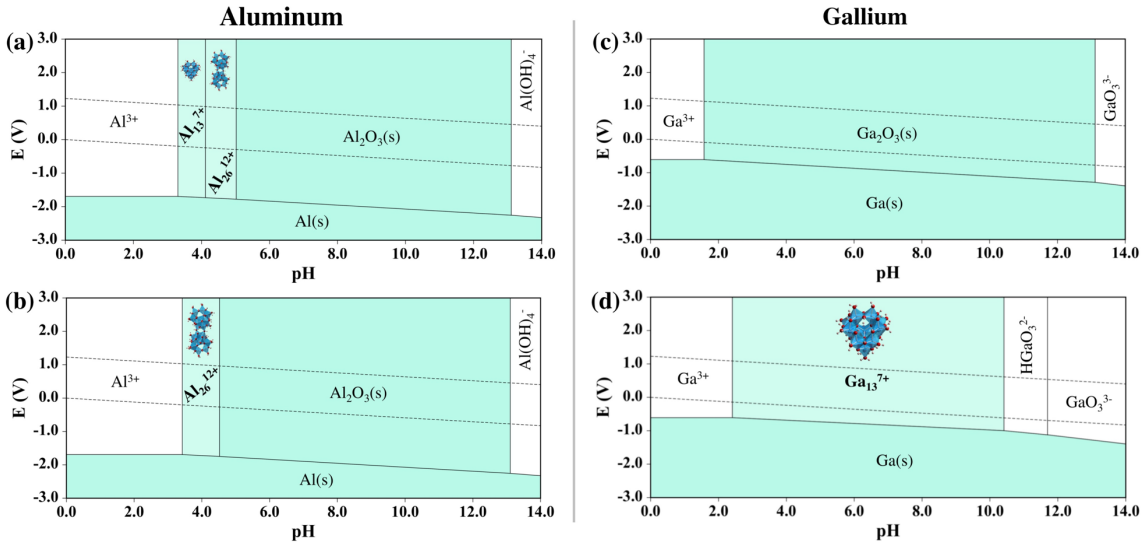

Figure 5.4. Al (a and b) and Ga (c and d) GA-Pourbaix diagrams incorporating solid phases from first-principles, aqueous ions from experiments and clusters from the GA method. In a) the respective concentrations are 10^{-8} M for both monomeric and cluster aluminum species and in b) 10^{-2} M for monomeric species and 10^{-3} M for the aluminum cluster species. In c) and d), the respective concentrations are 10^{-2} M for monomeric species and 10^{-3} M for the gallium cluster species. In c) all phases are included whereas in d) we simulate a situation where Ga_2O_3 is kinetically inhibited to nucleate which shows the stability regime of the Ga_{13} Keggin.

The new GA-Pourbaix formalism is able to quantitatively reproduce not only QM free energies, but also qualitatively the experimental free energies and speciation. To verify the accuracy, the equilibrium constant of the hydrolysis reaction leading to the Keggin aluminum or gallium tridecamer cluster was used to predict speciation. Specifically, the ratio of the monomer and Keggin concentrations was calculated with respect to pH and overall concentration of metal ions. As shown in Figure 5.2, the equilibria predicted from first-principles and the GA method robustly reproduce the reported experimental speciation behavior of both γ-Ga and ε-Al Keggin ions.

Figure 5.4 a-b show the two resulting GA-Pourbaix diagrams for aluminum which illustrates the evolution of stable species as a function of pH, standard hydrogen potential (SHE) - at two representative cluster concentrations. Similar to the well-known experimental aluminum Pourbaix diagram[40], for pH < 3, the monomer Al^{3+} is stable in solution, while at high pH, the $Al(OH)_4^-$ is preferred. Solid state Al_2O_3 is expected to

precipitate at neutral conditions and at reducing potentials lower than 2.0 V vs SHE, metallic aluminum represents the equilibrium state in aqueous solutions. However, in contrast to the known Pourbaix diagram, where only solid and monomeric species are considered, we also observe that multimeric aqueous cluster species are predicted to be thermodynamic ground states at slightly acidic conditions. At very low cluster concentration (10^{-8} M) we find that the ε-Al Keggin is the most stable species between 3.5 < pH < 4.1, while a 'dimer-Keggin' cluster (Al_{26}^{12+} in 5.4a) becomes stable at higher pH = 4.1-5.2. This dimer-Keggin resembles a dimer ε-Keggin, but is actually a dimer of δ-Keggins. The δ-Keggin cluster differs from the ε-Keggin by a 60° rotation of one of the four trimeric groups around the exterior of the ε-Keggin cluster. At higher cluster concentrations (10^{-3} M) the dimer-Keggin outcompetes the ε-Keggin, and stabilizes between 3.3 < pH < 4.7. This trend may be interpreted as a route towards nucleation, where larger oligomeric clusters are favored at higher cluster concentrations. Indeed, the δ-Keggin form is known to polymerize leading to the formation of larger aluminum polycations, whereof Al_{30}^{k}, Al_{32}^{k} and possibly Al_{26}^{k}, as suggested here, are examples. From our results, further experiments and calculations are encouraged to elucidate the stability of these polymeric clusters, which may provide insight into alternative nucleation mechanisms.

Interestingly, for gallium, we find that while the Keggin Ga_{13}^{k} shows the expected stability regime and speciation with respect to the monomeric Ga^{3+} ions (see Figure 5.2), in the full Pourbaix diagram it is outcompeted by other species, primarily the solid Ga_2O_3 by approximately 166 meV/Ga at a representative pH = 3.0, and 0.001 M cluster concentration. Hence, at regular concentrations, the gallium Pourbaix diagram – including the clusters – is exactly the same as the traditional one without any included cluster energies (see Figure 5.4c). However, an advantage of the GA-Pourbaix formalism is that it allows us to simulate scenarios where specific phases are unable to form. For example, if Ga_2O_3 nucleation and growth is inhibited, the Ga_{13}^{k} cluster emerges as the most stable phase for 2.4 < pH < 10.4 (see Figure 5.4d). At lower pH, the monomeric

aqueous ion Ga^{3+} is stable, while for pH >= 10.4, first, the $HGa(OH)_3^{2-}$ and then GaO_3^{-3} form at successively more basic conditions (pH > 11.8).

5.5 Discussion

The two complementary techniques presented in this work provide a robust and efficient framework for evaluating the thermodynamic stability of clusters in controlled aqueous solutions. For Al, the resulting GA-Pourbaix diagrams strongly support the recently proposed non-classical nucleation models[3,7,8] by advocating the existence of stable nanoscale pre-nucleation clusters. Figure 5.4 shows an intuitive succession of the ε-Keggin ion to dimerization of a similar structure (δ-Keggin) as the concentrations of the clusters as well as the monomeric ions are increased. Furthermore, we note that the Al clusters are stabilized without any counter-ion or salt effects, which may be indirectly supported by the variety of different solutions in which Al Keggin clusters have been observed.[41–44]

For gallium we find that the Ga_{13} Keggin successfully competes with the Ga^{3+} monomeric aqueous ion, as the computed speciation diagram reproduces experimental trends (see Figure 5.2b). However, in the full GA-Pourbaix diagram, other species such as the aqueous ion $Ga(OH)_2^+$ and the solid Ga_2O_3 phase are thermodynamically more stable for the pH range where the Ga clusters may emerge. Hence, the dilute Ga Pourbaix diagram – including cluster energies from 16 Ga clusters – is the same as the traditional experimental Pourbaix diagram.[40] However, our methodology allows us to simulate the stability of species under conditions where we assume one or more phases are inhibited to form. For example, if we assume that Ga_2O_3 nucleation is kinetically hindered, we obtain the GA-Pourbaix diagram in Figure 5.4d), where the Ga_{13}^k Keggin stability regime is evident.

The combined results of the aluminum and gallium GA-Pourbaix diagrams lead us to make the following comments. First of all, it is important to note that the results

displayed in Figure 5.4 assume non-interacting, dilute conditions and do not include any counter-ion effects, which are expected to selectively influence the stability of different clusters. Al Keggin clusters are clearly thermodynamically stable even under these conditions, while Ga clusters may be dependent on salt effects to outcompete the stable phases in the Ga Pourbaix diagram. For example, we stress that the energy difference between the Ga_{13}^{k} and Ga_2O_3 as well as monomeric aqueous specie $Ga(OH)_2^+$ is 166 and 72 meV/Ga; respectively, which is within the energy of counter-ion interactions. In general, analyzing the free energy difference between competing clusters as well as other possible species opens up the possibility to rationally influence cluster stability by tuning the solution composition. For example, the "flat" Al_{13} cluster is predicted to be thermodynamically unstable with respect to the ε-Keggin by 30 meV/Al. However, this cluster has been synthesized and observed under several different conditions.[5,45] In addition, the intermediates that have been suggested to give rise to the "flat" Al_{13} cluster are not stable from these QM or GA calculations.[5] We speculate that there are many more metastable clusters that may be stabilized by strong salt association and ion-pairing in solution. Available experimental results also suggest that different cluster structures, that may or may not be related to the macroscopic bulk,[5,46] form under different aqueous conditions. In particular, pre-nucleation clusters exhibiting building units resembling metastable bulk materials may pre-condition the synthesis of target nanoparticles,[5,10,12] thin films[2] and bulk materials with select structure and functionality.[18]

Finally, we would also like to emphasize that no kinetic effects are included, which are known to be important in many of the observed nucleation processes, and for determining the specific condition-dependent mechanism by which the final crystal and its morphology is formed. Nevertheless, the presented results provide a rigorous thermodynamic framework for the analysis of stable species in solution against which comparison and interpretation of experimental results can be made.

5.6 Conclusion

A general predictive computational framework to predict the vast array of aqueous metal clusters found in natural ecosystems, technological applications, and biology is a long-standing challenge. In this work we present the results of combining two procedures to improve our ability to predict and interpret cluster formation in aqueous solutions. Firstly, we disclose a general robust group additivity method to calculate the free energy of inorganic clusters, which reproduces experimental equilibrium constants & speciation, rival the accuracy of quantum mechanically computed values, and - once developed for a particular chemical system - can be performed in seconds. The speciation diagrams comparing group additivity, quantum mechanics, and experimental results show that the group additivity method is a general, accurate, and expedient method to predict the stabilities of group 13 metal aqua-oxo/hydroxo clusters. Furthermore, we import the resulting cluster thermodynamic data into the Persson Pourbaix framework, which provides a hybrid approach to classical Pourbaix diagrams – allowing for computed and experimental species to be evaluated within a single reference state system. The result supports the emerging experimental evidences[3,7–9,11,18] highlighting the role of thermodynamically stable solvated clusters in nucleation processes, and hence supports an alternative to classical nucleation theory. In the case of Al, we find that the ε-Keggin and 'dimer' δ-Keggin outcompetes monomeric aqueous species at mildly acidic conditions and low cluster concentrations, whereas higher concentrations favor the dimer-Keggin alone. In the case of Ga, we find no cluster species to be more stable than the monomeric ions and the bulk Ga_2O_3 solid under dilute, salt-free water conditions. However, the Keggin Ga_{13} cluster is found to be more stable than the monomeric Ga^{3+} under mildly acid conditions and between $2.4 < pH < 10.4$ is the second most stable species, after bulk Ga_2O_3. We emphasize that the current framework does not include interactions with other species in solution, such as counter-ions, which are likely to provide an excellent tuning parameter to change the hierarchy of stable clusters and promote nucleation of metastable structures. We also stress that kinetic factors are beyond the current analysis. Nevertheless this methodology will contribute towards

improved understanding on nucleation by providing a quantitative framework to aid analysis and ultimately guide rational synthesis of metastable clusters and structures in solution.

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Chapter 6. Theoretical Study of Peroxide Substitution into the Hafnium Hydroxide Tetramer

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Unpublished Manuscript

6.1 Abstract

Aqueous metal hydroxo clusters have gathered interest for their wide variety of applications in materials chemistry, geochemistry, and medicinal chemistry. Hafnium hydroxo clusters are particularly interesting for the application as a precursor to the patternable material HfSOx. In aqueous solutions of Hf ions, the Hf tetramer is one of the dominant cluster species formed and recently this tetramer has been shown to bind with peroxide in solution. In this work, we examine the structure of the Hf tetramer with bound peroxide and seek to understand what modes of substitution for existing ligands are most stable.

6.2 Introduction

Aqueous metal oxo and hydroxo clusters are popular precursors for the "green" deposition of high quality functional oxide films.[1-4] Hafnium clusters are of particular interest for their applications in nanolithography.[5-6] Previous studies of hafnium cluster chemistry have shown the existence of multiple cluster species, most ranging in size from four to six Hf ions, with one larger Hf_{18} cluster.[6-7] The solution chemistry of hafnium is dominated by these moderate-sized tetrameric, pentameric, and hexameric clusters.[7-8] The Hf_{18} cluster, on the other hand, has been shown to only exist via precipitation and crystallization; it does not exist in solution.[6]

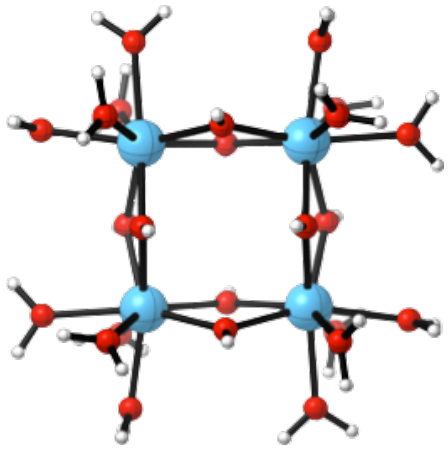

Figure 6.1. The structure of Hafnium hydroxide tetramer, $Hf_4(OH)_8(H_2O)_{16}^{8+}$.

Of the species that have been demonstrated to exist in solution, the Hf tetramer, $Hf_4(OH)_8(H_2O)_{16}^{8+}$, is of particular interest for a couple of reasons. First, this cluster has long been known to exist, both as a Hf cluster and as a Zr analogue, but has only recently been proven to dominate the solution speciation under certain pH and concentration conditions.[6,9-11] Second, this cluster has been shown via small-angle X-ray scattering (SAXS) to bind with peroxide in up to a 2:1 ratio of $Hf:O_2$, making it an appealing target for use as a thin film precursor.[6] However, little is known about the structure of the tetramer with peroxide, particularly where the peroxide binds with the cluster.

Herein, we use quantum mechanical computations to determine the structure of the Hf tetramer with two bound peroxide ligands per tetramer. The main research question here concerns whether the peroxide binds in the sites normally occupied by a pair of bringing hydroxide ligands (a bridging peroxide) or in the sites normally occupied by capping water molecules (a terminal peroxide).

6.3 Methods

The structures and absolute energies of each cluster were computed using B3LYP/lanl2dz for hafnium and B3LYP/6-31G(d) for all other elements in Gaussian 09. Solvation was modeled and compared using two implicit solvation models for water, PCM and CPCM.[13-14] Herein, the energy values will reflect the calculations performed with CPCM, unless otherwise noted. To examine the mode of peroxide binding to the Hf tetramer, we examined the structures of bridging and terminal peroxides bound to the tetramer with three levels of structural complexity. We examined the bare clusters with no counterions or explicit water molecules around the cluster. We examined the clusters with Cl^- counterions (using the amount needed for charge balance between counterions and the cluster) but no explicit water molecules to test the effect of counterions on peroxide binding. Finally, we also examined clusters with counterions and explicit water molecules to test the combined effect of counterions and the ability of the implicit solvation model to reproduce accurate structures.

6.4 Results

6.4.1 Clusters Only

The substitution of 2 bridging peroxides into the Hf tetramer can be achieved in only one of two ways, with the bridging peroxides on opposite sides of the tetramer or neighboring each other on the tetramer, with one Hf center in common (Figure 6.2).

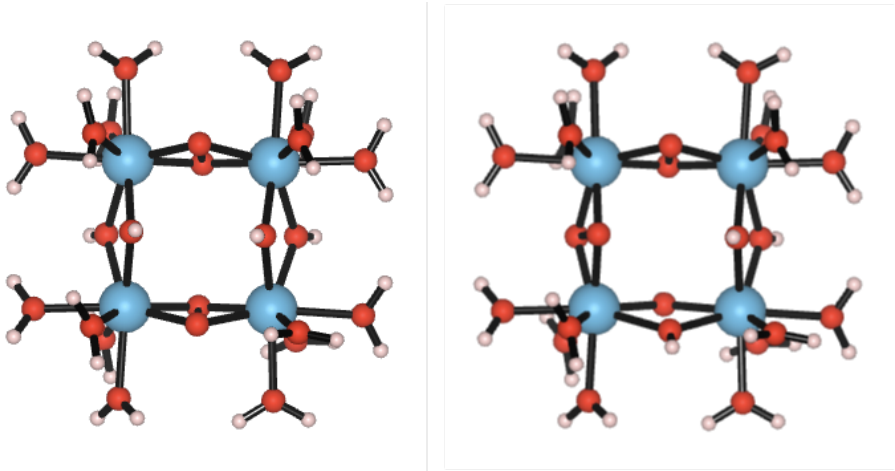

Figure 6.2. The binding modes of bridging peroxide. The pair of peroxides can either bind on opposite sides of the tetramer (left) or neighboring each other on the tetramer, with one Hf center in common (right).

The substitution of two terminal peroxides into the Hf tetramer, however, is more structurally complicated. For each Hf ion, there are five ways that one peroxide ligand can substitute for a pair of water molecules. Some of these are symmetrically equivalent for only one peroxide substitution, but the substitution of the second peroxide breaks this symmetry. The addition of the second peroxide can occur at one of two Hf centers, either the neighboring Hf or the Hf in the opposite corner of the molecule (Figure 6.3). Each of these substitutions can occur in one of five ways as well. This brings the total number of peroxide substitutions up to 50 combinations. We can reduce this by half based on symmetry, so for the terminal peroxides, we must consider 25 different modes of peroxide substitution.

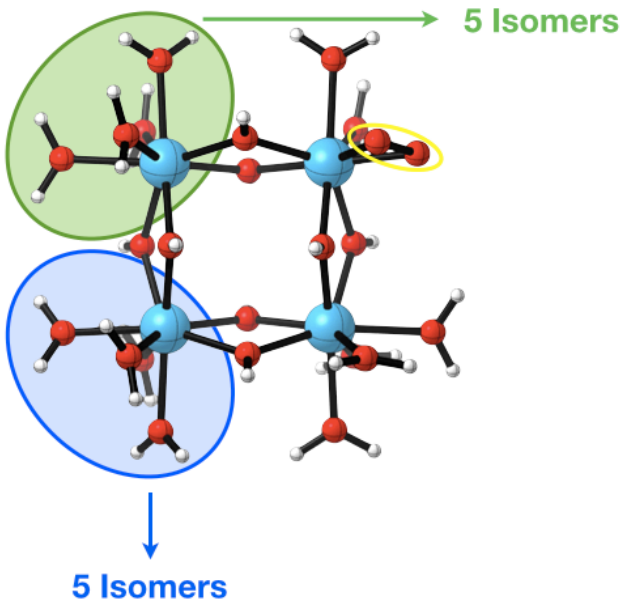

Figure 6.3. The determination of the total number of terminal peroxide combinations is determined based on the five ways a peroxide can add to each Hf center and the ability of the two peroxides to add to either neighboring Hf centers or Hf centers on opposite corners of the cluster.

Of the two bridging peroxide structures, the isomer with peroxides on opposite sides of the cluster was shown to be more stable. Of the 25 terminal peroxide isomers, the peroxides were most stable when they were on Hf centers in opposite corners of the tetramer. Based on optimizations of the two bridging peroxide and 25 terminal peroxide isomers, we found that terminal peroxides are highly favored. However, the charges of the bridging and terminal peroxide clusters are not the same; a di-subtituted terminal peroxide cluster is +4 in charge whereas a di-substituted bridging peroxide cluster is +8.

To assess if charge is a factor in stability, we also ran 6 structures corresponding to a Hf tetramer with two bridging peroxides and 4 deprotonated water molecules with an overall charge of +4. Deprotonation of water molecules resulted in a significantly more stable cluster. With deprotonation, the relative stability of the bridging and terminal peroxides

switched. The most stable bridging peroxide isomer was 12.8 kcal/mol more stable than the most stable terminal peroxide isomer (Figure 6.4).

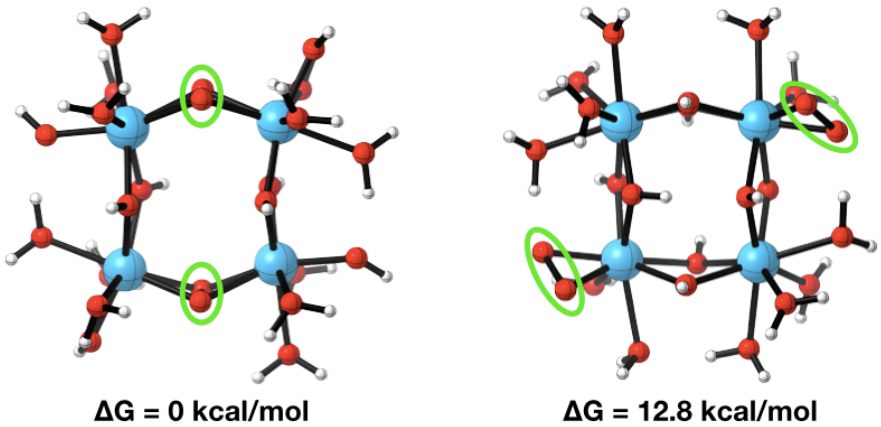

Figure 6.4. The most stable isomers of the Hf tetramer with bridging peroxides (left) and terminal peroxides (right). The green circles indicate the positions of the peroxides.

When we examined the optimized geometries of these clusters, however, there was cause for concern. With implicit solvation only, these clusters were clearly distorting their bond angles during optimization to form more favorable intramolecular hydrogen bonds. This is likely not a realistic picture of the clusters in solution, where intermolecular hydrogen bonding with the water solvent should dominate.

6.4.2 Clusters and Counterions

The Hf tetramer isomers for bridging and terminal peroxides described in the previous section were also examined with charge-balancing counterions surrounding the clusters. The inclusion of counterions reduces the symmetry of the tetramer, so we examined multiple possible positions for the counterions. In total, we examined 66 terminal peroxide isomers and 16 bridging peroxide isomers (including those with deprotonations). Once again, deprotonation of the tetramer with bridging peroxides was found to be favorable. With deprotonations of 4 water ligands on the bridging peroxide teramer, the bridging peroxides were favored over terminal peroxides by 6.6 kcal/mol.

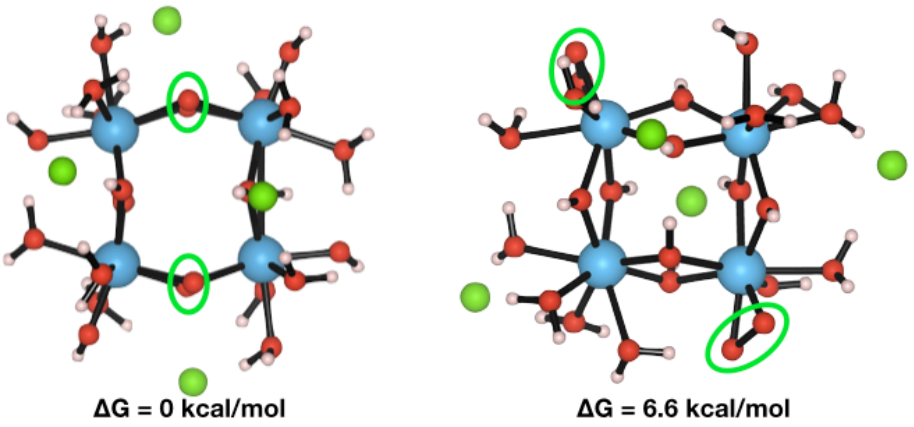

Figure 6.5. The most stable bridging (left) and terminal (right) peroxide isomers for the Hf tetramer with counterions included in the structure. The green circles indicate the positions of the peroxides.

Examination of the optimized structures yields the same concerns as for the clusters optimized with no counterions. The clusters are clearly distorting their structure to form more favorable intramolecular hydrogen bonding networks. This is slightly disrupted by the inclusion of counterions, as the cluster is also distorting due to attraction to the Cl^- ions. However, the structures still seem distorted beyond what would be reasonable in solution.

6.4.3. Clusters with Counterions and Explicit Waters

Finally, we optimized Hf tetramer structures with peroxide in the presence of both counterions and 15 explicit water molecules. The goal of this set of calculations was to understand the limitations of the implicit solvent model and compare the optimized structures of the clusters with varying levels of complexity. We computed 87 terminal peroxide and 17 bridging peroxide isomers. Surprisingly, the inclusion of 15 explicit water molecules reversed the relative stability of terminal vs. bridging peroxide clusters and favored terminal peroxide coordination. With these explicit waters, the most stable terminal peroxide isomer was 9.8 kcal/mol more stable than the most stable bridging peroxide isomer.

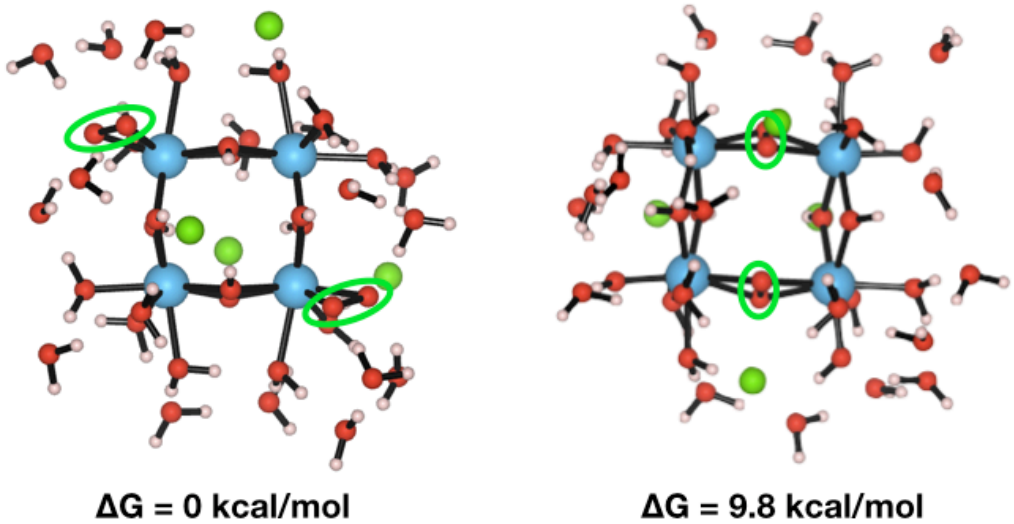

Figure 6.6. The most stable terminal (left) and bridging (right) peroxide Hf tetramer isomers for optimizations performed using counterions and explicit water molecules. The green circles indicate the positions of the peroxides.

It is notable that the structures obtained from optimization with counterions and 15 explicit water molecules look much less distorted than previous results. The presence of some explicit water molecules removes some of the propensity for the clusters to undergo intramolecular hydrogen bonding, instead preferring intermolecular hydrogen bonding with those explicit water molecules. The energies obtained from these calculation are likely more accurate as well, since they are based on more structures that are closer to what should be observed in solution.

6.4.4 Solvation: PCM vs. CPCM

We tested two solvation models in this study. The results above describe the energies and structures obtained from CPCM. However, we were also interested to understand if CPCM was a significant improvement over PCM, as has been suggested in the literature.[15] Our results indicate that the structures obtained from optimization with PCM solvation are extremely similar to the structures obtained using CPCM. In addition, while

there are some minor changes in cluster energies, the energies are largely similar and the relative stability of terminal vs. bridging peroxide ligands remains largely unchanged.

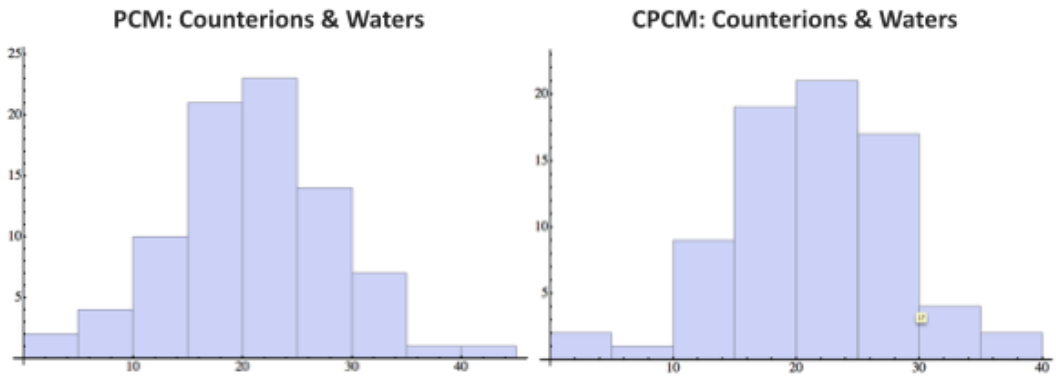

Figure 6.7. The distribution of cluster energies with counterions and explicit water molecules were similar between the clusters optimized with CPCM and PCM.

The overall distribution of the cluster energies was fairly similar between PCM and CPCM, as well. While Figure 6.7 shows the distribution of energies for the tetramers optimized with counterions and explicit waters, this trend was true for the clusters optimized without explicit waters and without counterions and explicit waters.

6.5 Conclusions

The objective of this study was to determine the way that peroxide binds into the Hf tetramer, $Hf_4(OH)_8(H_2O)_{16}^{8+}$. As an unexpected result, however, this study shows the importance of accurately modeling the solvent system for aqueous Hf clusters. The Hf tetramer studied here has a structure that can easily deform to undergo intramolecular hydrogen bonding during quantum mechanical optimization with either PCM or CPCM solvation. These deformations in structure are yield optimized cluster geometries that are not accurate compared to the structures of clusters in solution or in the solid state. Only with the inclusion of explicit water molecules does the optimized geometry accurately reflect the expected structure in solution. Based on the energies of Hf tetramers optimized with counterions and 15 explicit water molecules, peroxide addition to the Hf tetramer

prefers to occur through substitution of the peroxide ligands for pairs of terminal water ligands.

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Chapter 7. The Effect of Counterions on the Speciation of Aqueous Aluminum Oxo and Hydroxo Clusters

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Unpublished Manuscript

7.1 Abstract

Metal hydroxo and oxo clusters exist in a vast array of structural forms under aqueous conditions, and some of these clusters have recently been used in sustainable techniques for making metal oxide thin films. Understanding the vast array of metal hydroxo and oxo clusters formed in aqueous solutions is a long-standing challenge in geochemistry with broad consequences for the environment and technology. There is no universal understanding for the formation of specific clusters over others, and discovery of new clusters is still rare and serendipitous. Quantum mechanical calculations can be used to understand the stability of clusters; however, computing the stability of different cluster species is complicated by a lack of understanding of cluster protonation state and counterion affinity in solution. In this study, we examine the effect that counterions have on the stability of different aluminum hydroxo and oxo clusters using quantum mechanical (QM) computations. Our results show that the inclusion of counterions in computational models is essential, and the inclusion of counterions can provide a more accurate picture of the stability trends that dictate the stability of clusters.

7.2 Introduction

The identity, stability, and relative abundance of metal hydroxide and oxide clusters in solution is an intricate function of pH, pE, temperature, and concentration. [1,2] In medicine, these metal clusters have been implicated in several neurodegenerative disorders, including Alzheimer's and Parkinson's diseases.[3-7] The thermodynamic stabilities and kinetic viabilities of these clusters in water are important for understanding bioavailability, environmental fate, transport, and chemical toxicity.[2] In materials, aqueous solutions of these clusters are used to deposit high-quality thin films. This low-temperature solution process has introduced a new era of environmentally sustainable oxide materials through facile, large-area fabrication of directly imaged inorganic resists, optical devices, and thin-film transistors.[8-13] Given the diverse interests in metal hydroxide and oxide clusters, it is remarkable that very little is understood about the thermodynamics and kinetics that give rise to the existence of specific clusters. In fact,

discovery of new clusters is rare and serendipitous.[15] Aluminum clusters are of particular interest because they represent diverse environmental and geochemical profiles and an incalculable number of applications in commercial, industrial, and technological settings.[14-23]

Previous theoretical work has show that the stability of any arbitrary aluminum cluster can be understood by simply considering the types of ligands in the cluster.[**Error! Reference source not found.**] In this group additivity (GA) method, the overall free energy needed to make a cluster from the aluminum monomer can be calculated based on the total number of each type of oxo, hydroxo, or aquo ligands and a free energy value associated with each of these ligands. This method was shown to accurately reproduce the experimental speciation of aluminum clusters, particularly with respect to the formation of the aluminum Keggin clusters (Al forms three different isomers of the five possible Keggin clusters ε-, δ-, and γ- but not α- or β-).[24-29] However, this method does not account for the effect of cluster-cluster interactions or the interactions of clusters with counterions in solution. Some experimentally-observed clusters were predicted to be unstable based on this method. The flat aluminum tridecamer ($Al_{13}(OH)_{24}(H_2O)_{24}^{15+}$) has gathered recent interest for its technological applications as a thin film precursor.[14] While this cluster has been isolated experimentally, computations without counterions predict that this cluster should not be stable. However, compared to the Al Keggin clusters ($Al_{13}O_4(OH)_{24}(H_2O)_{12}^{7+}$), which are predicted to be stable, the flat Al tridecamer has a high overall charge when fully protonated.

To fully understand the speciation of Al clusters, we must understand how counterions affect the stability of Al clusters and if the presence of counterions stabilizes clusters with a high overall charge. Herein, we examine the effect of counterions on aluminum cluster stability and formation, with particular emphasis on the equilibria that form the flat and Keggin tridecamers.

7.3 Methods

Electrostatic potential maps were generated for each Al cluster structure and the Al monomer. These potential maps were generated for clusters quantum mechanically optimized without counterions at the HF/6-31G(d,p) level of theory with the PCM solvation model for water in Gaussian 09.[30,31] The electrostatic potential maps were generated from a charge calculation run in Gaussian 09 at the B3LYP/6-31G(d) level of theory in the gas phase.

Electrostatic potential maps were used to determine initial guesses for the locations of counterions surrounding each Al cluster. Since Al clusters are generally positively charged overall, the negatively charged counterions should be most strongly attracted to the parts of the cluster with the most positive charge and favorable hydrogen bonding networks for the counterions. Figure 1 shows the flat Al cluster along with the corresponding electrostatic potential map. These potential maps were used to generate initial counterion positions based on the charge distribution and hydrogen bonding networks of each cluster.

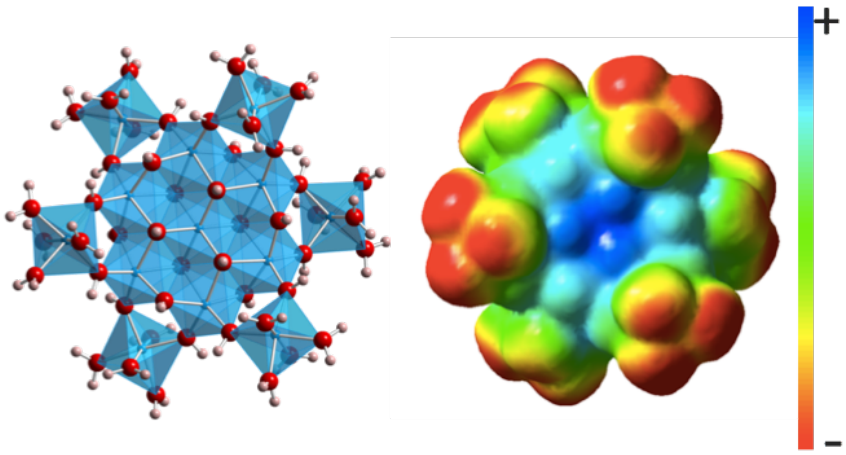

Figure 7.1. The structure and electrostatic potential map of the flat aluminum tridecamer, $Al_{13}(OH)_{24}(H_2O)_{24}^{15+}$. The electrostatic potential map was generated based on charge calculations in Gaussian 09 with B3LYP/6-31G(d).

The initial counterion positions and cluster structures were quantum mechanically (QM) optimized using B3LYP/6-31G(d) with the CPCM solvation model for water.[32] Energy refinements for the optimized structures were computed at the B3LYP/def2-SVP with CPCM solvation for water. This process was used to create QM optimized cluster structures for clusters with Cl^-, NO_3^-, and ClO_4^- counterions.

7.4 Results

The stability and predominance of different cluster products in solution is determined by the energy of hydrolysis for each cluster product. Generally, hydrolysis of aluminum clusters follows the reaction scheme shown below.

$$x\,Al(H_2O)_6^{3+} \rightleftharpoons Al_xO_w(OH)_y(H_2O)_z^{(3x-2w-y)+} + (6x-3w-2y-z)H_2O + (2w+y)H_3O^+$$

Many different hydrolysis products are possible for aluminum. We computed the hydrolysis free energy for 21 different aluminum clusters, ranging in size from two to thirteen aluminum ions (Figure 7.2).

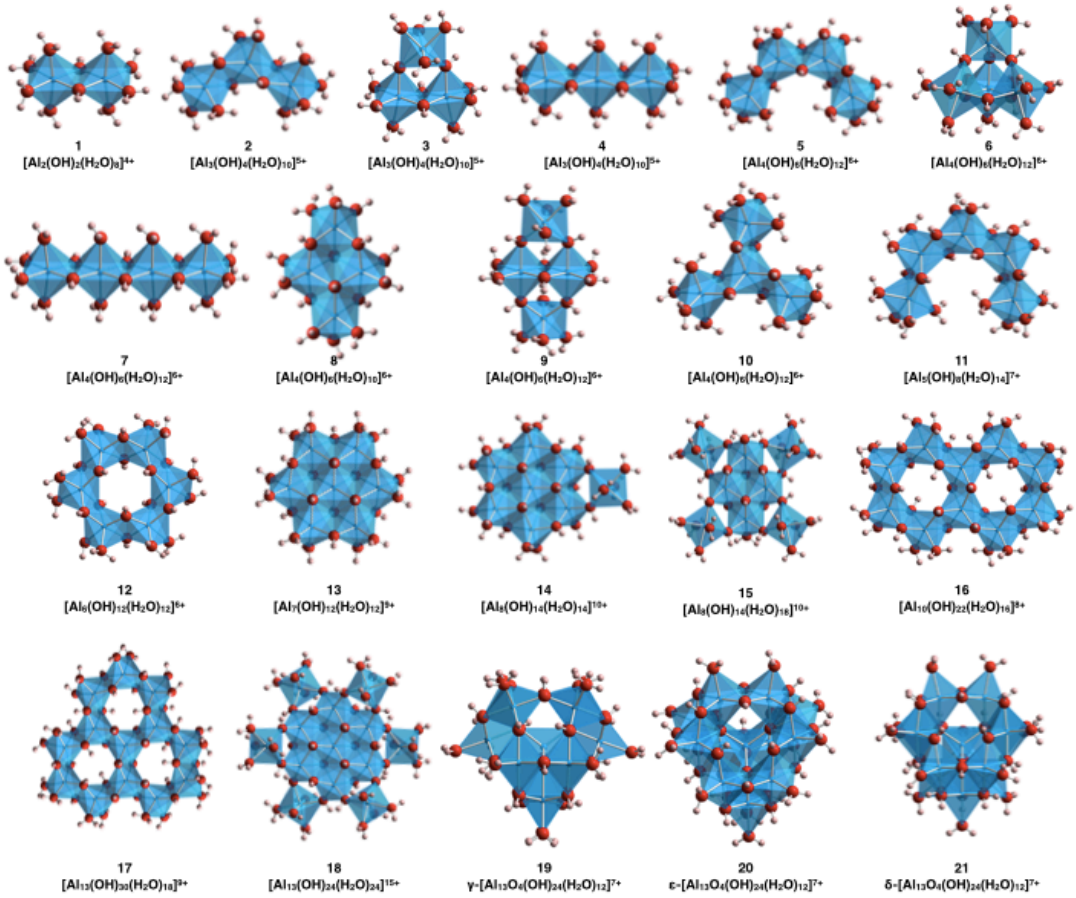

Figure 7.2. The 21 aluminum hydroxide clusters used for examining the effect of counterions on aluminum speciation.

The free energy of hydrolysis is tabulated below for each of these clusters (Table 7.1). We have also included the free energy of hydrolysis without any counterions computed in our previous work.**Error! Reference source not found.**

Table 7.1. The hydrolysis free energies of 21 Al clusters with different counterions

Cluster #	Formula	ΔG (No Counterions)	ΔG (Cl^-)	ΔG (NO_3^-)	ΔG (ClO_4^-)
1	$Al_2(OH)_2(H_2O)_8^{4+}$	42.0	15	4.2	14.9
2	$Al_3(OH)_4(H_2O)_{10}^{5+}$	61.5	9.9	4.0	15.7

3	$Al_3(OH)_4(H_2O)_{10}^{5+}$	62.2	-5.5	-9.9	14.1
4	$Al_3(OH)_4(H_2O)_{10}^{5+}$	63.5	13.8	4.6	29.7
5	$Al_4(OH)_6(H_2O)_{12}^{6+}$	82.4	12.8	-15.8	29.1
6	$Al_4(OH)_6(H_2O)_{12}^{6+}$	79.9	-8.7	-18.3	6.9
7	$Al_4(OH)_6(H_2O)_{12}^{6+}$	82.6	42.3	-6.4	44.7
8	$Al_4(OH)_6(H_2O)_{10}^{6+}$	78.2	3.0	-7.5	30.9
9	$Al_4(OH)_6(H_2O)_{12}^{6+}$	83.6	8.8	-9.2	18.9
10	$Al_4(OH)_6(H_2O)_{12}^{6+}$	82.6	12.2	-5.2	19.7
11	$Al_5(OH)_8(H_2O)_{14}^{7+}$	106.0	24.0	-17.9	24.4
12	$Al_6(OH)_{12}(H_2O)_{12}^{6+}$	93.9	37.5	-3.2	58.2
13	$Al_7(OH)_{12}(H_2O)_{12}^{9+}$	128.9	25.3	-2.6	74.4
14	$Al_8(OH)_{14}(H_2O)_{14}^{10+}$	149.1	11.0	-20.2	63.8
15	$Al_8(OH)_{14}(H_2O)_{18}^{10+}$	155.6	-7.0	-49.8	12.0
16	$Al_{10}(OH)_{22}(H_2O)_{16}^{8+}$	156.9	48.2	-20.9	97.8
17	$Al_{13}(OH)_{30}(H_2O)_{18}^{9+}$	196.5	84.8	-25.9	156.1
18	$Al_{13}(OH)_{24}(H_2O)_{24}^{15+}$	244.7	6.9	-86.1	49.9
19	$Al_{13}O_4(OH)_{24}(H_2O)_{12}^{7+}$	123.1	60.7	-36.2	153.4
20	$Al_{13}O_4(OH)_{24}(H_2O)_{12}^{7+}$	121.1	80.4	-14.9	167.1
21	$Al_{13}O_4(OH)_{24}(H_2O)_{12}^{7+}$	122.2	76.6	-35.4	158.7

Calculations of hydrolysis free energies without counterions demonstrated a general trend that clusters of increasing overall charge were predicted to be less stable. The inclusion of counterions to the structures used to calculate hydrolysis free energies completely

eliminates this trend. The presence of counterions that charge balance the cluster clearly has a large effect on stabilizing high charge clusters in solution.

In regards to the formation of the flat vs. Keggin tridecamers, the inclusion of counterions around both structures leads to significant stabilization of the flat tridecamer compared to the Keggin cluster. Across all three counterions tested, the hydrolysis free energy values for the flat tridecamer are significantly lower than the Keggin tridecamer. To understand how this affects speciation in solution, however, we need to consider the pH of the solution. Since hydronium is a side-product of hydrolysis, solution pH can drive the formation of certain clusters under different pH conditions.

The free energy of hydrolysis over the pH range 0-14 was examined for each of the clusters. The goal of this examination was to determine the most stable clusters at different pH values and to further understand the equilibrium between the flat and Keggin tridecamers. For Cl^- ions, these calculations suggest that three clusters dominate the speciation of aluminum, a Keggin cluster, the flat tridecamer, and the octamer, which has previously been crystallized in experiments.[33] From pH = 0-1.5, the octamer had the most favorable hydrolysis energy and should therefore dominate the speciation. From pH = 1.5-4.5, the flat tridecamer has the most favorable hydrolysis energy, and at pH conditions greater than pH = 4.5, the Keggin clusters should predominate.

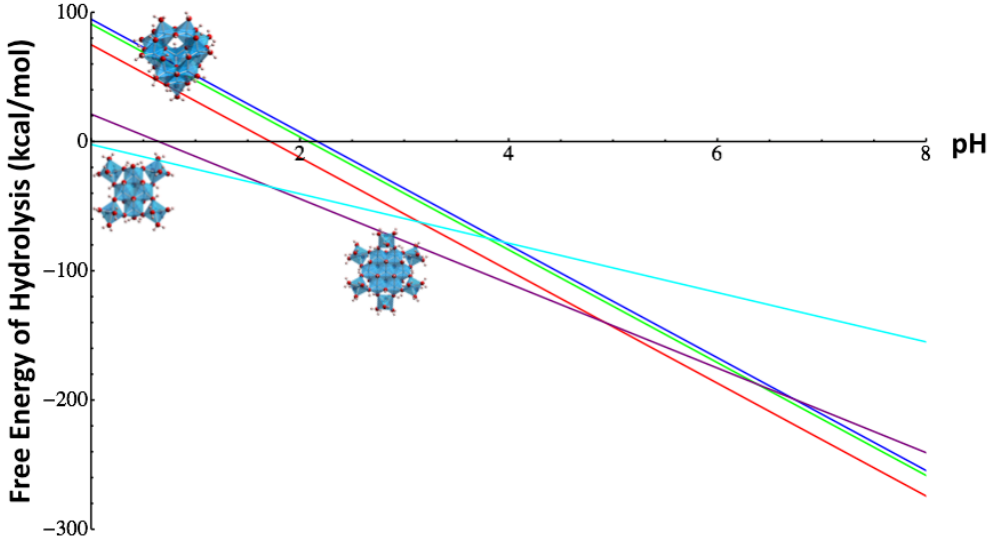

Figure 7.3. The hydrolysis free energy values of the most stable aluminum clusters with Cl^- counterions as a function of the solution pH.

For NO_3^- counterions, only the Keggin and flat tridecamers are predicted to predominate over a broad pH range. The octamer with NO_3^- counterions is predicted to overall be less stable than the flat tridecamer under all pH conditions. The pH where the most stable cluster transitions from the flat tridecamer to one of the Keggin tridecamers is roughly the same as for chloride counterions at approximately 4.5. This result is qualitatively consistent with ^{27}Al-NMR titration experiments showing that the formation of the Keggin cluster starts to occur around the same pH for both NO_3^- and Cl^- counterions and below that pH, the flat tridecamer dominates. However, in these experiments, the pH where this transition happens is approximately pH = 3 rather than 4.5.

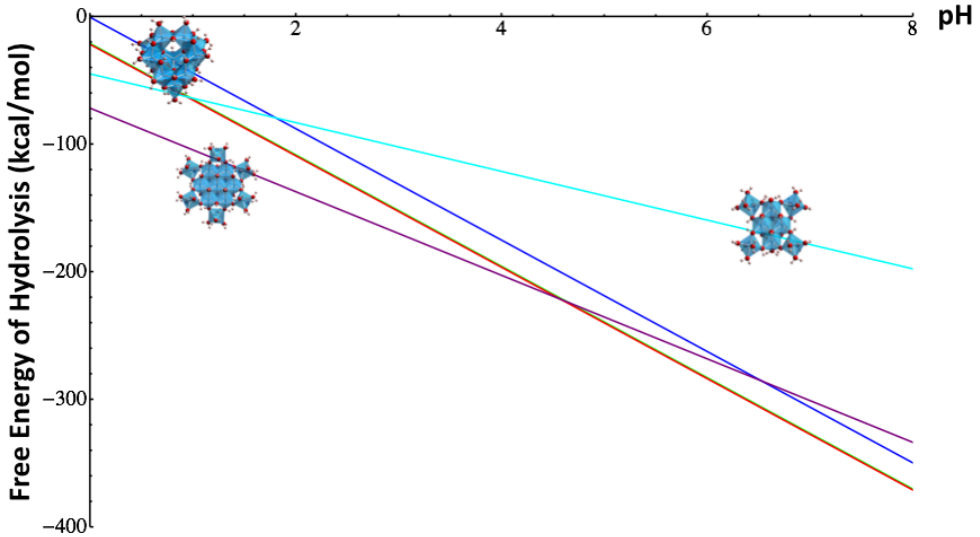

Figure 7.4. The hydrolysis free energy values of the most stable aluminum clusters with NO_3^- counterions as a function of the solution pH.

The behavior of aluminum clusters in an aqueous solution with ClO_4^- counterions is somewhat similar to the solution with Cl^- counterions. The primary difference is that the pH values where the octamer, flat tridecamer, and Keggin tridecamers transition in relative stability are higher than for Cl^-. The octamer is most stable up to pH = 3.5. The flat and Keggin tridecamers dominate at pH values higher than 3.5, with the flat tridecamer being the most stable cluster between pH = 3.5 and 9. The Keggin cluster should dominate above pH = 9.

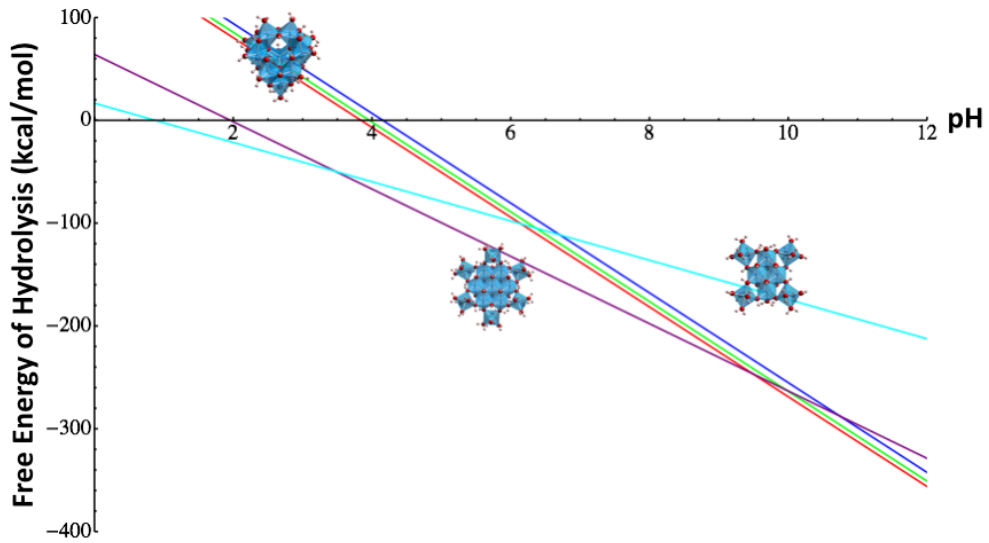

Figure 7.5. The hydrolysis free energy values of the most stable aluminum clusters with ClO_4^- counterions as a function of the solution pH.

There are a few additional things to note about these results. First, the speciation of clusters will vary to some degree depending on the concentration of Al cations in solution. Particularly, cluster formation is more likely to occur at high concentrations of Al cations. Second, there are other monomer species (most significantly, $Al(OH)_4^-$) that start to compete with cluster formation at high pH values. From this, we know that cluster formation is unlikely to occur above pH = 10.

7.5 Conclusions

The computations disclosed in this study show that inclusion of counterions in computations is essential for understanding the speciation of aqueous metal hydroxo clusters. Without counterions, known, stable clusters are predicted to be unstable due likely to the high charge of some clusters. With counterions, we show that these clusters are in fact stable and reproduce experimental speciation with moderate success. We compared the computationally predicted pH where the flat Al tridecamer transitions to the Keggin Al tridecamers with results from ^{27}Al-NMR experiments and found that computations predicted a pH value of 4.5 while NMR experiments show this happening

around pH = 3. Further calculations could be performed to improve the computational prediction of this equilibrium. However, even without improvements, these results show that the inclusion of counterions is vitally important to understand the stability of Al clusters, particularly the flat Al tridecamer.

Follow up studies should focus on improving the quantitative predictions of Al speciation, particularly the equilibrium between the flat and Keggin tridecamers. Different computational methods could be explored to improve the accuracy of the hydrolysis free energy values. In addition, the protonation states of Al clusters should be further studied. With cluster charges varying greatly and some clusters having very high charge, it is likely that some clusters may be partially deprotonated in solution to reduce charge.

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Chapter 8. Conclusion

In this dissertation, quantum mechanical computations have been used to understand the spectroscopic properties and stability of aqueous metal hydroxo clusters. Previously, there has been no broad understanding of why particular clusters form in solution over others and characterization of clusters through spectroscopy requires detailed analysis for each new system. The work disclosed in this dissertation makes a key contribution to general understandings of inorganic spectroscopy and cluster stability.

Computations have proven to be an invaluable analytical tool for understanding the spectroscopy of metal hydroxo clusters. Unlike organic chemistry, where particular functional groups have distinct and well-characterized frequencies and intensities, inorganic chemistry does not have a broad understanding of how to identify clusters from their vibrational or NMR spectra. I have shown that computations can be used to help bridge this knowledge gap and lay the groundwork needed to start making generalizations about the ^{1}H-NMR and vibrational signals of Group 13 metal hydroxo clusters.

Cluster stability is complicated by the dynamic nature of cluster speciation in solution. The identity of stable cluster species is a complicated function of pH, electrochemical potential, and ion concentration/identity. The studies disclosed in this dissertation show that computations can be used to accurately predict cluster stability and speciation, but often require a proper understanding of the counterions in solution with the cluster products. Because clusters can have varying overall charges, the presence of counterions serves to significantly stabilize some cluster products and are hence essential to understanding the stability of clusters formed through hydrolysis.

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Appendices

Appendix 1: Supporting information for Chapter 2

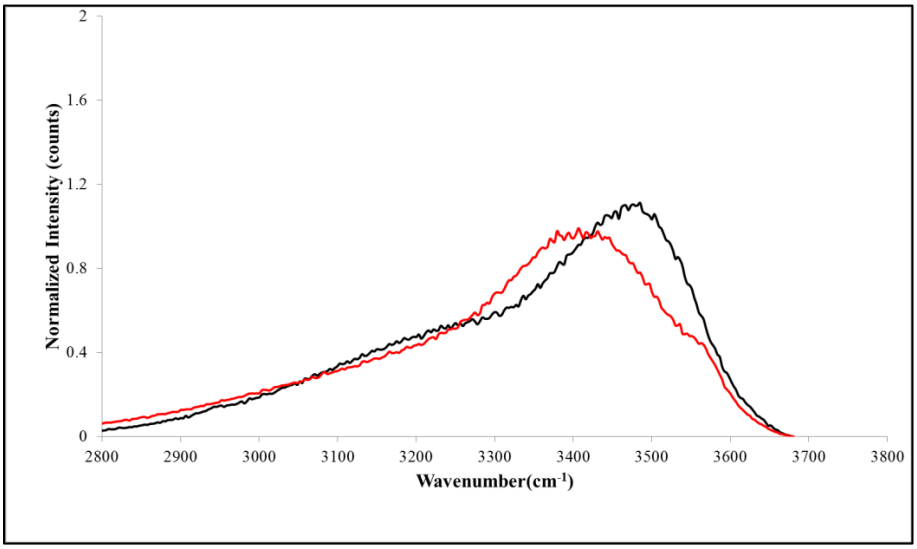

Figure A1.1. From 2600-3800 cm^{-1} displays the different types of waters associated with each of the cluster. Red = Ga13; Black =Al13

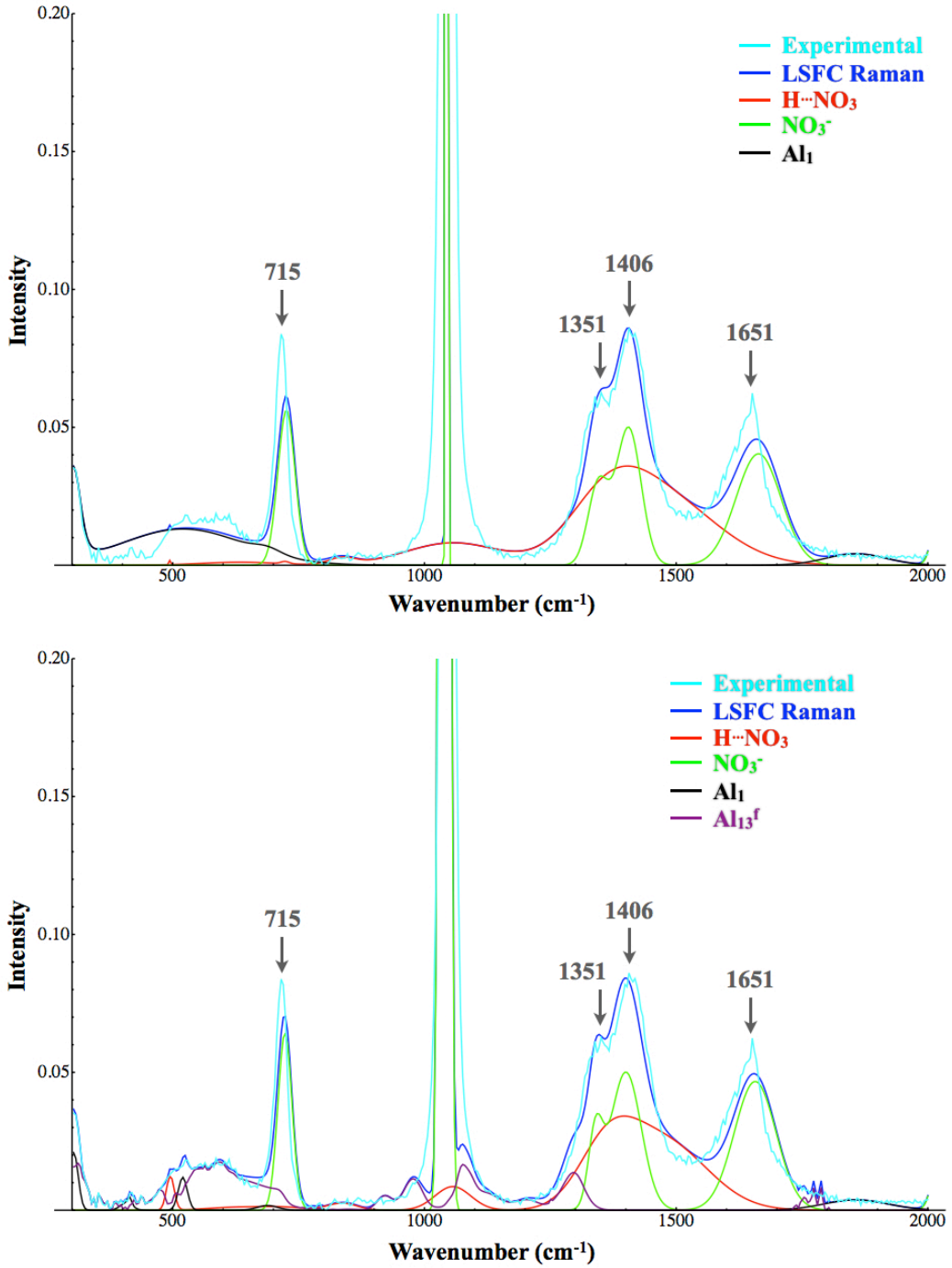

Figure A1.2. Solution phase Raman of the flat Al_{13} cluster. Top: LSFC Raman spectrum computed using the aluminum monomer (Al_1). This LSFC spectrum has an RMSD of 0.64 %. Bottom: LSFC Raman spectrum computed using Al_1 and the aluminum tridecamer (Al_{13}^f). This LSFC spectrum has an RMSD of 0.48 %.

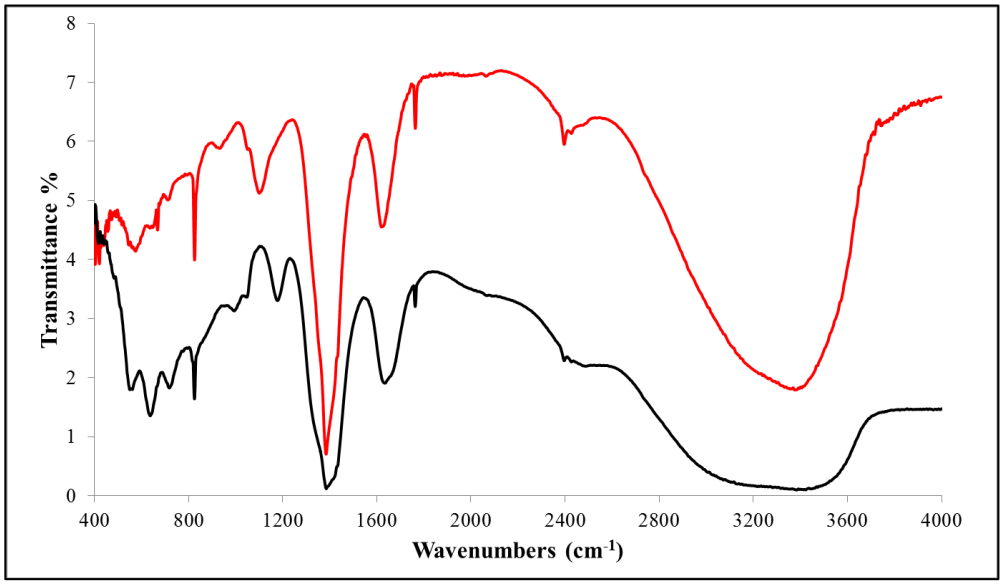

Figure A1.3. IR overlay of Al_{13} (black) and Ga_{13} (red) clusters.

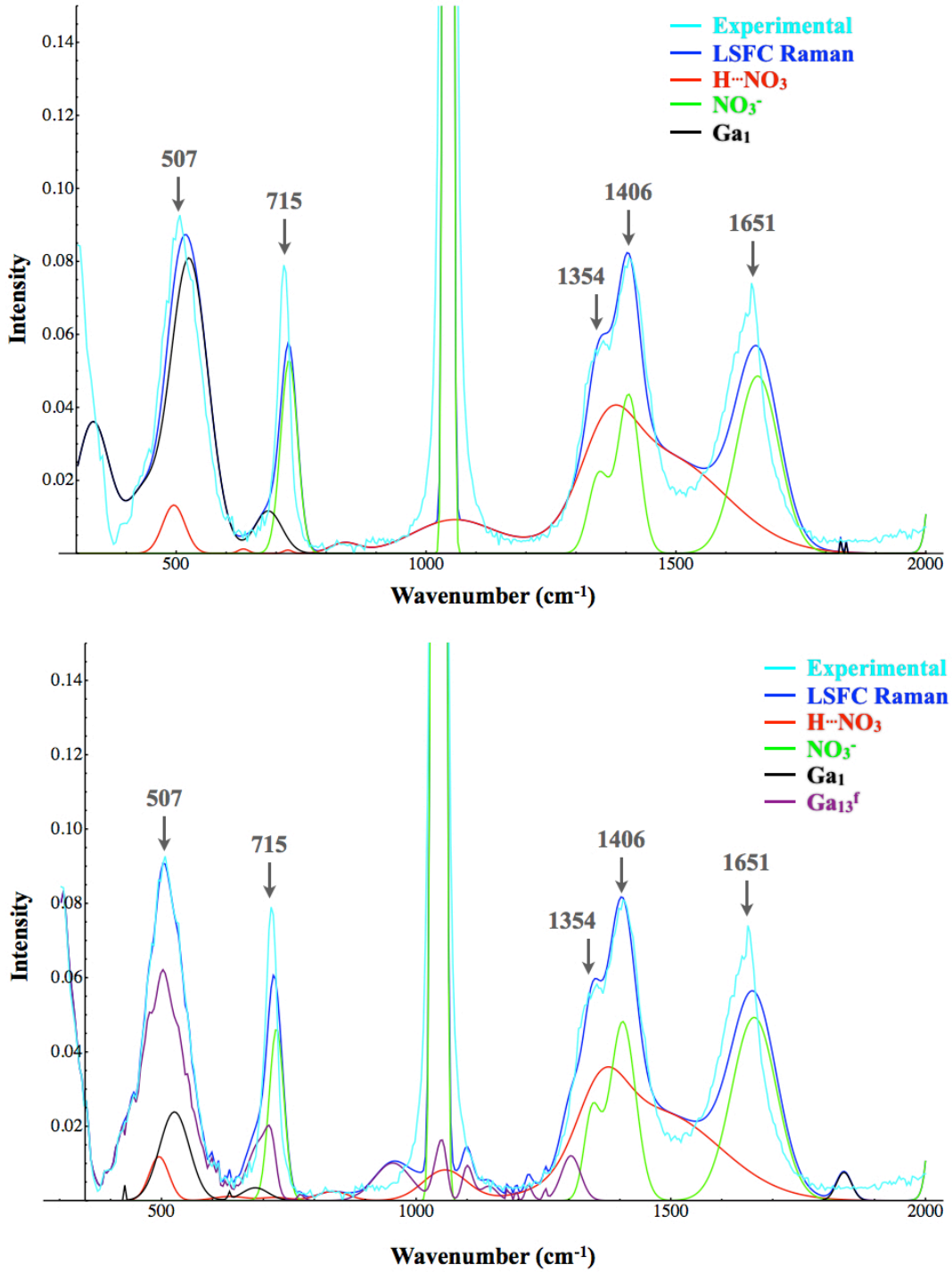

Figure A1.4. Solution phase Raman of the flat Ga_{13} cluster. Top: LSFC Raman spectrum computed using the gallium monomer (Al_1). This LSFC spectrum has an RMSD of

0.92 %. Bottom: LSFC Raman spectrum computed using Ga_1 and the gallium tridecamer (Ga_{13}^{f}). This LSFC spectrum has an RMSD of 0.48 %.

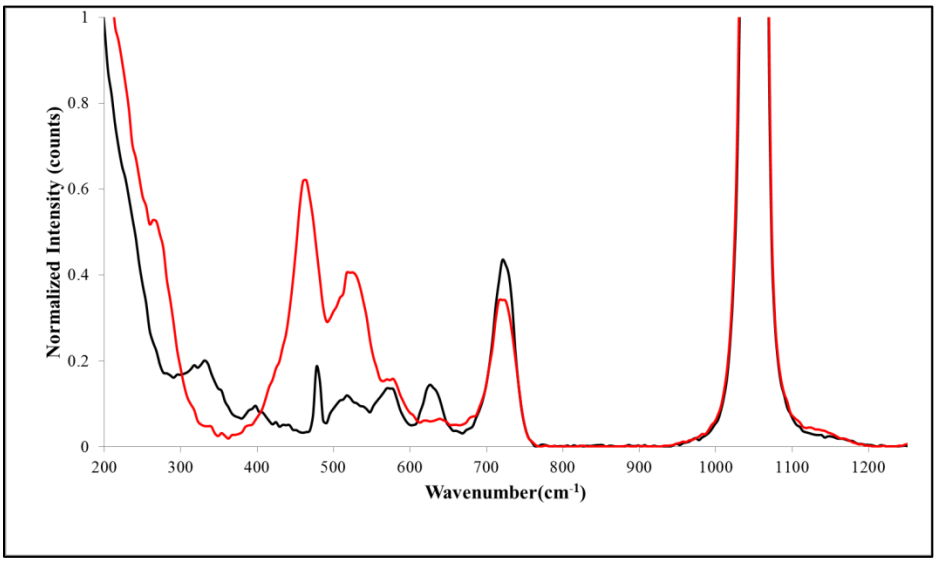

Figure A1.5. Raman overlay of Al_{13} (black) and Ga_{13} (red) clusters with normalized intensity

Table A1.1. Raman and IR spectral data for the Al_{13} in solid state and aqueous solution at 25°C

Raman Table		
Al_{13} Solid	**Al_{13} (0.1M)**	**Peak Assignments**
		Computational Analysis
313, w	**-**	**Al-O**
380, w	**-**	**Al-O**
424, w	**-**	**Al-O**
478, w		**Al-O**
517, w	**-**	**Al-O**
-	**525, v, br**	**Al-O**
574, w	**-**	**Al-O**
626, w	**-**	**Al-O**
725, m	**715, m**	**NO_3^{-1}, asy**
1048, vs	**1048, vs**	**NO_3^{-1}, sym**

1101, vw, sh	**-**	**μ_2-OH**
1340, m	**1341, m**	**NO3-1 asy**
1401, m	**1400, m**	**NO3-1 asy**
1637, m	**1626, m**	**H_2O•••NO_3^{-1} , d**
3271, s, br	**-**	**OH**
3455, s, br	**-**	**OH**

Infrared Table

Al_{13} Solid	**Peak Assignments**
	Computational Analysis
550, w	**Al-O**
636, m	**Al-O**
717	**Al-O•••ηH_2O**
824	**NO_3^{-1}, sym**
994	**μ_3-OH**
1048	**μ_3-OH core**
1178	**μ_3-OH and μ_2-OH shell**
1380, vs	**NO_3^{-1}, asy**

1634, m, br	**H_2O•••NO_3^{-1}, d**
1657, m, br	**H_2O•••NO_3^{-1}, d**
3291	**OH**

s=strong, m=medium, w=weak, v=very, br=broad, sh=shoulder, asy = asymmetric, sym = symmetric, b = bend, d = deformation, str = stretch; The numbers in table are in wavenumbers (cm^{-1})

Table A1.2. Raman and IR data of Ga_{13} in Solid and Solution phase at 25°C

Raman Table		
Ga_{13} Single Crystal	**Ga_{13} 0.1M**	**Peak Assignments Computational Analysis**
420,w, sh	**-**	**Ga-O**
464, s	**-**	**Ga-O, sym**
	507, m, br	**Ga-O, sym**
525,m	**-**	**Ga-O**
574,w	**-**	**Ga-O**
630, vw	**-**	**Ga-O**
716, s	**716, m**	**NO_3^{-1} asy**
1048, vs	**1048, vs**	**NO_3^{-1} sym**
1110, w,sh	**-**	**μ2-OH**
1330, m	**1330m**	**NO_3^{-1} asy**
1395, m	**1394,m**	**NO_3^{-1} asy**
1621, m	**1621, m**	**H_2O•NO_3^{-1}, d**
3234, br	**-**	**OH**

3388, br	**-**	**OH**
3533, sh	**-**	**OH**

Infrared Table	
Ga_{13}	**Peak Assignments**
Single crystal	**Computational Analysis**
420	**Ga-O**
574	**Ga-O**
635	**Ga-O**
713	**Al-O••ηH_2O**
824	**NO_3^{-1}, sym**
913	**μ_3-OH core**
1051	**μ_3-OH and μ_2-OH shell**
1101	**μ_2-OH shell**
1381	**NO_3^{-1}, asy**
1620	**H_2O••NO_3^{-1} , d**
3359	**OH**

s=strong, m=medium, w=weak, v=very, br=broad, sh=shoulder, asy = asymmetric, sym = symmetric, b = bend, d = deformation, str = stretch; The numbers in table are wavenumbers (cm^{-1})

Full authorship of Gaussian 09

Gaussian 09, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

Cartesian coordinates of Al and Ga tridecamers.

Structures and thermodynamic energies were computed by HF/6-31G(d,p)/PCM-UFF (H2O, Gaussian 09).

1. $[Al_{13}(OH)_{24}(H_2O)_{24}]^{15+}$

Supporting Information: Al13p.log

```
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 Using  Gaussian 09:  AM64L-G09RevB.01 12-Aug-2010
=============================================================================
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 # HF 6-31G** OPT(CalcFC,maxcycles=200,RFO) SCRF=(Solvent=water)
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 #N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RHF/6-31G(d,p) Freq
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133
 Charge = 15   Multiplicity = 1
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 Optimization completed.          {Found       1       times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
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 Displ      0.12275 ||  0.00180   [ NO ]       0.12275 ||  0.00180   [ NO ]
-----------------------------------------------------------------------------
     Atomic          Coordinates (Angstroms)
      Type          X           Y        Z
-----------------------------------------------------------------------------
      Al       0.000629      0.001954     -0.026546
      Al       2.746024     -1.274422     -0.050675
      Al       0.267732     -3.018799      0.010024
      Al      -2.473543     -1.729653     -0.023126
      Al      -2.750355      1.282771     -0.011175
      Al      -0.266430      3.018938      0.012138
      Al       2.479910      1.743342     -0.045983
      Al       3.038684     -4.212797      1.665169
      Al      -2.223941     -4.752552     -1.585280
      Al      -5.214107     -0.467639      1.590330
      Al      -3.001083      4.298917     -1.605450
      Al       2.205697      4.699589      1.673805
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H	-0.698886	4.904588	-1.412937
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H	4.155869	-1.711542	-1.933985
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H	2.993861	-6.840051	1.844934
H	2.527426	-6.255270	3.204203
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Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -6781.56580449 Predicted Change= -2.727151D-04
Zero-point correction (ZPE)= -6780.4645 1.10130
Internal Energy (U)= -6780.3662 1.19959
Enthalpy (H)= -6780.3652 1.20053
Gibbs Free Energy (G)= -6780.5760 0.98970

Frequencies -- 23.2052 27.2815 37.3857

2. $[Ga_{13}(OH)_{24}(H_2O)_{24}]^{15+}$

Supporting Information: Ga13p.log

Using Gaussian 09: AM64L-G09RevB.01 12-Aug-2010

==========

#HF/6-31G(d,p) scf=(maxcycle=300,direct,tight,xqc) density=current
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#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RHF/6-31G(d,p) Freq

---

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Charge = 15 Multiplicity = 1

SCF Energy= -28612.2252477 Predicted Change= -1.176400D-04

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Optimization completed. {Found 1 times}

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Ga	0.177154	-3.047913	0.005512
Ga	-2.549200	-1.671282	-0.015201
Ga	-2.734332	1.377315	-0.004388
Ga	-0.180474	3.052077	0.013545
Ga	2.550254	1.685257	-0.029783
Ga	2.942097	-4.398925	1.669558
Ga	-2.397170	-4.748206	-1.621657
Ga	-5.307081	-0.324095	1.624440
Ga	-2.915355	4.450783	-1.633809
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H	4.810718	5.826612	1.631103
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H	6.235041	0.959331	0.720679
H	7.292892	2.061226	-1.699040
H	6.640827	2.058326	-3.107665
H	7.525825	-0.735392	-2.632895
H	6.714475	-1.949874	-2.125785

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -28612.2252477 Predicted Change= -1.176400D-04
Zero-point correction (ZPE)= -28611.1378 1.08742
Internal Energy (U)= -28611.0345 1.19065
Enthalpy (H)= -28611.0336 1.19159
Gibbs Free Energy (G)= -28611.2572 0.96794

Frequencies -- 23.8500 30.8270 39.7484

Appendix 2. Supporting Information for Chapter 3

Validation of Computational Methods: To ensure the accuracy of the *ab initio* computations, the equilibrium energies from computations were compared to experimental equilibria (Figure S4). The speciation diagram shown in Figure S4 was generated by considering the equilibrium that produces any arbitrary cluster product in solution, shown below.

$$x\,Al(H_2O)_6^{3+} \rightleftharpoons Al_xO_w(OH)_y(H_2O)_z{}^{(3x-2w-y)+} + (6x-3w-2y-z)H_2O + (2w+y)H_3O^+$$

Due to the limited studies on the speciation of aluminum in water, the most suitable equilibrium reaction for comparison was the formation of the Keggin aluminum tridecamer, $[Al_{13}O_4(OH)_{24}(H_2O)_{12}]^{7+}$ ($Al_{13}{}^{k}$), from aluminum monomer, $Al(H_2O)_6{}^{3+}$ (Al_1). For the Keggin aluminum tridecamer, the hydrolysis reaction leading to the cluster product is:

$$13\,Al(H_2O)_6^{3+} \rightleftharpoons Al_{13}O_4(OH)_{24}(H_2O)_{12}{}^{7+} + 6H_2O + 32H_3O^+$$

Experimentally, the free energy associated with this reaction is determined by using a hydrogen sensitive electrode in conjunction with a titration over a broad pH range. In this titration, an acidic or basic solution of aluminum cations is titrated by addition a base or acid, respectively (the addition of base to an already acidic solution is most common). As the titrant is added to the solution of aluminum cations, the pH of the solution is monitored by a potentiometer. For any point in the titration, the theoretical pH can be calculated using amounts of acid and base that have been added to the solution. The actual pH of the solution will differ from the theoretical pH due to the hydrolysis reactions occurring in the solution. A comparison of the solution's actual pH to the calculated theoretical pH over a broad pH range then reveals the stoichiometry of the hydrolysis products present in solution and their respective stabilities. To fully

characterize the structures of these clusters in addition to the stoichiometries, further experimentation is required, such as X-ray diffraction experiments. In computing these clusters from quantum mechanics, we must take advantage of the structures obtained from crystallography in addition to the stabilities obtained through potentiometry.

In previous studies of aluminum systems, potentiometric pH titrations have revealed the existence of several small aluminum species, including several deprotonated forms of the aluminum monomer, an aluminum dimer, an aluminum trimer, and the Keggin aluminum tridecamer. Using the experimental equilibrium constants for these species and the generic equation for hydrolysis reactions (shown above), the concentration of each of these species can be calculated for a full range of pH conditions and initial aluminum ion concentration. Likewise, when using computed quantum mechanical stabilities, the hydrolysis free energy can be used to calculate the value of the equilibrium constant and, consequently, the concentrations of each species in solution.

In Figure S4, the calculated concentration of Al^{3+} cations in the fully protonated monomer is compared to the concentration of Al^{3+} cations in the Keggin cluster. This Figure shows an overlay of the predictions from the experimental equilibrium constants with the predictions from the quantum mechanical equilibrium constants.

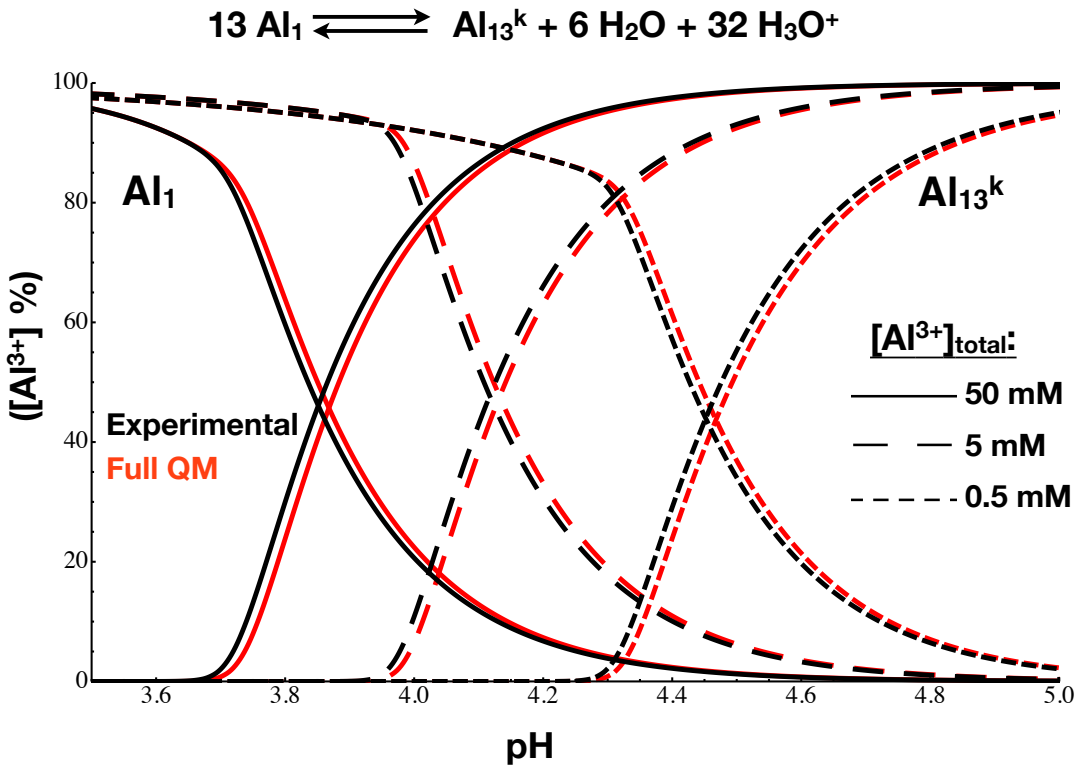

Figure A2.1. Speciation diagram for the predominant aluminum species as a function of pH and Al^{3+} concentration for the hydrolysis equilibrium between Al_1 and Al_{13}^k. Al_1 predominates at lower pH, while Al_{13}^k is the primary species at higher pH.

The agreement between the experimental and computed results shows that the computational methods used here are an accurate reflection of experimental thermodynamics and equilibrium behavior, and therefore confirms the accuracy of these methods as they apply to spectral analysis.

Computational Methods for FSR Raman Spectral Analysis:

- To ensure accurate predictions of the intermediates present in solution, multiple Least-Squares Fitted Computed (LSFC) Raman spectrum were computed and juxtaposed with the positive signal of the differential FSR (pH = 3.18), which reflect the emerging species during the electrolysis process.
- The LSFC Raman spectra for each Al clusters listed in Figure 5 are shown in Figures S10-S16. These clusters include:
    - The "flat" Al_{13}, harvested from the cathode solution at pH = 2.7-3.2 range
    - Three possible intermediates, Al_6, Al_7 and Al_{7+1}, similar to the Al_7 core of the "flat" Al_{13}
    - Al_2 and Al_8, whose crystal structure been reported and may exist in the solution
    - Al_1 cluster
    - Note: The Keggin Al_{13} is excluded here since solution ^{27}Al NMR studies (Fig. S1) of the final cathode solution (pH = 3.18) indicate that only ~0.05% of the Al atoms occupy a highly symmetric tetrahedral site.
- The root mean squared deviation (RMSD) values of the LSFC Raman spectra show that "flat" Al_{13}, Al_7 and Al_{7+1} are the most likely species in the cathode solution because they have the smallest RMSD values at 900-1300 cm^{-1} region (6.6%, 6.6% and 6.2%, respectively). The LSFC Raman RMSD of Al_8, Al_6 and Al_2 and Al_1 (Figure S13-S16) are suggestively worse, 7.1%, 7.9%, 8.8% and 16.3%, respectively.
- The LSFC Raman spectra computed from varying combinations of "flat" Al_{13}, Al_7 and Al_{7+1} are shown in Figures S6 to S9. The three-component LSFC Raman of Al_{13}, Al_7 and Al_{7+1} has the smallest RMSD value for the entire spectrum (350-1300 cm^{-1}) and for the region corresponding to hydroxide vibrations (900-1300 cm^{-1}). We therefore used this LSFC for further analysis. The computed parameters for this three-component LSFC Raman spectrum are listed in Table S2.

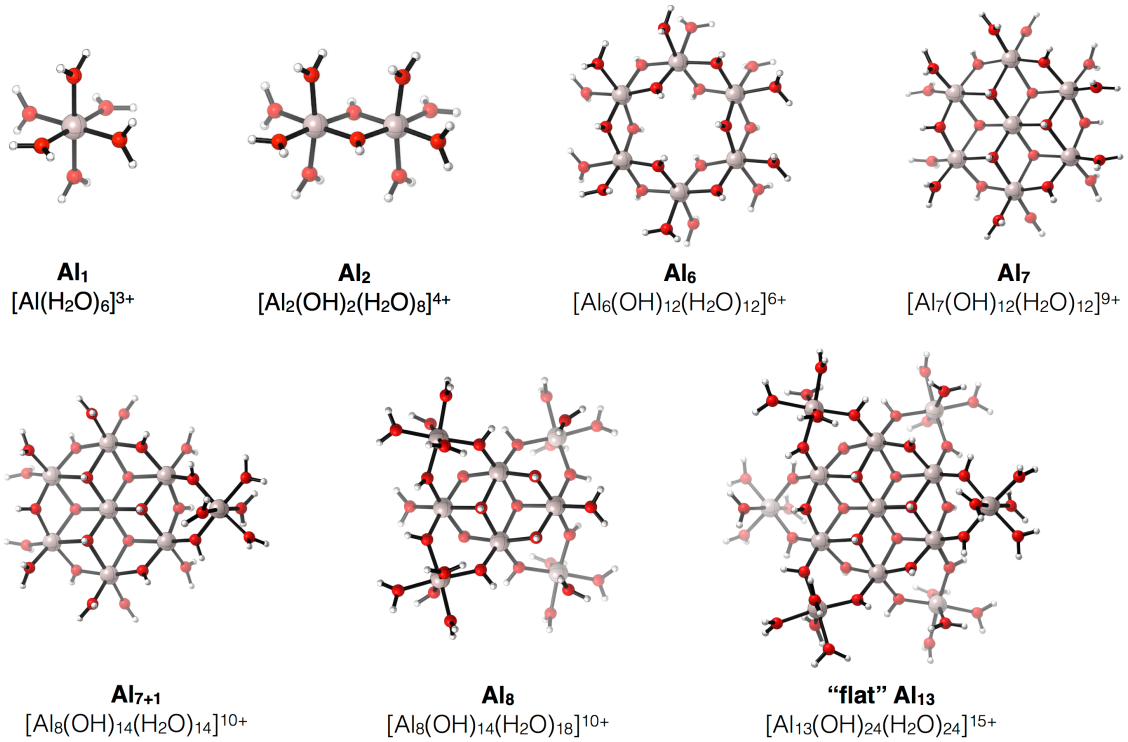

Figure A2.2. The geometries of clusters whose Raman spectra were computed and used as reference for assignment of experimental spectrum.

Table A2.1. The coefficients of the component Gaussian functions of the LSFC-Raman The Least-Squares Fitted Computed (LSFC) Raman spectrum, which is composed by Gaussian functions generated from the computed vibrational frequencies, Raman intensities and additional three scaling factors, is formulized as followed:

$$\sum_{n}(i_n)\exp\left[-(x-v_n)^2 \Big/ 2\left(w_n/6\right)^2\right]$$

v_n = the computed Raman vibrational frequencies.

i_n = the normalized computed Raman vibrational intensities.

w_n = the widths of the constituent Gaussian functions.

	v_n	i_n	w_n		v_n	i_n	w_n
1	317.7531306	0.049181621	49.6051	34	505.8136201	0.028887075	8.14626
2	318.6882579	0.043146738	49.4841	35	508.7334676	0.01163299	14.6835
3	321.0503272	0.047549331	48.6126	36	509.5696498	0.015903416	16.5205
4	329.5237052	0.068964787	36.916	37	511.1178481	0.010253571	23.6918
5	331.8052605	0.027007614	37.3731	38	515.9525723	0.022196933	29.8551
6	341.5435824	0.128112161	12.6221	39	521.8786016	0.025823626	41.0469
7	343.5738949	0.010489216	15.8673	40	525.1263257	0.008006298	48.1646
8	349.4436614	0.081471393	-0.0194797	41	533.6976786	0.002189809	48.1271
9	357.1225693	0.113128895	-0.0575216	42	534.9645626	0.004856664	44.9604
10	367.3730771	0.110352334	0.0194669	43	543.3031038	0.004960117	28.9631
11	374.5630803	0.03196775	24.9144	44	546.3995002	0.026340955	18.5121
12	378.4946889	0.01140887	29.8266	45	553.2596868	0.025915641	8.05312
13	381.5416128	0.048290718	27.1434	46	555.1280011	0.020938279	1.15064
14	388.573498	0.054992385	39.2441	47	561.3877273	0.015110228	-0.208638
15	390.869604	0.067171579	6.64363	48	577.536133	0.005908461	4.50579
16	401.3616539	0.199875816	-0.017121	49	583.513575	0.006730356	9.25098

17	404.4464098	0.026139761	3.98496	50	586.2335924	0.00039658	44.9027
18	406.3477058	0.058590327	0.502959	51	590.1021478	0.008707532	82.52
19	412.805322	0.002494431	35.2321	52	596.9060715	0.02108191	90.5388
20	416.9794428	0.008437374	-4.42088	53	600.3157937	0.000206911	53.2259
21	446.1701574	0.033174727	44.1794	54	605.3745992	0.018472587	69.8249
22	447.5767284	0.034985223	0.0372487	55	607.4611746	0.003149646	64.286
23	456.4555869	0.005856734	19.8485	56	609.4711162	0.019587611	58.0563
24	458.8360871	0.004011774	35.3192	57	632.2682377	0.619629714	-0.475607
25	467.3560275	0.047578082	0.0597022	58	632.70961	7.4718E-05	49.7292
26	473.3674212	0.000620733	49.1229	59	644.7149364	0.000505783	44.1984
27	476.6277559	0.017547232	16.242	60	648.1838317	8.62128E-05	49.4128
28	483.1755866	0.022857954	-0.0797976	61	669.6578064	0.001149506	57.7365
29	490.4014816	0.010690409	14.4348	62	674.8611492	0.001396652	67.9249
30	496.3158704	0.010420251	33.7313	63	676.7556549	0.002908251	80.2134
31	498.5217618	0.005253246	46.411	64	682.954268	0.004029018	106.94
32	502.821989	0.016368944	38.5498	65	686.4619652	0.000620733	68.6916
33	504.1800576	0.019627825	-5.58623	66	689.9648121	5.17277E-05	51.2166

Table A2.1. The coefficients of all the component Gaussian functions of the LSFC-Raman (continued)

	ν_n	i_n	w_n		ν_n	i_n	w_n
67	734.1864359	0.004333641	49.6755	110	367.8590716	0.011943827	-1.94758
68	749.5665628	0.000293124	49.894	111	369.9572876	0.026373122	-15.4663
69	756.3287744	0.001143756	55.2862	112	373.2816455	0.026195262	9.72938
70	761.5369675	0.00183921	66.7863	113	378.6469866	0.012308473	26.6418
71	766.5530908	0.004247425	78.5112	114	379.5792037	0.015435716	27.3652
72	767.4920983	0.00574753	81.4823	115	382.9413935	0.002890822	39.569
73	773.148454	0.002528913	53.5223	116	386.7575663	0.05129637	33.1361
74	778.9609876	0.0119376	44.1538	117	389.661893	0.062281016	-0.017311
75	786.4992384	0.047899917	79.0687	118	395.4142835	0.059315958	-8.60329
76	799.3155258	0.063515763	20.078	119	397.4736976	0.015834214	-3.32851
77	802.3925212	0.066205576	0.074032	120	403.2678002	0.022298018	0.459694
78	833.3351442	0.000218406	50.3612	121	408.6535123	0.021012506	0.38971
79	934.7042946	0.040824676	78.2642	122	410.4287019	0.038578079	-0.077212
80	939.7737707	0.030783762	97.024	123	415.6475656	0.017457485	0.0002547
81	994.5330368	0.009523647	68.0391	124	419.3162909	0.024106006	-0.602511
82	997.4043818	0.044284688	47.5041	125	426.4946535	0.005284083	-5.23898
83	999.0534651	0.04158335	45.9693	126	435.1203292	0.013749421	-0.020078
84	1006.290031	0.188542169	46.5165	127	444.8431303	0.014075861	50.5109
85	1078.655686	0.084747376	41.6954	128	449.6613637	0.002330215	31.1688
86	1100.12287	0.036169212	-0.83774	129	455.9715325	0.014636435	22.6279
87	1125.732164	0.01008119	48.3053	130	462.0362788	0.012713719	48.639
88	1131.358448	0.017110393	-12.7126	131	468.9187765	0.006004536	24.4761
89	1148.01419	0.027605371	55.8276	132	474.1182391	0.013918247	10.4716

90	1149.488664	0.090811072	121.038	133	479.0897402	0.00265217	43.4907
91	1154.600822	0.013414735	29.3047	134	486.2739231	0.005684834	26.0784
92	1157.966892	0.060280119	44.8991	135	490.9097873	0.007735884	13.2183
93	1166.736135	0.052618646	92.621	136	494.6609668	0.013907035	7.49035
94	1176.456026	0.050767935	22.0927	137	498.9670143	0.003996275	46.8993
95	1281.163115	0.01033406	15.3789	138	500.110702	0.003255555	48.0745
96	1292.638795	0.010132867	53.7258	139	502.011028	0.004187643	47.0232
97	320.8223657	0.016637958	49.3461	140	504.6447111	0.004322725	40.4018
98	322.3579532	0.007276593	49.4722	141	507.3860695	0.000497564	48.5309
99	324.2485787	0.015818431	47.9926	142	509.4697348	0.00423717	31.9123
100	327.9017833	0.050276451	39.8964	143	517.9091611	0.008717498	39.2362
101	331.0010898	0.021654174	38.5162	144	529.3547693	0.004351995	48.7727
102	332.9508883	0.011502552	38.6317	145	536.0500474	0.00142965	47.1209
103	335.5845714	0.029898863	27.6714	146	537.2364174	0.009505492	37.4944
104	338.1173693	0.011155758	27.8824	147	545.6855442	0.002287438	28.0614
105	344.9639751	0.010813568	10.9759	148	548.2707248	0.003514464	18.7012
106	349.1022042	0.016412857	1.73954	149	556.9390826	0.003690082	-3.5269
107	356.5191988	0.026773905	-0.86762	150	564.7586476	0.010766294	-0.875908
108	358.6426361	0.020807652	-0.43040	151	570.1841317	0.015278102	-0.2994
109	365.9771766	0.043805898	-0.15023	152	572.1804925	0.001544475	10.8622

Table A2.1. The coefficients of all the component Gaussian functions of the LSFC-Raman (continued)

	ν_n	i_n	w_n		ν_n	i_n	w_n
153	583.0925737	0.007670585	6.89343	194	983.0670576	0.000231896	52.0567
154	589.1223983	0.004372263	48.3424	195	996.279125	0.090394531	95.2189
155	592.7368009	0.009892734	99.2223	196	1012.779658	0.049889164	70.8919
156	593.8572075	0.029869582	96.0045	197	1027.485601	0.010041336	126.439
157	601.3440456	0.000990624	67.268	198	1100.675798	0.00327357	55.4543
158	607.9578397	0.009831953	61.2659	199	1124.888221	0.011378681	47.5242
159	614.6453575	0.003352366	51.8519	200	1129.02063	0.021645139	37.8347
160	624.9589185	0.073540398	273.845	201	1132.047183	0.033471844	0.010058
161	632.3953141	0.003525719	14.6368	202	1140.360503	0.010554659	68.977
162	638.0827114	0.108849403	0.30183	203	1143.173645	0.019272113	75.5075
163	648.2740462	0.002208641	5.41634	204	1145.870381	0.030873718	82.36
164	651.8574072	0.021406541	258.26	205	1195.439885	0.009305122	91.3088
165	655.693951	0.006234186	105.86	206	1198.185124	0.002255926	54.042
166	660.6363507	0.006436809	54.7303	207	1219.623207	0.022728082	114.893
167	663.1235563	0.002442787	56.4731	208	1256.853687	0.012538145	94.2841
168	667.1725408	0.002812026	55.8045	209	1343.110444	0.010203434	50.0122
169	672.5068403	0.004944114	63.9215	210	1351.33646	0.001344094	50
170	678.559946	0.002132099	85.1029	211	318.2788972	0.06832678	49.0097
171	680.340956	0.001123456	79.9952	212	319.1480611	0.071516812	48.5671
172	682.7912998	0.004818034	108.049	213	321.1104702	0.021021071	48.9915
173	686.3707806	0.005862694	124.682	214	321.6866793	0.042580589	47.7604
174	696.8065677	0.001765113	79.2878	215	322.6324771	0.016089807	48.6499
175	700.3666476	0.004052561	95.2255	216	325.2079572	0.052715518	43.4095

176	708.670267	0.003210524	51.1338	217	327.2964727	0.047039957	40.6689
177	724.7430089	0.005804166	49.9891	218	328.192798	0.022928467	42.3344
178	728.3622617	0.001749351	49.9825	219	330.7255959	0.024490261	37.7416
179	739.790409	0.000184616	49.9309	220	331.4764138	0.072646743	31.3815
180	744.938459	0.002336975	48.2981	221	334.9821709	0.023034784	29.6088
181	755.4780414	0.00099963	55.1074	222	337.1948527	0.022051202	25.1528
182	757.6509512	0.00250358	72.2682	223	337.9602214	0.122677239	7.16632
183	763.4402036	0.003233034	82.3848	224	340.3397516	0.032857466	16.9752
184	764.9903419	0.002165864	72.6246	225	340.4192956	0.119792991	-5.07586
185	777.7406659	0.004730236	43.7547	226	342.784275	0.032923964	11.4387
186	782.5113669	0.006312982	56.3912	227	344.3033718	0.047611466	6.11604
187	794.6049678	0.031695531	155.641	228	345.7235235	0.004213513	19.6796
188	799.3388069	0.028000965	-0.025660	229	348.8761828	0.071244411	-2.62248
189	810.8261272	0.004320472	-1.26627	230	349.6299108	0.006493084	-1.01231
190	825.5844527	0.00329608	39.5314	231	351.2072105	0.005296816	12.9894
191	870.0311278	0.004903589	49.9038	232	351.6010504	0.037489623	-0.449817
192	906.8464275	0.00160751	58.0688	233	352.6787748	0.065189893	0.0955639
193	958.2726051	0.026017402	47.1513	234	354.7905715	0.125734276	0.133988

Table A2.1. The coefficients of all the component Gaussian functions of the LSFC-Raman (continued)

	ν_n	i_n	w_n		ν_n	i_n	w_n
235	356.3533204	0.010666726	4.11612	276	465.0055988	0.020456186	-0.042833
236	358.9433513	0.054489865	-0.340867	277	468.9827997	0.014607758	13.6335
237	361.2268466	0.050907788	0.0455184	278	472.8843368	0.068160669	0.0593148
238	363.1262026	0.040088117	0.0797467	279	473.6312745	0.029953188	-2.73557
239	365.9936674	0.043205242	0.213774	280	476.9459319	0.017744645	0.489291
240	368.8135998	0.008872322	11.2702	281	478.985945	0.04295928	-0.190928
241	369.2578823	0.00853337	16.7246	282	482.9941874	0.069908577	0.260014
242	370.4112706	0.063634802	0.497872	283	486.9093052	0.075690427	-16.2953
243	372.8373631	0.083213775	0.508112	284	490.7904713	0.060756963	12.2882
244	374.5291286	0.033714729	-24.5804	285	492.6966175	0.095276077	-0.148574
245	376.9717119	0.072241346	-19.7965	286	495.6310158	0.060079164	-0.0846453
246	380.7209513	0.004446123	32.4706	287	497.4537378	0.014335276	37.5631
247	381.2108261	0.033568647	27.4211	288	499.4617393	0.034459025	-0.592939
248	383.8988318	0.07864785	-23.0602	289	504.4089892	0.068386601	1.41099
249	387.7596269	0.135749829	-38.0644	290	506.6527125	0.121733449	8.16367
250	388.3125548	0.087407152	-38.6507	291	508.621912	0.040819328	14.0959
251	392.0889556	0.05991973	0.0648294	292	511.9530602	0.03780876	19.8163
252	392.850444	0.184138706	-45.3919	293	513.4003733	0.011783224	26.3422
253	393.5052271	0.028757026	-4.63374	294	517.09529	0.059461187	27.53
254	395.879907	0.03844009	0.147202	295	520.3701754	0.030484905	35.9994
255	399.9415022	0.03093677	3.05876	296	521.0957721	0.109531475	32.5373
256	403.0398387	0.017963955	0.174297	297	523.7604967	0.027846352	42.2872
257	405.0148585	0.081419399	-0.040016	298	525.4813636	0.01515272	46.2669

258	406.4612015	0.029541115	0.661831	299	527.0305318	0.014388448	47.0401
259	407.6359309	0.049651805	0.608922	300	531.7410898	0.020024189	43.1396
260	409.0871242	0.21140714	0.0293623	301	532.2484254	0.011224988	44.4618
261	412.0283128	0.090424397	-0.31229	302	536.8028055	0.016601521	35.5673
262	416.6903682	0.034904482	0.258849	303	540.910963	0.083453061	24.7042
263	423.1916366	0.030245619	0.0495917	304	543.1139443	0.020044112	24.0488
264	423.575776	0.048262825	0.112991	305	545.4614628	0.014747323	20.7489
265	427.2027893	0.046308747	-0.030533	306	546.59351	0.028597324	17.78
266	431.8929762	0.024742793	0.249696	307	548.9080469	0.020834984	14.6044
267	433.8146432	0.139444872	0.0318339	308	552.2430754	0.008367232	10.3201
268	434.027084	0.032372218	-0.257296	309	554.7584125	0.004186941	-1.31898
269	434.206543	0.013883357	-0.740546	310	556.8702091	0.049884414	0.936362
270	437.4047946	0.049246408	-0.204362	311	561.4168288	0.005795257	0.206295
271	439.8046958	0.067728565	-0.25903	312	564.252282	0.051665437	-0.078797
272	441.491611	0.017698123	0.147679	313	565.4454423	0.057533815	0.0774078
273	449.0259816	0.105258247	-0.200861	314	569.7631304	0.006081037	-0.074447
274	458.5314918	0.058298141	0.173001	315	571.3530407	0.015617939	0.313432
275	459.9691044	0.010806291	41.9531	316	576.4962405	0.012839927	0.093404

Table A2.1. The coefficients of all the component Gaussian functions of the LSFC-Raman (continued)

	ν_n	i_n	w_n		ν_n	i_n	w_n
317	580.2338393	0.049425872	-3.83456	360	748.4713775	0.016076508	105.516
318	585.3974101	0.057075273	11.3331	361	759.4562123	0.009503679	120.32
319	586.7671193	0.082994252	111.225	362	766.1107485	0.004326506	85.5787
320	588.9031672	0.158126523	103.793	363	766.4366849	0.024530133	112.486
321	597.0409083	0.012992792	90.3396	364	776.4475906	0.013192179	39.7155
322	601.0394503	0.026889475	82.3466	365	779.6720335	0.010832864	47.6548
323	606.8733249	0.0073637	64.3783	366	787.2141645	0.00440625	64.3673
324	618.7709759	0.017492086	48.2889	367	793.8551199	0.022549643	109.445
325	619.4635909	0.008480198	47.0697	368	794.7378645	0.016216073	92.1433
326	621.7490264	0.006951653	43.2409	369	800.9151366	0.02347343	1.5574
327	629.3590608	0.012707011	0.096163	370	805.6916578	0.000844033	42.4703
328	632.0043844	0.018555439	-0.076569	371	817.5699078	0.004127119	35.2307
329	632.6669278	0.037961518	0.105796	372	846.7189102	0.007170963	77.6706
330	634.4372673	0.049904176	-0.195224	373	870.2086468	0.00246564	49.961
331	636.8798507	0.021167286	0.055622	374	890.2993316	0.000525029	49.0639
332	638.6967524	0.024769392	0.279931	375	921.2312841	0.11779912	69.6282
333	640.053851	0.013790313	0.565263	376	949.3035321	0.166115091	85.9556
334	640.5650668	0.027640448	-0.047515	377	971.4361701	0.022091074	22.7592
335	644.5859199	0.029979894	-0.305354	378	977.5474788	0.25687171	-0.5097
336	647.1439391	0.128492472	0.099302	379	1029.289892	0.012447829	137.659
337	647.7735009	0.233265471	0.384292	380	1049.389308	0.032585065	49.782
338	652.842007	0.033754788	-0.0016189	381	1054.714877	0.034133479	49.9742
339	656.6513894	0.015857198	220.936	382	1069.517824	0.038194127	49.703

340	660.9254253	0.037130694	56.5491	383	1071.157207	0.11948053	48.3591
341	671.2001843	0.003322975	61.3468	384	1074.241963	0.051931429	47.5786
342	676.7847564	0.001395645	75.7454	385	1086.939905	0.18633848	24.1592
343	688.576672	0.008334009	136.896	386	1090.034361	0.003582157	41.0141
344	690.4954289	0.006021216	142.76	387	1104.914912	0.079285856	0.12898
345	692.3433723	0.005230344	146.562	388	1126.84772	0.076873503	53.3795
346	696.9084229	0.008606491	173.689	389	1176.873147	0.100725704	71.9091
347	697.939585	0.00368185	125.094	390	1193.858705	0.063196022	52.4655
348	698.6438405	0.0044129	135.325	391	1200.028217	0.065415825	-11.047
349	704.0926058	0.004771776	65.8236	392	1204.286732	0.081459191	0.123424
350	706.0705357	0.011643658	87.2223	393	1220.457449	0.001674774	53.1016
351	709.4278753	0.013205452	55.2221	394	1251.702727	0.079478674	108.605
352	713.955094	0.018183264	50.7722	395	1262.014348	0.092332007	92.2636
353	717.0000778	0.017232904	50.1576	396	1265.331916	0.026211543	74.21
354	727.6715868	0.022616087	49.821	397	1266.040051	0.071483697	66.637
355	730.6282962	0.009669817	49.7477	398	1270.288866	0.092883486	0.09004
356	731.4518678	0.018940914	49.3471	399	1290.184571	0.074999275	0.00237
357	736.1507851	0.008387154	48.6932	400	1291.736649	0.03938388	53.0961
358	743.4067516	0.032000204	34.1044	401	1293.385733	0.104288018	69.4383
359	743.6647847	0.025061796	36.2792	402	1300.234279	0.09579444	0.36618

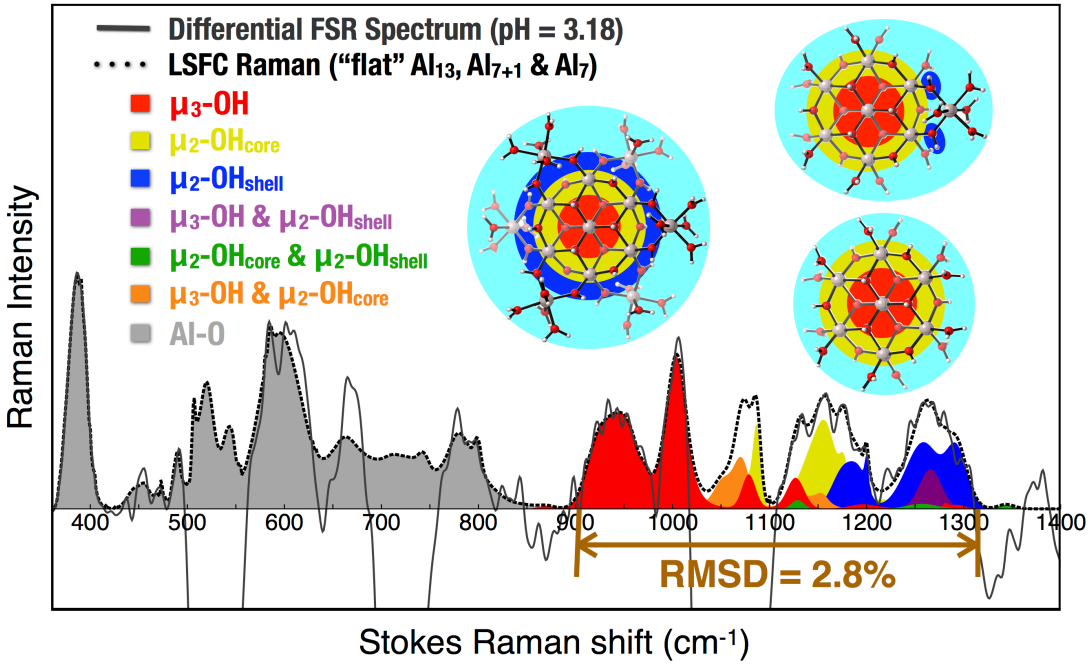

Figure A2.3. The experimental differential FSR spectrum (pH = 3.18) and the LSFC Raman spectrum, composing 402 Raman vibrational modes, generated from the computed Raman vibrational frequencies and intensities of "flat" Al_{13} (192 vibrational modes), Al_{7+1} (114 vibrational modes) and Al_7 (96 vibrational modes). In addition, the Raman contributions of each hydroxyl ligands in each polycation are also shown. The RMSD between the LSFC Raman and differential FSR spectrum (positive peaks) spectra are 4.5% for 350~1305 cm^{-1} and 2.8% for 907~1300 cm^{-1}. In the LSFC Raman spectrum, a universal scaling factor (0.9700) i1s used to modulate the frequencies of all the species and three intensity scaling factors are used for "flat" Al_{13} (0.066459), Al_{7+1} (0.022514) and Al_7 (0.057475), respectively. The normalized factor for the experimental differential FSR spectrum is 0.000235.

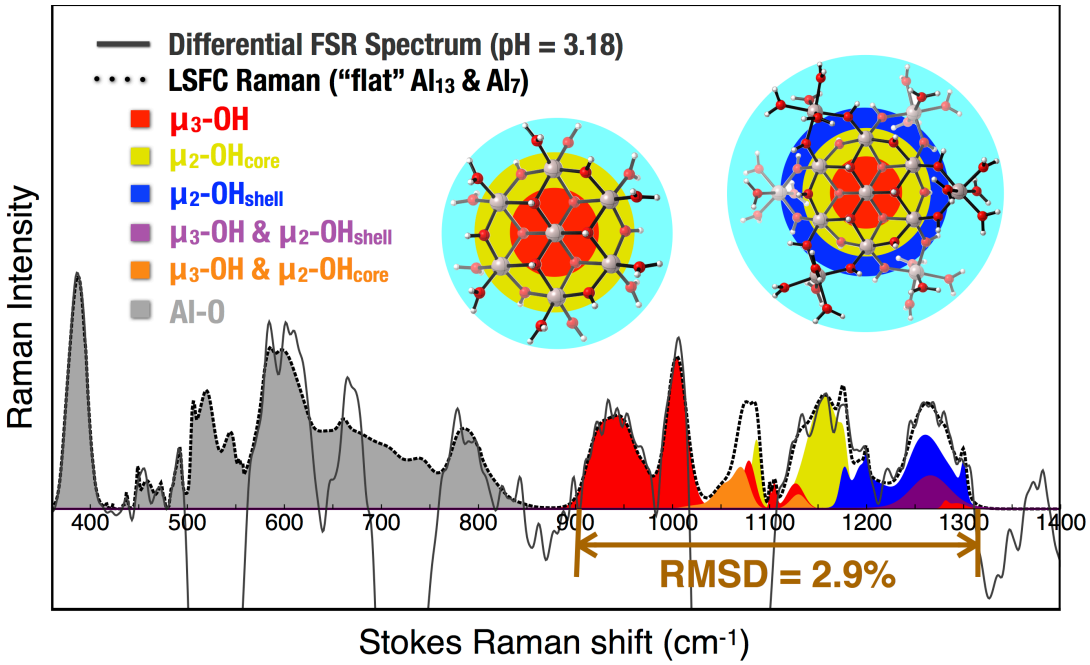

Figure A2.4. The experimental differential FSR spectrum (pH = 3.18) and the LSFC Raman spectrum, composing 288 Raman vibrational modes, generated from the computed Raman vibrational frequencies and intensities of "flat" Al_{13} (192 vibrational modes) and Al_7 (96 vibrational modes). In addition, the Raman contributions of each hydroxyl ligands in each polycation are also shown. The RMSD between the LSFC Raman and differential FSR spectrum (positive peaks) spectra are 4.9% for 350~1305 cm^{-1} and 2.9% for 907~1300 cm^{-1}. In the LSFC Raman spectrum, a universal scaling factor (0.9700) is used to modulate the frequencies of all the species and two intensity scaling factors are used for "flat" Al_{13} (0.054674) and Al_7 (0.081381), respectively. The normalized factor for the experimental differential FSR spectrum is 0.000235.

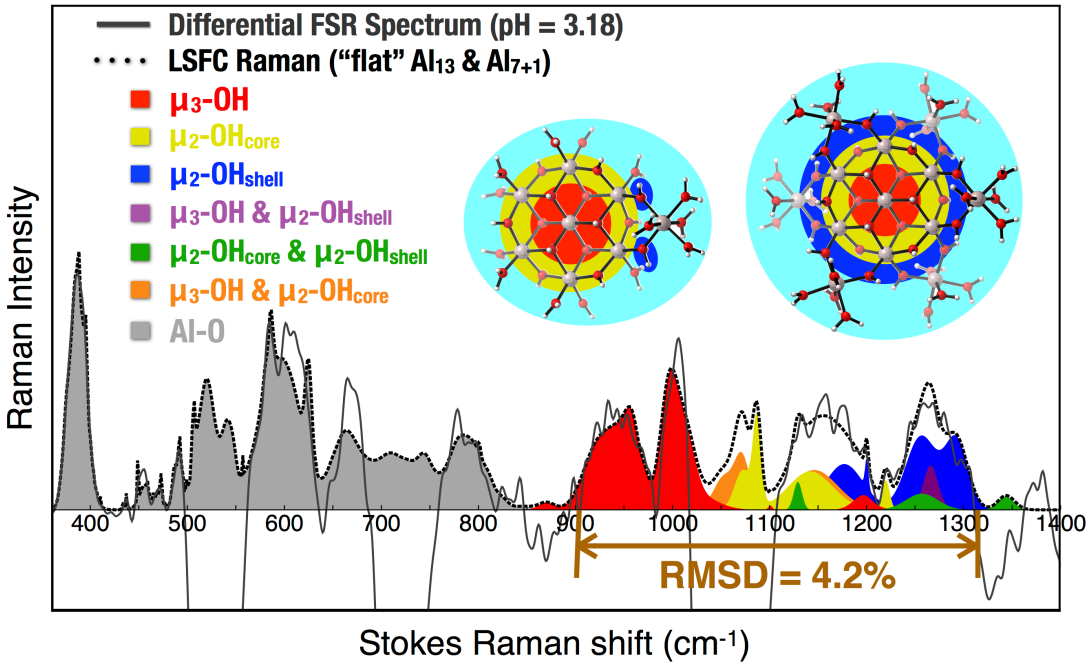

Figure A2.5. The experimental differential FSR spectrum (pH = 3.18) and the LSFC Raman spectrum, composing 306 Raman vibrational modes, generated from the computed Raman vibrational frequencies and intensities of "flat" Al_{13} (192 vibrational modes) and Al_{7+1} (114 vibrational modes). In addition, the Raman contributions of each hydroxyl ligands in each polycation are also shown. The RMSD between the LSFC Raman and differential FSR spectrum (positive peaks) spectra are 4.9% for 350~1305 cm^{-1} and 4.2% for 907~1300 cm^{-1}. In the LSFC Raman spectrum, a universal scaling factor (0.9702) is used to modulate the frequencies of all the species and two intensity scaling factors are used for "flat" Al_{13} (0.074789) and Al_{7+1} (0.072037), respectively. The normalized factor for the experimental differential FSR spectrum is 0.000235.

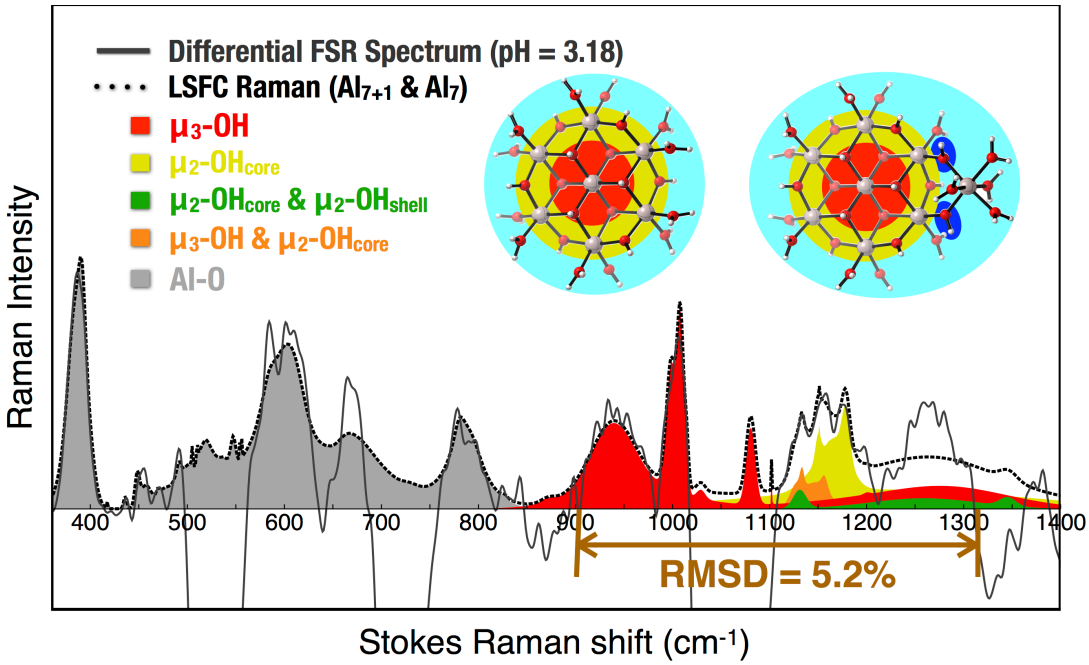

Figure A2.6. The experimental differential FSR spectrum (pH = 3.18) and the LSFC Raman spectrum, composing 210 Raman vibrational modes, generated from the computed Raman vibrational frequencies and intensities of Al_{7+1} (114 vibrational modes) and Al_7 (96 vibrational modes). In addition, the Raman contributions of each hydroxyl ligands in the polycation are also shown. The RMSD between the LSFC Raman and differential FSR spectrum (positive peaks) spectra are 5.7% for 350~1305 cm^{-1} and 5.2% for 907~1300 cm^{-1}. In the LSFC Raman spectrum, a universal scaling factor (0.9719) is used to modulate the frequencies of all the species and two intensity scaling factors are used for Al_{7+1} (0.047637) and Al_7 (0.128482), respectively. The normalized factor for the experimental differential FSR spectrum is 0.000235.

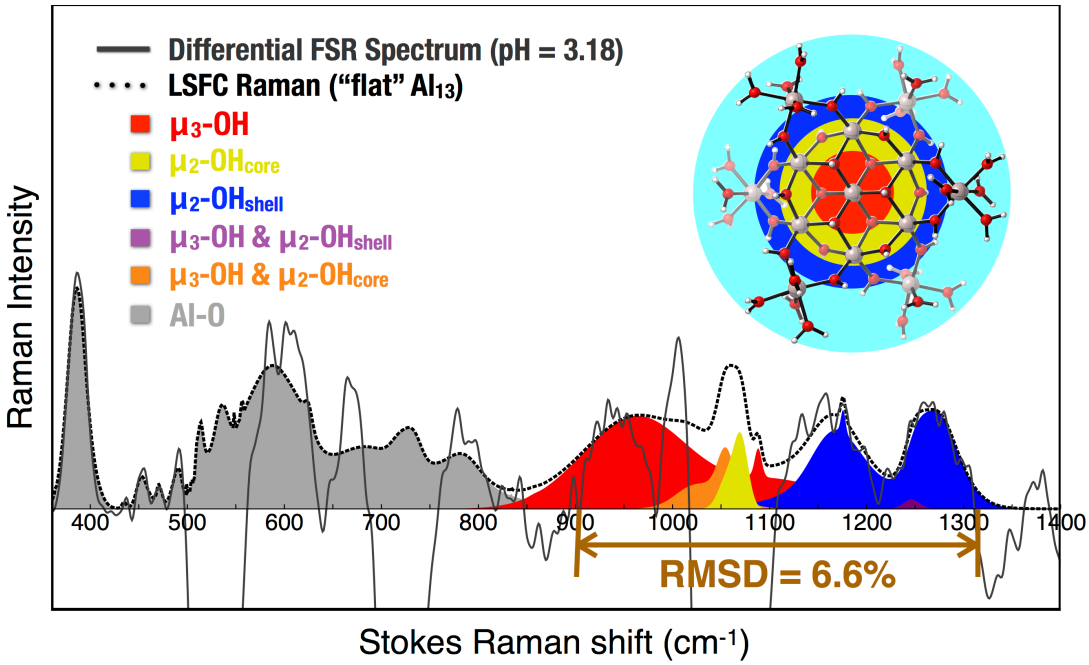

Figure A2.7. The experimental differential FSR spectrum (pH = 3.18) and the LSFC Raman spectrum generated from the computed Raman vibrational frequencies and intensities of "flat" Al_{13} (192 Raman vibrational modes). In addition, the Raman contributions of each hydroxyl ligands in the polycation are also shown. The RMSD between the LSFC Raman and differential FSR spectrum (positive peaks) spectra are 7.3% for 350~1305 cm^{-1} and 6.6% for 907~1300 cm^{-1}. In the LSFC Raman spectrum, two universal scaling factors are used to modulate the computed Raman frequencies (0.9555) and intensities (0.059155) of "flat" Al_{13}. The normalized factor for the experimental differential FSR spectrum is 0.000235.

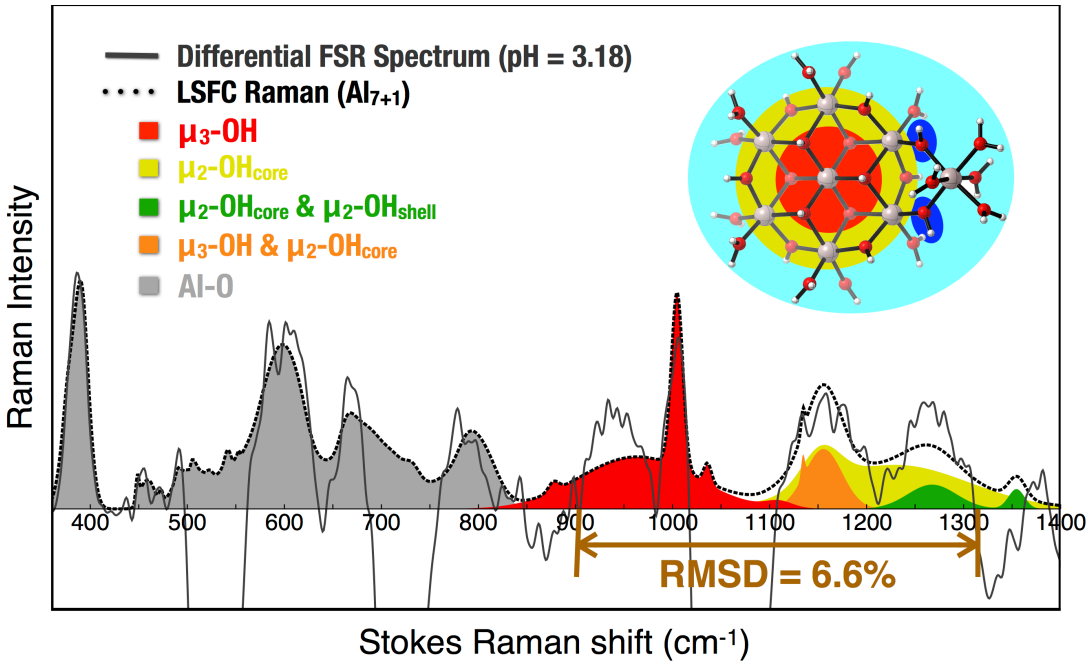

Figure A2.8. The experimental differential FSR spectrum (pH = 3.18) and the LSFC Raman spectrum generated from the computed Raman vibrational frequencies and intensities of Al_{7+1} (114 Raman vibrational modes). In addition, the Raman contributions of each hydroxyl ligands in the polycation are also shown. The RMSD between the LSFC Raman and differential FSR spectrum (positive peaks) spectra are 6.3% for 350~1305 cm^{-1} and 6.6% for 907~1300 cm^{-1}. In the LSFC Raman spectrum, two universal scaling factors are used to modulate the computed Raman frequencies (0.9783) and intensities (0.108066) of Al_{7+1}. The normalized factor for the experimental differential FSR spectrum is 0.000235.

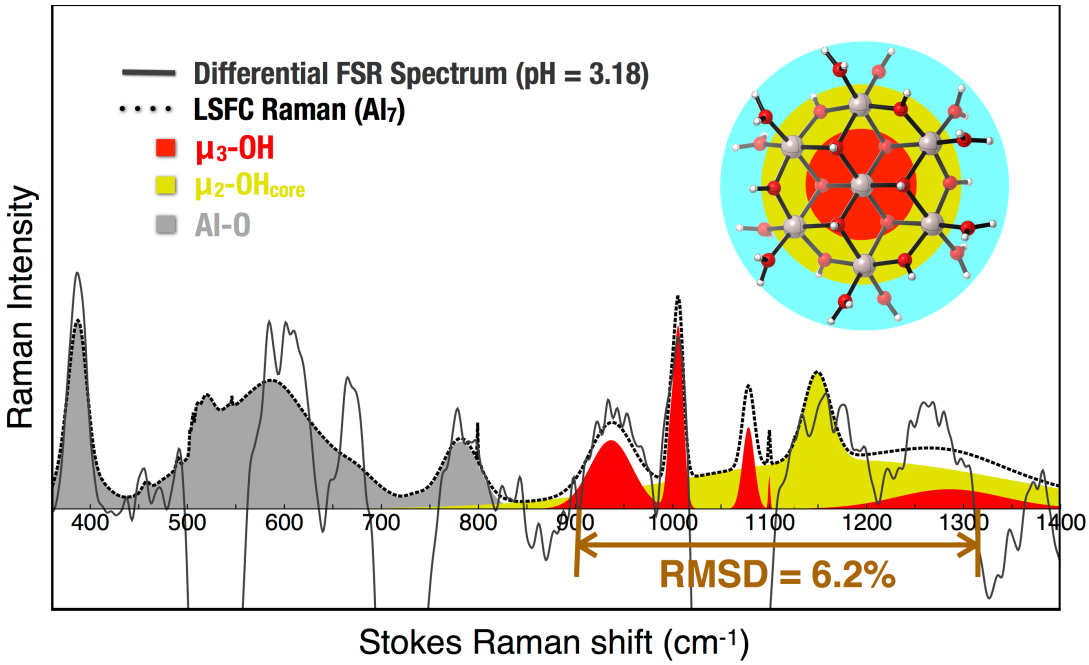

Figure A2.9. The experimental differential FSR spectrum (pH = 3.18) and the LSFC Raman spectrum generated from the computed Raman vibrational frequencies and intensities of Al_7 (96 Raman vibrational modes). In addition, the Raman contributions of each hydroxyl ligands in the polycation are also shown. The RMSD between the LSFC Raman and differential FSR spectrum (positive peaks) spectra are 7.9% for 350~1305 cm^{-1} and 6.2% for 907~1300 cm^{-1}. In the LSFC Raman spectrum, two universal scaling factors are used to modulate the computed Raman frequencies (0.9697) and intensities (0.137532) of Al_7. The normalized factor for the experimental differential FSR spectrum is 0.000235.

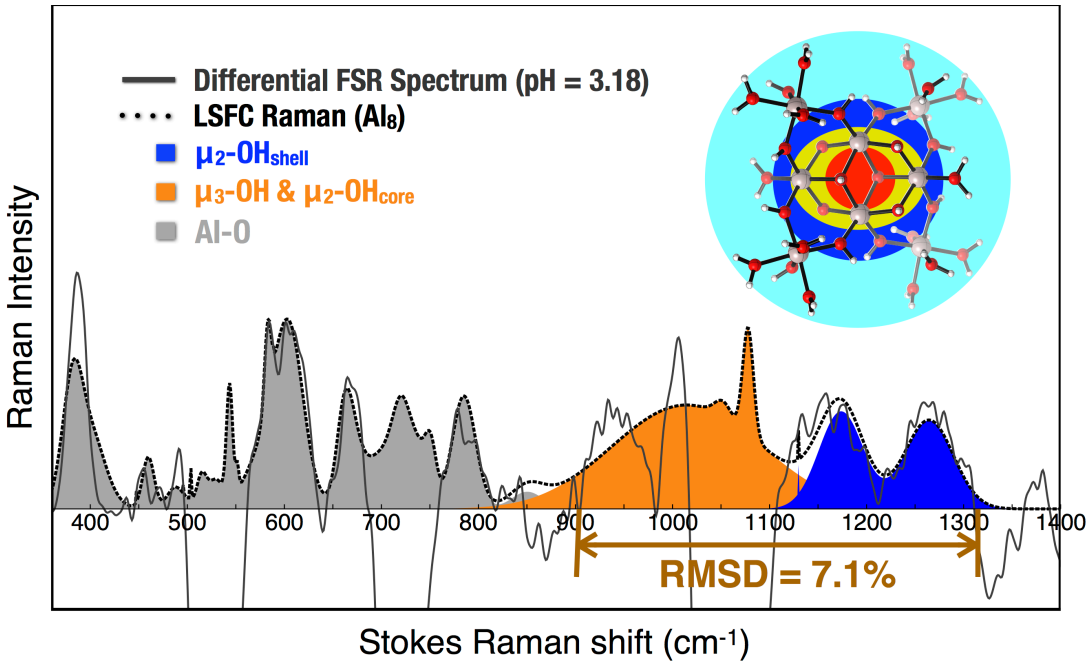

Figure A2.10. The experimental differential FSR spectrum (pH = 3.18) and the LSFC Raman spectrum generated from the computed Raman vibrational frequencies and intensities of Al_8 (67 Raman vibrational modes). In addition, the Raman contributions of each hydroxyl ligands in the polycation are also shown. The RMSD between the LSFC Raman and differential FSR spectrum (positive peaks) spectra are 6.8% for 350~1305 cm^{-1} and 7.1% for 907~1300 cm^{-1}. In the LSFC Raman spectrum, two universal scaling factors are used to modulate the computed Raman frequencies (0.9538) and intensities (0.095485) of Al_8. The normalized factor for the experimental differential FSR spectrum is 0.000235.

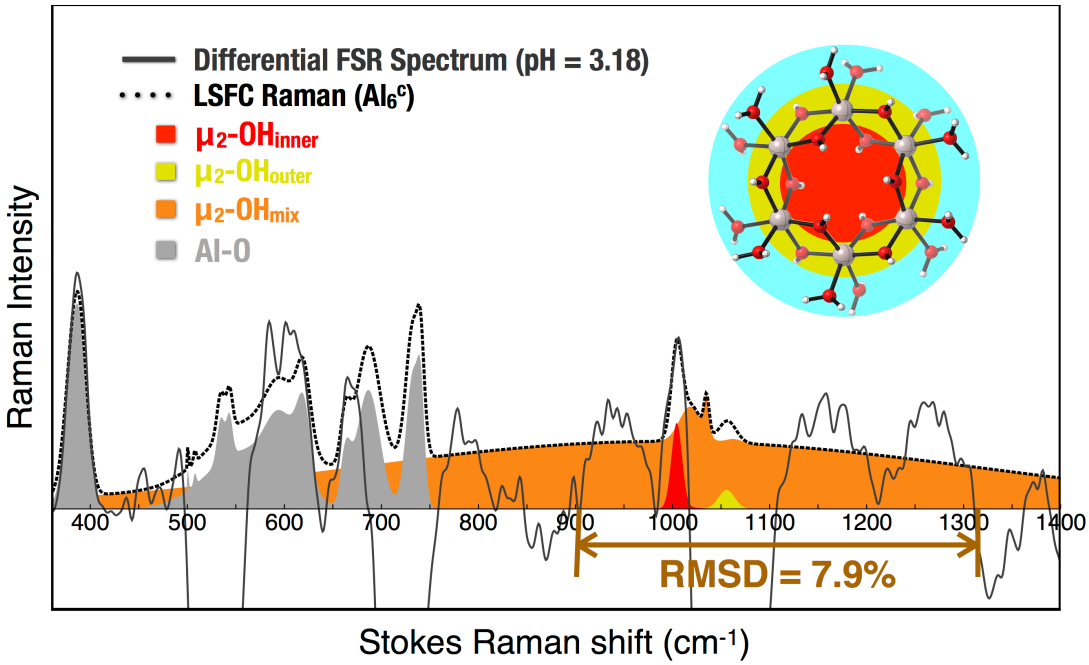

Figure A2.11. The experimental differential FSR spectrum (pH = 3.18) and the LSFC Raman spectrum generated from the computed Raman vibrational frequencies and intensities of Al_6^c (73 Raman vibrational modes). In addition, the Raman contributions of each hydroxyl ligands in the polycation are also shown. The RMSD between the LSFC Raman and differential FSR spectrum (positive peaks) spectra are 8.0% for 350~1305 cm^{-1} and 7.9% for 907~1300 cm^{-1}. In the LSFC Raman spectrum, two universal scaling factors are used to modulate the computed Raman frequencies (0.9809) and intensities (0.072053) of Al_6^c. The normalized factor for the experimental differential FSR spectrum is 0.000235.

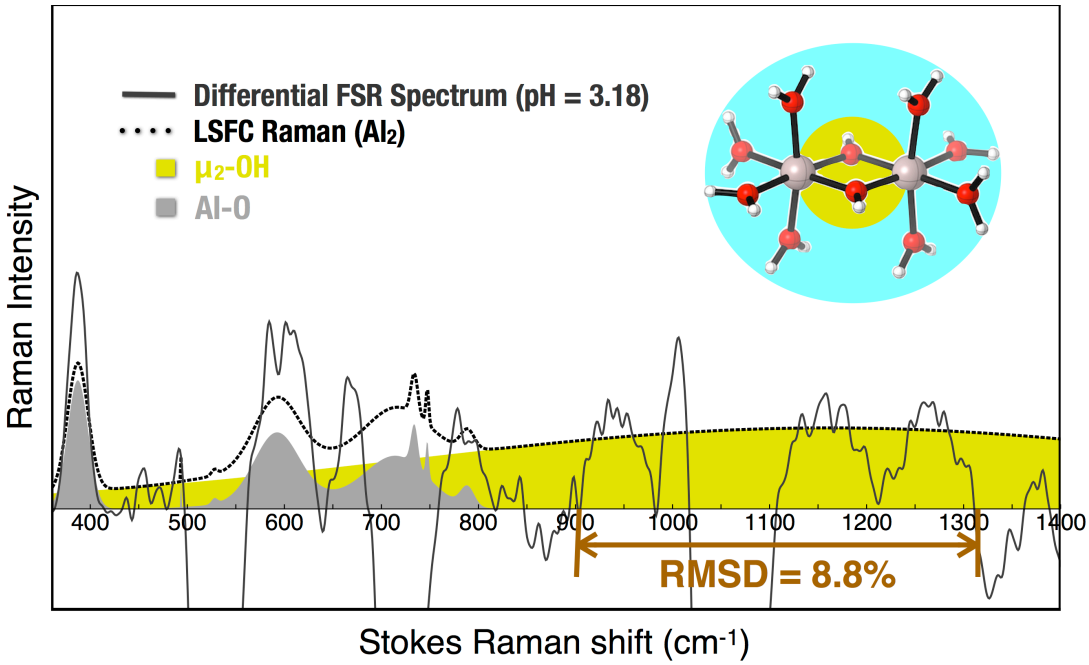

Figure A2.12. The experimental differential FSR spectrum (pH = 3.18) and the LSFC Raman spectrum generated from the computed Raman vibrational frequencies and intensities of Al_2 (17 Raman vibrational modes). The RMSD between the LSFC Raman and differential FSR spectrum (positive peaks) spectra are 9.7% for 350~1305 cm^{-1} and 8.8% for 907~1300 cm^{-1}. In the LSFC Raman spectrum, two universal scaling factors are used to modulate the computed Raman frequencies (1.0347) and intensities (0.115939) of Al_2. The normalized factor for the experimental differential FSR spectrum is 0.000235.

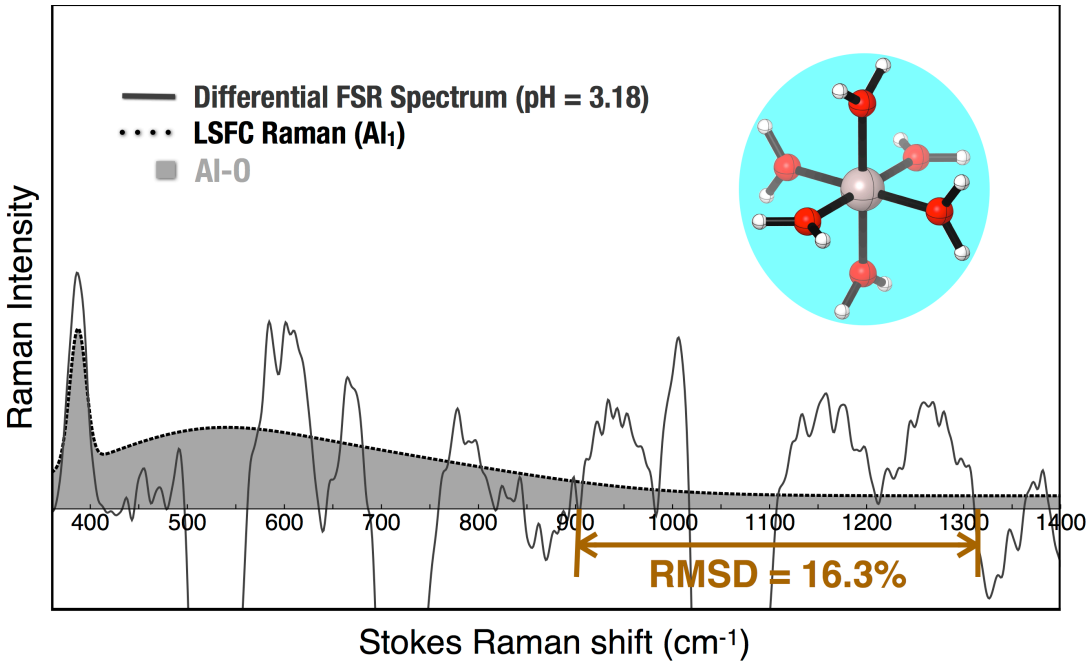

Figure A2.13. The experimental differential FSR spectrum (pH = 3.18) and the LSFC Raman spectrum generated from the computed Raman vibrational frequencies and intensities of Al_1 (9 Raman vibrational modes). The RMSD between the LSFC Raman and differential FSR spectrum (positive peaks) spectra are 14.4% for 350~1305 cm^{-1} and 16.3% for 907~1300 cm^{-1}. In the LSFC Raman spectrum, two universal scaling factors are used to modulate the computed Raman frequencies (1.0325) and intensities (0.086834) of Al_1. The normalized factor for the experimental differential FSR spectrum is 0.000235.

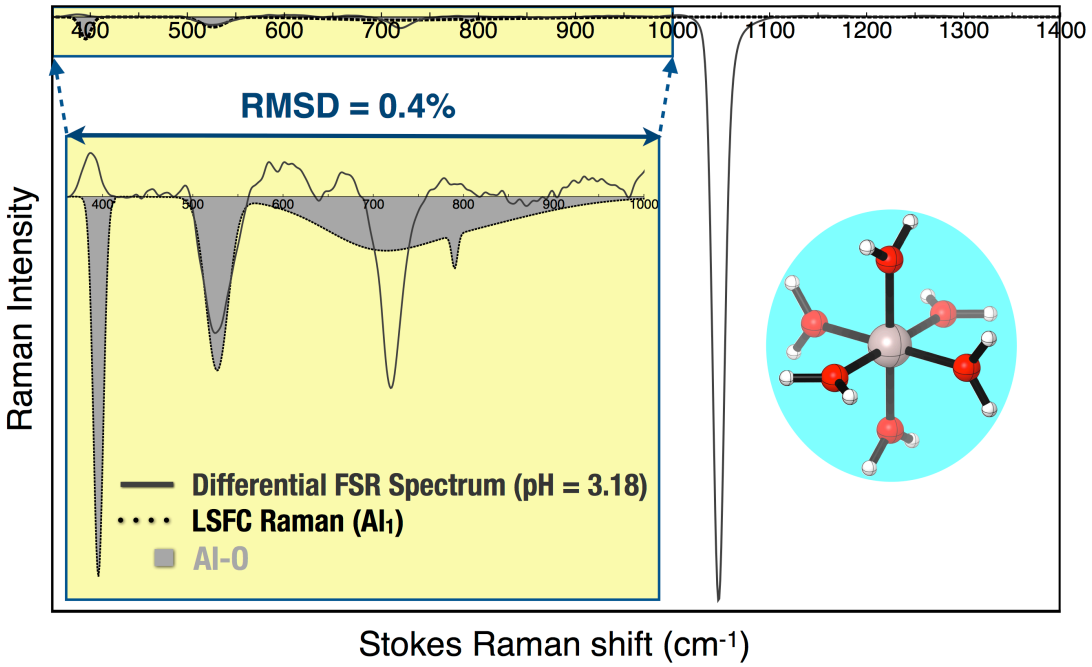

Figure A2.14. The experimental differential FSR spectrum (pH = 3.18) and the LSFC Raman spectrum generated from the computed Raman vibrational frequencies and intensities of Al_1 (9 Raman vibrational modes). The RMSD between the LSFC Raman and differential FSR spectrum (negative peaks) spectra are 18.9% for 350~1107 cm^{-1} and 0.4% for 350~820 cm^{-1}. In the LSFC Raman spectrum, two universal scaling factors are used to modulate the computed Raman frequencies (1.0539) and intensities (-0.009743) of Al_1. The normalized factor for the experimental differential FSR spectrum is 0.031701.

Table A2.2. Al_1, $[Al(H_2O)_6]^{3+}$

Supporting Information: Al1.log

```
-----------------------------------------------------------------------------
 Using  Gaussian 09:  AM64L-G09RevB.01 12-Aug-2010
=============================================================================
===============
 # HF 6-31G** SCRF=(Solvent=water) guess=read geom=check Freq
-----------------------------------------------------------------------------
 Pointgroup= CI   Stoichiometry= AlH12O6(3+)   CI[O(Al),X(H12O6)]  #Atoms= 19
 Charge = 3     Multiplicity = 1
-----------------------------------------------------------------------------
 SCF Energy= -697.911852594         Predicted Change= -9.657759D-08
=============================================================================
===============
 Optimization completed.            {Found       1       times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00001 ||  0.00045   [ YES ]      0.00000 ||  0.00030   [ YES ]
 Displ      0.00173 ||  0.00180   [ YES ]      0.00173 ||  0.00180   [ YES ]
-----------------------------------------------------------------------------
     Atomic          Coordinates (Angstroms)
      Type          X           Y        Z
-----------------------------------------------------------------------------
      Al       0.000000      0.000000      0.000000
      O       -1.116085      1.054169      1.113137
      O        0.780315     -0.796505      1.537478
      H       -0.900746      1.916485      1.453890
      H       -1.981347      0.796468      1.414029
      H        1.461459     -1.461055      1.522633
      H        0.547435     -0.593731      2.437744
      O        1.325878      1.358324      0.029911
      H        1.371201      2.094733     -0.571504
      H        2.033756      1.417159      0.663475
      O        1.116085     -1.054169     -1.113137
      O       -0.780315      0.796505     -1.537478
      H        0.900746     -1.916485     -1.453890
      H        1.981347     -0.796468     -1.414029
      H       -1.461459      1.461055     -1.522633
      H       -0.547435      0.593731     -2.437744
      O       -1.325878     -1.358324     -0.029911
      H       -1.371201     -2.094733      0.571504
      H       -2.033756     -1.417159     -0.663475
-----------------------------------------------------------------------------
```

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm
==========
SCF Energy= -697.911852594 Predicted Change= -9.657759D-08
Zero-point correction (ZPE)= -697.7463 0.16552
Internal Energy (U)= -697.7316 0.18024
Enthalpy (H)= -697.7306 0.18118
Gibbs Free Energy (G)= -697.7832 0.12864

Frequencies -- 133.7650 152.7680 176.2020

Table A2.3. Al_2, $[Al_2(OH)_2(H_2O)_8]^{4+}$

Supporting Information: Al2.log

Using Gaussian 09: AM64L-G09RevB.01 12-Aug-2010
==========
HF 6-31g(d,p) SCRF=(Solvent=water) guess=read geom=check Freq
---
Pointgroup= C1 Stoichiometry= Al2H18O10(4+) C1[X(Al2H18O10)] #Atoms= 30
Charge = 4 Multiplicity = 1

SCF Energy= -1242.91402345 Predicted Change= -3.198302D-07
==========
Optimization incomplete.

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001 ||	0.00045	[YES]	0.00000 ||	0.00030	[YES]
Displ	0.00385 ||	0.00180	[NO]	0.00385 ||	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
Al	-1.435203	0.000034	-0.011300
Al	1.435218	0.000170	0.011295
O	0.019191	0.000096	-1.162798
H	0.066615	0.000404	-2.106366
O	-0.019186	0.000020	1.162794
H	-0.066621	-0.000081	2.106361
O	2.860747	-0.000363	-1.285743

H	3.219021	0.777258	-1.697353
H	3.218564	-0.778324	-1.697106
O	2.747100	-0.000034	1.405560
H	2.593355	0.000631	2.343468
H	3.683768	-0.000542	1.239134
O	-2.747111	0.000079	-1.405545
H	-3.683772	0.000022	-1.239082
H	-2.593400	0.000000	-2.343460
O	-2.860743	-0.000150	1.285741
H	-3.218740	-0.777977	1.697198
H	-3.218846	0.777603	1.697249
O	1.609152	-1.933502	-0.063064
H	1.211914	-2.486290	-0.725317
H	2.096106	-2.469325	0.551890
O	1.609495	1.933624	-0.063238
H	1.212538	2.486396	-0.725680
H	2.097168	2.469362	0.551227
O	-1.609209	-1.933564	0.063030
H	-1.212254	-2.486354	0.725455
H	-2.096580	-2.469320	-0.551656
O	-1.609442	1.933566	0.063264
H	-1.212280	2.486340	0.725578
H	-2.096702	2.469360	-0.551476

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1242.91402345 Predicted Change= -3.198302D-07
Zero-point correction (ZPE)= -1242.6593 0.25467
Internal Energy (U)= -1242.6349 0.27911
Enthalpy (H)= -1242.6339 0.28006
Gibbs Free Energy (G)= -1242.7074 0.20662

Frequencies -- 56.5790 64.6349 94.7748

Table A2.4. Al_6, $[Al_6(OH)_{12}(H_2O)_{12}]^{6+}$
Supporting Information: Al6c.log

Using Gaussian 09: AM64L-G09RevB.01 12-Aug-2010

==========

#HF/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current Guess=Read Geom=Check
#SCRF=(PCM,SOLVENT=H2O) opt=(maxcycle=250,RFO,ReadFC) IOp(1/8=3) freq
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RHF/6-31G(d,p) Freq

---

Pointgroup= C1 Stoichiometry= Al6H36O24(6+) C1[X(Al6H36O24)] #Atoms= 66
Charge = 6 Multiplicity = 1

SCF Energy= -3269.98839168 Predicted Change= -1.471099D-04

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00018 ||	0.00045	[YES]	0.00004 ||	0.00030	[YES]
Displ	0.06660 ||	0.00180	[NO]	0.06660 ||	0.00180	[NO]

Atomic Type	Coordinates (Angstroms) X	Y	Z
Al	-2.232142	1.875169	0.036624
Al	0.509985	2.855381	-0.041990
Al	2.747470	0.991103	0.043328
Al	2.232153	-1.875193	-0.036625
Al	-0.509971	-2.855382	0.041955
Al	-2.747502	-0.991119	-0.043328
O	1.306103	1.505044	-1.026708
O	-1.306136	-1.505083	1.026702
O	-1.983088	0.371140	-1.039905
O	-0.663269	1.870721	1.022576
O	1.983119	-0.371181	1.039938
O	0.663288	-1.870696	-1.022566
O	-1.129547	3.033097	-0.925319
O	2.067979	2.496205	0.922356
O	3.207366	-0.542742	-0.918914
O	1.129512	-3.033016	0.925394
O	-2.068044	-2.496286	-0.922305
O	-3.207357	0.542731	0.918916
H	1.078353	1.170348	-1.876039
H	-1.078034	-1.170019	1.875785
H	-1.600231	0.342366	-1.899246
H	-0.486508	1.501155	1.869442
H	1.600492	-0.342516	1.899386
H	0.486786	-1.501583	-1.869686
H	-1.254296	3.391441	-1.788486

H	2.307550	2.779756	1.789222
H	3.563024	-0.607016	-1.790014
H	1.254330	-3.391948	1.788307
H	-2.306959	-2.779210	-1.789561
H	-3.563313	0.607102	1.789884
O	3.865228	-2.440002	0.928222
H	3.906277	-3.028397	1.671324
H	4.588949	-1.827324	0.976799
O	-1.414365	-4.137233	1.299918
H	-1.548392	-3.916457	2.212735
H	-1.269808	-5.072363	1.228781
O	-4.024083	-2.133050	0.946072
H	-4.579330	-1.872437	1.669259
H	-3.844533	-3.063287	1.007337
O	-4.311555	-0.867618	-1.294722
H	-4.201192	-0.626962	-2.205654
H	-5.044710	-1.465227	-1.220197
O	-3.865044	2.440022	-0.928365
H	-4.589012	1.827691	-0.977493
H	-3.906633	3.030202	-1.670013
O	-2.872633	3.297634	1.305301
H	-3.752995	3.644970	1.236941
H	-2.614001	3.296027	2.217997
O	0.164482	4.536873	0.941282
H	0.666140	4.881890	1.668395
H	-0.730981	4.845765	1.004129
O	-0.164656	-4.536760	-0.941434
H	-0.667682	-4.883335	-1.666850
H	0.730643	-4.845935	-1.005049
O	2.872711	-3.297695	-1.305208
H	2.614293	-3.296204	-2.217962
H	3.752941	-3.645306	-1.236536
O	4.024015	2.133031	-0.946133
H	3.844381	3.063226	-1.007766
H	4.579916	1.872302	-1.668775
O	4.311592	0.867611	1.294659
H	5.044745	1.465218	1.220100
H	4.201260	0.626985	2.205603
O	1.414407	4.137301	-1.299827
H	1.548319	3.916805	-2.212729
H	1.270070	5.072440	-1.228347

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

```
=================================================================
================
SCF Energy=     -3269.98839168      Predicted Change= -1.471099D-04
Zero-point correction (ZPE)=              -3269.4555  0.53289
Internal Energy (U)=                -3269.4016  0.58673
Enthalpy (H)=                              -3269.4007   0.58767
Gibbs Free Energy (G)=                    -3269.5343    0.45407
-----------------------------------------------------------------------
Frequencies --     9.2376              36.5716              45.6516
```

Table A2.5. Al_7, $[Al_7(OH)_{12}(H_2O)_{12}]^{9+}$
Supporting Information: Al7.log

```
-----------------------------------------------------------------------
Using  Gaussian 09:  AM64L-G09RevB.01 12-Aug-2010
=================================================================
================
#HF/6-31G(d,p) scf=(maxcycle=300,direct,tight) density=current
#SCRF=(PCM,SOLVENT=H2O) opt=(maxcycle=250,RFO) IOp(1/7=200,1/8=5) freq
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RHF/6-31G(d,p) Freq
-----------------------------------------------------------------------
Pointgroup= C1   Stoichiometry= Al7H36O24(9+)   C1[X(Al7H36O24)]  #Atoms= 67
Charge = 9     Multiplicity = 1
-----------------------------------------------------------------------
SCF Energy= -3511.54477817         Predicted Change= -3.143734D-04
=================================================================
================
Optimization completed.            {Found        1        times}
Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
Force      0.00028 ||  0.00045   [ YES ]      0.00005 ||  0.00030   [ YES ]
Displ      0.06172 ||  0.00180   [ NO ]       0.06172 ||  0.00180   [ NO ]
-----------------------------------------------------------------------
     Atomic          Coordinates (Angstroms)
      Type          X            Y        Z
-----------------------------------------------------------------------
      Al        0.000059      -0.000086      -0.000613
      Al        0.245074      -3.023841       0.014356
      Al        2.740827      -1.303207      -0.013895
      Al        2.499385       1.720030       0.011198
      Al       -0.245942       3.023957      -0.015846
      Al       -2.741314       1.302101       0.018037
      Al       -2.498594      -1.720294      -0.013606
      O         1.657753       0.130339       0.946754
```

O	-1.656802	-0.128880	-0.946909
O	-0.717446	-1.496103	0.949086
O	0.937939	-1.369172	-0.943835
O	0.718063	1.495913	-0.951136
O	-0.934385	1.369287	0.945093
O	1.859534	-2.681458	0.823416
O	3.243343	0.264958	-0.834121
O	1.393420	2.946335	0.817246
O	-1.862789	2.681928	-0.817140
O	-3.240484	-0.268651	0.834852
O	-1.389444	-2.941288	-0.825556
H	1.668655	0.121889	1.901077
H	-1.668839	-0.120967	-1.901263
H	-0.742729	-1.502740	1.903313
H	0.934495	-1.382430	-1.897740
H	0.748646	1.504397	-1.905179
H	-0.927779	1.382750	1.898942
H	2.238658	-3.228745	1.498465
H	3.902157	0.315494	-1.514118
H	1.684746	3.550306	1.487328
H	-2.241258	3.233131	-1.489453
H	-3.907457	-0.325516	1.506287
H	-1.677638	-3.547447	-1.494979
O	3.249057	2.967461	-1.202477
H	3.480478	3.855726	-0.948248
H	3.573439	2.810681	-2.083708
O	0.235218	4.324511	-1.309817
H	0.001554	4.338532	-2.232806
H	0.704580	5.127110	-1.101169
O	-4.189398	1.329196	-1.201256
H	-5.087961	1.136357	-0.949048
H	-4.184007	1.635095	-2.102647
O	-3.875174	-1.941841	-1.298762
H	-3.780990	-2.182231	-2.215416
H	-4.802569	-1.934004	-1.080624
O	-3.252828	-2.971839	1.194587
H	-3.492758	-2.840842	2.106369
H	-3.537321	-3.840833	0.927407
O	-0.246918	-4.320729	1.304966
H	-0.751599	-5.103241	1.102940
H	0.033953	-4.365023	2.213788
O	0.931843	-4.284918	-1.217043
H	1.534739	-4.982055	-0.975495
H	0.671870	-4.405815	-2.124644

O	3.618838	-2.398824	-1.290004
H	3.801057	-2.206535	-2.204908
H	4.059008	-3.211375	-1.057289
O	-3.621130	2.387492	1.302707
H	-4.084486	3.188139	1.073445
H	-3.779070	2.198647	2.222887
O	-0.924489	4.291429	1.212277
H	-0.637249	4.439354	2.107656
H	-1.551609	4.968980	0.976481
O	4.186612	-1.323129	1.208678
H	4.182225	-1.626504	2.110879
H	5.084051	-1.124777	0.956894
O	3.876184	1.941367	1.297768
H	4.802726	1.948392	1.076076
H	3.782712	2.166456	2.218319

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -3511.54477817 Predicted Change= -3.143734D-04
Zero-point correction (ZPE)= -3510.9916 0.55311
Internal Energy (U)= -3510.9433 0.60145
Enthalpy (H)= -3510.9423 0.60240
Gibbs Free Energy (G)= -3511.0612 0.48349

Frequencies -- 29.6353 61.8939 66.8044

Table A2.6. Al_{7+1}, $[Al_8(OH)_{14}(H_2O)_{14}]^{10+}$
Supporting Information: Al7-1.log

Using Gaussian 09: AM64L-G09RevB.01 12-Aug-2010

==========

HF 6-31G** OPT(maxcycles=200)
SCRF=(Solvent=water) IOp(1/8=15) Freq
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RHF/6-31G(d,p) Freq

---

Pointgroup= C1 Stoichiometry= Al8H42O28(10+) C1[X(Al8H42O28)] #Atoms= 78
Charge = 10 Multiplicity = 1

SCF Energy= -4056.55203136 Predicted Change= -4.894787D-07

==========
==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001 ||	0.00045	[YES]	0.00000 ||	0.00030	[YES]
Displ	0.01513 ||	0.00180	[NO]	0.01513 ||	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
Al	-0.848713	0.002791	-0.162267
Al	-0.819930	-3.017603	-0.124522
Al	1.785991	-1.483431	-0.556221
Al	1.796110	1.505255	-0.501736
Al	-0.828040	3.021341	-0.122246
Al	-3.437949	1.517665	0.259401
Al	-3.430211	-1.521627	0.282371
Al	4.608602	-0.016642	0.672601
O	0.908124	-0.009588	0.524820
O	-2.637002	-0.001648	-0.826158
O	-1.518181	-1.420959	0.933995
O	-0.207897	-1.455674	-1.210850
O	-0.194191	1.471385	-1.190521
O	-1.525791	1.426844	0.929823
O	0.928982	-2.795814	0.415823
O	2.118209	0.032080	-1.546945
O	0.911734	2.810059	0.461074
O	-2.571121	2.828065	-0.696207
O	-3.929149	0.004138	1.181751
O	-2.569014	-2.829428	-0.679814
O	3.386741	-1.400241	0.361532
O	3.309233	1.326904	0.533551
O	4.362618	-0.155780	2.586076
O	5.131388	0.073478	-1.176174
O	6.053082	-1.287944	0.930803
O	5.910857	1.367176	1.030950
H	1.055159	-0.022206	1.466148
H	-2.780451	-0.003677	-1.769300
H	-1.363941	-1.391399	1.874792
H	-0.370878	-1.474069	-2.150481
H	-0.324724	1.493813	-2.134736
H	-1.379139	1.394330	1.871551
H	1.350092	-3.297931	1.100595
H	2.470831	0.049047	-2.424597

H	1.327114	3.398218	1.077816
H	-3.003111	3.436412	-1.281148
H	-4.494032	0.008168	1.943076
H	-3.006421	-3.440741	-1.257523
H	3.737985	-2.240231	0.632328
H	3.313609	1.877037	1.307560
H	4.845157	0.345178	3.234642
H	3.711757	-0.694343	3.022089
H	5.138875	-0.647255	-1.795767
H	5.651428	0.787649	-1.528936
H	6.678368	-1.573988	0.274034
H	6.264650	-1.693919	1.764312
H	5.787385	2.300857	0.900466
H	6.830344	1.196442	1.204769
O	2.428623	2.735334	-1.804501
H	2.788066	3.585529	-1.570801
H	2.645241	2.555142	-2.712772
O	-0.438554	4.360459	-1.411122
H	-0.760541	4.421918	-2.304786
H	0.138040	5.099291	-1.241744
O	-5.016187	1.646883	-0.788923
H	-5.894040	1.513768	-0.444204
H	-5.083066	1.875458	-1.710549
O	-5.032747	-1.689179	-0.716342
H	-5.127867	-1.892180	-1.641656
H	-5.898246	-1.579599	-0.333432
O	-4.062372	-2.681726	1.646307
H	-4.046942	-2.552277	2.589312
H	-4.442554	-3.535800	1.462144
O	-1.193527	-4.295273	1.236161
H	-1.775091	-5.039839	1.112530
H	-0.870773	-4.308050	2.131266
O	-0.457361	-4.376205	-1.398381
H	0.128389	-5.106818	-1.223696
H	-0.771123	-4.439886	-2.294761
O	2.336408	-2.681121	-1.940086
H	2.388111	-2.506666	-2.874160
H	2.712765	-3.540272	-1.775129
O	-4.093460	2.687638	1.602115
H	-4.467032	3.542357	1.407918
H	-4.090309	2.563725	2.545871
O	-1.218171	4.316322	1.215719
H	-0.920067	4.328475	2.119458
H	-1.799404	5.058109	1.075707

```
---------------------------------------------------------------------------
Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin      Pressure= 1.00000 Atm
===========================================================================
===============
SCF Energy=     -4056.55203136      Predicted Change= -4.894787D-07
Zero-point correction (ZPE)=              -4055.9045  0.64751
Internal Energy (U)=                -4055.8491  0.70292
Enthalpy (H)=                              -4055.8481   0.70386
Gibbs Free Energy (G)=                    -4055.9785   0.57346
---------------------------------------------------------------------------
Frequencies --    52.6672             58.6053             70.0203
```

Table A2.7. Al_8, $[Al_8(OH)_{14}(H_2O)_{18}]^{10+}$
Supporting Information: Al8.log

```
---------------------------------------------------------------------------
Using  Gaussian 09:  AM64L-G09RevB.01 12-Aug-2010
===========================================================================
===============
# HF 6-31G** OPT(tight,ReadFC,maxcycles=200)
# SCRF=(Solvent=water) guess=read geom=check Freq
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RHF/6-31G(d,p) Freq
---------------------------------------------------------------------------
Pointgroup= C1   Stoichiometry= Al8H50O32(10+)   C1[X(Al8H50O32)]  #Atoms= 90
Charge = 10   Multiplicity = 1
---------------------------------------------------------------------------
SCF Energy= -4360.80171560         Predicted Change= -3.191544D-11
===========================================================================
===============
Optimization completed.           {Found       2       times}
Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
Force      0.00000 ||  0.00001   [ YES ]      0.00000 ||  0.00001   [ YES ]
Displ      0.00003 ||  0.00006   [ YES ]      0.00003 ||  0.00006   [ YES ]
---------------------------------------------------------------------------
     Atomic          Coordinates (Angstroms)
      Type          X            Y        Z
---------------------------------------------------------------------------
      Al       -0.163851      -1.551329       0.004743
      Al        0.163852       1.551328      -0.004741
      Al       -2.285470       0.238041       1.032969
      Al        2.285471      -0.238043      -1.032966
      Al       -3.351134      -2.756464      -0.288129
```

Al	-2.685099	3.389024	-0.291620
Al	3.351133	2.756467	0.288122
Al	2.685099	-3.389025	0.291626
O	-1.118206	0.106936	-0.529048
O	1.118206	-0.106937	0.529051
O	-1.198597	-1.235629	1.544226
O	-0.928898	1.472624	1.523517
O	1.198598	1.235627	-1.544224
O	0.928899	-1.472626	-1.523514
O	0.936574	-2.901218	0.680654
O	-1.546344	-2.609627	-0.688511
O	-0.936574	2.901216	-0.680651
O	1.546345	2.609628	0.688510
O	-3.516252	-1.016902	0.336922
O	-3.208111	1.686218	0.239523
O	3.516251	1.016901	-0.336920
O	3.208112	-1.686220	-0.239519
O	-3.182045	0.372453	2.728627
O	3.182047	-0.372456	-2.728623
O	-4.519166	3.979111	-0.000041
O	-2.250523	4.003915	1.478820
O	-3.214168	3.099566	-2.136388
O	-2.334078	5.229304	-0.833030
O	3.007868	3.518455	-1.451007
O	3.870431	2.335334	2.110555
O	3.352921	4.608777	0.917747
O	5.265612	3.029158	-0.027798
O	3.214167	-3.099566	2.136394
O	2.250525	-4.003919	-1.478814
O	4.519167	-3.979112	0.000048
O	2.334078	-5.229305	0.833037
O	-3.870425	-2.335318	-2.110560
O	-3.007873	-3.518462	1.450996
O	-3.352922	-4.608770	-0.917765
O	-5.265614	-3.029155	0.027782
H	-1.520737	0.147785	-1.387251
H	1.520738	-0.147785	1.387254
H	-0.797610	-1.260479	2.402034
H	-0.542248	1.417263	2.386150
H	0.797610	1.260474	-2.402031
H	0.542250	-1.417266	-2.386147
H	0.481662	-3.556303	1.193091
H	-1.245736	-3.344311	-1.208237
H	-0.481663	3.556301	-1.193088

H	1.245737	3.344310	1.208239
H	-4.409106	-0.702089	0.314267
H	-3.934947	1.397471	-0.296053
H	4.409105	0.702086	-0.314255
H	3.934948	-1.397473	0.296057
H	-3.521531	-0.370986	3.213679
H	-3.622064	1.161090	3.024970
H	3.521541	0.370982	-3.213671
H	3.622061	-1.161096	-3.024968
H	-5.154721	3.507391	0.526086
H	-4.837320	4.860380	-0.160509
H	-2.859067	4.467645	2.042843
H	-1.689627	3.448328	2.008789
H	-2.651623	2.720543	-2.801424
H	-4.079157	3.251502	-2.499735
H	-1.928617	5.880539	-0.272369
H	-2.459588	5.588999	-1.703495
H	3.661217	3.945728	-1.992620
H	2.389677	3.059937	-2.009314
H	3.257109	2.058226	2.781508
H	4.747654	2.071067	2.363445
H	3.105730	5.364294	0.397036
H	3.551786	4.881411	1.805789
H	5.733558	3.780552	0.320286
H	5.782803	2.655313	-0.732432
H	2.651621	-2.720541	2.801429
H	4.079156	-3.251501	2.499741
H	2.859070	-4.467648	-2.042837
H	1.689628	-3.448334	-2.008784
H	4.837322	-4.860380	0.160518
H	5.154722	-3.507391	-0.526079
H	1.928618	-5.880540	0.272376
H	2.459587	-5.588999	1.703502
H	-3.257099	-2.058223	-2.781514
H	-4.747644	-2.071035	-2.363450
H	-3.661226	-3.945736	1.992606
H	-2.389685	-3.059947	2.009307
H	-3.105744	-5.364292	-0.397055
H	-3.551789	-4.881400	-1.805808
H	-5.733558	-3.780544	-0.320314
H	-5.782809	-2.655317	0.732417

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

```
=================================================================
================
 SCF Energy=     -4360.80171560      Predicted Change= -3.191544D-11
 Zero-point correction (ZPE)=              -4360.0484  0.75331
 Internal Energy (U)=                -4359.9817  0.81993
 Enthalpy (H)=                              -4359.9808   0.82088
 Gibbs Free Energy (G)=                    -4360.1328    0.66889
-------------------------------------------------------------------------
 Frequencies --    29.1511              44.7078              47.7004
```

Table A2.8. "flat" Al_{13}, $Al_{13}(OH)_{24}(H_2O)_{24}]^{15+}$

```
            Supporting Information: Al13p.log
-------------------------------------------------------------------------
 Using  Gaussian 09:  AM64L-G09RevB.01 12-Aug-2010
=================================================================
================
 # HF 6-31G** OPT(CalcFC,maxcycles=200,RFO) SCRF=(Solvent=water)
 # Freq
 #N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RHF/6-31G(d,p) Freq
-------------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= Al13H72O48(15+)   C1[X(Al13H72O48)]  #Atoms=
133
 Charge = 15   Multiplicity = 1
-------------------------------------------------------------------------
 SCF Energy= -6781.56580449         Predicted Change= -2.727151D-04
=================================================================
================
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 Displ      0.12275 ||  0.00180   [ NO ]       0.12275 ||  0.00180   [ NO ]
-------------------------------------------------------------------------
      Atomic          Coordinates (Angstroms)
       Type          X            Y        Z
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Statistical Thermodynamic Analysis
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Full authorship of Gaussian 09

Gaussian 09, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

Appendix 3. Supporting Information for Chapter 4

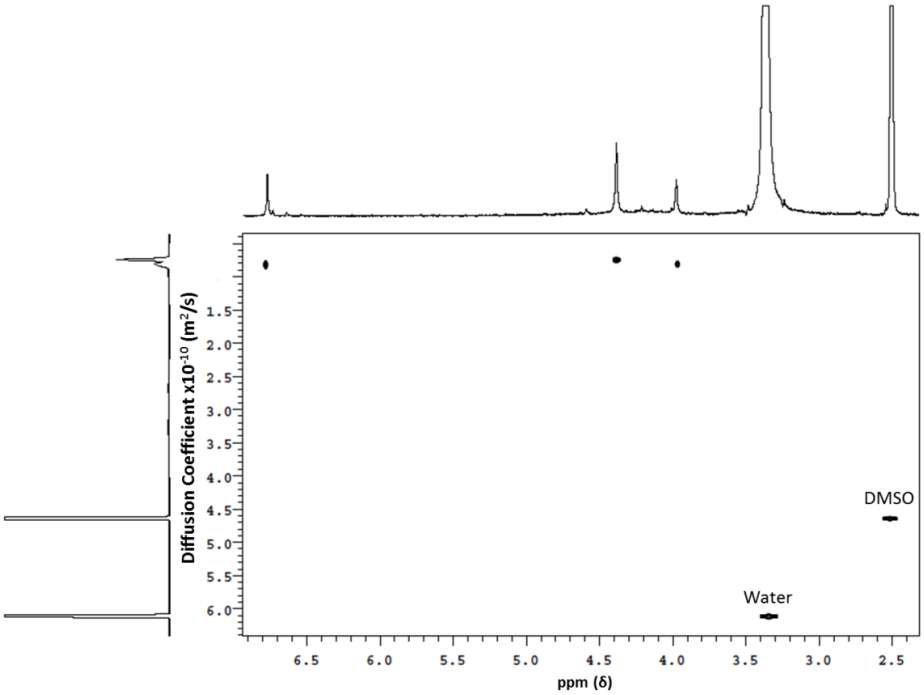

Figure A3.1. Representative DOSY of 2 mM Ga_7In_6 in d_6-DMSO.

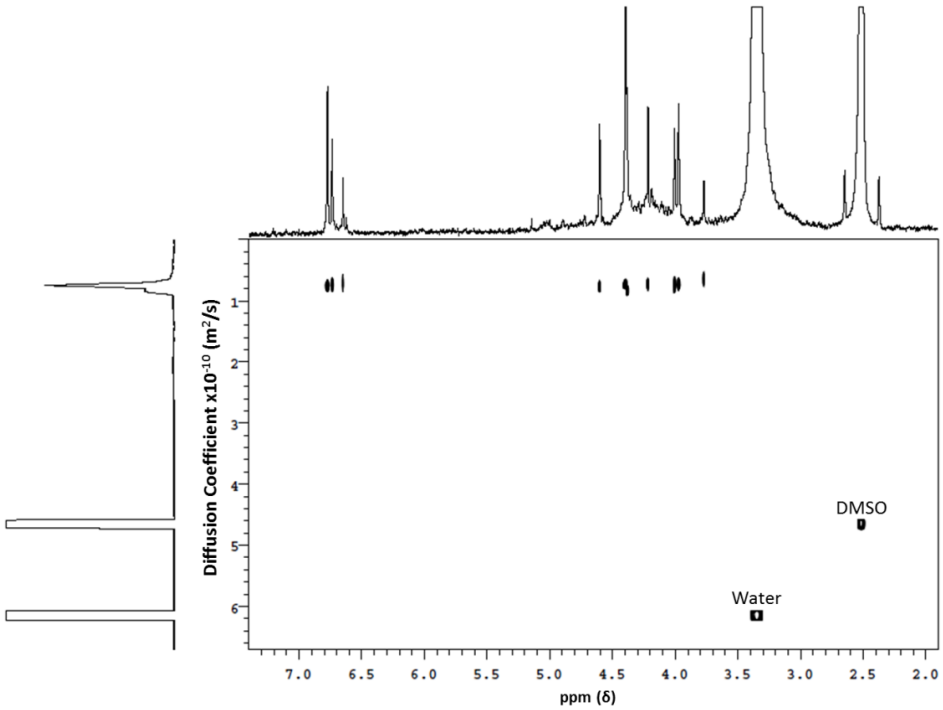

Figure A3.2. Representative DOSY of 2 mM Ga_8In_5 in d_6-DMSO.

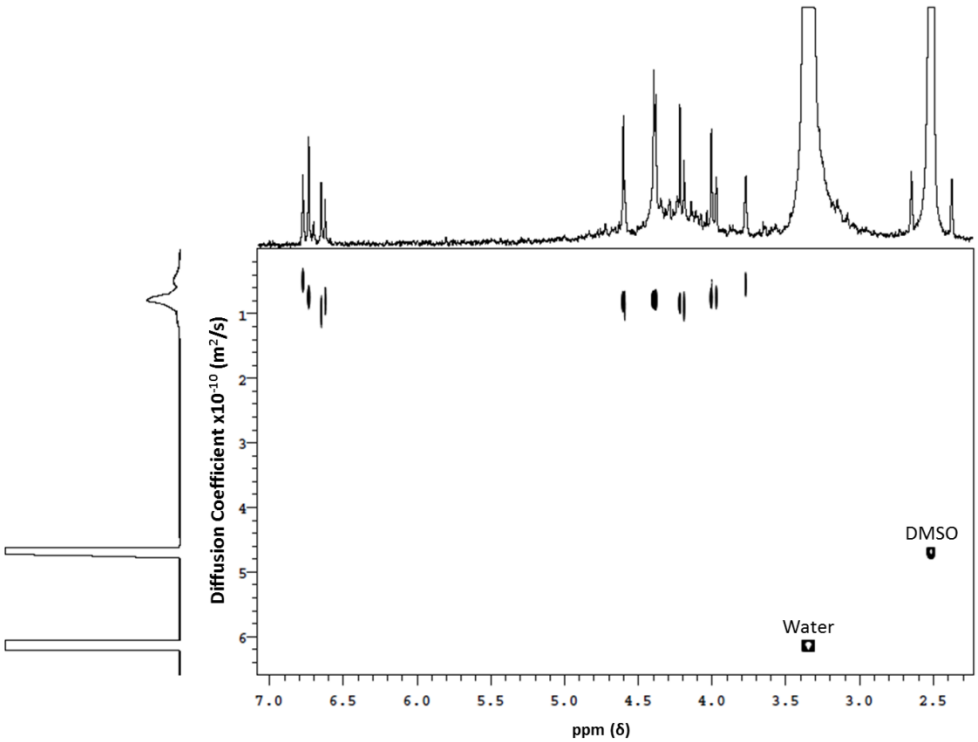

Figure A3.3. Representative DOSY of 2 mM Ga_9In_4 in d_6-DMSO.

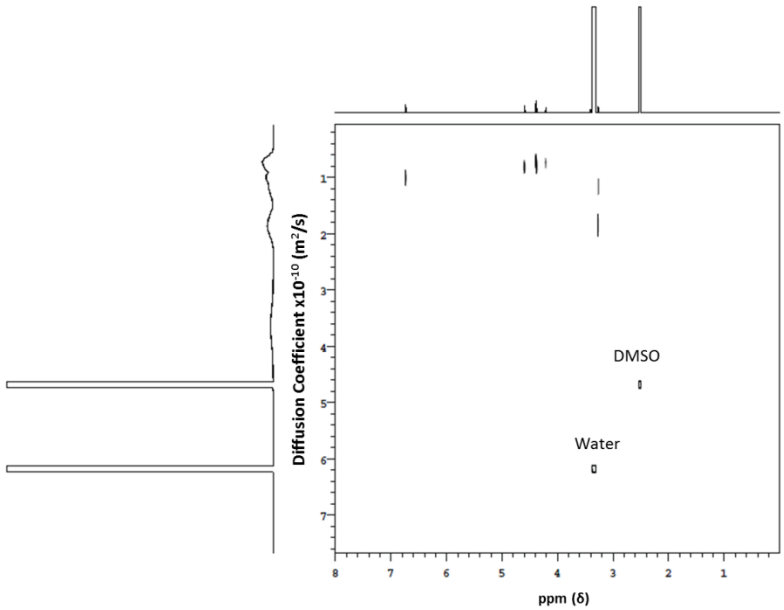

Figure A3.4. Representative DOSY of 2 mM $Ga_{10}In_3$ in d_6-DMSO.

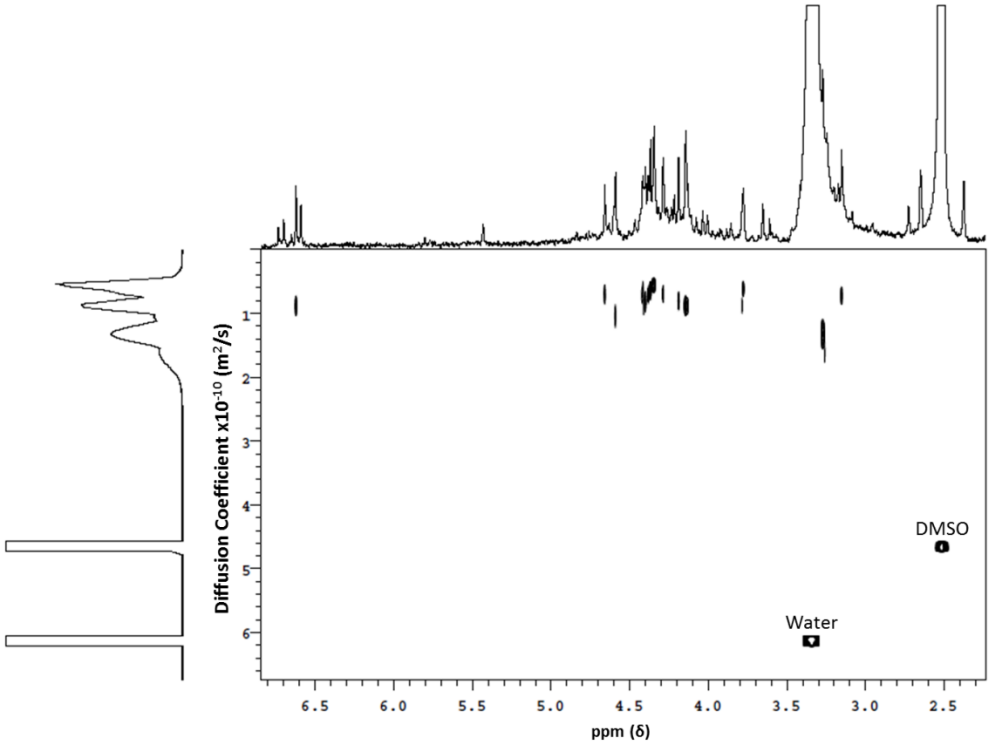

Figure A3.5. Representative DOSY of 2 mM $Ga_{11}In_2$ in d_6-DMSO.

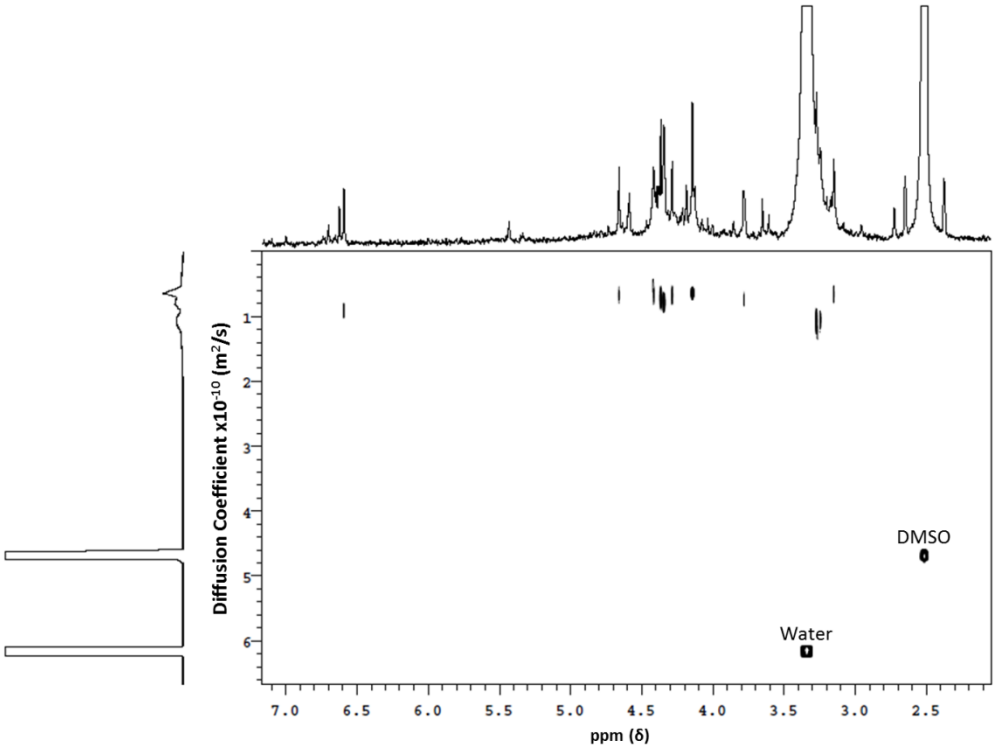

Figure A3.6. Representative DOSY of 2 mM $Ga_{12}In_1$ in d_6-DMSO.

Table A3.1. Diffusion Data and Radii of $Ga_{13-x}In_x$ Clusters. T = 298 K; $\eta = 2.03 \times 10^{-3}$ Pa·s; Concentration = 2 mM; Solvent d_6-DMSO; 500 MHz NMR

Species	**Average Diffusion Coefficient x 10^{-10} (m^2/s)**	**Average Radius (Å)**
Ga_7In_6	0.99 ± 0.12	11.1 ± 1.1
Ga_8In_5	1.16 ± 0.04	9.4 ± 0.4
Ga_9In_4	0.92 ± 0.11	11.7 ± 1.5
$Ga_{10}In_3$	1.09 ± 0.17	9.9 ± 1.6
$Ga_{11}In_2$	0.97 ± 0.13	11.1 ± 1.4
$Ga_{12}In_1$	0.90 ± 0.14	12.0 ± 1.9
Ga_{13}	0.96 ± 0.06	11.2 ± 0.8

Initially, the clusters of interest were optimized with full quantum mechanics. The computed shifts were then scaled with constant scaling factors (F) for each type of proton and plotted against the experimental results. These results look extremely good, with nearly all peaks accounted for. However, these predictions get the ordering of the internal and external μ_2-OH protons wrong.

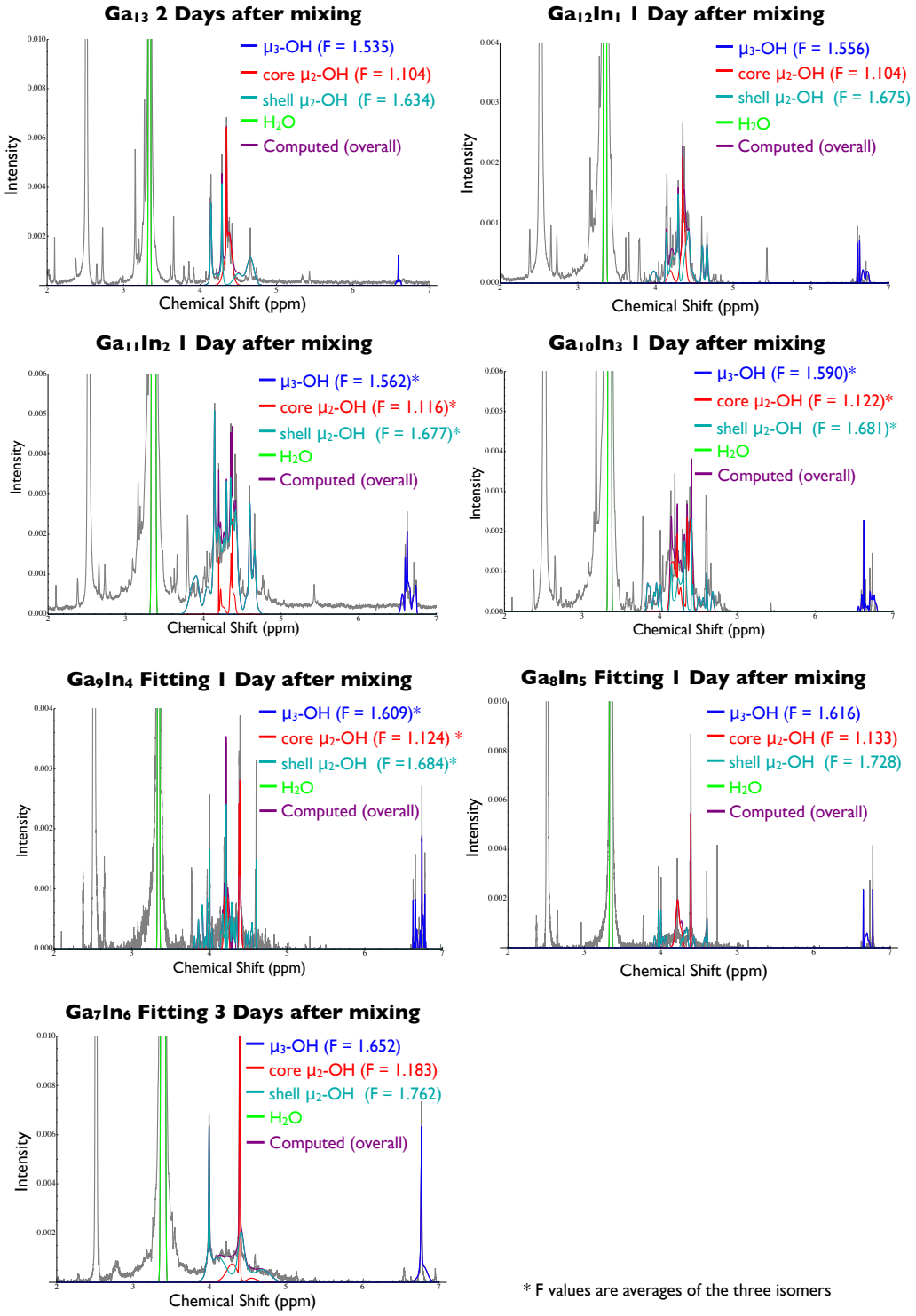

Figure S7: Experimental vs. computed spectra for quantum optimized cluster structures without counterions.

XYZ of Ga_7In_6

193

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H	-2.035660	4.339166	1.187920
O	-4.513582	5.295369	-3.248080
O	-5.193672	4.196425	-0.696080
O	-6.387771	2.990523	-3.103080
O	-2.305563	-6.667812	-3.097080
O	-1.577546	-6.454872	-0.339080
O	0.523400	-7.115044	-2.294080
O	6.538091	1.304462	-6.309080
H	-4.112851	2.012336	-4.892080
H	-3.186738	3.391260	-4.960080
H	-6.752843	2.103553	-3.130080
H	-6.929709	3.740567	-3.360080
H	-5.236563	5.525428	-3.836080
H	-3.860527	5.957315	-3.008080
H	-5.893708	3.749482	-0.216080
H	-4.865602	5.045398	-0.387080
H	-2.073613	-7.272831	-0.423080
H	-1.411515	-6.080886	0.529920
H	0.181327	-8.007016	-2.382080
H	1.471413	-6.961122	-2.294080
H	-2.501635	-7.549796	-2.773080
H	-2.765535	-6.325775	-3.866080
H	-0.528465	-5.466958	-4.838080
H	0.240646	-4.115021	-4.251080
H	-5.597253	-2.883542	3.474920
H	-4.764135	-1.449611	3.363920
H	-8.263178	-1.974323	1.372920
H	-7.615054	-0.456377	1.568920
H	-7.083379	-4.419420	0.462920
H	-6.043402	-4.705506	1.727920
H	-6.940255	-2.917432	-1.447080
H	-6.236135	-1.446490	-1.767080
H	2.116490	6.167825	3.455920
H	1.852590	7.391847	2.360920
H	-2.120458	6.802173	1.883920
H	-0.833372	7.849067	1.971920
H	-0.891691	3.957072	3.840920
H	-0.122580	5.309009	4.426920

H	0.761470	5.921936	-0.939080
H	1.423568	7.113882	0.012920
H	5.584090	1.287540	1.356920
H	6.289210	2.758483	1.037920
H	5.390357	4.547556	-2.136080
H	6.433334	4.260471	-0.874080
H	6.965008	0.297427	-1.979080
H	7.613133	1.816374	-1.783080
H	4.114090	1.290661	-3.775080
H	4.947207	2.724593	-3.885080
H	6.278664	-3.898517	2.950920
H	6.101798	-2.261502	2.720920
H	4.217557	-5.202347	-0.022080
H	5.244663	-3.906432	-0.192080
H	3.210482	-6.116265	2.597920
H	4.587518	-5.684378	3.424920
H	2.535693	-3.550209	4.548920
H	3.462806	-2.171286	4.481920

XYZ of Ga_8In_5

193

In	4.873787	2.031745	-1.197722
In	-5.537755	-2.329641	0.725042
In	-4.417078	3.213365	-2.424610
In	3.752112	-3.511254	1.950928
In	0.079189	5.188439	1.793958
Ga	-0.332493	-0.148457	-0.236329
Ga	2.752062	-0.547103	0.101465
Ga	-3.418047	0.250171	-0.574125
Ga	-1.530739	2.738874	-0.354598
Ga	0.864751	-3.035831	-0.117062
Ga	-2.191401	-2.629585	-0.658668
Ga	1.526433	2.331672	0.185986
O	4.155990	0.095900	-1.022736
O	-4.820975	-0.392814	0.550079
O	-2.475600	3.567719	-1.793326
O	1.809615	-3.864651	1.320667
O	-2.109839	-3.945162	-2.041900
O	1.444889	3.646249	1.569193
O	3.039200	2.909530	-0.817574
O	-3.704168	-3.207444	0.344892
O	-4.386535	1.212904	-1.902514
O	3.720548	-1.509861	1.430854
O	0.818489	-4.432853	-1.413585
O	-1.484458	4.134897	0.941900
O	6.826903	1.321231	-1.742473
O	-7.492886	-1.618137	1.268813
O	3.943354	-5.524115	2.681127
O	1.526624	6.398574	2.823746
O	5.653520	4.028611	-1.369042
O	-6.319490	-4.326567	0.897357
O	5.776026	-3.183933	2.600719
O	-1.309026	6.816073	2.026818
O	1.355986	0.521745	-0.969108
O	-2.019936	-0.820641	0.496404
O	-1.526667	0.933963	-1.348138
O	0.862699	-1.231859	0.875459
O	-0.426138	-1.787098	-1.305937
O	-0.238845	1.490209	0.832281
O	2.620118	1.075107	1.110155

O	-3.285086	-1.373020	-1.582837
O	-3.084794	1.876399	0.359649
O	2.418829	-2.174305	-0.833333
O	-0.892841	-3.502917	0.446605
O	0.228873	3.205021	-0.919285
O	5.703796	2.028498	0.791623
O	-6.368783	-2.325437	-1.263281
O	4.610532	-4.349840	0.161204
O	0.807434	6.242052	0.060392
O	4.563100	2.098447	-3.320394
O	-5.228067	-2.396361	2.847712
O	-3.827294	2.787007	-4.443657
O	3.161328	-3.084913	3.969973
O	-0.184459	-4.881677	-4.248902
O	-0.481524	4.584771	3.775242
O	-4.633010	-5.339229	-4.310019
O	7.066750	-1.527580	-2.554607
O	-2.110601	6.803868	-3.481966
O	4.807247	0.234518	3.367537
O	-5.472232	-0.531432	-3.840194
O	-3.934709	4.321321	2.331707
O	3.269741	-4.619235	-2.804389
O	-3.032375	-5.338878	2.071475
O	2.367408	5.040964	-2.544157
O	3.968040	5.041290	3.838336
N	-5.333766	-4.605995	-3.596934
N	6.607123	-2.457070	-1.874682
N	-1.264649	6.909212	-2.582210
N	4.105511	0.966760	4.079595
N	-4.771476	-1.264666	-4.553279
N	-4.394333	3.391855	3.010633
N	3.728350	-3.688762	-3.484292
N	-2.185423	-5.233516	2.971234
N	1.521455	4.935620	-3.443913
N	4.667796	4.308039	3.125249
O	-6.544357	-4.434441	-3.823327
O	7.086310	-3.603049	-1.921380
O	-0.506839	7.890027	-2.505964
O	2.895899	1.139306	3.854229
O	-3.561882	-1.436213	-4.327888
O	-3.915148	2.245852	2.964935
O	3.250181	-2.543766	-3.437617
O	-1.428631	-4.251720	3.047502
O	0.762663	3.953789	-3.520187
O	5.878372	4.137509	3.350667

O	-7.183414	-1.804510	5.813250
O	2.884794	-4.895186	7.070987
O	8.317175	-0.153404	0.057366
O	-2.684281	5.695522	4.942680
O	-4.821450	-4.017826	-2.634779
O	5.639415	-2.249536	-1.130340
O	-1.158178	6.011440	-1.734211
O	4.617826	1.554929	5.041749
O	-5.283794	-1.852860	-5.514433
O	-5.362041	3.599390	3.754974
O	4.697073	-3.897303	-4.227656
O	-2.079968	-6.130281	3.818255
O	1.414983	5.833367	-4.290912
O	4.156480	3.719888	2.163097
O	-7.809873	-0.718991	4.055543
O	2.672138	-6.082631	5.279200
O	6.787310	-0.454643	1.548976
O	-4.215151	5.394215	6.436288
O	7.143905	0.421060	-4.528228
N	-7.879671	-1.753288	4.758693
N	3.418297	-5.585265	6.155557
N	7.767988	-0.905766	0.912592
N	-3.233470	4.943135	5.798906
N	7.214688	1.456399	-5.232350
O	-8.583557	-2.689461	4.415598
O	4.627489	-5.749912	6.105033
O	8.186077	-2.029546	1.135404
O	-2.814364	3.818372	6.021695
O	7.919589	2.391565	-4.888278
H	2.638767	1.043016	1.845623
H	-3.303754	-1.339956	-2.317281
H	-3.238997	1.951826	1.075432
H	2.573029	-2.249757	-1.548116
H	-1.053462	-3.631469	1.153259
H	0.388477	3.334555	-1.625916
H	4.529565	-0.437819	-1.102329
H	-5.195550	0.140887	0.629669
H	-2.180613	4.151325	-1.840076
H	1.514645	-4.449256	1.367391
H	-2.734777	-3.982181	-2.239244
H	2.069792	3.685267	1.766587
H	1.427616	0.582103	-1.611644
H	-2.092602	-0.879018	1.138987
H	-1.460911	0.930279	-1.994292
H	0.795928	-1.227168	1.520636

H	-0.301831	-1.765990	-1.942341
H	-0.364134	1.468084	1.468656
H	2.870297	3.479003	-1.223796
H	-3.536284	-3.775960	0.752136
H	-4.693469	0.759984	-2.368677
H	4.029481	-1.056906	1.897022
H	1.458625	-4.501637	-1.735024
H	-2.123575	4.202724	1.262317
O	-4.608320	5.226226	-3.154809
O	-5.274502	4.051918	-0.632883
O	-6.441996	2.885976	-3.072404
O	-2.190590	-6.696445	-3.297425
O	-1.472402	-6.539966	-0.533074
O	0.644056	-7.114011	-2.498501
O	6.518429	1.507596	-6.285907
H	-4.146357	1.992954	-4.879386
H	-3.244492	3.389169	-4.910452
H	-6.791354	1.993700	-3.122538
H	-6.996483	3.632613	-3.311968
H	-5.333960	5.458243	-3.738750
H	-3.967529	5.893294	-2.896622
H	-5.967608	3.580886	-0.166041
H	-4.962083	4.898500	-0.301885
H	-1.953825	-7.364132	-0.638805
H	-1.314856	-6.185023	0.345441
H	0.317913	-8.009356	-2.609681
H	1.589213	-6.943546	-2.492180
H	-2.371822	-7.589573	-2.996106
H	-2.654840	-6.343356	-4.058822
H	-0.431119	-5.421374	-5.003200
H	0.312825	-4.071301	-4.380557
H	-5.562541	-3.136344	3.358604
H	-4.754531	-1.685699	3.285687
H	-8.239486	-2.221594	1.273075
H	-7.618583	-0.697910	1.508680
H	-7.014903	-4.622063	0.305259
H	-5.972797	-4.921491	1.565410
H	-6.894081	-3.070400	-1.566184
H	-6.215246	-1.579786	-1.847446
H	1.990854	6.046460	3.586168
H	1.707841	7.292726	2.521452
H	-2.253181	6.645650	2.019501
H	-0.984898	7.712407	2.137019
H	-0.978810	3.774369	3.907897
H	-0.234863	5.124467	4.529541

H	0.649886	5.887085	-0.817123
H	1.288857	7.066218	0.166123
H	5.548279	1.281837	1.374758
H	6.228111	2.772444	1.094499
H	5.304808	4.624474	-2.036075
H	6.349937	4.324174	-0.778941
H	6.953615	0.399996	-1.981362
H	7.574501	1.924680	-1.745732
H	4.089565	1.387811	-3.759368
H	4.897573	2.838430	-3.831286
H	6.330496	-3.929569	2.840308
H	6.125367	-2.290656	2.650878
H	4.299078	-5.194405	-0.169742
H	5.303601	-3.876833	-0.304589
H	3.302561	-6.191207	2.423940
H	4.669995	-5.756114	3.265070
H	2.578527	-3.687075	4.436768
H	3.481390	-2.290868	4.406704
Ga	-0.744157	-5.486353	-2.266640

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193

In	5.02800	1.71500	-1.15100
In	-5.61100	-2.08000	0.72800
In	-4.17800	3.34700	-2.49500
In	0.37200	5.15900	1.74000
Ga	-0.29200	-0.18200	-0.21100
Ga	2.76500	-0.73200	0.16600
Ga	-3.34900	0.36700	-0.58800
Ga	-1.34000	2.76000	-0.38700
Ga	0.75600	-3.12500	-0.03400
Ga	-2.27000	-2.57200	-0.61500
Ga	1.68700	2.20600	0.19200
O	4.21100	-0.17900	-0.95300
O	-4.79400	-0.18600	0.53100
O	-2.22700	3.61200	-1.84800
O	1.64300	-3.97700	1.42600
O	-2.24200	-3.91200	-1.97600
O	1.65900	3.54500	1.55400
O	3.23700	2.69000	-0.80400
O	-3.82000	-3.05600	0.38200
O	-4.25400	1.35600	-1.94100
O	3.67000	-1.72100	1.52000
O	0.65100	-4.53800	-1.30900
O	-1.23500	4.17200	0.88800
O	6.94800	0.89700	-1.66400
O	-7.53200	-1.26200	1.24000
O	3.67600	-5.72100	2.83500
O	1.86900	6.31000	2.76700
O	5.91100	3.66600	-1.34500
O	-6.49500	-4.03200	0.92300
O	5.62600	-3.47900	2.73800
O	-0.93400	6.85800	1.93300
O	1.43600	0.38900	-0.93600
O	-2.01800	-0.75600	0.51400
O	-1.41800	0.94100	-1.35200
O	0.83600	-1.30700	0.93000
O	-0.45800	-1.83100	-1.25600
O	-0.12500	1.46600	0.83300
O	2.70600	0.91100	1.14800
O	-3.28900	-1.27700	-1.57000

O	-2.94300	1.98900	0.32400
O	2.35900	-2.35500	-0.74700
O	-1.02900	-3.49300	0.51800
O	0.44700	3.12700	-0.94000
O	5.83800	1.70100	0.84700
O	-6.42100	-2.06600	-1.26800
O	4.42700	-4.62300	0.30400
O	1.17000	6.14600	-0.00200
O	4.74200	1.76300	-3.27700
O	-5.32600	-2.12900	2.85500
O	-3.59000	2.85900	-4.50100
O	3.00600	-3.22500	4.07700
O	-0.34600	-4.98100	-4.14800
O	-0.23800	4.61600	3.72500
O	-4.81100	-5.21200	-4.24900
O	7.05000	-1.97300	-2.42900
O	-1.68100	6.79800	-3.58300
O	4.82500	-0.00400	3.44100
O	-5.40800	-0.36100	-3.86300
O	-3.68600	4.50500	2.24900
O	3.10300	-4.87100	-2.67100
O	-3.27500	-5.19100	2.14800
O	2.69200	4.82500	-2.57000
O	4.22800	4.84700	3.82800
N	-5.48000	-4.43300	-3.55500
N	6.53700	-2.86700	-1.73900
N	-0.83900	6.87500	-2.67600
N	4.15500	0.77500	4.13400
N	-4.73900	-1.14100	-4.55700
N	-4.19900	3.61200	2.93700
N	3.61500	-3.97600	-3.36000
N	-2.43300	-5.11500	3.05500
N	1.85100	4.74900	-3.47700
N	4.89600	4.06700	3.13400
O	-6.67800	-4.20400	-3.79700
O	6.95800	-4.03600	-1.76300
O	-0.03300	7.81700	-2.60700
O	2.95800	1.00500	3.89300
O	-3.54200	-1.37000	-4.31600
O	-3.77900	2.44200	2.91400
O	3.19600	-2.80800	-3.33700
O	-1.62800	-4.17100	3.12400
O	1.04400	3.80600	-3.54600
O	6.09400	3.83900	3.37500
O	-7.27700	-1.39100	5.79000

O	2.60700	-4.96900	7.20300
O	8.34300	-0.62200	0.17500
O	-2.39300	5.85600	4.85100
O	-4.94800	-3.85600	-2.59700
O	5.57400	-2.59900	-1.00900
O	-0.78700	5.98700	-1.81300
O	4.68700	1.35200	5.09200
O	-5.27100	-1.71700	-5.51500
O	-5.16200	3.88000	3.66800
O	4.57900	-4.24600	-4.09000
O	-2.38200	-6.00200	3.91700
O	1.79900	5.63700	-4.33900
O	4.36500	3.49100	2.17600
O	-7.83000	-0.30300	4.00900
O	2.35200	-6.17200	5.42700
O	6.78500	-0.82200	1.65400
O	-3.95200	5.65700	6.33300
O	7.24600	-0.06300	-4.43100
N	-7.96000	-1.32100	4.72700
N	3.11400	-5.70000	6.30400
N	7.74800	-1.33200	1.03600
N	-2.98800	5.14600	5.71300
N	7.37700	0.95600	-5.15100
O	-8.70700	-2.22600	4.39100
O	4.31400	-5.92600	6.26900
O	8.10600	-2.47200	1.28000
O	-2.62900	4.00500	5.95800
O	8.12500	1.86000	-4.81400
H	2.71600	0.89000	1.88400
H	-3.29900	-1.25400	-2.30500
H	-3.10000	2.08400	1.03700
H	2.51600	-2.45000	-1.45900
H	-1.20300	-3.60100	1.22500
H	0.62000	3.23700	-1.64700
H	4.55800	-0.73200	-1.02100
H	-5.14200	0.36800	0.59800
H	-1.90200	4.18000	-1.90100
H	1.31800	-4.54500	1.47900
H	-2.86600	-3.92100	-2.18000
H	2.28300	3.55600	1.75800
H	1.51700	0.43600	-1.57900
H	-2.10000	-0.80000	1.15700
H	-1.34600	0.92400	-1.99800
H	0.76300	-1.28900	1.57400
H	-0.32700	-1.82700	-1.89100

H	-0.25700	1.46100	1.46800
H	3.10200	3.26100	-1.22100
H	-3.68600	-3.62600	0.79900
H	-4.57900	0.91200	-2.40400
H	3.99700	-1.27700	1.98200
H	1.29000	-4.64500	-1.62300
H	-1.87300	4.27800	1.20100
O	-4.25900	5.35500	-3.25800
O	-5.00900	4.25700	-0.72500
O	-6.21000	3.11300	-3.15900
O	-2.45100	-6.67600	-3.19000
O	-1.75300	-6.51200	-0.42100
O	0.35100	-7.22400	-2.35400
O	6.69400	1.02600	-6.21200
H	-3.94500	2.07500	-4.92700
H	-2.97300	3.42300	-4.97000
H	-6.60400	2.23900	-3.19900
H	-6.72300	3.88300	-3.41600
H	-4.96600	5.61400	-3.85300
H	-3.58700	5.99300	-3.00300
H	-5.72900	3.82900	-0.25900
H	-4.65700	5.09200	-0.40400
H	-2.27500	-7.31200	-0.51900
H	-1.58600	-6.15100	0.45400
H	-0.02000	-8.10300	-2.45500
H	1.30300	-7.10200	-2.34100
H	-2.68100	-7.55300	-2.87700
H	-2.88900	-6.31200	-3.96200
H	-0.61200	-5.51900	-4.89600
H	0.19400	-4.19900	-4.28700
H	-5.70200	-2.84200	3.37400
H	-4.82100	-1.43600	3.28700
H	-8.30800	-1.82600	1.24600
H	-7.61300	-0.33300	1.46400
H	-7.19800	-4.30100	0.32900
H	-6.18500	-4.63300	1.60400
H	-6.98000	-2.78800	-1.56500
H	-6.22300	-1.33800	-1.86200
H	2.30700	5.94700	3.53900
H	2.09800	7.18900	2.45200
H	-1.88500	6.73600	1.91800
H	-0.56500	7.73900	2.03300
H	-0.77800	3.83400	3.86500
H	0.02800	5.15500	4.47300
H	1.00300	5.78500	-0.87500

H	1.69200	6.94600	0.09700
H	5.63800	0.97300	1.44000
H	6.39600	2.42200	1.14400
H	5.59900	4.26800	-2.02500
H	6.61500	3.93500	-0.75200
H	7.03000	-0.03300	-1.88700
H	7.72500	1.46100	-1.66800
H	4.23800	1.07000	-3.71000
H	5.11900	2.47700	-3.79600
H	6.13900	-4.24800	2.99500
H	6.02000	-2.60400	2.77800
H	4.07600	-5.45600	-0.01700
H	5.14700	-4.19300	-0.16200
H	3.00400	-6.35900	2.58100
H	4.38400	-5.98000	3.43000
H	2.38900	-3.78900	4.54700
H	3.36200	-2.44100	4.50500
Ga	-0.95500	-5.52400	-2.16300
Ga	3.59400	-3.71300	2.07100

XYZ of Ga_9In_4-m

193

In	-5.36900	-2.52400	0.76900
In	-4.50500	3.04200	-2.42100
In	3.97200	-3.31300	1.92200
In	-0.05900	5.22600	1.74800
Ga	-0.26600	-0.13500	-0.24900
Ga	2.83500	-0.40400	0.06500
Ga	-3.36900	0.13400	-0.56300
Ga	-1.58400	2.70000	-0.37300
Ga	1.05000	-2.96900	-0.12400
Ga	-2.02400	-2.69300	-0.64200
Ga	1.49200	2.42300	0.14400
O	4.20100	0.29000	-1.07500
O	-4.73400	-0.56000	0.57700
O	-2.57400	3.48000	-1.80800
O	2.04100	-3.75000	1.31000
O	-1.90000	-4.01200	-2.01800
O	1.36700	3.74100	1.52100
O	2.97100	3.05700	-0.87600
O	-3.50400	-3.32700	0.37800
O	-4.38700	1.04800	-1.88800
O	3.85300	-1.31800	1.39100
O	1.05100	-4.37500	-1.41200
O	-1.58500	4.10400	0.91600
O	6.81300	1.62100	-1.82400
O	-7.34700	-1.89100	1.32500
O	4.25200	-5.31200	2.66200
O	1.34500	6.50100	2.75900
O	5.53200	4.28000	-1.45500
O	-6.06600	-4.55000	0.95900
O	5.98600	-2.89800	2.55300
O	-1.51200	6.79700	1.98400
O	1.38700	0.60000	-1.00000
O	-1.91800	-0.87200	0.50200
O	-1.51400	0.89100	-1.35600
O	0.98200	-1.16100	0.85900
O	-0.30100	-1.78200	-1.30900
O	-0.23200	1.51300	0.81000
O	2.64400	1.21800	1.06600
O	-3.17700	-1.48800	-1.56300

O	-3.09500	1.77800	0.35900
O	2.56100	-2.04900	-0.85800
O	-0.68200	-3.50500	0.45700
O	0.15000	3.23500	-0.95500
O	5.68300	2.29600	0.71600
O	-6.21600	-2.56600	-1.21200
O	4.84900	-4.12600	0.13000
O	0.61000	6.29900	0.00300
O	4.50600	2.29500	-3.38700
O	-5.03900	-2.56500	2.88900
O	-3.91400	2.62900	-4.44200
O	3.38100	-2.89900	3.94400
O	0.04400	-4.88100	-4.23600
O	-0.57800	4.61200	3.73800
O	-4.38200	-5.52300	-4.25700
O	7.16400	-1.22000	-2.62200
O	-2.35800	6.71900	-3.51800
O	4.88300	0.48200	3.30900
O	-5.41500	-0.75100	-3.80700
O	-4.02900	4.19700	2.32500
O	3.49700	-4.46800	-2.82300
O	-2.73000	-5.41900	2.11000
O	2.19700	5.14800	-2.60800
O	3.84900	5.25200	3.76100
N	-5.10600	-4.81500	-3.54200
N	6.74900	-2.16400	-1.93300
N	-1.50900	6.86400	-2.62600
N	4.15700	1.18800	4.02300
N	-4.69100	-1.45900	-4.52200
N	-4.44400	3.25300	3.01300
N	3.91100	-3.52300	-3.51200
N	-1.88100	-5.27300	3.00200
N	1.34900	5.00300	-3.50000
N	4.57300	4.54400	3.04600
O	-6.32500	-4.69500	-3.75900
O	7.27500	-3.28900	-1.97800
O	-0.79200	7.87600	-2.56100
O	2.94000	1.30900	3.80700
O	-3.47300	-1.57900	-4.30600
O	-3.91900	2.12800	2.97000
O	3.38600	-2.39900	-3.46700
O	-1.16500	-4.26100	3.06700
O	0.63100	3.99000	-3.56400
O	5.79100	4.42500	3.26200
O	-6.99300	-2.03700	5.86800

O	3.20500	-4.70100	7.05700
O	8.37800	0.22000	-0.02900
O	-2.81500	5.63700	4.91800
O	-4.61100	-4.20100	-2.58800
O	5.78000	-1.99200	-1.18200
O	-1.35900	5.97700	-1.77400
O	4.65300	1.80300	4.97800
O	-5.18600	-2.07300	-5.47500
O	-5.41400	3.42500	3.76400
O	4.88100	-3.69600	-4.26200
O	-1.73100	-6.16000	3.85300
O	1.19800	5.89000	-4.35100
O	4.07800	3.93000	2.09100
O	-7.67800	-0.98900	4.10900
O	3.02700	-5.90700	5.27400
O	6.87400	-0.13600	1.47800
O	-4.32000	5.28200	6.42600
O	7.14400	0.71800	-4.60700
N	-7.69900	-2.02100	4.81900
N	3.75900	-5.37400	6.14100
N	7.86800	-0.55000	0.83500
N	-3.32600	4.86800	5.78300
N	7.16600	1.75200	-5.31700
O	-8.36700	-2.98800	4.48700
O	4.97300	-5.48900	6.08100
O	8.33400	-1.65400	1.06100
O	-2.85900	3.76300	6.00800
O	7.83500	2.71700	-4.98500
H	2.67000	1.19100	1.80100
H	-3.20300	-1.46000	-2.29800
H	-3.24600	1.85100	1.07600
H	2.71300	-2.12200	-1.57400
H	-0.83100	-3.63600	1.16600
H	0.29800	3.36700	-1.66400
H	4.59600	-0.22800	-1.15400
H	-5.13000	-0.04200	0.65700
H	-2.30400	4.07500	-1.86100
H	1.77000	-4.34600	1.36300
H	-2.52400	-4.07600	-2.21000
H	1.99100	3.80700	1.71200
H	1.45100	0.66000	-1.64300
H	-1.98300	-0.92900	1.14500
H	-1.45300	0.88600	-2.00300
H	0.92000	-1.15600	1.50400
H	-0.18300	-1.76000	-1.94600

H	-0.35100	1.48900	1.44700
H	2.77500	3.61600	-1.28300
H	-3.30900	-3.88600	0.78700
H	-4.67900	0.58000	-2.34900
H	4.14700	-0.84900	1.85200
H	1.69100	-4.41900	-1.73900
H	-2.22400	4.14700	1.24100
O	-4.78500	5.04100	-3.16000
O	-5.38100	3.85500	-0.62700
O	-6.52000	2.62800	-3.05000
O	-1.87700	-6.77200	-3.25800
O	-1.14300	-6.57000	-0.50100
O	0.97900	-7.06700	-2.48100
O	6.46000	1.76800	-6.36500
H	-4.20400	1.82000	-4.87100
H	-3.36100	3.25200	-4.91700
H	-6.83200	1.72100	-3.09200
H	-7.10600	3.34900	-3.28900
H	-5.52500	5.24000	-3.74000
H	-4.17000	5.73600	-2.91100
H	-6.05000	3.35900	-0.15100
H	-5.10100	4.71600	-0.30300
H	-1.59100	-7.41400	-0.59800
H	-0.99300	-6.20300	0.37500
H	0.68900	-7.97600	-2.58400
H	1.91600	-6.85800	-2.48300
H	-2.01900	-7.67000	-2.95000
H	-2.36200	-6.44300	-4.01700
H	-0.18600	-5.43500	-4.98500
H	0.50700	-4.05200	-4.37700
H	-5.33800	-3.31500	3.40700
H	-4.59200	-1.83300	3.31900
H	-8.06800	-2.52400	1.33900
H	-7.50900	-0.97500	1.56100
H	-6.75300	-4.87800	0.37400
H	-5.68900	-5.12600	1.62700
H	-6.71200	-3.33300	-1.50700
H	-6.09800	-1.81800	-1.80200
H	1.83000	6.17300	3.52000
H	1.48700	7.40000	2.45000
H	-2.44800	6.58700	1.98600
H	-1.22400	7.70600	2.08700
H	-1.04000	3.78200	3.87900
H	-0.34800	5.16600	4.48700
H	0.46000	5.93300	-0.87100

H	1.05800	7.14300	0.10000
H	5.56300	1.54700	1.30400
H	6.17800	3.06300	1.01000
H	5.15300	4.85700	-2.12300
H	6.22000	4.60700	-0.87300
H	6.97600	0.70400	-2.05900
H	7.53500	2.25500	-1.83700
H	4.05900	1.56200	-3.81800
H	4.80600	3.04500	-3.90400
H	6.57300	-3.61900	2.79200
H	6.29800	-1.99100	2.59500
H	4.57100	-4.98400	-0.19400
H	5.51800	-3.62700	-0.34400
H	3.63800	-6.00600	2.41400
H	4.99300	-5.51000	3.24100
H	2.82700	-3.52200	4.41900
H	3.67100	-2.09000	4.37300
Ga	-0.47300	-5.49700	-2.24600
Ga	4.83700	2.25300	-1.26600

XYZ of Ga_9In_4-p

193

In	4.87200	2.13000	-1.12800
In	-5.53400	-2.28600	0.69800
In	-4.42000	3.32500	-2.33200
In	3.75800	-3.48000	1.90100
Ga	-0.33100	-0.07700	-0.21500
Ga	2.75400	-0.47900	0.11500
Ga	-3.41700	0.32400	-0.54500
Ga	-1.53400	2.81000	-0.27200
Ga	0.87000	-2.96500	-0.15700
Ga	-2.18700	-2.55200	-0.69100
Ga	1.52400	2.39600	0.26100
O	4.15700	0.19000	-0.99500
O	-4.82000	-0.34500	0.56500
O	-2.47900	3.66800	-1.69300
O	1.81600	-3.82300	1.26300
O	-2.10300	-3.83700	-2.10200
O	1.44000	3.68000	1.67200
O	3.03600	2.99700	-0.73000
O	-3.69900	-3.15300	0.30000
O	-4.38700	1.31300	-1.85300
O	3.72300	-1.46800	1.42400
O	0.82600	-4.33400	-1.48300
O	-1.49000	4.17800	1.05400
O	6.82600	1.43400	-1.68800
O	-7.49000	-1.58900	1.25700
O	3.95200	-5.50800	2.58800
O	1.51800	6.40500	2.98500
O	5.64900	4.13100	-1.25700
O	-6.31200	-4.28700	0.82800
O	5.78100	-3.16400	2.55800
O	-1.31800	6.83600	2.19600
O	1.35600	0.61100	-0.93300
O	-2.01800	-0.76800	0.50300
O	-1.52700	1.02700	-1.30400
O	0.86500	-1.18300	0.87400
O	-0.42200	-1.69300	-1.31900
O	-0.24000	1.53800	0.88800
O	2.61900	1.12100	1.15800
O	-3.28200	-1.27700	-1.58800

O	-3.08700	1.93000	0.42400
O	2.42300	-2.08600	-0.85500
O	-0.88700	-3.44700	0.39600
O	0.22500	3.29100	-0.82600
O	5.70200	2.08600	0.86100
O	-6.36400	-2.24100	-1.28900
O	4.61800	-4.27900	0.09400
O	0.79900	6.30700	0.21900
O	4.56200	2.24200	-3.24900
O	-5.22400	-2.39800	2.81900
O	-3.83000	2.94200	-4.35900
O	3.16600	-3.09800	3.92800
O	-0.17600	-4.72400	-4.32800
O	-0.48800	4.56900	3.89700
O	-4.62400	-5.18600	-4.40000
O	7.07000	-1.39600	-2.56100
O	-2.11900	6.94000	-3.31200
O	4.80700	0.23600	3.39700
O	-5.47000	-0.39100	-3.82700
O	-3.94000	4.33100	2.44700
O	3.27800	-4.48700	-2.87700
O	-3.02400	-5.32000	1.98100
O	2.36200	5.16400	-2.41100
O	3.96100	5.03000	3.97100
N	-5.32600	-4.46900	-3.67100
N	6.61200	-2.34100	-1.90100
N	-1.27300	7.02700	-2.41000
N	4.10400	0.95200	4.12500
N	-4.76800	-1.10700	-4.55600
N	-4.39900	3.38700	3.10600
N	3.73500	-3.54200	-3.53700
N	-2.17800	-5.23300	2.88300
N	1.51600	5.07700	-3.31300
N	4.66200	4.31300	3.24200
O	-6.53600	-4.29500	-3.89400
O	7.09300	-3.48500	-1.97200
O	-0.51700	8.00700	-2.31200
O	2.89400	1.12700	3.90300
O	-3.55800	-1.28200	-4.33400
O	-3.91800	2.24300	3.03600
O	3.25500	-2.39900	-3.46600
O	-1.42200	-4.25200	2.98000
O	0.75900	4.09600	-3.41000
O	5.87300	4.14000	3.46400
O	-7.18100	-1.87200	5.79600

O	2.89100	-4.97500	6.99000
O	8.31800	-0.07600	0.08000
O	-2.69200	5.65100	5.08700
O	-4.81400	-3.90100	-2.69700
O	5.64400	-2.15000	-1.15200
O	-1.16600	6.11200	-1.58100
O	4.61600	1.52000	5.09900
O	-5.27900	-1.67600	-5.52900
O	-5.36700	3.57700	3.85500
O	4.70400	-3.73300	-4.28400
O	-2.07100	-6.14700	3.71000
O	1.40800	5.99200	-4.14000
O	4.15200	3.74500	2.26800
O	-7.80900	-0.75000	4.06200
O	2.68100	-6.12400	5.17300
O	6.78900	-0.41200	1.56500
O	-4.22300	5.31600	6.57400
O	7.14500	0.59400	-4.49200
N	-7.87700	-1.80000	4.74300
N	3.42600	-5.64400	6.06000
N	7.77000	-0.84800	0.91900
N	-3.24100	4.88000	5.92700
N	7.21400	1.64500	-5.17400
O	-8.58000	-2.72900	4.38000
O	4.63600	-5.80600	6.00600
O	8.19000	-1.97500	1.11800
O	-2.82000	3.75100	6.12600
O	7.91800	2.57300	-4.81000
H	2.63800	1.07300	1.89300
H	-3.30000	-1.22800	-2.32200
H	-3.24100	1.99000	1.14100
H	2.57700	-2.14600	-1.57100
H	-1.04800	-3.59000	1.10000
H	0.38500	3.43600	-1.53000
H	4.53100	-0.34100	-1.08600
H	-5.19500	0.18600	0.65600
H	-2.18500	4.25300	-1.72700
H	1.52200	-4.40900	1.29700
H	-2.72800	-3.87100	-2.30000
H	2.06500	3.71600	1.87000
H	1.42800	0.68500	-1.57400
H	-2.09100	-0.84000	1.14400
H	-1.46100	1.03700	-1.95000
H	0.79800	-1.19200	1.51900
H	-0.29800	-1.65800	-1.95500

H	-0.36600	1.50200	1.52400
H	2.86600	3.57500	-1.12400
H	-3.53000	-3.73000	0.69500
H	-4.69300	0.87000	-2.32800
H	4.03200	-1.02500	1.89900
H	1.46600	-4.39500	-1.80600
H	-2.12900	4.23800	1.37600
O	-4.61400	5.35200	-3.01900
O	-5.27900	4.12300	-0.52300
O	-6.44500	3.00800	-2.98700
O	-2.17900	-6.56100	-3.41600
O	-1.46200	-6.46300	-0.64900
O	0.65600	-6.99200	-2.62500
O	6.51800	1.71700	-6.22600
H	-4.14700	2.15700	-4.81200
H	-3.24800	3.55500	-4.81300
H	-6.79300	2.11700	-3.05600
H	-7.00000	3.75900	-3.21000
H	-5.34000	5.59600	-3.59800
H	-3.97500	6.01500	-2.74600
H	-5.97200	3.64100	-0.06600
H	-4.96800	4.96300	-0.17400
H	-1.94200	-7.28500	-0.77200
H	-1.30500	-6.12600	0.23700
H	0.33100	-7.88500	-2.75600
H	1.60100	-6.82000	-2.61500
H	-2.35900	-7.46100	-3.13400
H	-2.64400	-6.19300	-4.17000
H	-0.42200	-5.24700	-5.09400
H	0.32000	-3.91000	-4.44200
H	-5.55800	-3.14900	3.31400
H	-4.75200	-1.69600	3.27200
H	-8.23600	-2.19400	1.24800
H	-7.61700	-0.67500	1.51600
H	-7.00700	-4.57100	0.22900
H	-5.96500	-4.89600	1.48300
H	-6.88800	-2.98000	-1.60800
H	-6.21200	-1.48200	-1.85800
H	1.98200	6.03800	3.74000
H	1.69800	7.30600	2.70200
H	-2.26200	6.66400	2.18500
H	-0.99500	7.73000	2.32600
H	-0.98400	3.75500	4.01200
H	-0.24200	5.09200	4.66300
H	0.64200	5.97100	-0.66600

H	1.28000	7.12900	0.34200
H	5.54700	1.32600	1.42800
H	6.22500	2.82400	1.17900
H	5.29900	4.74100	-1.91100
H	6.34500	4.41500	-0.66000
H	6.95400	0.51900	-1.94600
H	7.57300	2.03900	-1.67800
H	4.08900	1.54000	-3.70300
H	4.89500	2.99300	-3.74400
H	6.33700	-3.91400	2.78200
H	6.12900	-2.27200	2.62700
H	4.30700	-5.11700	-0.25500
H	5.31000	-3.79500	-0.36200
H	3.31200	-6.17000	2.31600
H	4.67900	-5.75200	3.16700
H	2.58400	-3.71100	4.38200
H	3.48500	-2.31300	4.38200
Ga	-0.73500	-5.37100	-2.35900
Ga	0.07200	5.21500	1.92900

XYZ of $Ga_{10}In_3$-a

193

In	-5.459691	-2.255648	0.770072
In	-4.253182	3.204908	-2.489959
In	0.262171	5.201813	1.697833
Ga	-0.221729	-0.169244	-0.223520
Ga	2.856090	-0.604881	0.129677
Ga	-3.300549	0.266390	-0.576722
Ga	-1.378234	2.731868	-0.403826
Ga	0.933771	-3.070364	-0.042218
Ga	-2.115118	-2.631722	-0.599273
Ga	1.671663	2.292234	0.152229
O	4.271414	-0.005229	-1.004152
O	-4.714872	-0.333259	0.557113
O	-2.308138	3.544391	-1.861486
O	1.863680	-3.882882	1.414441
O	-2.049548	-3.976470	-1.955031
O	1.606096	3.635982	1.507982
O	3.194631	2.827687	-0.859392
O	-3.638086	-3.167175	0.412347
O	-4.252388	1.215363	-1.926868
O	3.807925	-1.553859	1.480823
O	0.870182	-4.492924	-1.309917
O	-1.314642	4.153428	0.863868
O	6.961096	1.166784	-1.742551
O	-7.405550	-1.505271	1.294506
O	3.970599	-5.544352	2.813700
O	1.724660	6.412052	2.706003
O	5.825854	3.897748	-1.427513
O	-6.270314	-4.237243	0.981464
O	5.836776	-3.232730	2.689641
O	-1.103060	6.853548	1.893972
O	1.477694	0.461577	-0.965896
O	-1.920146	-0.802062	0.518852
O	-1.397965	0.907051	-1.360121
O	0.955510	-1.246536	0.913082
O	-0.336628	-1.828009	-1.259509
O	-0.106826	1.489526	0.811469
O	2.745313	1.039428	1.104563
O	-3.188769	-1.378916	-1.551608
O	-2.945964	1.906533	0.324282

O	2.501514	-2.246020	-0.772331
O	-0.831498	-3.500620	0.526752
O	0.389043	3.161135	-0.973791
O	5.842988	1.941933	0.773840
O	-6.286451	-2.280425	-1.219879
O	4.659754	-4.431745	0.271805
O	1.009029	6.209079	-0.055253
O	4.711936	1.943673	-3.341435
O	-5.155391	-2.283161	2.894391
O	-3.665384	2.728779	-4.498435
O	3.220934	-3.068266	4.050386
O	-0.133215	-4.985533	-4.137796
O	-0.311239	4.647046	3.689751
O	-4.587729	-5.380659	-4.200039
O	7.161781	-1.701245	-2.495508
O	-1.893309	6.739620	-3.615284
O	4.915491	0.214241	3.383882
O	-5.358949	-0.552729	-3.830922
O	-3.764845	4.403344	2.243757
O	3.321390	-4.742832	-2.690802
O	-3.000482	-5.272065	2.183873
O	2.557027	4.932577	-2.630918
O	4.144270	5.041167	3.753995
N	-5.279383	-4.622996	-3.503805
N	6.687475	-2.609911	-1.797748
N	-1.047801	6.851334	-2.715879
N	4.222845	0.970906	4.079107
N	-4.667295	-1.310392	-4.527156
N	-4.239146	3.494682	2.940517
N	3.794692	-3.833169	-3.388561
N	-2.153974	-5.160348	3.083283
N	1.711518	4.820863	-3.530323
N	4.834923	4.283500	3.057756
O	-6.486921	-4.438856	-3.736533
O	7.150289	-3.763334	-1.819795
O	-0.276175	7.822584	-2.657976
O	3.016299	1.156044	3.847388
O	-3.460753	-1.494531	-4.295433
O	-3.776337	2.341254	2.919470
O	3.332882	-2.680743	-3.366514
O	-1.383351	-4.188101	3.141186
O	0.938896	3.848610	-3.588235
O	6.042462	4.100365	3.289489
O	-7.108198	-1.602642	5.842530
O	2.912063	-4.810313	7.187218

O	8.426352	-0.291697	0.090679
O	-2.500269	5.812896	4.828944
O	-4.760688	-4.022562	-2.552709
O	5.721300	-2.373328	-1.060112
O	-0.955962	5.969744	-1.849393
O	4.741540	1.571340	5.030203
O	-5.185995	-1.910831	-5.477252
O	-5.205321	3.731265	3.678153
O	4.761866	-4.070753	-4.125197
O	-2.063134	-6.040937	3.948769
O	1.619675	5.702449	-4.395809
O	4.317228	3.683069	2.106665
O	-7.715395	-0.544627	4.061448
O	2.686129	-6.031161	5.419668
O	6.889240	-0.540347	1.584531
O	-4.038391	5.564234	6.324791
O	7.270940	0.205135	-4.508497
N	-7.801463	-1.563157	4.785499
N	3.437520	-5.526603	6.287402
N	7.864670	-1.018409	0.959856
N	-3.061955	5.086180	5.699121
N	7.358009	1.224674	-5.233539
O	-8.517978	-2.496032	4.460016
O	4.644331	-5.709507	6.243126
O	8.266152	-2.143232	1.206661
O	-2.659471	3.960360	5.945927
O	8.075522	2.156547	-4.907056
H	2.761976	1.022191	1.840578
H	-3.205439	-1.360684	-2.286618
H	-3.100553	1.998844	1.038001
H	2.656098	-2.338336	-1.485050
H	-0.995409	-3.612319	1.235512
H	0.551951	3.273831	-1.682552
H	4.637468	-0.545751	-1.071896
H	-5.081926	0.207260	0.624852
H	-2.004723	4.122640	-1.919499
H	1.560268	-4.462131	1.472450
H	-2.674542	-4.008605	-2.153051
H	2.231084	3.670117	1.706012
H	1.551513	0.507693	-1.609364
H	-1.994972	-0.846181	1.162324
H	-1.330929	0.889155	-2.005907
H	0.887476	-1.227638	1.557867
H	-0.210712	-1.821757	-1.895916
H	-0.233738	1.482271	1.447867

H	3.034747	3.391048	-1.277608
H	-3.479210	-3.729544	0.831564
H	-4.564813	0.757391	-2.384367
H	4.122350	-1.095881	1.938331
H	1.509932	-4.577434	-1.628362
H	-1.953384	4.236946	1.181314
O	-4.414050	5.204869	-3.261745
O	-5.102214	4.092255	-0.717845
O	-6.281236	2.893235	-3.135690
O	-2.167110	-6.751532	-3.154043
O	-1.452484	-6.548567	-0.391791
O	0.659600	-7.193041	-2.340016
O	6.664739	1.264154	-6.289570
H	-3.994889	1.930580	-4.918538
H	-3.073049	3.312838	-4.976103
H	-6.643239	2.005197	-3.168338
H	-6.824471	3.642635	-3.391831
H	-5.135080	5.435180	-3.852037
H	-3.764303	5.867879	-3.015780
H	-5.802964	3.640861	-0.243080
H	-4.778384	4.940910	-0.403544
H	-1.945447	-7.367771	-0.481733
H	-1.291689	-6.177937	0.479628
H	0.320893	-8.085731	-2.433578
H	1.607087	-7.035998	-2.334957
H	-2.361745	-7.635601	-2.834896
H	-2.624675	-6.407565	-3.923618
H	-0.386020	-5.537034	-4.881446
H	0.375901	-4.185218	-4.284869
H	-5.501491	-3.007639	3.419562
H	-4.672629	-1.570487	3.318815
H	-8.160727	-2.097787	1.309379
H	-7.518545	-0.578608	1.515148
H	-6.968661	-4.534879	0.393907
H	-5.933566	-4.823208	1.662397
H	-6.821741	-3.023876	-1.508680
H	-6.121036	-1.549202	-1.818852
H	2.182216	6.069081	3.476583
H	1.919296	7.297125	2.385860
H	-2.049542	6.696514	1.887918
H	-0.766351	7.747236	1.986529
H	-0.820359	3.846727	3.837825
H	-0.058434	5.198548	4.433402
H	0.848230	5.838445	-0.925672
H	1.501991	7.028283	0.034688

H	5.675581	1.209707	1.371798
H	6.377281	2.684380	1.062631
H	5.487098	4.484701	-2.107451
H	6.525210	4.195395	-0.841952
H	7.075089	0.239120	-1.962192
H	7.717269	1.759299	-1.756419
H	4.229178	1.231004	-3.766859
H	5.058035	2.668151	-3.866606
H	6.380008	-3.981131	2.945786
H	6.198776	-2.343693	2.722293
H	4.336917	-5.278396	-0.042482
H	5.360493	-3.978355	-0.201951
H	3.320847	-6.207367	2.568736
H	4.692629	-5.774661	3.403997
H	2.628598	-3.652325	4.528054
H	3.551434	-2.270068	4.471494
Ga	-0.705626	-5.541301	-2.144878
Ga	3.809731	-3.544392	2.041915
Ga	5.017236	1.916163	-1.217112

XYZ of $Ga_{10}In_3$-b

193

In	5.022072	1.839058	-1.085373
In	-5.592574	-2.065968	0.703195
In	-4.193561	3.437829	-2.403592
Ga	-0.285738	-0.112942	-0.191081
Ga	2.774308	-0.649721	0.177004
Ga	-3.346784	0.423864	-0.559179
Ga	-1.353562	2.825259	-0.305924
Ga	0.781073	-3.051146	-0.075251
Ga	-2.248066	-2.506997	-0.646792
Ga	1.676564	2.280115	0.264601
O	4.217381	-0.063910	-0.928735
O	-4.788857	-0.161974	0.546574
O	-2.245212	3.702506	-1.749906
O	1.672737	-3.928363	1.367732
O	-2.209950	-3.817843	-2.036381
O	1.638422	3.589961	1.654159
O	3.224177	2.795405	-0.719720
O	-3.795679	-3.022288	0.337529
O	-4.257294	1.435352	-1.892334
O	3.684805	-1.661238	1.511160
O	0.686954	-4.438127	-1.379938
O	-1.259470	4.211241	0.998732
O	6.947557	1.045396	-1.613437
O	-7.520018	-1.271222	1.230264
O	3.716078	-5.687733	2.741372
O	1.828464	6.329534	2.924789
O	5.891297	3.800221	-1.237354
O	-6.463813	-4.027106	0.856149
O	5.651375	-3.430762	2.693311
O	-0.977150	6.876443	2.100333
O	1.438574	0.485429	-0.902274
O	-2.009104	-0.713338	0.520065
O	-1.418734	1.027022	-1.309387
O	0.848231	-1.253931	0.927209
O	-0.440340	-1.740354	-1.270713
O	-0.131122	1.514501	0.887552
O	2.703484	0.971592	1.193251
O	-3.274987	-1.198474	-1.575442
O	-2.951908	2.028939	0.387086

O	2.379421	-2.255765	-0.770290
O	-1.001460	-3.442678	0.467242
O	0.430958	3.215768	-0.849420
O	5.829623	1.788879	0.912566
O	-6.401112	-2.014793	-1.293728
O	4.461751	-4.531401	0.235194
O	1.132886	6.219126	0.153176
O	4.737550	1.930274	-3.210801
O	-5.309053	-2.157157	2.828609
O	-3.601505	2.996009	-4.418646
O	3.029018	-3.222835	4.035442
O	-0.304259	-4.827594	-4.228126
O	-0.268202	4.601768	3.844953
O	-4.767794	-5.087068	-4.338701
O	7.069717	-1.807081	-2.438825
O	-1.719032	6.927830	-3.416582
O	4.826762	0.023348	3.468866
O	-5.398238	-0.249232	-3.851027
O	-3.713900	4.499087	2.363636
O	3.142398	-4.725970	-2.745827
O	-3.237619	-5.190178	2.059222
O	2.666117	4.963296	-2.441414
O	4.196278	4.860155	3.957509
N	-5.443030	-4.327111	-3.628980
N	6.562063	-2.718717	-1.768965
N	-0.878995	6.990970	-2.507382
N	4.150514	0.782363	4.177543
N	-4.723002	-1.009189	-4.560747
N	-4.221541	3.587480	3.032497
N	3.649079	-3.813307	-3.415671
N	-2.396582	-5.127065	2.968436
N	1.826080	4.900155	-3.350614
N	4.870514	4.100225	3.247775
O	-6.642323	-4.100882	-3.867171
O	6.990492	-3.884569	-1.816978
O	-0.079348	7.936807	-2.417695
O	2.952234	1.009535	3.940396
O	-3.524695	-1.235361	-4.323569
O	-3.793126	2.421598	2.985483
O	3.221624	-2.648481	-3.367675
O	-1.597908	-4.180202	3.058139
O	1.025406	3.953346	-3.440344
O	6.069847	3.875025	3.484997
O	-7.268126	-1.494256	5.776605
O	2.639143	-5.034814	7.123252

O	8.351550	-0.503025	0.193791
O	-2.432054	5.803173	4.995253
O	-4.915568	-3.767147	-2.658221
O	5.596528	-2.472255	-1.033728
O	-0.821547	6.085057	-1.663312
O	4.677977	1.342327	5.148303
O	-5.250478	-1.569182	-5.530508
O	-5.187075	3.833943	3.767734
O	4.615573	-4.060825	-4.149925
O	-2.340094	-6.031922	3.811523
O	1.768618	5.806039	-4.193684
O	4.344052	3.540235	2.277029
O	-7.826895	-0.373091	4.018452
O	2.393428	-6.202527	5.322747
O	6.793848	-0.743697	1.667485
O	-3.990784	5.562467	6.470933
O	7.254393	0.146235	-4.400657
N	-7.950019	-1.406838	4.715065
N	3.151394	-5.743211	6.209678
N	7.760385	-1.234629	1.038981
N	-3.023233	5.071539	5.841442
N	7.378557	1.180985	-5.098225
O	-8.690943	-2.309112	4.359365
O	4.352580	-5.961069	6.170994
O	8.125856	-2.376966	1.259937
O	-2.656789	3.928175	6.062381
O	8.120440	2.082202	-4.741543
H	2.712762	0.934965	1.928686
H	-3.284251	-1.160878	-2.309847
H	-3.110328	2.107489	1.101611
H	2.537826	-2.334344	-1.483816
H	-1.175229	-3.567573	1.171437
H	0.603754	3.341689	-1.553598
H	4.567784	-0.613261	-1.007350
H	-5.140260	0.387404	0.625175
H	-1.924175	4.272683	-1.790296
H	1.351674	-4.499539	1.408092
H	-2.833750	-3.826102	-2.240507
H	2.262275	3.600219	1.858346
H	1.519733	0.545820	-1.543673
H	-2.091208	-0.771703	1.161512
H	-1.346242	1.023712	-1.954822
H	0.774780	-1.249566	1.571662
H	-0.308365	-1.721542	-1.905642
H	-0.264123	1.494716	1.522438

H	3.085055	3.373869	-1.124528
H	-3.657545	-3.599755	0.743353
H	-4.578945	0.998869	-2.364220
H	4.008455	-1.224809	1.983072
H	1.326844	-4.533600	-1.694986
H	-1.898372	4.305718	1.312764
O	-4.287566	5.460881	-3.124563
O	-5.032268	4.304461	-0.616373
O	-6.223890	3.203876	-3.074516
O	-2.398953	-6.556413	-3.307967
O	-1.704388	-6.446008	-0.535367
O	0.405634	-7.103356	-2.481525
O	6.696650	1.268372	-6.158766
H	-3.950713	2.219116	-4.862125
H	-2.987603	3.574096	-4.875913
H	-6.611871	2.328239	-3.133293
H	-6.742144	3.975580	-3.315759
H	-4.995878	5.727822	-3.714825
H	-3.620676	6.097548	-2.855927
H	-5.750552	3.862265	-0.159493
H	-4.686241	5.134658	-0.277396
H	-2.220678	-7.247461	-0.650751
H	-1.540755	-6.102877	0.346720
H	0.041368	-7.982776	-2.601116
H	1.357291	-6.975014	-2.464289
H	-2.622809	-7.442145	-3.013546
H	-2.838870	-6.179212	-4.072243
H	-0.566437	-5.351975	-4.987974
H	0.229824	-4.039412	-4.350022
H	-5.681466	-2.884165	3.331823
H	-4.809251	-1.470435	3.275498
H	-8.292620	-1.840984	1.223295
H	-7.607407	-0.347557	1.473904
H	-7.165207	-4.288451	0.255115
H	-6.151037	-4.640213	1.524502
H	-6.955598	-2.734173	-1.606292
H	-6.208406	-1.273723	-1.872086
H	2.268393	5.953301	3.690095
H	2.052361	7.216295	2.629400
H	-1.927793	6.748104	2.082111
H	-0.614842	7.756947	2.218928
H	-0.802299	3.813556	3.967847
H	-0.006024	5.126148	4.604800
H	0.969239	5.875965	-0.727912
H	1.649176	7.020579	0.268560

H	5.634905	1.046894	1.489868
H	6.383082	2.507288	1.225087
H	5.576535	4.414350	-1.904704
H	6.593719	4.061598	-0.638306
H	7.035905	0.120675	-1.856096
H	7.721144	1.615100	-1.605456
H	4.237762	1.243582	-3.658689
H	5.109964	2.657282	-3.714014
H	6.169655	-4.201467	2.934584
H	6.039381	-2.554126	2.752118
H	4.116777	-5.359626	-0.103709
H	5.180075	-4.087237	-0.220626
H	3.049174	-6.324431	2.473735
H	4.425390	-5.954702	3.331648
H	2.415115	-3.800921	4.492708
H	3.379211	-2.445999	4.479933
Ga	-0.911535	-5.416927	-2.255271
Ga	3.622072	-3.664682	2.020401
Ga	0.340033	5.190044	1.873080

XYZ $Ga_{10}In_3$-c

193

In	-5.576068	-2.145786	0.689759
In	3.682516	-3.464435	2.009006
In	0.168016	5.293495	1.626113
Ga	-0.325990	-0.080625	-0.284069
Ga	2.748532	-0.526366	0.084889
Ga	-3.401512	0.365116	-0.653037
Ga	-1.471214	2.824137	-0.477152
Ga	0.818225	-2.985389	-0.089996
Ga	-2.226386	-2.537261	-0.662678
Ga	1.574406	2.375010	0.094538
O	4.171376	0.065364	-1.043678
O	-4.823356	-0.226615	0.475540
O	-2.391252	3.636300	-1.941259
O	1.738272	-3.797550	1.373111
O	-2.159187	-3.885648	-2.014736
O	1.507207	3.722398	1.446594
O	3.104081	2.902465	-0.911148
O	-3.756061	-3.064716	0.343007
O	-4.343506	1.314078	-2.010077
O	3.690517	-1.475330	1.442929
O	0.755570	-4.410905	-1.354417
O	-1.408559	4.248653	0.787267
O	6.868727	1.225892	-1.772177
O	-7.521697	-1.387140	1.203029
O	3.832538	-5.463006	2.786556
O	1.630020	6.501038	2.638211
O	5.741798	3.961681	-1.469395
O	-6.394788	-4.123933	0.902245
O	5.707560	-3.158388	2.665608
O	-1.192201	6.950588	1.811603
O	1.379198	0.542245	-1.019912
O	-2.030178	-0.705496	0.451779
O	-1.492937	0.996998	-1.428958
O	0.841957	-1.159248	0.860826
O	-0.441904	-1.741576	-1.316437
O	-0.210067	1.580328	0.747299
O	2.639014	1.120781	1.055115
O	-3.290994	-1.283031	-1.623255
O	-3.045341	2.006248	0.245538

O	2.392370	-2.168496	-0.814688
O	-0.951263	-3.407898	0.471626
O	0.300283	3.245648	-1.039758
O	5.741443	2.011373	0.736905
O	-6.393432	-2.172626	-1.304044
O	4.537767	-4.359280	0.245197
O	0.926815	6.293663	-0.125909
O	4.630001	2.006780	-3.383707
O	-5.281981	-2.169031	2.815567
O	-3.738849	2.818898	-4.582599
O	3.085879	-2.981146	4.013449
O	-0.236118	-4.907053	-4.185805
O	-0.416852	4.745805	3.616657
O	-4.691674	-5.286414	-4.268298
O	7.062709	-1.644725	-2.516984
O	-1.956627	6.825595	-3.701055
O	4.795346	0.293593	3.346814
O	-5.447326	-0.454843	-3.914953
O	-3.864389	4.510801	2.154828
O	3.212409	-4.673051	-2.722969
O	-3.134446	-5.167398	2.122819
O	2.482466	5.005148	-2.690959
O	4.039685	5.124162	3.701157
N	-5.383912	-4.524531	-3.577269
N	6.581833	-2.549928	-1.819221
N	-1.115014	6.936554	-2.797912
N	4.102117	1.054479	4.036832
N	-4.755088	-1.216727	-4.605982
N	-4.345256	3.605599	2.851592
N	3.692285	-3.766847	-3.420740
N	-2.291832	-5.056439	3.025971
N	1.640852	4.894189	-3.594103
N	4.730923	4.362279	3.010119
O	-6.589661	-4.336664	-3.816212
O	7.040607	-3.705050	-1.836172
O	-0.340195	7.905183	-2.738763
O	2.897360	1.243343	3.798900
O	-3.550330	-1.404591	-4.368048
O	-3.886490	2.450476	2.835640
O	3.234510	-2.612726	-3.403781
O	-1.518013	-4.086810	3.085113
O	0.865033	3.924560	-3.653263
O	5.936681	4.175414	3.248064
O	-7.246343	-1.474107	5.752648
O	2.755840	-4.714165	7.153125

O	8.320004	-0.233189	0.071665
O	-2.607085	5.922338	4.742477
O	-4.867600	-3.923558	-2.625217
O	5.613012	-2.308035	-1.086794
O	-1.030461	6.056829	-1.928793
O	4.618430	1.655451	4.988884
O	-5.271410	-1.817701	-5.557034
O	-5.314076	3.847493	3.584018
O	4.662096	-4.009743	-4.152159
O	-2.208270	-5.935162	3.894083
O	1.556291	5.773912	-4.462222
O	4.215610	3.761306	2.058076
O	-7.841260	-0.418422	3.966048
O	2.533944	-5.938650	5.387580
O	6.774918	-0.472578	1.558789
O	-4.153189	5.682946	6.231592
O	7.188280	0.256172	-4.534198
N	-7.934424	-1.434810	4.692228
N	3.283001	-5.434594	6.257621
N	7.751590	-0.955696	0.939971
N	-3.175508	5.199830	5.611784
N	7.282454	1.273561	-5.261367
O	-8.652722	-2.365936	4.365669
O	4.489345	-5.621921	6.219558
O	8.147857	-2.081320	1.191504
O	-2.778242	4.073205	5.863324
O	8.001742	2.203685	-4.933801
H	2.652112	1.105340	1.791241
H	-3.304101	-1.266593	-2.358380
H	-3.202993	2.100911	0.958278
H	2.550013	-2.263161	-1.526428
H	-1.118945	-3.517224	1.179875
H	0.466965	3.355974	-1.748013
H	4.535808	-0.476632	-1.108322
H	-5.188788	0.315382	0.540174
H	-2.085493	4.213313	-1.999272
H	1.432513	-4.375563	1.431122
H	-2.783343	-3.916049	-2.215653
H	2.131363	3.754799	1.647515
H	1.456243	0.586475	-1.663133
H	-2.108223	-0.747725	1.094995
H	-1.422893	0.977233	-2.074369
H	0.770923	-1.138482	1.505231
H	-0.312939	-1.737379	-1.952250
H	-0.340031	1.575131	1.383100

H	2.948210	3.465338	-1.331531
H	-3.601199	-3.626590	0.764383
H	-4.655390	0.856074	-2.467913
H	4.004401	-1.017326	1.900783
H	1.396521	-4.498503	-1.669596
H	-2.048501	4.335252	1.101454
O	-4.484508	5.300757	-3.355696
O	-5.188756	4.197028	-0.812328
O	-6.360550	2.996136	-3.232758
O	-2.280991	-6.663287	-3.207342
O	-1.578795	-6.455913	-0.442232
O	0.540212	-7.112840	-2.378744
O	6.594364	1.312856	-6.320787
H	-4.069211	2.020825	-5.002268
H	-3.142157	3.399631	-5.058898
H	-6.725575	2.109318	-3.264907
H	-6.899869	3.746825	-3.493361
H	-5.201891	5.532155	-3.949995
H	-3.833566	5.962060	-3.108297
H	-5.893371	3.749339	-0.339781
H	-4.863384	5.045309	-0.498613
H	-2.074258	-7.273574	-0.532471
H	-1.420821	-6.083665	0.429014
H	0.198756	-8.004548	-2.471684
H	1.488221	-6.959173	-2.369561
H	-2.480311	-7.545847	-2.886914
H	-2.733652	-6.319629	-3.979949
H	-0.487357	-5.459521	-4.929270
H	0.276558	-4.108936	-4.332454
H	-5.633172	-2.890940	3.340894
H	-4.798692	-1.457019	3.240501
H	-8.279056	-1.976915	1.215784
H	-7.632418	-0.459527	1.420808
H	-7.091393	-4.420551	0.312112
H	-6.063387	-4.709378	1.586241
H	-6.930003	-2.914884	-1.593530
H	-6.222548	-1.443511	-1.904050
H	2.082672	6.158378	3.411820
H	1.829350	7.384601	2.316784
H	-2.139201	6.796922	1.801430
H	-0.852735	7.843298	1.903527
H	-0.929537	3.947686	3.764306
H	-0.165613	5.298273	4.360122
H	0.768832	5.921412	-0.996154
H	1.422278	7.111324	-0.035670

H	5.568568	1.281261	1.335891
H	6.277014	2.752632	1.026380
H	5.408389	4.548125	-2.152408
H	6.439422	4.258303	-0.881253
H	6.980438	0.297276	-1.988948
H	7.627077	1.815665	-1.783923
H	4.146722	1.294770	-3.809642
H	4.981192	2.728690	-3.909035
H	6.246880	-3.908077	2.926213
H	6.072586	-2.270570	2.697759
H	4.213395	-5.205562	-0.068505
H	5.242373	-3.909593	-0.226347
H	3.181586	-6.124310	2.540157
H	4.550920	-5.694404	3.380864
H	2.489186	-3.561879	4.489748
H	3.417231	-2.183075	4.434127
Ga	-0.819996	-5.455746	-2.194254
Ga	4.925088	1.983536	-1.257890
Ga	-4.334487	3.302187	-2.578147

XYZ of $Ga_{11}In_2$-o

193

In	-5.445286	-2.230993	0.743041
In	-4.265169	3.302475	-2.401670
Ga	-0.217619	-0.097311	-0.203247
Ga	2.862208	-0.524312	0.142919
Ga	-3.298447	0.329682	-0.549420
Ga	-1.389025	2.800917	-0.323863
Ga	0.952781	-2.995572	-0.081637
Ga	-2.098014	-2.561169	-0.631535
Ga	1.662783	2.365548	0.225015
O	4.275067	0.106141	-0.977193
O	-4.710306	-0.300762	0.570698
O	-2.322276	3.638828	-1.764917
O	1.886037	-3.833457	1.358417
O	-2.024692	-3.877014	-2.014973
O	1.589470	3.680393	1.608428
O	3.183546	2.929825	-0.774178
O	-3.618777	-3.125446	0.367658
O	-4.254401	1.301658	-1.880155
O	3.818157	-1.496313	1.474655
O	0.897298	-4.391714	-1.378746
O	-1.333533	4.196059	0.973220
O	6.959074	1.307163	-1.689154
O	-7.395308	-1.501767	1.281654
O	4.000715	-5.512823	2.724206
O	1.692960	6.431469	2.864114
O	5.809525	4.025068	-1.318063
O	-6.245760	-4.220723	0.912537
O	5.854970	-3.189511	2.649628
O	-1.136534	6.875183	2.059508
O	1.478946	0.557613	-0.931146
O	-1.913169	-0.754226	0.524606
O	-1.398750	0.996348	-1.317987
O	0.964520	-1.191961	0.911472
O	-0.323324	-1.734697	-1.273654
O	-0.111909	1.540101	0.866159
O	2.742351	1.098729	1.151779
O	-3.177582	-1.294350	-1.558299
O	-2.952885	1.952502	0.385809
O	2.516659	-2.148106	-0.793334

O	-0.810567	-3.446703	0.477026
O	0.376337	3.251090	-0.883541
O	5.835504	2.023917	0.842070
O	-6.270748	-2.218563	-1.247565
O	4.685580	-4.343940	0.206522
O	0.979998	6.282392	0.098735
O	4.706853	2.105577	-3.273055
O	-5.142084	-2.301198	2.866535
O	-3.673745	2.871348	-4.419224
O	3.237519	-3.066952	4.011699
O	-0.101889	-4.830459	-4.216967
O	-0.334344	4.635855	3.809467
O	-4.554261	-5.247203	-4.290504
O	7.175046	-1.543477	-2.501569
O	-1.922976	6.872012	-3.451470
O	4.915445	0.237439	3.414906
O	-5.350684	-0.432061	-3.821400
O	-3.785800	4.404506	2.356327
O	3.350569	-4.600127	-2.762847
O	-2.971314	-5.263477	2.095380
O	2.536084	5.067856	-2.501900
O	4.119025	5.051557	3.884983
N	-5.250234	-4.507796	-3.579111
N	6.705045	-2.468925	-1.823222
N	-1.078581	6.969323	-2.549350
N	4.218485	0.975864	4.125268
N	-4.654711	-1.171468	-4.532793
N	-4.255795	3.479084	3.033674
N	3.819561	-3.673688	-3.441174
N	-2.125919	-5.166157	2.997506
N	1.691689	4.970544	-3.404020
N	4.813998	4.312141	3.173585
O	-6.458573	-4.325085	-3.808785
O	7.173838	-3.619232	-1.868978
O	-0.312028	7.943128	-2.470689
O	3.011133	1.159558	3.896625
O	-3.447366	-1.354162	-4.304125
O	-3.787008	2.328751	2.988917
O	3.351777	-2.524372	-3.395437
O	-1.360375	-4.191361	3.076186
O	0.924145	3.995732	-3.482712
O	6.022334	4.130455	3.402284
O	-7.100104	-1.692361	5.826865
O	2.935847	-4.875565	7.111338
O	8.430796	-0.181619	0.114299

O	-2.530045	5.766389	4.971194
O	-4.735208	-3.924642	-2.615352
O	5.737229	-2.252758	-1.081483
O	-0.982683	6.070353	-1.701358
O	4.733511	1.559018	5.089027
O	-5.169742	-1.754647	-5.495552
O	-5.223612	3.695250	3.775413
O	4.788381	-3.890871	-4.181933
O	-2.031025	-6.064110	3.844517
O	1.595786	5.869489	-4.251012
O	4.299973	3.728996	2.209832
O	-7.711734	-0.600608	4.067797
O	2.717266	-6.060462	5.318577
O	6.894122	-0.469283	1.601584
O	-4.067729	5.478667	6.460474
O	7.275504	0.404978	-4.474323
N	-7.792949	-1.634437	4.770409
N	3.465530	-5.570224	6.197154
N	7.872378	-0.929178	0.967757
N	-3.088467	5.018805	5.825652
N	7.357715	1.439841	-5.177903
O	-8.504434	-2.564015	4.425064
O	4.673297	-5.745930	6.149910
O	8.279535	-2.056812	1.191348
O	-2.680303	3.890180	6.049223
O	8.070203	2.368402	-4.831579
H	2.758675	1.066244	1.887286
H	-3.193919	-1.260891	-2.292781
H	-3.108365	2.029120	1.101189
H	2.672135	-2.224749	-1.507714
H	-0.974311	-3.573994	1.183191
H	0.539072	3.379373	-1.589686
H	4.643955	-0.430955	-1.055932
H	-5.080194	0.236325	0.649431
H	-2.021825	4.219719	-1.810659
H	1.585595	-4.415349	1.404134
H	-2.649396	-3.908243	-2.214051
H	2.214157	3.713622	1.807557
H	1.552901	0.617509	-1.573461
H	-1.988140	-0.812131	1.166966
H	-1.331247	0.992260	-1.963959
H	0.896013	-1.186856	1.556464
H	-0.197072	-1.714534	-1.909705
H	-0.239153	1.518930	1.502180
H	3.020991	3.500946	-1.180675

H	-3.457235	-3.695602	0.775175
H	-4.564184	0.851713	-2.347313
H	4.129940	-1.046351	1.941823
H	1.537661	-4.466264	-1.698442
H	-1.972883	4.269643	1.291896
O	-4.435941	5.317228	-3.131726
O	-5.119816	4.148302	-0.612037
O	-6.291206	2.993856	-3.055154
O	-2.127186	-6.627057	-3.271628
O	-1.415229	-6.478013	-0.505255
O	0.701298	-7.070829	-2.465028
O	6.664865	1.497739	-6.233360
H	-3.998868	2.080386	-4.856095
H	-3.084163	3.468286	-4.884210
H	-6.648587	2.104834	-3.106548
H	-6.838164	3.745616	-3.295999
H	-5.157810	5.556064	-3.717589
H	-3.789779	5.978315	-2.871551
H	-5.818496	3.683499	-0.147264
H	-4.800567	4.991883	-0.279897
H	-1.903890	-7.297699	-0.612587
H	-1.256862	-6.124798	0.373808
H	0.367273	-7.963113	-2.577404
H	1.647957	-6.909035	-2.456045
H	-2.317426	-7.518578	-2.971106
H	-2.586077	-6.269495	-4.034185
H	-0.351402	-5.367641	-4.972121
H	0.403161	-4.024634	-4.346981
H	-5.484733	-3.038241	3.376257
H	-4.663265	-1.595040	3.306049
H	-8.147416	-2.098357	1.283656
H	-7.513228	-0.580500	1.521478
H	-6.942214	-4.509652	0.318425
H	-5.906379	-4.819004	1.581346
H	-6.802012	-2.958588	-1.552163
H	-6.108772	-1.474172	-1.831057
H	2.151838	6.074881	3.627696
H	1.883197	7.324016	2.562617
H	-2.082187	6.713422	2.049530
H	-0.804512	7.768475	2.170899
H	-0.839400	3.830004	3.940481
H	-0.084832	5.173037	4.564622
H	0.821626	5.929152	-0.779329
H	1.468659	7.102078	0.206067
H	5.671542	1.278534	1.424526

H	6.365777	2.762934	1.146637
H	5.468130	4.624307	-1.985857
H	6.506989	4.314056	-0.725945
H	7.077998	0.384879	-1.927998
H	7.712177	1.903736	-1.690151
H	4.228040	1.399445	-3.713569
H	5.049503	2.842620	-3.782777
H	6.401920	-3.940271	2.890498
H	6.212343	-2.299489	2.701047
H	4.367314	-5.185514	-0.125562
H	5.384238	-3.877163	-0.257201
H	3.354548	-6.173937	2.465031
H	4.723584	-5.751652	3.310074
H	2.647938	-3.663890	4.476685
H	3.563637	-2.276007	4.449575
Ga	-0.672575	-5.430587	-2.236457
Ga	3.829943	-3.498071	1.994150
Ga	5.011055	2.035380	-1.149556
Ga	0.237345	5.234966	1.829937

XYZ of $Ga_{11}In_2$-m

193

In	-5.647425	-1.870839	0.688736
In	0.489948	5.254372	1.570885
Ga	-0.281136	-0.115230	-0.258544
Ga	2.759958	-0.723903	0.152260
Ga	-3.323229	0.493499	-0.669368
Ga	-1.261591	2.844742	-0.511017
Ga	0.698300	-3.075130	-0.005091
Ga	-2.310678	-2.469107	-0.619280
Ga	1.748350	2.237649	0.102206
O	4.225075	-0.230472	-0.969458
O	-4.787348	0.000012	0.452371
O	-2.119924	3.682061	-1.998245
O	1.556653	-3.912465	1.481138
O	-2.304216	-3.841405	-1.948746
O	1.741832	3.608949	1.431687
O	3.315286	2.663052	-0.894417
O	-3.877615	-2.894510	0.377344
O	-4.197019	1.470379	-2.051988
O	3.633728	-1.700768	1.535880
O	0.569929	-4.515802	-1.247172
O	-1.133276	4.284415	0.731078
O	6.990020	0.767064	-1.685865
O	-7.553271	-0.997483	1.167757
O	3.540597	-5.667348	2.944650
O	2.005993	6.395963	2.580012
O	6.013307	3.565564	-1.439659
O	-6.576654	-3.796951	0.923564
O	5.541584	-3.472126	2.808070
O	-0.778227	6.986908	1.714440
O	1.463511	0.400216	-0.984917
O	-2.024897	-0.632728	0.467879
O	-1.374601	1.006043	-1.433655
O	0.813271	-1.237556	0.916603
O	-0.478142	-1.784152	-1.265453
O	-0.084111	1.553677	0.747366
O	2.731772	0.942657	1.094710
O	-3.294101	-1.174114	-1.611783
O	-2.886054	2.127146	0.206809
O	2.322747	-2.358563	-0.724902

O	-1.097630	-3.389889	0.543163
O	0.536300	3.158376	-1.060215
O	5.881924	1.655145	0.797415
O	-6.444217	-1.885589	-1.313502
O	4.332316	-4.646593	0.394101
O	1.321196	6.181886	-0.188216
O	4.814898	1.643542	-3.334908
O	-5.377227	-1.874999	2.817835
O	-3.483165	2.896599	-4.641248
O	2.919858	-3.128016	4.123155
O	-0.418191	-5.003356	-4.081300
O	-0.145060	4.772937	3.563192
O	-4.886821	-5.137385	-4.208118
O	7.032402	-2.121852	-2.382409
O	-1.490965	6.812833	-3.803810
O	4.814985	0.035797	3.423600
O	-5.377257	-0.266257	-3.940687
O	-3.584914	4.704457	2.066398
O	3.022586	-4.935915	-2.583471
O	-3.392018	-4.998479	2.197486
O	2.829690	4.767022	-2.714559
O	4.324472	4.905943	3.692045
N	-5.542941	-4.327068	-3.537243
N	6.494873	-2.987409	-1.675739
N	-0.653946	6.892119	-2.893093
N	4.157830	0.845156	4.093469
N	-4.721137	-1.076574	-4.611562
N	-4.122423	3.838886	2.772068
N	3.559172	-4.069305	-3.290175
N	-2.554000	-4.919249	3.108224
N	1.992670	4.687736	-3.625276
N	4.979594	4.095681	3.021149
O	-6.733875	-4.076890	-3.792788
O	6.889095	-4.166227	-1.669017
O	0.172692	7.817327	-2.840684
O	2.967930	1.096293	3.838930
O	-3.531181	-1.326712	-4.357038
O	-3.728221	2.660083	2.779790
O	3.165893	-2.891541	-3.296863
O	-1.728305	-3.992987	3.160597
O	1.164979	3.761585	-3.677691
O	6.170604	3.846486	3.275680
O	-7.330543	-1.023990	5.721010
O	2.461637	-4.787806	7.286219
O	8.338951	-0.739133	0.197386

O	-2.278346	6.087162	4.645193
O	-5.004065	-3.739807	-2.589146
O	5.533369	-2.680255	-0.958285
O	-0.627318	6.023615	-2.009110
O	4.696706	1.432418	5.041565
O	-5.260033	-1.663820	-5.558659
O	-5.083927	4.146040	3.489523
O	4.521598	-4.377498	-4.006596
O	-2.528295	-5.786714	3.991172
O	1.966023	5.556255	-4.508259
O	4.441717	3.508365	2.073073
O	-7.847422	0.033137	3.911132
O	2.190634	-6.027306	5.538092
O	6.767575	-0.868106	1.670573
O	-3.850759	5.958275	6.120358
O	7.284096	-0.264539	-4.428226
N	-8.004312	-0.964360	4.652380
N	2.957368	-5.551016	6.408377
N	7.722370	-1.414631	1.070653
N	-2.894946	5.411679	5.519460
N	7.442059	0.733886	-5.170467
O	-8.769656	-1.859688	4.332653
O	4.151811	-5.805286	6.386967
O	8.053022	-2.556092	1.344629
O	-2.563351	4.269164	5.793470
O	8.208326	1.628175	-4.849705
H	2.736329	0.938738	1.831090
H	-3.298622	-1.169182	-2.347177
H	-3.045631	2.242188	0.916114
H	2.482305	-2.473590	-1.433207
H	-1.278477	-3.478016	1.251127
H	0.716204	3.247556	-1.768214
H	4.559571	-0.792765	-1.021295
H	-5.122842	0.562361	0.504188
H	-1.782078	4.240264	-2.062020
H	1.218751	-4.471666	1.544926
H	-2.926971	-3.840620	-2.156200
H	2.364698	3.610161	1.639113
H	1.549582	0.429440	-1.627851
H	-2.111854	-0.659899	1.110764
H	-1.299045	0.971729	-2.077834
H	0.736792	-1.202204	1.559747
H	-0.342530	-1.797638	-1.899751
H	-0.220777	1.566220	1.381658
H	3.195226	3.226619	-1.325489

H	-3.758517	-3.457008	0.809380
H	-4.529016	1.022762	-2.505937
H	3.967722	-1.253262	1.989870
H	1.208289	-4.643884	-1.553638
H	-1.770673	4.411428	1.036579
O	-4.102905	5.435875	-3.462723
O	-4.893666	4.415095	-0.910154
O	-6.104931	3.240739	-3.324165
O	-2.567303	-6.627491	-3.098064
O	-1.883525	-6.413344	-0.328857
O	0.215878	-7.218351	-2.230513
O	6.768271	0.793531	-6.238097
H	-3.852849	2.111133	-5.051807
H	-2.850287	3.435504	-5.119996
H	-6.518175	2.375022	-3.346250
H	-6.599087	4.015638	-3.602830
H	-4.800138	5.696642	-4.068726
H	-3.418935	6.064234	-3.218587
H	-5.626885	4.014909	-0.438507
H	-4.525079	5.249203	-0.606388
H	-2.422562	-7.203779	-0.411604
H	-1.714249	-6.035977	0.538053
H	-0.173472	-8.091259	-2.313033
H	1.170798	-7.117143	-2.213065
H	-2.818541	-7.492256	-2.765833
H	-2.992159	-6.272231	-3.881142
H	-0.691899	-5.553370	-4.818625
H	0.139416	-4.237315	-4.234888
H	-5.773326	-2.567592	3.350637
H	-4.859682	-1.183809	3.236765
H	-8.342235	-1.544237	1.181377
H	-7.614689	-0.061683	1.369402
H	-7.282441	-4.064399	0.330409
H	-6.285338	-4.388370	1.620545
H	-7.018045	-2.601784	-1.597129
H	-6.226960	-1.177085	-1.923124
H	2.430885	6.041716	3.364076
H	2.257306	7.261711	2.246767
H	-1.732129	6.885630	1.696012
H	-0.390797	7.860910	1.795905
H	-0.702687	4.006911	3.717780
H	0.128648	5.322951	4.300518
H	1.151901	5.804534	-1.054126
H	1.860234	6.972321	-0.105470
H	5.662635	0.945738	1.406010

H	6.454699	2.370397	1.081035
H	5.720031	4.158107	-2.135695
H	6.720132	3.832926	-0.848482
H	7.052360	-0.169774	-1.886475
H	7.779962	1.313778	-1.698464
H	4.297373	0.952336	-3.754838
H	5.210997	2.336134	-3.867710
H	6.035796	-4.246026	3.086721
H	5.954884	-2.605411	2.830142
H	3.964839	-5.478759	0.090328
H	5.065627	-4.244395	-0.076574
H	2.856607	-6.295691	2.701514
H	4.238828	-5.928170	3.550674
H	2.286980	-3.666922	4.601903
H	3.290520	-2.342590	4.534734
Ga	-1.052276	-5.485830	-2.087959
Ga	3.509640	-3.676725	2.133580
Ga	5.086094	1.639326	-1.205788
Ga	-4.071949	3.445252	-2.651652

XYZ of $Ga_{11}In_2$-p

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In	5.071626	1.605111	-1.081065
In	-5.752993	-1.715366	0.628023
Ga	-0.341143	-0.054590	-0.226530
Ga	2.681976	-0.738913	0.197679
Ga	-3.365259	0.629809	-0.650768
Ga	-1.255183	2.931202	-0.416373
Ga	0.571871	-3.040314	-0.035717
Ga	-2.417201	-2.354456	-0.663008
Ga	1.734837	2.244278	0.209937
O	4.168311	-0.250662	-0.898091
O	-4.850598	0.141481	0.445031
O	-2.080662	3.822440	-1.890810
O	1.397379	-3.931544	1.437721
O	-2.427198	-3.694262	-2.025192
O	1.744757	3.583087	1.572110
O	3.320272	2.659319	-0.761481
O	-4.002636	-2.769497	0.308409
O	-4.204216	1.658360	-2.017397
O	3.520904	-1.767472	1.565307
O	0.424749	-4.447624	-1.313455
O	-1.108138	4.337515	0.861354
O	6.960973	0.703443	-1.564393
O	-7.644227	-0.812538	1.110305
O	3.328653	-5.763763	2.876703
O	2.057509	6.335332	2.789982
O	6.042304	3.515796	-1.259598
O	-6.725694	-3.625905	0.807498
O	5.377635	-3.609911	2.811925
O	-0.704722	7.007268	1.913117
O	1.421236	0.440096	-0.923956
O	-2.102680	-0.551349	0.470902
O	-1.398647	1.118071	-1.384268
O	0.717279	-1.228327	0.931225
O	-0.564099	-1.694184	-1.275339
O	-0.118158	1.585012	0.821279
O	2.680386	0.904763	1.179898
O	-3.362749	-1.014941	-1.632969
O	-2.901675	2.232064	0.268732
O	2.218344	-2.342156	-0.722831

O	-1.235712	-3.329028	0.488031
O	0.554345	3.218772	-0.941073
O	5.847901	1.555536	0.929248
O	-6.530216	-1.664725	-1.381309
O	4.167153	-4.699530	0.359087
O	1.395485	6.202703	0.011134
O	4.821506	1.666327	-3.211889
O	-5.503869	-1.776505	2.758817
O	-3.434459	3.130468	-4.564618
O	2.751128	-3.240560	4.110518
O	-0.545748	-4.845411	-4.167622
O	-0.137505	4.736316	3.713533
O	-5.014766	-4.879187	-4.339198
O	6.948051	-2.168160	-2.330253
O	-1.366813	6.981239	-3.614119
O	4.720640	-0.102809	3.505421
O	-5.402927	-0.006372	-3.958482
O	-3.563171	4.778577	2.183596
O	2.880808	-4.888755	-2.636667
O	-3.580301	-4.926610	2.081515
O	2.897938	4.816432	-2.534586
O	4.332373	4.769001	3.887126
N	-5.659863	-4.071137	-3.655031
N	6.385117	-3.038541	-1.649776
N	-0.537266	7.020427	-2.694005
N	4.074498	0.704331	4.188549
N	-4.757829	-0.814423	-4.642649
N	-4.126076	3.908205	2.863074
N	3.442823	-4.017300	-3.317163
N	-2.749758	-4.887500	3.001658
N	2.068391	4.777244	-3.454701
N	4.976474	3.961028	3.202930
O	-6.842574	-3.789067	-3.915508
O	6.753809	-4.225471	-1.667930
O	0.308525	7.925922	-2.611527
O	2.892832	0.987311	3.929111
O	-3.576085	-1.096406	-4.383200
O	-3.757413	2.721266	2.845919
O	3.075050	-2.831444	-3.298990
O	-1.904886	-3.980930	3.084118
O	1.221526	3.870830	-3.537218
O	6.159291	3.679964	3.462418
O	-7.466848	-0.953170	5.663455
O	2.226273	-4.965445	7.228072
O	8.258638	-0.876493	0.294301

O	-2.252555	6.070252	4.807150
O	-5.117819	-3.518656	-2.688024
O	5.423442	-2.727868	-0.934067
O	-0.538006	6.130581	-1.831099
O	4.616543	1.256812	5.155556
O	-5.299903	-1.366912	-5.608656
O	-5.087751	4.218877	3.578782
O	4.405387	-4.329055	-4.031854
O	-2.751388	-5.776263	3.863546
O	2.069102	5.667082	-4.316606
O	4.435426	3.408469	2.235952
O	-7.943072	0.158083	3.874974
O	1.945855	-6.156441	5.448004
O	6.670460	-1.006603	1.749257
O	-3.841788	5.940203	6.264077
O	7.259712	-0.268183	-4.328074
N	-8.128651	-0.853273	4.590363
N	2.714073	-5.717958	6.336657
N	7.619125	-1.559196	1.145186
N	-2.892097	5.387541	5.659035
N	7.446394	0.744101	-5.044423
O	-8.909898	-1.723819	4.241949
O	3.902923	-5.997546	6.320206
O	7.922445	-2.713823	1.394508
O	-2.587859	4.231840	5.908376
O	8.228531	1.613564	-4.694992
H	2.677625	0.883071	1.915978
H	-3.359941	-0.992260	-2.368039
H	-3.065699	2.333488	0.979099
H	2.382339	-2.443589	-1.432199
H	-1.425356	-3.430171	1.191941
H	0.743069	3.320990	-1.645002
H	4.491130	-0.818688	-0.960414
H	-5.174413	0.709585	0.507325
H	-1.730278	4.374537	-1.937906
H	1.046918	-4.484638	1.484806
H	-3.047725	-3.674960	-2.238349
H	2.365439	3.565779	1.785288
H	1.514225	0.482866	-1.565165
H	-2.196511	-0.592047	1.112105
H	-1.317522	1.097597	-2.028358
H	0.635265	-1.206769	1.574298
H	-0.422586	-1.695386	-1.908490
H	-0.260745	1.585294	1.454390
H	3.216600	3.235548	-1.179879

H	-3.899912	-3.344659	0.727789
H	-4.541289	1.229092	-2.485118
H	3.859970	-1.338358	2.033085
H	1.063185	-4.582159	-1.616982
H	-1.745626	4.470984	1.163900
O	-4.010987	5.653594	-3.330774
O	-4.848549	4.589266	-0.811131
O	-6.061025	3.499803	-3.264026
O	-2.738847	-6.445579	-3.244024
O	-2.077849	-6.312881	-0.464205
O	0.022329	-7.117454	-2.365189
O	6.784562	0.843989	-6.116515
H	-3.816901	2.363305	-4.997493
H	-2.785466	3.666825	-5.024272
H	-6.492556	2.644054	-3.310906
H	-6.535640	4.291726	-3.528431
H	-4.696465	5.943927	-3.936743
H	-3.316091	6.260895	-3.065146
H	-5.594802	4.193907	-0.356150
H	-4.465109	5.407632	-0.483845
H	-2.632923	-7.089198	-0.571074
H	-1.909018	-5.960201	0.413123
H	-0.384876	-7.979460	-2.472436
H	0.978988	-7.037476	-2.336416
H	-3.011875	-7.312404	-2.935178
H	-3.148253	-6.062472	-4.022189
H	-0.823968	-5.371488	-4.920561
H	0.029687	-4.088206	-4.297426
H	-5.919986	-2.472914	3.270988
H	-4.975718	-1.106984	3.199154
H	-8.444864	-1.342182	1.103345
H	-7.687481	0.119266	1.333967
H	-7.431211	-3.863632	0.201504
H	-6.454024	-4.240077	1.492634
H	-7.116502	-2.361263	-1.687516
H	-6.291795	-0.946682	-1.971552
H	2.466963	5.953214	3.569157
H	2.330644	7.203162	2.480147
H	-1.660355	6.927221	1.883373
H	-0.299403	7.870434	2.019318
H	-0.712970	3.979103	3.844337
H	0.140714	5.262393	4.466472
H	1.226625	5.850015	-0.865195
H	1.950560	6.979020	0.118003
H	5.607439	0.836659	1.518423

H	6.433113	2.251154	1.235416
H	5.768690	4.131112	-1.943782
H	6.748876	3.753463	-0.655575
H	7.005118	-0.229444	-1.787038
H	7.762577	1.233001	-1.556406
H	4.293383	0.996815	-3.653225
H	5.237622	2.362736	-3.724060
H	5.852328	-4.400838	3.076341
H	5.809243	-2.753166	2.858817
H	3.784863	-5.515980	0.031852
H	4.913531	-4.302186	-0.094872
H	2.633727	-6.371072	2.612074
H	4.015127	-6.054174	3.482701
H	2.102135	-3.776917	4.570172
H	3.134537	-2.473483	4.544422
Ga	-1.209609	-5.361697	-2.192529
Ga	3.348483	-3.754042	2.113812
Ga	0.527245	5.251519	1.739458
Ga	-4.030817	3.643873	-2.567883

XYZ of $Ga_{12}In_1$

193

In	-5.623284	-1.870232	0.667283
Ga	-0.273861	-0.042794	-0.238644
Ga	2.772749	-0.629080	0.163765
Ga	-3.321471	0.543538	-0.641074
Ga	-1.283614	2.911653	-0.433849
Ga	0.734872	-2.997200	-0.042460
Ga	-2.279390	-2.409227	-0.648227
Ga	1.731621	2.322640	0.170933
O	4.233999	-0.099000	-0.946217
O	-4.781722	0.013412	0.468928
O	-2.148764	3.769566	-1.905307
O	1.600043	-3.855109	1.427998
O	-2.257849	-3.754875	-2.004506
O	1.710035	3.667289	1.527207
O	3.295239	2.783255	-0.815196
O	-3.843008	-2.869842	0.337903
O	-4.203579	1.538758	-2.005208
O	3.654836	-1.624305	1.528899
O	0.622182	-4.414276	-1.312884
O	-1.170970	4.327730	0.836569
O	6.989556	0.940030	-1.639437
O	-7.538257	-1.025568	1.161129
O	3.599948	-5.618659	2.859006
O	1.945138	6.433583	2.730625
O	5.984652	3.723236	-1.339242
O	-6.533440	-3.809782	0.862927
O	5.579017	-3.401308	2.768205
O	-0.843970	7.013689	1.873500
O	1.466282	0.504279	-0.952583
O	-2.013098	-0.591911	0.475304
O	-1.377289	1.090494	-1.392728
O	0.830520	-1.177127	0.915455
O	-0.453139	-1.693392	-1.278530
O	-0.094563	1.607809	0.800242
O	2.726936	1.018182	1.138883
O	-3.274705	-1.104769	-1.616177
O	-2.901549	2.163848	0.267701
O	2.352803	-2.250384	-0.746016
O	-1.058378	-3.340630	0.497292

O	0.511608	3.253997	-0.974565
O	5.870106	1.767804	0.859535
O	-6.417850	-1.853397	-1.335823
O	4.384015	-4.539893	0.330061
O	1.265336	6.267383	-0.042118
O	4.807457	1.827146	-3.273506
O	-5.355226	-1.913733	2.796212
O	-3.501389	3.022877	-4.564950
O	2.952643	-3.109414	4.086636
O	-0.358127	-4.855613	-4.157280
O	-0.190574	4.770075	3.678971
O	-4.825061	-5.031701	-4.292150
O	7.061540	-1.934003	-2.392803
O	-1.549313	6.941500	-3.647972
O	4.816742	0.086351	3.451954
O	-5.364465	-0.171939	-3.929242
O	-3.628046	4.696837	2.176937
O	3.080277	-4.783424	-2.654230
O	-3.338246	-5.004388	2.116760
O	2.790477	4.917801	-2.594054
O	4.277271	4.945109	3.815856
N	-5.489935	-4.241377	-3.606213
N	6.531976	-2.818665	-1.704005
N	-0.714056	7.011137	-2.734851
N	4.150844	0.875727	4.136865
N	-4.699590	-0.962264	-4.615179
N	-4.157589	3.812179	2.864735
N	3.608888	-3.897717	-3.343043
N	-2.501990	-4.934796	3.029902
N	1.955220	4.848163	-3.507175
N	4.941147	4.154831	3.129898
O	-6.683052	-3.998099	-3.858218
O	6.937961	-3.993393	-1.720067
O	0.103233	7.943334	-2.663191
O	2.958751	1.119953	3.885886
O	-3.507452	-1.205491	-4.364194
O	-3.751624	2.637447	2.849672
O	3.203855	-2.724034	-3.326966
O	-1.685654	-4.001555	3.101547
O	1.136887	3.915014	-3.578862
O	6.134330	3.912557	3.380910
O	-7.319912	-1.139749	5.713238
O	2.507825	-4.835824	7.215771
O	8.351566	-0.589520	0.215362
O	-2.337999	6.041325	4.784102

O	-4.957926	-3.667601	-2.646058
O	5.566718	-2.535347	-0.981798
O	-0.679643	6.125658	-1.868148
O	4.682853	1.449503	5.097020
O	-5.231621	-1.536044	-5.574335
O	-5.122846	4.095497	3.586942
O	4.575078	-4.182084	-4.064236
O	-2.468509	-5.819226	3.895590
O	1.920786	5.733638	-4.372878
O	4.410136	3.581009	2.169764
O	-7.845495	-0.052303	3.923948
O	2.251012	-6.043208	5.443197
O	6.780060	-0.763231	1.683806
O	-3.910545	5.867650	6.254524
O	7.296727	-0.034238	-4.401262
N	-7.993154	-1.065757	4.645175
N	3.012058	-5.576567	6.323642
N	7.740883	-1.288249	1.074379
N	-2.948702	5.342591	5.644119
N	7.445453	0.980174	-5.123463
O	-8.749180	-1.962191	4.306913
O	4.209006	-5.818432	6.298671
O	8.082657	-2.431540	1.326178
O	-2.605976	4.198255	5.895933
O	8.202410	1.875558	-4.784186
H	2.730782	0.999770	1.875047
H	-3.278526	-1.085363	-2.351336
H	-3.062991	2.263264	0.978944
H	2.514224	-2.349806	-1.456258
H	-1.239055	-3.444518	1.203159
H	0.691332	3.358930	-1.680447
H	4.574155	-0.656794	-1.008733
H	-5.122876	0.571252	0.531424
H	-1.816453	4.332264	-1.957643
H	1.267686	-4.418805	1.480328
H	-2.880369	-3.756209	-2.212661
H	2.332647	3.670621	1.735373
H	1.552711	0.547049	-1.594710
H	-2.100434	-0.632637	1.117422
H	-1.300737	1.069662	-2.037367
H	0.753035	-1.155245	1.559079
H	-0.316754	-1.692998	-1.912806
H	-0.231993	1.606461	1.434491
H	3.169987	3.353996	-1.235208
H	-3.718730	-3.439543	0.758899

H	-4.530620	1.096900	-2.468305
H	3.983875	-1.182539	1.992037
H	1.262102	-4.529905	-1.621041
H	-1.809916	4.442319	1.143742
O	-4.147696	5.532077	-3.337299
O	-4.930806	4.453255	-0.806334
O	-6.127806	3.314763	-3.244519
O	-2.491887	-6.520212	-3.208898
O	-1.813105	-6.353970	-0.435176
O	0.296180	-7.100281	-2.349794
O	6.772189	1.054161	-6.190527
H	-3.862780	2.242020	-4.991378
H	-2.873446	3.577420	-5.032201
H	-6.532348	2.445570	-3.284186
H	-6.629403	4.090042	-3.508439
H	-4.846885	5.797787	-3.938886
H	-3.470293	6.162287	-3.079980
H	-5.660466	4.036538	-0.343568
H	-4.570890	5.284840	-0.485720
H	-2.344125	-7.147957	-0.534160
H	-1.648494	-5.992123	0.439217
H	-0.084336	-7.975231	-2.449997
H	1.250022	-6.989912	-2.329191
H	-2.734801	-7.393832	-2.894103
H	-2.919477	-6.153816	-3.985330
H	-0.625568	-5.393665	-4.905648
H	0.191947	-4.081162	-4.295044
H	-5.744920	-2.620629	3.314761
H	-4.845047	-1.225819	3.229329
H	-8.321726	-1.580331	1.162997
H	-7.609236	-0.094591	1.381126
H	-7.235913	-4.072497	0.263752
H	-6.236934	-4.411912	1.548455
H	-6.984197	-2.569543	-1.634226
H	-6.207070	-1.130861	-1.931081
H	2.372753	6.068182	3.508062
H	2.188119	7.308208	2.414836
H	-1.796792	6.903279	1.851918
H	-0.465384	7.889735	1.972667
H	-0.740669	3.995619	3.817735
H	0.076868	5.308128	4.427339
H	1.100705	5.905531	-0.915511
H	1.796356	7.061370	0.056866
H	5.657303	1.044365	1.453745
H	6.435408	2.482997	1.157911

H	5.686173	4.326451	-2.023806
H	6.688165	3.985915	-0.742046
H	7.061468	0.008004	-1.858419
H	7.774003	1.494743	-1.640285
H	4.297299	1.139237	-3.707623
H	5.197152	2.534042	-3.792055
H	6.080661	-4.175589	3.032130
H	5.983605	-2.531117	2.807877
H	4.025189	-5.369525	0.009479
H	5.113745	-4.121182	-0.131694
H	2.922525	-6.248875	2.602686
H	4.300136	-5.884415	3.460613
H	2.324699	-3.663956	4.553886
H	3.315012	-2.328607	4.514084
Ga	-0.989384	-5.383655	-2.174620
Ga	3.549909	-3.612818	2.087338
Ga	0.441615	5.297068	1.697326
Ga	-4.097657	3.526236	-2.565632
Ga	5.076514	1.783599	-1.144556

XYZ of Ga_{13}

193

Ga	-0.348120	-0.085005	-0.227292
Ga	2.724445	-0.529519	0.159038
Ga	-3.421686	0.359509	-0.613637
Ga	-1.493515	2.819320	-0.425870
Ga	0.796259	-2.989332	-0.027729
Ga	-2.245235	-2.542344	-0.617608
Ga	1.548994	2.371335	0.163022
O	4.153440	0.063245	-0.961184
O	-4.849681	-0.233255	0.506601
O	-2.405547	3.631601	-1.894911
O	1.708307	-3.801611	1.440313
O	-2.169727	-3.890218	-1.969741
O	1.473486	3.718208	1.515153
O	3.084146	2.899826	-0.833734
O	-3.780387	-3.070836	0.379148
O	-4.356346	1.308540	-1.975691
O	3.659090	-1.478553	1.522092
O	0.741450	-4.414422	-1.292994
O	-1.438706	4.243410	0.839393
O	6.854386	1.225226	-1.673872
O	-7.551612	-1.395234	1.218274
O	3.795216	-5.466647	2.865088
O	1.588267	6.496475	2.708439
O	5.724534	3.960408	-1.376549
O	-6.421790	-4.131420	0.922949
O	5.669874	-3.161157	2.755657
O	-1.229394	6.945073	1.865908
O	1.360960	0.538883	-0.953174
O	-2.056200	-0.710893	0.498602
O	-1.508997	0.992512	-1.378434
O	0.813756	-1.163522	0.923863
O	-0.457406	-1.745637	-1.260895
O	-0.238819	1.575629	0.805312
O	2.608663	1.117232	1.129210
O	-3.304903	-1.288241	-1.583795
O	-3.071374	2.000476	0.287539
O	2.374149	-2.171484	-0.743139
O	-0.976216	-3.412825	0.523641
O	0.280975	3.241815	-0.978212

O	5.712461	2.009310	0.829018
O	-6.408717	-2.179322	-1.282602
O	4.514438	-4.361699	0.328186
O	0.900931	6.289779	-0.059720
O	4.624542	2.005702	-3.297868
O	-5.320783	-2.176712	2.843282
O	-3.737694	2.814550	-4.544186
O	3.040469	-2.985557	4.088585
O	-0.233853	-4.909994	-4.130169
O	-0.463373	4.739987	3.674570
O	-4.688696	-5.291295	-4.238208
O	7.053888	-1.645038	-2.418582
O	-1.962309	6.821718	-3.651065
O	4.752256	0.290176	3.432877
O	-5.448497	-0.460186	-3.887460
O	-3.902412	4.503982	2.193018
O	3.206171	-4.674992	-2.647603
O	-3.168000	-5.173881	2.161728
O	2.471759	5.002871	-2.616313
O	3.992441	5.120283	3.784623
N	-5.385203	-4.529966	-3.550868
N	6.569442	-2.550704	-1.723895
N	-1.125910	6.932725	-2.743097
N	4.054765	1.050508	4.119200
N	-4.751990	-1.221515	-4.574800
N	-4.386842	3.598319	2.886705
N	3.689617	-3.768326	-3.342303
N	-2.330600	-5.062873	3.069712
N	1.635360	4.891864	-3.524282
N	4.687947	4.358954	3.097267
O	-6.589652	-4.342547	-3.796618
O	7.028819	-3.705616	-1.738641
O	-0.351871	7.901676	-2.679184
O	2.851300	1.238925	3.874467
O	-3.548526	-1.408932	-4.330066
O	-3.927481	2.443404	2.872959
O	3.231240	-2.614414	-3.327544
O	-1.557562	-4.092923	3.133611
O	0.860321	3.921913	-3.588212
O	5.892412	4.172537	3.342020
O	-7.302174	-1.483709	5.769358
O	2.693297	-4.719847	7.225711
O	8.295770	-0.233874	0.177698
O	-2.660514	5.915148	4.788298
O	-4.874596	-3.929106	-2.595673

O	5.596352	-2.309501	-0.996921
O	-1.045925	6.052726	-1.873823
O	4.565372	1.651367	5.074395
O	-5.262613	-1.822377	-5.528996
O	-5.359932	3.839521	3.613679
O	4.663691	-4.010531	-4.068265
O	-2.251601	-5.941870	3.937973
O	1.555360	5.771861	-4.392556
O	4.178340	3.758094	2.142087
O	-7.887359	-0.427647	3.979770
O	2.482018	-5.943796	5.458493
O	6.742334	-0.474478	1.655900
O	-4.214980	5.674539	6.268484
O	7.190119	0.256637	-4.434370
N	-7.984212	-1.444336	4.705046
N	3.225877	-5.439722	6.332972
N	7.722734	-0.956943	1.042491
N	-3.233565	5.192077	5.654091
N	7.287986	1.274329	-5.160629
O	-8.700222	-2.375663	4.374064
O	4.432502	-5.626501	6.301723
O	8.118060	-2.082482	1.295879
O	-2.837240	4.065538	5.907492
O	8.004981	2.204653	-4.828634
H	2.617569	1.101533	1.865393
H	-3.313825	-1.271545	-2.318977
H	-3.233131	2.094813	0.999402
H	2.535890	-2.265823	-1.454002
H	-1.147886	-3.522479	1.230883
H	0.451645	3.352469	-1.685466
H	4.518475	-0.478567	-1.023941
H	-5.215716	0.308557	0.569342
H	-2.099719	4.208769	-1.950975
H	1.402478	-4.379779	1.496374
H	-2.792713	-3.920822	-2.174225
H	2.096472	3.750813	1.719642
H	1.441653	0.583377	-1.595930
H	-2.137894	-0.753387	1.141347
H	-1.435264	0.973010	-2.023443
H	0.739039	-1.143018	1.567859
H	-0.324819	-1.741155	-1.895960
H	-0.372406	1.570147	1.440360
H	2.930425	3.462781	-1.254799
H	-3.627681	-3.632793	0.801201
H	-4.665410	0.850562	-2.435460

H	3.970154	-1.020574	1.981892
H	1.384227	-4.501624	-1.604543
H	-2.080467	4.329614	1.149955
O	-4.491441	5.295639	-3.320673
O	-5.209694	4.190687	-0.781756
O	-6.367130	2.990144	-3.209257
O	-2.283493	-6.667482	-3.164010
O	-1.597172	-6.460789	-0.394866
O	0.533138	-7.116085	-2.319494
O	6.605933	1.313699	-6.223942
H	-4.065302	2.016481	-4.966016
H	-3.138553	3.395716	-5.016867
H	-6.731572	2.103177	-3.243803
H	-6.905287	3.740688	-3.472666
H	-5.205525	5.526933	-3.918971
H	-3.842215	5.957141	-3.069330
H	-5.916794	3.742517	-0.313395
H	-4.886493	5.039000	-0.465888
H	-2.091749	-7.278637	-0.488220
H	-1.444335	-6.088783	0.477399
H	0.192613	-8.007910	-2.414697
H	1.481011	-6.962002	-2.304849
H	-2.484245	-7.550246	-2.845038
H	-2.731892	-6.323747	-3.939064
H	-0.480601	-5.462306	-4.875250
H	0.279297	-4.111598	-4.273607
H	-5.674643	-2.898965	3.366341
H	-4.840241	-1.464639	3.271220
H	-8.308769	-1.985348	1.226499
H	-7.663985	-0.467747	1.435748
H	-7.114886	-4.428135	0.328747
H	-6.094036	-4.716964	1.608616
H	-6.943298	-2.921714	-1.575408
H	-6.234737	-1.449916	-1.881364
H	2.036651	6.153738	3.484496
H	1.789034	7.380240	2.388470
H	-2.176252	6.790992	1.850278
H	-0.890854	7.837900	1.960084
H	-0.976538	3.941588	3.819008
H	-0.216625	5.292299	4.419652
H	0.748079	5.917771	-0.930985
H	1.395508	7.107627	0.033635
H	5.536496	1.278906	1.426748
H	6.246043	2.750702	1.121807
H	5.394765	4.546949	-2.061245

H	6.418660	4.257127	-0.784333
H	6.967744	0.296737	-1.890334
H	7.612529	1.815338	-1.681083
H	4.144016	1.293631	-3.726805
H	4.978402	2.727955	-3.820927
H	6.208031	-3.910700	3.019067
H	6.034316	-2.273189	2.790205
H	4.192237	-5.208012	0.012337
H	5.221523	-3.911532	-0.139171
H	3.145974	-6.128151	2.614745
H	4.510299	-5.697940	3.463401
H	2.441327	-3.566724	4.561267
H	3.369062	-2.187491	4.511430
Ga	-0.828836	-5.459658	-2.142175
Ga	3.648744	-3.467864	2.087407
Ga	0.132596	5.288648	1.687590
Ga	-4.344970	3.296857	-2.542992
Ga	4.907509	1.981826	-1.170411
Ga	-5.602750	-2.152836	0.715840

Appendix 4. Supporting Information for Chapter 5

The computed ligand energy and the detailed results of Gibbs free energy and hydrolysis energy obtained from QM computation and group additivity method

The ground-state structures and Gibbs free energy are computed by HF/6-31G(d,p) with IEFPCM-UFF continuum solvation model for water. The electronic energy was refined using B3LYP/6-311+G(d) single point, and the solvation energy was recomputed using HF/6-311+G(d) with CPCM-UAKS for water.

Table A4.1. The Gibbs free energies of metal cation (M^{3+}) and m_4-O, m_3-OH, m_2-$OH_{edge,O}$, m_2-$OH_{edge,OH}$, m_2-$OH_{edge,core\text{-}links}$, m_2-OH_{corner}, and h-H_2O in Al and Ga aquo-oxo/hydroxo clusters.

	$[Al_mO_x(OH)_y(H_2O)_z]^{(3m-2x-y)}$ (a.u.)	$Ga_mO_x(OH)_y(H_2O)_z]^{(3m-2x-y)}$ (a.u.)
M^{3+}	-241.278336	-1923.603085
μ_4-O	-76.143619	-76.166418
μ_3-OH	-76.450168	-76.442767
μ_2-$OH_{edge,O}$	-76.359781	-76.340185
μ_2-$OH_{edge,OH}$	-76.313202	-76.305428
μ_2-$OH_{edge,core\text{-}links}$	-76.315207	-76.308287
μ_2-OH_{corner}	-76.313110	-76.308385
η-H_2O	-76.587968	-76.584082

Table A4.2. The species and their quantities contained in each aluminum hydroxyl cluster studied in this manuscript.

	μ_4-O	μ_3-OH	μ_2-OH (edge,O^{2-})	μ_2-OH (edge,OH^-)	μ_2-OH (edge, core-links)	μ_2-OH (corner)	η-H_2O	Ref.
a_1, a_2		2		4			10	[1,2]
b_1, b_2				2		4	12	[3–5]
c_1, c_2				6			12	[6]
d_1, d_2		6		6		2	14	
e_1, e_2	4		11	2		10	14	
f_1, f_2	4		12	6		6	12	[7–9]

g_1, g_2				22		16	10,11
1, 21			2			8	12
2, 22			4			10	13
3, 23			4			10	10
4, 24			2		2	10	3,4,13
5, 25					6	12	14
6, 26			6			12	
7, 27			6			12	
8, 28			8			14	
9, 29				12		12	10,11,15
10, 30		6	6			12	16–19
11, 31		2	4		8	18	20
12		6	6	10		16	21,22
13		12	10			16	22,23
14, 32		6	6		12	24	22,24–27
15, 33	4	12	12			12	9,28,29
16, 34	4	12	2		10	12	9,30
17, 35				30		18	31
18		6	6	18		18	21,22
19		12	10	8		18	21,22
20, 36				38		20	10,11
37		6	6		12	24	32
38		6	6		12	24	32
39	4	12	12			12	33,34
40	4	12	12			12	

Equations for Solving for GA Ligand Energies

$$G_a - 4G_{M^{3+}} = 2G_{\mu_3-OH} + 4G_{\mu_2-OH_{edge,OH}} + 10G_{\eta-H_2O}$$

$$G_b - 4G_{M^{3+}} = 2G_{\mu_2-OH_{edge,OH}} + 4G_{\mu_2-OH_{corner}} + 12G_{\eta-H_2O}$$

$$G_c - 4G_{M^{3+}} = 6G_{\mu_2-OH_{edge,OH}} + 12G_{\eta-H_2O}$$

$$G_d - 8G_{M^{3+}} = 6G_{\mu_3-OH} + 6G_{\mu_2-OH_{edge,OH}} + 2G_{\mu_2-OH_{corner}} + 14G_{\eta-H_2O}$$

$$G_e - 13G_{M^{3+}} = 4G_{\mu_4-O} + 11G_{\mu_2-OH_{edge,O}} + 2G_{\mu_2-OH_{edge,OH}} + 10G_{\mu_2-OH_{corner}} + 14G_{\eta-H_2O}$$

$$G_f - 13G_{M^{3+}} = 4G_{\mu_4-O} + 12G_{\mu_2-OH_{edge,O}} + 6G_{\mu_2-OH_{edge,OH}} + 6G_{\mu_2-OH_{corner}} + 12G_{\eta-H_2O}$$

$$G_g - 10G_{M^{3+}} = 22G_{\mu_2-OH_{edge,core-links}} + 16G_{\eta-H_2O}$$

Detailed information on ligands: These seven basis ligands are η–H_2O (the aqua ligands that fill the peripheral coordination sites); μ_4-O; μ_3-OH; μ_2-OH_{corner} (binds two metallic cations which share one common hydroxo ligand at the corner sites of the metallic octahedral structure), μ_2-$OH_{edge,O}$ (binds two metallic cations which share one common hydroxo ligand and one common oxo ligand at the same edge of the metallic octahedral structure), μ_2-$OH_{edge,OH}$ (binds two metallic cations which share two common hydroxo ligand at the same edge of the metallic octahedral structure), and μ_2-$OH_{edge,\ core-links}$, (μ_2-$OH_{edge,OH}$ ligands in gibbsite-like core-links structures).

GA of Group 13 Clusters: GA method is also robust for heterometallic clusters. The Gibbs free energies of heterometallic flat and Keggin tridecamers are predicted and the results are shown in Figure B. In computing the GA energy for heterometallic clusters,

the ligand energies of homometallic clusters are used for ligands attached to only one type of metal cation. If the ligand bridges two different cations, the ligand energy is computed from the energies of that species of ligand in both of the homometallic clusters by specific weighting ratio.

$$G_{ligand,M_xN_y} = \alpha G_{ligand,M_{(x+y)}} + \beta G_{ligand,N_{(x+y)}} \quad (4)$$

The weighting ratios differ from species of ligands and are closely related to the cluster structures. For bridging μ_2-OH_{corner} ligands in the heterometallic flat tridecamers (x = 7, y = 6), $\alpha = \beta = 0.5$; for bridging μ_4-O ligand in Keggin tridecamers (x = 1, y = 12), $\alpha = 0$ and $\beta = 1$.

The above assumption gave good predictions for the Gibbs free energy of Ga_7Al_6 ($\Delta G_{total,GA\text{-}QM}$ = 1.3 kcal/mol), $GaAl_{12}$ ($\Delta G_{total,GA\text{-}QM}$ = 0.1 kcal/mol) and $AlGa_{12}$ ($\Delta G_{total,GA\text{-}QM}$ = 0.0 kcal/mol). The error of Al_7Ga_6 is somewhat larger ($\Delta G_{total,GA\text{-}QM}$ = 11.0 kcal/mol). The origin of rather larger error in this case is the μ_2-OH_{corner} ligand, which is overestimated by 0.91 kcal/mol. These ligands in Al_7Ga_6 are slightly closer to the $[Al_7(OH)_{12}]^{9+}$ core (1.86 Å in average) than the analogous ligands are to the $[Ga_7(OH)_{12}]^{9+}$ core in Ga_7Al_6 (1.92 Å in average). Hence, the μ_2-OH_{corner} ligands in Al_7Ga_6 experience stronger electrostatic attraction from $[Al_7(OH)_{12}]^{9+}$ core and is consequently slightly lower in energy than the μ_2-OH_{corner} ligands of flat Al_{13} and Ga_{13}. In Keggin tridecamers, the available space that the μ_4-O ligands can occupy is strictly confined by the central tetrahedral cation and the outer octahedral cations. Since the cluster size of Keggin tridecamers only has negligible change with substitution of the cation in the tetrahedral core and both Ga and Al cations are trivalent, it is not surprising that the energy of bridging μ_4-O ligand is determined exclusively by the outer octahedral metallic cations.

The difference between the GA predicted and QM computed Gibbs free energies ($\Delta G_{total,GA\text{-}QM}$) of 40 clusters are shown in Figure B. The mean absolute error (MAE) is

4.0 kcal/mol (standard deviation = 6.3 kcal/mol). The mean absolute percent error (MAPE) for the absolute energies of the cluster is 0.0001% (standard deviation = 0.00017%). Among all the clusters, $[Al_{12}(OH)_{22}(H_2O)_{16}]^{14+}$ (cluster **13** in Figure B), has the largest error, -31.6 kcal/mol or 0.00087% of the total energy. The MAPE for the hydrolysis energies of the clusters is 2.9% (standard deviation = 2.9 %).

The regression plot comparing the GA predicted and QM computed hydrolysis energies is shown in Figure A. The linearity between the QM energy and GA predicted energy (R^2 value =0.99) shows that the GA method robustly and accurately reproduces the QM computed hydrolysis reaction energies of Al, Ga and Al/Ga aqueous oxo/hydroxo clusters.

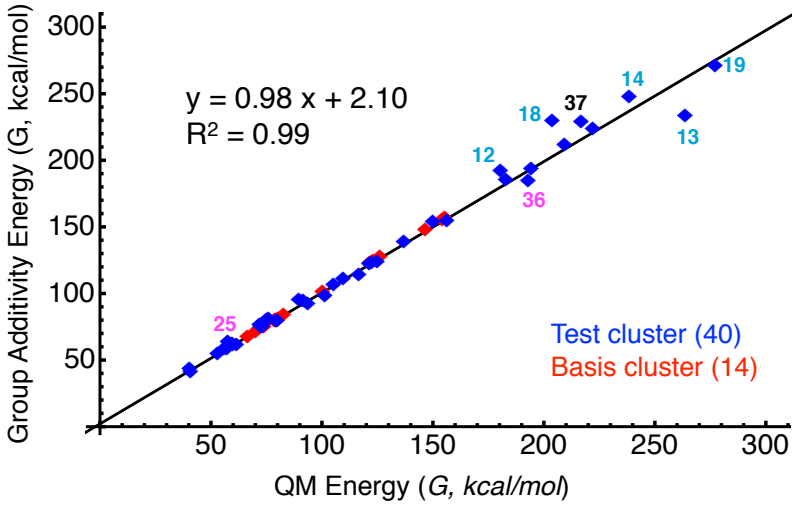

Figure A4.1. GA predicted versus QM computed hydrolysis energies. The slope of the linear regression line is near unity (0.98), the intercept is 2.10 and the R^2 value is 0.99. Clusters whose error are larger than 5 kcal/mol are labeled. Al clusters are in cyan, Ga in magenta, and heterometallic clusters in black

Equilibrium Constants: Table S3 lists the experimental QM computed and predicted equilibrium constants of selected clusters. The GA method reproduces QM computed and experimental data.

Table S3. The QM computed and GA predicted equilibrium constants of $[Al(OH)_4]^-$, $[Ga(OH)_4]^-$, Al_{13}^k and Ga_{13}^k clusters as well as H_2O disproportionation**.**

	Exp.	QM	GA
Al_{13}^k	98.73[35]		
ε-isomer		99.32	99.28
δ-isomer		99.53	99.53
γ-isomer		100.15	99.70
Ga_{13}^k	62.34[36]		
γ-isomer		63.11	65.63
ε-isomer		76.13	79.23
δ-isomer		71.07	71.07
$[Al(OH)_4]^-$	23.0[37]	25.06	—
$[Ga(OH)_4]^-$	16.6[37]	16.72	—
H_2O	14.0[35]	14.49	—

GA of Heterometallic Group 13 Clusters: GA method is also robust for heterometallic clusters. The Gibbs free energies of heterometallic flat and Keggin tridecamers are predicted and the results are shown in Figure B. In computing the GA energy for heterometallic clusters, the ligand energies of homometallic clusters are used for ligands attached to only one type of metal cation. If the ligand bridges two different cations, the ligand energy is computed from the energies of that species of ligand in both of the homometallic clusters by specific weighting ratio.

$$G_{ligand,M_xN_y} = \alpha G_{ligand,M_{(x+y)}} + \beta G_{ligand,N_{(x+y)}} \quad (4)$$

The weighting ratios differ from species of ligands and are closely related to the cluster structures. For bridging μ_2-OH_{corner} ligands in the heterometallic flat tridecamers (x = 7, y = 6), $\alpha = \beta = 0.5$; for bridging μ_4-O ligand in Keggin tridecamers (x = 1, y = 12), $\alpha = 0$ and $\beta = 1$.

The above assumption gave good predictions for the Gibbs free energy of Ga_7Al_6 ($\Delta G_{total,GA\text{-}QM}$ = 1.3 kcal/mol), $GaAl_{12}$ ($\Delta G_{total,GA\text{-}QM}$ = 0.1 kcal/mol) and $AlGa_{12}$ ($\Delta G_{total,GA\text{-}QM}$ = 0.0 kcal/mol). The error of Al_7Ga_6 is somewhat larger ($\Delta G_{total,GA\text{-}QM}$ = 11.0 kcal/mol). The origin of rather larger error in this case is the μ_2-OH_{corner} ligand, which is overestimated by 0.91 kcal/mol. These ligands in Al_7Ga_6 are slightly closer to the $[Al_7(OH)_{12}]^{9+}$ core (1.86 Å in average) than the analogous ligands are to the $[Ga_7(OH)_{12}]^{9+}$ core in Ga_7Al_6 (1.92 Å in average). Hence, the μ_2-OH_{corner} ligands in Al_7Ga_6 experience stronger electrostatic attraction from $[Al_7(OH)_{12}]^{9+}$ core and is consequently slightly lower in energy than the μ_2-OH_{corner} ligands of flat Al_{13} and Ga_{13}.

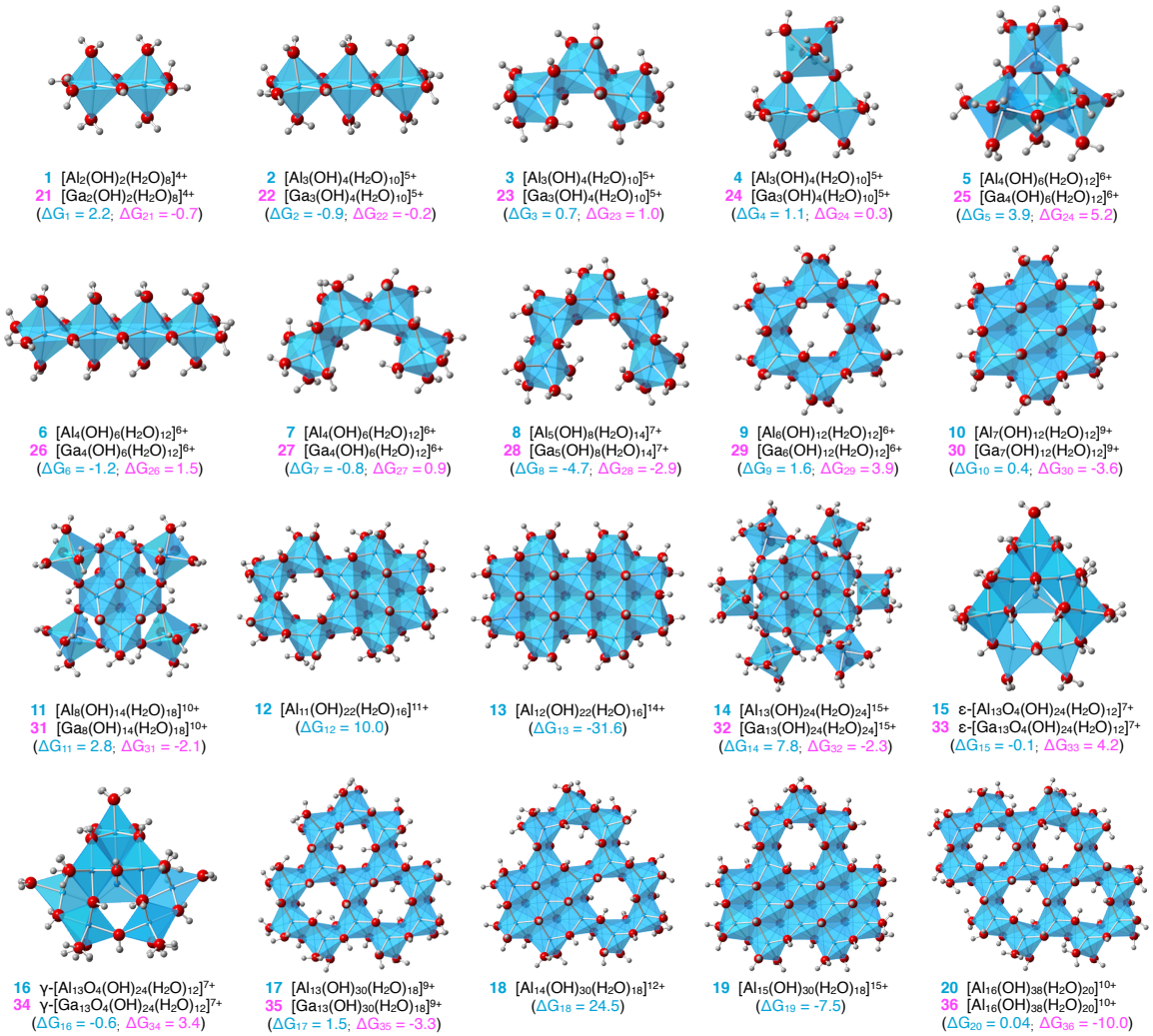

Figure A4.2. The structures of the 36 test clusters with difference between the GA predicted and QM computed Gibbs free energies ($\Delta G_{total,GA\text{-}QM}$). Energies shown here are obtained by QM level of theory I and are in the unit of kcal/mol. The notation for Al clusters are shown in cyan, magenta notation represents Ga clusters, and the black for heterometallic clusters.

Table S4. The chemical potential ($\mu_{cluster}^{ref}$) of all the clusters at the standard state (room temperature 25 °C, atmospheric pressure, and 1 M concentration).

	$\mu_{cluster}^{ref}$ kcal/mol		$\mu_{cluster}^{ref}$ kcal/mol
1	-753.33	20	-4896.56
2	-1076.41	21	-605.55
3	-1076.41	22	-854.79
4	-1076.31	23	-854.79
5	-1399.18	24	-858.49
6	-1399.48	25	-1115.22
7	-1399.48	26	-1104.02
8	-1722.66	27	-1104.02
9	-1953.85	28	-1353.36
10	-2024.27	29	-1517.01
11	-2576.70	30	-1523.28
12	-3222.29	31	-2006.38
13	-3295.30	32	-3040.99
14	-3962.32	33	-2685.67
15 - Al_{13}^{7+}	-3633.79	34 -	-2704.27
16	-3633.29	35	-3079.99
17	-4024.22	36	-3735.02
18	-4094.63	37 -	-7155.00
19	-4167.64		

Appendix 5. Supporting Information for Chapter 6

Optimized geometries of Hf tetramers with no counterions or explicit water

64
Hf4_8_2_bridging_peroxide_conf1.log Energy: -1269008.3318996

Hf	-2.01036	1.71506	0.02707
O	-2.42613	-0.06647	1.05975
O	-1.50459	-0.04089	-1.06869
O	-2.57542	2.17321	-2.08122
O	-2.25076	2.35091	2.17385
O	-2.15068	3.95263	-0.14790
O	-4.19035	2.11757	0.31984
Hf	1.91175	1.80832	-0.06186
O	-0.08503	2.37640	-0.66104
O	-0.02588	1.90607	0.76856
O	2.24122	2.53937	2.05642
O	2.21849	2.50679	-2.14989
O	4.06766	2.31931	0.03640
O	2.08939	4.05669	-0.03138
Hf	-1.89704	-1.81750	-0.02399
O	0.05704	-2.48992	-0.56039
O	0.05773	-1.91145	0.83291
O	-2.23009	-2.48651	2.11443
O	-2.40535	-2.33329	-2.12855
O	-4.08516	-2.10574	-0.01814
O	-2.16415	-4.05391	-0.22518
Hf	2.00911	-1.73684	0.01186
O	2.48856	0.06407	0.99975
O	1.46348	-0.00851	-1.09414
O	2.52993	-2.19770	-2.11872
O	2.32575	-2.32947	2.16346
O	2.24562	-3.97239	-0.11747
O	4.20160	-2.11924	0.25402
H	-3.16084	1.59665	-2.60875
H	-1.51906	2.73980	2.68716
H	-1.32822	4.42446	-0.38328
H	-4.72837	2.69172	-0.25796
H	3.12584	2.67950	2.44335
H	1.50391	2.61970	-2.80529
H	4.80863	1.68800	-0.04131
H	1.85086	4.60828	-0.79948
H	-3.04132	-2.88381	2.48424

H	-2.56266	-1.73920	-2.88521
H	-4.72382	-1.63447	0.54922
H	-2.95850	-4.51145	0.11033
H	3.19553	-1.66669	-2.59789
H	3.18120	-2.59179	2.55266
H	2.75377	-4.51592	0.51364
H	4.72023	-2.72708	-0.30724
H	-1.41636	-4.67255	-0.13095
H	-2.35580	-3.25243	-2.45286
H	2.64278	-3.12225	-2.41370
H	1.48615	-4.51258	-0.40611
H	4.80534	-1.40731	0.54202
H	1.61522	-2.67958	2.73135
H	-1.47924	-2.86809	2.60657
H	-4.54996	-2.34680	-0.84297
H	-1.09254	0.02545	-1.94612
H	-2.58424	-0.08797	2.02111
H	1.34566	-0.05152	-2.05957
H	2.69433	0.07667	1.95150
H	1.59375	2.48814	2.78311
H	1.88514	4.55338	0.78265
H	3.05189	2.37372	-2.64149
H	-3.08915	2.65949	2.56619
H	-2.66090	4.53665	0.44453
H	-4.79186	1.44459	0.69168
H	-2.72612	3.09417	-2.36909
H	4.39653	3.22018	-0.14745

64
Hf4_8_2_bridging_peroxide_conf2.log Energy: -1269009.2360968

Hf	-2.66067	-0.29185	-0.10363
O	-1.80843	1.61412	-0.73967
O	-1.64423	1.35041	0.72804
O	-3.52472	-0.02319	1.97778
O	-3.34516	-0.20670	-2.23269
O	-4.38512	-1.71376	0.08159
O	-4.51587	0.96891	-0.20171
Hf	0.15193	-2.46057	0.07113
O	-1.59953	-1.71838	1.04709
O	-0.94060	-1.03245	-1.07860
O	-0.07027	-3.37092	-1.98407
O	0.51475	-3.22933	2.18673
O	1.60942	-4.18566	-0.08266
O	-0.95139	-4.43616	0.41906

Hf	-0.13767	2.66828	0.06056
O	1.88544	2.02820	0.09558
O	1.09281	1.27852	-0.94570
O	-0.32311	3.60053	-1.91974
O	-0.12538	2.97661	2.25072
O	-1.63738	4.28073	0.36686
O	1.01847	4.53169	0.30514
Hf	2.66404	0.04310	-0.05643
O	1.79242	-1.62578	-1.00724
O	1.04474	-0.73869	1.02691
O	3.38590	0.14926	2.02911
O	3.31721	0.25387	-2.18790
O	4.42711	1.46372	0.02646
O	4.54388	-1.18095	-0.16848
H	-3.12582	0.50626	2.69244
H	-3.57586	-1.01704	-2.72661
H	-4.31772	-2.67828	-0.05674
H	-4.80030	1.48714	0.57402
H	0.31331	-4.24068	-2.20391
H	0.27917	-2.78279	3.02095
H	2.57343	-4.10060	-0.20380
H	-1.12617	-4.69659	1.34305
H	0.29403	4.29352	-2.22519
H	-0.47463	2.33203	2.89562
H	-2.07267	4.42922	1.22758
H	0.63243	5.42184	0.41428
H	3.12412	-0.40485	2.78795
H	4.13971	0.72878	-2.41490
H	5.36868	1.21603	-0.03295
H	4.92523	-1.58361	0.63528
H	1.98781	4.61009	0.22016
H	0.56534	3.50541	2.69438
H	4.06294	0.78923	2.31955
H	4.34738	2.42902	-0.08622
H	4.74958	-1.77532	-0.91503
H	2.65666	0.50090	-2.86420
H	-0.65217	3.12569	-2.70710
H	-2.25540	4.55033	-0.33845
H	-0.62128	-0.70319	-1.93598
H	-1.97067	-2.03610	1.88807
H	0.75269	-0.40000	1.89001
H	2.02107	-1.94527	-1.89834
H	-0.86560	-3.24507	-2.53461
H	-1.71940	-4.71682	-0.11322

H	1.36607	-3.67896	2.34840
H	-3.03213	0.44837	-2.88577
H	-5.28267	-1.43155	-0.18129
H	-4.79502	1.44238	-1.00749
H	-4.22305	-0.58553	2.36154
H	1.39403	-5.11551	0.11943

60
Hf4_4_2_bridging_peroxide_conf1_deprot1.log Energy: -1267998.8343307

Hf	1.32635	-2.12722	-0.01585
O	1.56623	-0.38816	1.12160
O	1.61608	-0.39255	-1.20334
O	1.59418	-2.83602	-2.21458
O	1.55530	-2.78960	2.20340
O	1.03947	-4.43313	-0.11628
O	3.29575	-2.48461	0.10354
Hf	-2.33102	-1.28218	0.01476
O	-0.68912	-2.42267	-0.77214
O	-0.68617	-2.45233	0.73065
O	-2.98605	-1.62877	2.22761
O	-2.98704	-1.67186	-2.19236
O	-4.13906	0.00559	-0.22363
O	-3.64059	-2.77543	0.14355
Hf	2.32858	1.28423	-0.00742
O	0.68076	2.47020	-0.70701
O	0.70042	2.42719	0.79552
O	2.90823	1.54747	2.23913
O	2.96559	1.62864	-2.23018
O	4.15580	0.01275	0.20402
O	3.63307	2.78143	-0.15076
Hf	-1.31787	2.12479	0.01717
O	-1.70074	0.41852	1.19895
O	-1.51089	0.37841	-1.14874
O	-1.58613	2.78453	-2.19018
O	-1.58668	2.87783	2.19018
O	-1.09212	4.43122	-0.18996
O	-3.30084	2.48188	0.10947
H	2.50546	-3.01117	-2.51205
H	0.88228	-3.34042	2.64041
H	0.17679	-4.74113	0.21722
H	3.88085	-3.18056	-0.22975
H	-3.54093	-2.42890	2.12247
H	-2.37462	-2.14645	-2.78243
H	-3.99993	0.99536	-0.06756

H	-4.06705	-3.08817	-0.66940
H	3.81032	1.25777	2.46622
H	2.29169	1.86259	-2.89352
H	4.00509	-0.98455	0.14512
H	4.13467	3.16049	0.58490
H	-2.35697	2.43126	-2.66840
H	-2.44065	3.30110	2.39058
H	-1.63285	5.04755	0.33487
H	-3.79755	3.14888	-0.38881
H	3.52921	2.42108	-2.10667
H	-1.59858	3.75307	-2.30188
H	-0.16825	4.73629	-0.12229
H	-0.88823	3.37592	2.65056
H	2.76243	2.40228	2.68146
H	4.95868	0.24400	-0.29351
H	1.80685	-0.50277	-2.14750
H	1.60673	-0.42224	2.09052
H	-1.02157	0.27216	-1.97907
H	-1.99816	0.57531	2.10958
H	-2.31826	-1.83192	2.90693
H	-3.29173	-0.88396	-2.67675
H	2.42665	-3.17273	2.41006
H	1.71106	-5.05402	0.21749
H	1.09693	-3.65843	-2.38038
H	-4.96848	-0.27416	0.19966

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Hf4_4_2_bridging_peroxide_conf1_deprot2.log Energy: -1267979.0456879

Hf	-1.56997	-2.07693	-0.19906
O	-2.98020	-0.55441	-0.60406
O	-1.25138	-0.38009	1.01812
O	-2.24649	-2.98965	1.39588
O	-1.39797	-2.10982	-2.53250
O	-0.96207	-4.21483	-0.87775
O	-3.40530	-3.12437	-1.20263
Hf	2.33721	-1.39541	0.22034
O	0.58451	-2.52711	0.51902
O	0.48356	-1.72334	-0.75379
O	3.19457	-2.31413	-1.30478
O	2.25787	-1.72101	2.57308
O	4.26121	-0.50672	1.02752
O	3.64698	-3.14490	0.98508
Hf	-2.32655	1.32539	0.23797
O	-0.58113	2.52512	0.07982

O	-0.48448	1.43219	-0.95891
O	-3.33434	1.88178	-1.36647
O	-2.07751	1.60177	2.53047
O	-4.33710	1.08628	1.28272
O	-2.97577	3.44448	0.97574
Hf	1.49973	2.09292	-0.26857
O	2.48869	0.36183	-1.02889
O	1.32946	0.39362	1.06240
O	2.12031	2.82242	1.46553
O	1.38543	2.31780	-2.58662
O	1.14217	4.37268	-0.59583
O	3.45014	3.10204	-0.98194
H	-0.70920	-1.56457	-2.95147
H	-0.17069	-4.45161	-0.35517
H	-3.33856	-4.09538	-1.25897
H	1.39616	-1.79981	3.01721
H	4.65175	0.23295	0.52799
H	3.34432	-3.66275	1.75147
H	-3.65231	2.78293	-1.52530
H	-1.47421	1.00359	3.00396
H	-4.98696	0.48791	0.87301
H	-3.93313	3.61417	1.03614
H	1.64301	3.11522	-3.08173
H	1.76269	4.93522	-1.09111
H	4.00222	3.33216	-0.21113
H	-2.57072	4.22076	0.55055
H	-1.97810	2.49879	2.89509
H	2.06231	3.77568	1.63708
H	0.23629	4.65771	-0.80745
H	4.04061	2.65135	-1.61284
H	0.46588	2.11018	-2.84198
H	-4.30060	0.87530	2.23383
H	-0.29759	-0.16214	1.17237
H	-3.54053	-0.45738	-1.39184
H	1.54448	0.68676	1.96542
H	2.72068	0.29696	-1.96897
H	2.97365	-2.17242	-2.23680
H	3.81631	-3.74758	0.23694
H	2.85956	-1.26913	3.19044
H	-2.19064	-2.06957	-3.09565
H	-0.67556	-4.21222	-1.81088
H	-4.25764	-2.93483	-0.77065
H	-2.61455	-3.88494	1.43342
H	4.97088	-1.15704	1.18721

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Hf4_4_2_bridging_peroxide_conf1_deprot3.log Energy: -1267990.3768209

Hf	0.11073	2.49224	0.05997
O	-1.15021	1.17887	1.13401
O	-1.20995	1.35952	-1.18246
O	0.23938	3.32499	-2.12499
O	0.31093	3.01706	2.31892
O	1.59254	4.27518	0.04842
O	-1.07209	4.08295	0.19102
Hf	2.63231	-0.28595	-0.06487
O	1.93010	1.64035	-0.79452
O	2.01869	1.65447	0.70394
O	3.57415	-0.13438	2.03880
O	3.40329	-0.15149	-2.24244
O	3.63758	-1.98818	-0.09350
O	4.67265	0.75539	-0.15731
Hf	-2.65610	0.27721	-0.05507
O	-1.92129	-1.62374	-0.77008
O	-2.01744	-1.66308	0.72909
O	-3.44430	0.22403	2.11639
O	-3.37462	0.24108	-2.27591
O	-3.98500	1.73624	0.04332
O	-4.58164	-1.01664	-0.27469
Hf	-0.09576	-2.47363	0.06573
O	1.12029	-1.12868	1.16430
O	1.04780	-1.17765	-1.16003
O	-0.21906	-3.26679	-2.12963
O	-0.23672	-3.05901	2.31311
O	-1.47622	-4.32344	0.05407
O	1.26280	-3.91252	0.12134
H	-0.17131	4.20970	-2.10990
H	1.18504	3.05754	2.74530
H	2.46161	4.11517	0.45727
H	3.93235	-0.94715	2.43697
H	2.96387	0.38827	-2.92303
H	4.86722	1.23852	-0.97976
H	-4.20345	0.82459	2.23327
H	-2.78975	-0.19576	-2.92156
H	-5.39337	-0.69682	0.15721
H	0.31736	-4.08037	-2.17407
H	0.25251	-3.87778	2.51184
H	-1.07239	-5.16500	0.33284
H	2.18676	-3.59048	0.06903

H	-4.49538	-1.96474	-0.06702
H	-4.20927	-0.26594	-2.29665
H	-1.12045	-3.51727	-2.40240
H	-2.33396	-4.24682	0.50855
H	-1.08988	-3.10777	2.77948
H	-3.66120	-0.61797	2.55391
H	-4.33365	2.19094	-0.73889
H	-1.29704	1.64142	-2.10659
H	-1.15998	1.15602	2.10393
H	1.03718	-1.33563	-2.11680
H	1.17067	-1.24701	2.12562
H	3.19021	0.40164	2.75487
H	4.90562	1.32837	0.59420
H	3.71687	-0.96829	-2.66938
H	-0.15336	3.84872	2.52487
H	1.24378	5.11101	0.40597
H	-2.03313	3.94745	0.14790
H	1.15757	3.45585	-2.42456
H	4.59062	-2.15777	-0.09620

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Hf4_4_2_bridging_peroxide_conf1_deprot4.log Energy: -1267990.5234761

Hf	2.14248	1.51732	-0.26360
O	1.94593	-0.35548	-1.28101
O	1.37543	-0.09894	1.03815
O	2.69529	1.98368	1.96268
O	2.87161	2.16205	-1.98952
O	3.14058	3.57419	0.02998
O	4.20342	0.65098	0.09973
Hf	-1.72485	2.03848	0.12383
O	0.40369	2.57508	0.42915
O	0.14588	1.98012	-0.93119
O	-2.23587	2.94439	-1.93413
O	-1.69440	2.53602	2.36452
O	-3.60008	2.38269	0.55304
O	-1.52014	4.34004	0.24073
Hf	1.67958	-1.95394	0.09940
O	-0.32564	-2.47133	0.71058
O	-0.27505	-2.24428	-0.77865
O	2.18325	-2.92300	-1.93112
O	1.99302	-2.34153	2.35812
O	3.69557	-1.93447	0.21390
O	1.70833	-4.21936	0.54892
Hf	-2.15283	-1.52155	0.00078

O	-2.24240	0.31068	-1.04623
O	-1.34417	0.17858	1.14511
O	-2.99188	-1.99762	1.73179
O	-2.42718	-2.02682	-2.29257
O	-2.73906	-3.74495	-0.14800
O	-4.38545	-1.51088	-0.67023
H	2.40744	1.20436	2.47396
H	2.77726	1.73415	-2.85259
H	2.70939	4.24174	0.59255
H	4.16589	-0.36207	0.15188
H	-3.10463	2.85601	-2.36400
H	-0.96472	3.06541	2.73392
H	-4.43037	2.22338	0.08292
H	-0.57969	4.59436	0.17976
H	3.08297	-3.26308	-2.08308
H	1.64084	-1.66544	2.96265
H	2.30912	-4.84229	0.10313
H	-3.57780	-1.40963	2.23313
H	-3.29328	-2.40958	-2.52001
H	-2.12296	-4.39347	-0.53343
H	-4.97242	-1.98883	-0.05666
H	0.82549	-4.63282	0.56734
H	1.73678	-3.21401	2.70564
H	-2.92011	-4.02686	0.76944
H	-4.78709	-0.63412	-0.80901
H	-1.74614	-2.56167	-2.73651
H	1.55941	-3.50365	-2.40172
H	4.13557	-2.34875	0.97431
H	0.42434	0.04093	1.27097
H	2.32877	-0.55069	-2.15102
H	-1.53177	0.16583	2.10012
H	-2.34956	0.28769	-2.01086
H	-1.55675	2.92364	-2.63234
H	-1.98804	4.80559	-0.47627
H	-2.52582	2.99785	2.58360
H	3.25534	3.95195	-0.86301
H	4.79644	0.86940	-0.64185
H	3.65562	2.06377	2.10762

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Hf4_4_2_bridging_peroxide_conf2_deprot1.log Energy: -1267987.9552807

Hf	2.37799	-1.27562	0.01491
O	2.31951	0.76958	0.70785
O	2.12893	0.68838	-0.78699

O	3.16645	-1.82662	-2.11291
O	2.93400	-1.79543	2.17778
O	2.30683	-3.50907	0.06902
O	4.36897	-1.18652	-0.04654
Hf	-1.06123	-2.14407	-0.00742
O	0.67439	-1.77327	-1.20889
O	0.53884	-1.43995	1.18969
O	-1.66775	-3.00227	2.10597
O	-1.68412	-3.14610	-2.04286
O	-3.28437	-2.69861	-0.01783
O	-0.25509	-4.03269	-0.04451
Hf	1.26477	2.52358	-0.00303
O	-0.69531	2.14475	-0.75227
O	-0.63363	1.93544	0.74926
O	1.64590	2.89817	2.18881
O	1.64619	2.94912	-2.19587
O	3.48139	3.10212	-0.05744
O	0.99565	4.44932	-0.00069
Hf	-2.45990	1.14190	-0.01001
O	-2.03391	-0.59674	1.15326
O	-1.66624	-0.45776	-1.22191
O	-3.37785	1.27723	-2.09493
O	-3.32657	1.50337	2.11333
O	-3.43057	2.87317	0.07410
O	-4.47494	-0.04818	0.02398
H	3.09445	-2.77307	-2.33578
H	2.20343	-1.81240	2.82082
H	1.34684	-3.85562	0.02301
H	-2.42988	-3.60820	2.13730
H	-1.80982	-2.69888	-2.89802
H	-3.86822	-1.90716	0.03035
H	1.16056	3.63676	2.59822
H	1.62221	2.23237	-2.85505
H	3.78218	3.45004	-0.91671
H	-3.08914	0.67441	-2.80229
H	-3.63617	2.42923	2.02518
H	-5.07930	0.18329	-0.70772
H	1.55749	5.19587	0.25210
H	1.16921	3.71199	-2.56959
H	-3.75229	2.07624	-2.50400
H	-3.43855	3.58441	-0.58270
H	-4.97707	0.07723	0.85313
H	-2.78351	1.45195	2.92025
H	1.66100	2.16716	2.83227

H	4.06494	2.35147	0.15992
H	0.27973	-0.71385	1.78137
H	0.75543	-2.07107	-2.12698
H	-0.99996	-0.22100	-1.88868
H	-2.34246	-0.83406	2.04145
H	-0.97982	-3.36733	2.68945
H	-0.53017	-4.71666	0.58493
H	-1.18632	-3.97088	-2.18947
H	3.72842	-1.46992	2.63459
H	2.74968	-3.93685	0.82301
H	4.95028	-0.73880	0.58548
H	4.11873	-1.66813	-1.93425
H	-3.51309	-3.17537	-0.83812

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Hf4_4_2_bridging_peroxide_conf2_deprot2.log Energy: -1267982.9134805

Hf	-2.72278	0.13521	-0.24725
O	-1.80307	2.05715	-0.42634
O	-1.46972	1.48701	0.92502
O	-4.04929	0.32647	1.21968
O	-2.68934	0.64009	-2.57414
O	-3.36599	-1.71926	-1.38867
O	-4.75460	0.74606	-1.09730
Hf	-0.24538	-2.36231	0.31507
O	-1.97964	-1.44643	1.07126
O	-0.89967	-0.71268	-0.87185
O	-1.13550	-3.37345	-1.21220
O	-0.13248	-2.70444	2.67399
O	1.28877	-3.98437	0.76808
O	-1.30557	-4.31333	1.06594
Hf	0.19124	2.62428	0.23060
O	2.11692	1.71882	-0.03858
O	1.08294	1.09317	-0.93879
O	0.22775	3.88463	-1.26905
O	0.42911	2.52338	2.54439
O	-1.01063	4.35040	1.19081
O	1.70379	4.17983	1.01853
Hf	2.67711	-0.35043	-0.27330
O	1.48124	-1.97408	-1.01660
O	1.16571	-0.90624	1.08265
O	3.87997	-0.48811	1.29615
O	2.86976	-0.06249	-2.55501
O	4.59877	0.95998	-0.72549
O	4.32367	-1.75227	-1.06517

H	-2.73698	-0.14274	-3.15121
H	-2.66261	-2.43333	-1.35305
H	-5.31595	1.11993	-0.39337
H	-0.45380	-2.04973	3.31770
H	2.03506	-4.01251	0.14313
H	-1.72302	-4.39135	1.94088
H	0.05921	1.79048	3.06618
H	-1.48637	4.14360	2.01527
H	1.25372	5.03275	1.16749
H	3.68251	-0.98137	2.10581
H	3.76718	0.12782	-2.88446
H	5.14602	0.83392	0.07434
H	4.88168	-2.04964	-0.32319
H	2.43088	4.35818	0.39464
H	1.28773	2.76367	2.93522
H	4.36408	1.90634	-0.73894
H	4.10500	-2.54191	-1.59085
H	2.28399	0.64605	-2.88228
H	-0.39656	3.83911	-2.00944
H	-1.64507	4.78986	0.59706
H	-0.37105	-0.40563	-1.61946
H	-2.60123	-1.84938	1.69660
H	1.23374	-0.69504	2.02469
H	1.49385	-2.20451	-1.95958
H	-0.85124	-3.26144	-2.13295
H	-1.90902	-4.66216	0.38506
H	0.68793	-3.08671	3.03270
H	-2.03607	1.24747	-2.96157
H	-4.23131	-2.13263	-1.22234
H	-4.79768	1.31009	-1.88915
H	-3.80382	0.26845	2.15519
H	0.91257	-4.88210	0.83203

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Hf4_4_2_term_perox_conf1_diconf10.log Energy: -1267986.5976012

Hf	-1.18342	-2.22931	-0.10572
O	-1.87549	-0.47732	-1.19978
O	-1.65943	-0.48572	1.19806
O	-1.72955	-3.16532	1.94683
O	-1.89780	-3.24971	-1.71244
O	-1.44023	-4.13841	-0.58735
O	-3.66212	-2.30378	-0.08743
Hf	2.19256	-1.24182	0.01558
O	0.67812	-2.33845	1.02663

O	0.64874	-1.89872	-1.26445
O	3.64065	-1.66426	-1.72020
O	3.30688	-1.81320	1.95885
O	4.11664	0.03225	0.20383
O	2.85715	-3.45225	-0.00057
Hf	-2.12460	1.21839	0.04903
O	-0.62003	2.18721	1.18304
O	-0.60507	2.02574	-1.19668
O	-3.24779	1.90227	-1.89854
O	-3.07241	1.51757	2.17784
O	-4.22201	0.34340	-0.08917
O	-3.12580	3.25140	0.27196
Hf	1.24686	2.19159	0.02038
O	1.85742	0.48195	-1.16655
O	1.48040	0.32559	1.16634
O	2.32170	2.96478	1.53232
O	1.99406	2.97638	-2.06254
O	0.75986	4.44416	-0.11622
O	3.20893	2.56120	0.38359
H	-2.29899	-2.71215	2.59272
H	-4.14769	-2.87771	0.53202
H	4.35271	-0.99999	-1.78299
H	3.46181	-2.76488	2.09918
H	3.86567	1.00152	0.37012
H	2.11241	-4.07736	0.06700
H	-2.83440	2.18700	-2.73210
H	-3.26990	0.72930	2.71358
H	-4.18177	-0.65271	-0.13464
H	-3.45097	3.62536	-0.56820
H	2.84480	3.42520	-1.89686
H	0.96659	4.87680	0.73216
H	-2.69714	3.96547	0.77746
H	-3.75751	2.18278	2.36771
H	-0.11105	4.76693	-0.40569
H	1.44517	3.61795	-2.54828
H	-4.08035	1.44170	-2.10802
H	-4.91820	0.58053	0.54792
H	-0.69889	2.28349	2.14596
H	-0.48364	1.59309	-2.05810
H	-1.12252	-0.36405	1.99668
H	-2.16468	-0.53089	-2.12440
H	0.51285	-1.42297	-2.10035
H	0.65062	-2.50276	1.98253
H	1.40956	0.37998	2.13150

H	2.18418	0.64539	-2.06530
H	3.38483	-1.92560	-2.62335
H	3.44934	-3.75756	-0.71104
H	3.26569	-1.38262	2.83054
H	-3.54868	-2.81177	-0.93397
H	-2.02187	-4.09335	1.90039
H	4.71882	-0.23711	0.92008

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Hf4_4_2_term_perox_conf1_diconf1.log Energy: -1267983.6543182

Hf	2.49832	-0.21622	0.01172
O	1.45442	1.21274	1.19873
O	1.11316	0.78036	-1.14229
O	3.41706	-0.38399	-2.09869
O	3.91917	-0.01502	1.80102
O	4.05452	-1.88607	-0.00561
O	3.65008	1.69660	-0.25328
Hf	-0.19992	-2.44042	0.08094
O	1.57804	-1.93295	-0.95541
O	1.28267	-1.44352	1.29302
O	-0.44285	-3.48879	2.14877
O	-0.36564	-3.57999	-2.01570
O	-2.23924	-3.33346	-0.22830
O	0.72192	-4.47961	0.13274
Hf	0.17581	2.48302	-0.05056
O	-1.49169	1.78477	-1.27478
O	-1.54509	1.84722	1.14240
O	0.56043	3.60465	1.98200
O	0.93125	3.59126	-1.56807
O	1.88452	3.55690	-0.41092
O	-1.03849	4.47111	-0.02903
Hf	-2.49674	0.28869	-0.05483
O	-1.38082	-1.08252	1.19939
O	-1.05164	-1.00811	-1.15828
O	-3.58952	-0.40816	-1.64410
O	-3.65556	0.17867	1.96223
O	-4.33675	1.68361	-0.23483
O	-3.79922	-1.24792	-0.41860
H	3.23200	0.29498	-2.77163
H	3.77159	-0.39332	2.68718
H	3.73268	-2.77766	-0.23128
H	4.39354	1.75595	-0.87820
H	-1.28146	-3.64880	2.61663
H	-0.08784	-3.27454	-2.89731

H	-2.94078	-2.57855	-0.35180
H	0.78721	-4.95043	-0.71943
H	-0.20175	4.10492	2.32566
H	-0.77426	4.91105	-0.85980
H	-4.38293	-0.46346	1.85610
H	-4.73115	1.26746	-1.03150
H	-2.00982	4.43891	-0.01212
H	-4.20810	2.62421	-0.44697
H	-4.08117	1.01323	2.23184
H	1.23507	4.27710	1.76590
H	-1.46420	1.75756	-2.24410
H	-1.40576	1.66887	2.08667
H	0.45952	0.23702	-1.62453
H	1.76495	1.58085	2.04176
H	0.89783	-0.90432	2.00650
H	1.74219	-2.02844	-1.90746
H	-1.45438	-1.20931	-2.02154
H	-1.58294	-1.13852	2.14648
H	0.24028	-3.35094	2.83035
H	0.48123	-5.11439	0.83204
H	-1.27337	-3.92759	-2.10712
H	4.33404	0.86048	1.91215
H	4.70776	-1.96240	0.71286
H	3.01125	2.49865	-0.42939
H	4.31375	-0.73339	-2.25106
H	-2.64945	-4.06185	0.26981

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Hf4_4_2_term_perox_conf1_diconf2.log Energy: -1267981.9086057

Hf	1.31921	2.05935	-0.04228
O	-0.50402	2.43427	0.92138
O	-0.27410	1.71271	-1.29644
O	2.12356	3.04665	-1.96994
O	1.97675	2.68771	2.13127
O	3.59838	2.22410	0.12983
O	1.31672	4.33026	0.16450
Hf	2.05253	-1.40495	0.00604
O	2.16811	0.39672	-1.14452
O	1.23919	0.25138	1.04829
O	2.88201	-1.53124	2.19539
O	3.19767	-2.06521	-1.89658
O	2.88313	-3.50637	0.21615
O	4.27392	-0.69086	0.19024
Hf	-2.19734	1.35078	-0.07288

O	-1.95114	-0.38727	-1.28892
O	-1.37560	-0.26733	1.16538
O	-2.98679	2.52007	1.78173
O	-4.11634	1.45072	-0.62844
O	-2.40711	3.44030	-1.00032
O	-4.00456	0.52835	0.53182
Hf	-1.42005	-2.15941	-0.11293
O	0.52595	-2.46030	0.98625
O	0.45219	-1.78717	-1.22520
O	-2.06509	-3.15407	-1.72220
O	-1.91413	-2.96432	2.05063
O	-3.64916	-1.98151	0.34760
O	-1.71551	-4.06692	-0.57052
H	1.63305	3.09624	-2.80940
H	1.86972	2.08208	2.88539
H	4.04545	1.35447	0.03253
H	1.62373	4.82704	-0.61694
H	3.11385	-2.35336	2.66348
H	3.12876	-1.63707	-2.76842
H	2.28417	-4.15650	0.62801
H	4.88210	-0.94621	-0.53030
H	-3.90037	2.17750	1.85311
H	-1.70430	3.68693	-1.62815
H	-1.71026	-3.91054	2.16434
H	-4.13335	-2.47366	-0.33925
H	-3.94003	-0.99445	0.30004
H	-2.88999	-2.90427	2.07743
H	-3.03640	3.49156	1.72865
H	-3.26229	3.60853	-1.43511
H	-2.54104	-0.51792	-2.04840
H	-1.67658	-0.35237	2.08584
H	-0.18304	1.13281	-2.06951
H	-0.56625	2.60712	1.87373
H	0.30036	0.07008	1.35445
H	2.58277	0.54396	-2.00888
H	0.37184	-1.45575	-2.13309
H	0.49661	-2.53393	1.95359
H	2.51564	-0.91211	2.85157
H	4.70930	-0.90338	1.03844
H	3.16265	-3.02574	-2.06207
H	1.88847	3.59825	2.46468
H	3.89593	2.60090	0.97951
H	0.46295	4.71531	0.43783
H	3.07410	3.14342	-2.16046

H	3.79707	-3.83962	0.28587

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Hf4_4_2_term_perox_conf1_diconf3.log Energy: -1267973.0528909

Hf	-1.85941	-1.64079	0.02532
O	-0.19304	-2.58464	0.89510
O	-0.18454	-1.29465	-1.11991
O	-2.60607	-2.28309	-2.05790
O	-2.67326	-1.82794	2.15664
O	-4.18257	-1.89215	0.03155
O	-2.47237	-3.82711	0.29090
Hf	-1.60418	1.89695	0.00162
O	-2.53517	0.19966	-0.88921
O	-1.21758	0.11643	1.08602
O	-2.29434	2.32914	2.13582
O	-2.22676	2.64374	-2.09974
O	-1.62229	4.17330	-0.05161
O	-3.78403	2.65574	0.01145
Hf	1.69752	-1.93027	-0.06030
O	2.46513	-0.19094	-1.06970
O	1.43132	-0.10918	1.16452
O	2.42198	-2.39611	2.21586
O	1.73073	-2.67980	-2.29121
O	2.42410	-3.83075	0.10146
O	3.46934	-2.81767	-0.28336
Hf	2.00086	1.68705	-0.05273
O	0.20464	2.51924	0.91122
O	0.06535	1.39667	-1.18855
O	2.54606	2.60046	-1.73934
O	2.70448	2.38720	2.07949
O	4.27499	1.24788	0.31028
O	2.81614	3.44654	-0.51623
H	-2.08041	-1.91051	-2.78997
H	-2.25143	-1.26585	2.83019
H	-4.71011	-1.75466	-0.77510
H	-3.39681	-4.11888	0.19060
H	-2.44554	3.20053	2.54484
H	-2.20192	2.10825	-2.91304
H	-0.84607	4.66279	0.27474
H	-4.27860	2.66998	-0.82793
H	2.67810	-3.29765	1.90683
H	0.84519	-2.86900	-2.64718
H	3.65577	2.19584	2.17582
H	4.75499	1.93550	-0.18928

H	2.21412	-3.52543	-2.25178
H	4.47940	0.39531	-0.11802
H	2.29497	2.14260	2.92740
H	1.77316	-2.52889	2.92835
H	2.75182	-0.22801	-1.99576
H	1.77827	-0.20550	2.06540
H	-0.09624	-0.38186	-1.48009
H	-0.25617	-3.23368	1.61269
H	-0.25918	0.04325	1.36484
H	-3.27231	0.23701	-1.51882
H	0.17437	1.75993	-2.08397
H	0.21929	2.86327	1.81818
H	-2.03238	1.70711	2.83703
H	-4.38522	2.33383	0.70796
H	-1.97472	3.55417	-2.34175
H	-2.85613	-2.69502	2.56287
H	-4.66932	-1.48972	0.77372
H	-1.88450	-4.58904	0.14097
H	-2.70882	-3.23217	-2.25725
H	-2.41622	4.72827	0.05707

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Hf4_4_2_term_perox_conf1_diconf5.log Energy: -1267985.5206443

Hf	-2.43784	0.56550	-0.09752
O	-0.85227	1.32895	-1.21920
O	-1.00375	1.40820	1.19343
O	-3.64720	1.07630	1.74428
O	-3.61899	0.83626	-2.03688
O	-4.39423	-0.66455	-0.00641
O	-2.91936	2.75803	-0.42127
Hf	-0.55627	-2.35148	0.08252
O	-2.03478	-1.18263	1.10608
O	-1.78328	-1.15811	-1.23130
O	-0.66829	-3.66193	-1.86606
O	-0.72294	-3.38917	2.22294
O	1.08994	-3.84283	0.39677
O	-2.18849	-3.91108	0.16146
Hf	0.61006	2.39302	0.07660
O	2.09572	1.19836	1.18952
O	1.95531	1.31457	-1.21145
O	0.26641	3.73966	-1.41274
O	0.60334	3.28919	2.24233
O	-0.64476	3.98318	-0.24704
O	2.25040	4.02825	0.29458

Hf	2.48342	-0.50647	-0.06404
O	0.88650	-1.47937	-1.17854
O	0.81966	-1.28767	1.17887
O	3.58422	-1.47515	1.32635
O	3.35271	-1.00836	-2.17073
O	4.58628	0.46219	-0.25163
O	3.23902	-2.40779	0.20121
H	-3.45027	1.77517	2.39216
H	-3.53176	0.28554	-2.83579
H	-4.25215	-1.58906	0.26768
H	-3.58672	3.20707	0.12586
H	0.11608	-4.02050	-2.31839
H	-0.92308	-3.00249	3.09367
H	2.00808	-3.34232	0.40837
H	-2.32744	-4.29768	1.04726
H	-0.28107	3.58730	2.52096
H	2.07383	4.55441	-0.51224
H	3.81672	-1.86125	-2.06431
H	5.09835	0.09466	0.49420
H	3.19417	3.79347	0.29241
H	1.16847	4.08484	2.24501
H	4.64266	1.43112	-0.18795
H	4.02978	-0.37859	-2.47941
H	2.07829	1.17534	2.15901
H	1.70758	1.23736	-2.14643
H	-0.79838	1.01837	2.05783
H	-0.95027	1.80797	-2.05972
H	-1.26954	-0.84480	-1.99614
H	-2.15717	-1.14359	2.06807
H	0.95120	-1.34073	2.13749
H	1.01968	-1.63559	-2.12590
H	-1.29430	-3.39678	-2.56514
H	-2.15743	-4.63888	-0.48692
H	0.05917	-3.96317	2.33368
H	-3.74602	1.76338	-2.31208
H	-4.97175	-0.66914	-0.79090
H	-2.05867	3.33796	-0.42078
H	-4.57512	0.79624	1.84147
H	1.20341	-4.70252	-0.04402

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Hf4_4_2_term_perox_conf1_diconf6.log Energy: -1267990.3353362

Hf	-1.02193	-2.26867	0.04631
O	0.76598	-1.79332	1.21871

O	0.53868	-1.30250	-1.14357
O	-1.12366	-3.72797	-1.31968
O	-1.54507	-3.42802	1.97373
O	-3.41527	-2.73341	0.16711
O	-0.10374	-4.05945	-0.26555
Hf	-2.28552	0.99948	-0.08763
O	-2.08271	-0.83201	-1.19410
O	-1.90586	-0.62170	1.20815
O	-3.48309	1.88001	1.63418
O	-3.29884	1.42212	-2.08947
O	-2.39657	3.25940	-0.54556
O	-4.33143	-0.04921	0.17928
Hf	2.29186	-0.99425	-0.06654
O	2.18502	0.87094	-1.10906
O	2.00035	0.62469	1.24516
O	3.57709	-1.84538	1.63392
O	3.00096	-1.40653	-2.26631
O	2.39872	-3.26807	-0.27164
O	4.46932	-0.33970	-0.23740
Hf	1.04873	2.29492	0.06977
O	-0.75694	1.78945	1.16516
O	-0.54586	1.41846	-1.19718
O	1.13219	3.65329	-1.39677
O	1.24911	3.27488	2.16899
O	3.22200	3.06920	0.41076
O	0.14187	4.07288	-0.34245
H	-1.65283	-3.08093	2.87701
H	-3.69491	-3.23545	-0.62163
H	-3.17122	2.43734	2.36809
H	-3.86990	0.86685	-2.64791
H	-1.45834	3.65782	-0.55965
H	-4.17523	-1.02689	0.18824
H	3.77550	-1.41244	2.48349
H	2.33403	-1.84845	-2.82264
H	1.46507	-3.66326	-0.40405
H	5.18549	-0.84111	0.19207
H	0.72462	4.09586	2.21624
H	3.49145	3.65607	-0.31994
H	4.84044	0.14633	-0.99429
H	3.87294	-1.74890	-2.53208
H	3.88112	2.35295	0.45521
H	2.17393	3.54234	2.32897
H	3.54838	-2.80882	1.77720
H	2.99255	-3.69728	-0.91143

H	2.26934	0.89073	-2.07592
H	1.61058	0.41550	2.10985
H	0.20707	-0.49092	-1.57559
H	0.98134	-2.25681	2.04317
H	-1.48799	-0.41136	2.05765
H	-2.02438	-0.83948	-2.16222
H	-0.57536	1.73741	-2.11490
H	-0.74409	1.81099	2.13410
H	-4.23860	1.34678	1.94250
H	-5.08070	0.12152	-0.41780
H	-3.48639	2.36081	-2.27548
H	-1.07475	-4.27965	2.03461
H	-3.59796	-3.31243	0.93176
H	-2.94568	3.82390	0.02626

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Hf4_4_2_term_perox_conf1_diconf7.log Energy: -1267987.2109038

Hf	1.42032	-2.11873	0.05301
O	1.86960	-0.27386	1.19473
O	1.74497	-0.32735	-1.17732
O	2.22853	-3.03069	-1.57658
O	2.05045	-2.98393	2.09162
O	2.07221	-3.94467	-0.40265
O	3.89531	-1.86559	0.01373
Hf	-2.05951	-1.46301	-0.02231
O	-0.41097	-2.36381	-1.03746
O	-0.49233	-1.95461	1.28852
O	-3.48839	-2.04053	1.68408
O	-3.02421	-2.09407	-2.02775
O	-4.08287	-0.38910	-0.28419
O	-2.46760	-3.73042	-0.03839
Hf	1.97370	1.42860	-0.05868
O	0.37399	2.21585	-1.20094
O	0.38581	2.08459	1.18947
O	3.02489	2.22320	1.89598
O	2.89962	1.88403	-2.18137
O	4.15976	0.80615	0.07918
O	2.72061	3.57848	-0.25794
Hf	-1.47387	2.05354	-0.01721
O	-1.93386	0.28703	1.18529
O	-1.44758	0.17212	-1.13283
O	-2.63253	2.73724	-1.50883
O	-2.33016	2.76202	2.05584
O	-1.20626	4.34115	0.13666

O	-3.46708	2.19448	-0.38075
H	2.38313	-3.89570	1.99676
H	3.84539	-2.36116	-0.84340
H	-4.30191	-1.50226	1.70699
H	-3.10175	-3.04522	-2.22225
H	-3.93935	0.60933	-0.42761
H	-1.66139	-4.26581	-0.15343
H	2.57940	2.47338	2.72426
H	3.33339	1.21069	-2.73418
H	4.22321	-0.19036	0.02955
H	3.04367	3.94886	0.58508
H	-3.17954	3.20514	1.87080
H	-1.38408	4.78148	-0.71342
H	2.17428	4.25564	-0.69615
H	3.40906	2.70732	-2.28938
H	-0.41719	4.75668	0.52523
H	-1.82232	3.37533	2.61658
H	3.89048	1.83326	2.11509
H	4.83377	1.17238	-0.51947
H	0.44877	2.31838	-2.16337
H	0.30829	1.62090	2.03970
H	1.66617	-0.38982	-2.14164
H	2.18564	-0.27999	2.11186
H	-0.44244	-1.33296	2.03426
H	-0.34473	-2.59648	-1.97743
H	-0.90624	0.10494	-1.93273
H	-2.43323	0.43807	2.00355
H	-3.22155	-2.22962	2.60176
H	-2.98603	-4.11379	0.69182
H	-2.91212	-1.61982	-2.87044
H	1.41118	-2.99997	2.82655
H	4.42456	-2.40274	0.63044
H	-4.60825	-0.71692	-1.03586

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Hf4_4_2_term_perox_conf1_diconf8.log Energy: -1267976.3224599

Hf	-0.35742	2.54513	0.05002
O	-2.06738	1.52024	0.93554
O	-1.04980	0.77810	-1.10821
O	-0.53838	3.21444	-2.21362
O	0.00796	3.28311	2.34334
O	0.06406	4.51535	-0.02258
O	-1.39799	4.24190	0.23035
Hf	2.49611	0.32754	-0.02963

O	1.50848	1.96750	-0.99575
O	0.98969	1.18436	1.19571
O	3.80608	0.25595	1.80339
O	3.48059	0.55146	-2.08621
O	3.76359	-1.52404	-0.68572
O	3.79677	2.23159	0.25403
Hf	-2.46937	-0.32974	-0.06939
O	-1.51180	-2.05559	-0.92087
O	-0.86550	-0.96990	1.12201
O	-3.47560	-0.58446	1.99289
O	-3.24169	-0.10461	-2.21418
O	-4.60644	0.60681	-0.08997
O	-4.11834	-1.93129	-0.28642
Hf	0.35775	-2.50608	0.08050
O	1.85577	-1.34990	1.16159
O	1.13420	-0.81836	-1.14094
O	0.98420	-3.45240	-1.62545
O	0.21593	-3.25921	2.25735
O	-0.48103	-4.69958	0.10656
O	2.00915	-3.50298	-0.53290
H	-1.37593	3.00218	-2.66103
H	0.13132	4.21993	2.08664
H	3.95167	-0.51972	2.37259
H	3.79855	1.36645	-2.51234
H	3.16818	-2.35282	-0.66560
H	3.34570	2.97111	-0.19631
H	-4.01256	-1.39318	2.08871
H	-2.59446	0.21849	-2.86556
H	-4.96548	1.00997	0.72067
H	-5.07064	-1.73638	-0.33745
H	0.10912	-4.22132	2.37251
H	-0.14128	-4.92762	-0.78727
H	-3.97277	-2.87753	-0.45819
H	-3.84940	-0.71941	-2.66307
H	-1.44742	-4.82155	0.08373
H	-0.50170	-2.83226	2.76078
H	-2.84245	-0.58723	2.73421
H	-4.80569	1.21098	-0.82837
H	-1.72628	-2.41401	-1.79740
H	-0.34993	-0.23178	1.50618
H	-0.30656	0.23767	-1.45797
H	-2.67872	1.94966	1.55392
H	1.14262	1.46495	2.11500
H	1.46746	2.07314	-1.96087

H	1.34033	-1.13866	-2.03832
H	1.70127	-1.25017	2.11367
H	4.28841	1.01718	2.17144
H	4.74627	2.28854	0.03934
H	4.11565	-0.16587	-2.27395
H	-0.76214	3.27086	2.93817
H	-0.51636	4.18345	-2.08808
H	4.56411	-1.73673	-0.17404

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Hf4_4_2_term_perox_conf1_diconf9.log Energy: -1267986.0248796

Hf	1.63260	-1.96189	-0.09033
O	-0.29002	-2.24744	-1.06653
O	-0.19524	-1.43745	1.15567
O	2.01189	-2.98841	1.91864
O	2.31907	-2.84332	-1.78848
O	4.07790	-1.68551	-0.28044
O	2.22067	-3.78332	-0.62696
Hf	1.92073	1.56347	0.07571
O	2.24867	-0.23758	1.15651
O	1.86562	-0.11300	-1.18538
O	2.71784	2.53434	-1.85173
O	2.89437	2.25154	2.00138
O	1.42751	3.76081	0.61811
O	4.17751	1.09524	-0.29500
Hf	-1.95578	-1.56763	0.06425
O	-2.44176	0.26153	1.04645
O	-1.86771	0.07761	-1.22388
O	-3.00293	-2.34261	-1.90019
O	-2.48556	-2.16001	2.26202
O	-2.10247	-3.85233	0.07944
O	-4.20627	-1.85651	0.32060
Hf	-1.62284	1.96199	-0.05862
O	0.24005	2.04503	-1.14950
O	0.11874	1.43783	1.17911
O	-2.01767	3.15466	1.51285
O	-2.10153	2.86110	-2.14893
O	-3.91334	2.33027	-0.33535
O	-1.23636	3.88897	0.45719
H	1.27439	-2.98694	2.55477
H	4.65863	-2.17346	0.33069
H	2.39625	3.36360	-2.24632
H	3.43636	1.79573	2.66795
H	0.41763	3.90105	0.62455

H	4.27737	0.10690	-0.31193
H	-3.04279	-1.83720	-2.73060
H	-1.75454	-2.41653	2.85017
H	-1.26878	-4.31127	-0.13368
H	-4.65722	-2.04017	-0.52520
H	-1.65064	3.70772	-2.32167
H	-4.16754	2.88181	0.42999
H	-4.73796	-1.19731	0.80183
H	-3.30436	-2.56514	2.59703
H	-4.50206	1.55485	-0.32250
H	-3.05721	3.04482	-2.22214
H	-2.95944	-3.28834	-2.12903
H	-2.53501	-4.35189	0.79451
H	-2.58700	0.26336	2.00654
H	-1.41015	-0.01771	-2.07480
H	-0.08798	-0.58091	1.61347
H	-0.26953	-2.62020	-1.96282
H	1.75814	-0.06746	-2.14813
H	2.20140	-0.27532	2.12368
H	0.03776	1.74345	2.09904
H	0.26534	1.94667	-2.11321
H	3.68691	2.49778	-1.95414
H	4.83187	1.43775	0.33922
H	2.71218	3.16356	2.29261
H	4.03043	-2.20236	-1.12055
H	2.33491	-3.90535	1.85478
H	1.82241	4.50973	0.13867

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Hf4_4_2_term_perox_conf2_diconf10.log Energy: -1267996.1646043

Hf	0.94096	2.26984	0.02260
O	-0.88858	1.98173	1.14921
O	-0.76095	1.71588	-1.25774
O	1.48060	3.51273	-1.85327
O	1.78808	3.28073	1.52799
O	2.81639	2.89567	0.49939
O	-0.39489	4.29799	-0.08353
Hf	2.38700	-0.97705	0.06258
O	1.97036	0.74379	-1.17939
O	1.26171	0.39444	1.11321
O	3.28168	-1.39241	2.14880
O	4.01483	-1.15683	-1.54566
O	3.31829	-3.08136	0.11336
O	4.01284	0.55696	0.52598

Hf	-2.27343	0.86339	-0.07206
O	-1.66336	-0.75024	-1.38476
O	-1.27774	-0.66217	0.97179
O	-3.42950	0.94926	1.88193
O	-3.58534	1.29234	-1.88148
O	-2.98073	3.02343	0.06185
O	-3.97737	-0.66002	-0.12185
Hf	-0.84760	-2.38446	-0.24519
O	0.93736	-2.35985	0.96886
O	1.00752	-1.72958	-1.32066
O	-1.06228	-3.35606	-2.29458
O	-2.69772	-1.42970	3.04815
O	-2.76298	-3.02605	-0.02241
O	-1.94606	-3.31630	1.20412
H	1.21063	3.33563	-2.77171
H	-0.15601	4.82926	-0.86685
H	3.58809	-2.28824	2.37705
H	4.71249	-0.47597	-1.52209
H	2.65733	-3.79141	0.20702
H	3.63255	1.49886	0.63615
H	-3.34552	0.18115	2.50526
H	-3.28372	1.72894	-2.69831
H	-2.19823	3.62628	0.06529
H	-4.72417	-0.54438	0.49225
H	-0.26249	-3.64620	-2.77025
H	-2.64366	-2.29454	2.56136
H	-3.63753	-1.61323	-0.03555
H	-4.24030	0.61042	-2.11920
H	-1.72947	-4.06096	-2.38773
H	-2.33528	-1.58050	3.93707
H	-3.51589	1.77204	2.39443
H	-3.61463	3.35157	-0.60080
H	-1.99908	-0.90212	-2.28258
H	-1.59396	-0.88541	1.89116
H	-0.54356	1.17981	-2.03795
H	-0.92120	1.98049	2.11813
H	0.41890	0.04805	1.47391
H	2.55860	0.98870	-1.91056
H	0.87957	-1.15789	-2.09625
H	0.92448	-2.54047	1.92224
H	2.94221	-0.96706	2.95667
H	4.53671	0.35423	1.32161
H	3.88305	-1.42718	-2.47237
H	-0.16960	4.84833	0.69075

H	2.39965	3.83630	-1.86965
H	3.97366	-3.35266	-0.55386

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Hf4_4_2_term_perox_conf2_diconf1.log Energy: -1267974.3356143

Hf	1.58585	1.90521	-0.00707
O	-0.20572	2.52383	0.89486
O	-0.07747	1.41092	-1.21953
O	2.20225	2.69278	-2.09438
O	2.29851	2.31924	2.14286
O	3.84835	2.43476	-0.07949
O	1.79000	4.17327	0.30650
Hf	1.86656	-1.63427	0.00917
O	2.49639	0.21102	-0.93371
O	1.24875	0.11088	1.09265
O	2.75585	-1.86625	2.11571
O	2.45195	-2.27396	-2.11162
O	2.49539	-3.83859	0.33212
O	4.17869	-1.89100	-0.10388
Hf	-2.00968	1.68722	-0.09302
O	-2.46421	-0.21131	-1.07620
O	-1.42159	-0.07653	1.16202
O	-2.59794	2.44263	2.06093
O	-2.61693	2.57271	-1.77208
O	-2.83265	3.44059	-0.55324
O	-4.20447	1.11031	0.41464
Hf	-1.69168	-1.92526	-0.02175
O	0.21264	-2.57061	0.91334
O	0.16411	-1.30897	-1.11387
O	-1.80073	-2.68983	-2.26919
O	-2.40556	-2.34203	2.26230
O	-3.46163	-2.82802	-0.24184
O	-2.41510	-3.81975	0.18904
H	1.63981	3.27359	-2.63875
H	2.12455	1.65599	2.83341
H	4.41376	1.65690	-0.24637
H	2.33190	4.77959	-0.22990
H	2.86384	-2.75631	2.49917
H	1.70181	-2.24367	-2.73292
H	1.88017	-4.55939	0.10458
H	4.67494	-1.45232	-0.81834
H	-3.43117	2.02951	2.35562
H	-4.81177	1.80008	0.08728
H	-1.01020	-3.13695	-2.61559

H	-2.65758	-3.25330	1.97915
H	-4.38502	0.30341	-0.10521
H	-2.50374	-3.36316	-2.20557
H	-1.75243	-2.45050	2.97501
H	-2.76808	3.40268	2.08108
H	-2.71534	-0.27669	-2.01108
H	-1.73494	-0.12398	2.07959
H	-0.15637	1.64251	-2.16042
H	-0.27937	2.67198	1.85240
H	0.29234	0.03639	1.37451
H	2.80281	0.23212	-1.85647
H	0.07015	-0.40170	-1.47958
H	0.28373	-3.21948	1.63044
H	2.39106	-1.28634	2.80768
H	4.63207	-1.66207	0.72963
H	2.99025	-3.05092	-2.34703
H	2.28654	3.20229	2.55450
H	4.21200	2.86054	0.71930
H	0.92247	4.59963	0.43944
H	3.11258	3.03656	-2.16710
H	3.39276	-4.12423	0.07980

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Hf4_4_2_term_perox_conf2_diconf2.log Energy: -1267973.4535870

Hf	0.76501	2.34275	0.07762
O	-1.13600	2.21855	0.96154
O	-0.57274	1.29225	-1.18594
O	0.98830	3.38725	-1.97745
O	1.29851	2.89494	2.24743
O	2.68192	3.65585	0.07038
O	0.17399	4.52846	0.53056
Hf	2.33616	-0.82408	-0.07120
O	2.23578	1.15859	-0.94028
O	1.16149	0.52311	1.09466
O	3.26821	-0.83048	2.02965
O	3.11716	-1.01066	-2.24245
O	3.75018	-2.63697	0.02230
O	4.58286	-0.19518	-0.15436
Hf	-2.50904	0.80033	-0.15507
O	-2.28383	-1.15795	-0.97059
O	-1.16038	-0.55002	1.14029
O	-3.90332	-0.36017	1.32517
O	-3.11344	1.53466	-1.88839
O	-3.87604	2.35995	0.95365

O	-4.27226	0.94773	-1.15091
Hf	-0.86034	-2.42926	0.05012
O	1.22237	-2.40403	0.77667
O	0.58681	-1.14091	-1.12727
O	-0.60466	-3.30312	-2.08024
O	-1.17239	-2.94692	2.38337
O	-2.21954	-3.88001	-0.00751
O	-0.87393	-4.45608	0.33912
H	0.22598	3.81177	-2.41314
H	1.39760	2.17803	2.89813
H	3.47207	3.15121	-0.20143
H	0.55811	5.30494	0.08468
H	3.73213	-1.61720	2.37096
H	3.77679	-1.68737	-2.48151
H	3.46788	-3.54469	-0.18876
H	4.86790	0.40190	-0.86924
H	-4.27159	-1.16819	0.92490
H	-3.55886	3.26370	1.12657
H	0.24333	-3.07845	-2.50034
H	-1.11551	-3.90750	2.16693
H	-0.61483	-4.26858	-1.93650
H	-0.45422	-2.75949	3.01200
H	-4.65997	0.15726	1.65450
H	-4.55345	2.40684	0.24315
H	-2.73679	-1.40600	-1.79170
H	-1.57365	-0.69056	2.00939
H	-0.67368	1.49750	-2.13072
H	-1.24280	2.33437	1.92049
H	0.27234	0.09599	1.34551
H	2.50989	1.32879	-1.85721
H	0.15912	-0.31476	-1.44752
H	1.56857	-3.01705	1.44344
H	2.69740	-0.49025	2.74163
H	4.90898	0.19192	0.67987
H	2.38533	-1.11454	-2.87876
H	0.93658	3.67863	2.69941
H	2.90612	4.05031	0.93465
H	-0.79034	4.66747	0.57045
H	1.73458	4.00949	-2.06817
H	4.70372	-2.55747	-0.16232

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Hf4_4_2_term_perox_conf2_diconf3.log Energy: -1267969.2330587

Hf	-1.95041	-1.50944	-0.00482

O	-0.37391	-2.60236	0.87159
O	-0.21963	-1.29403	-1.11125
O	-2.71527	-2.05285	-2.11676
O	-2.81737	-1.70050	2.11015
O	-4.29483	-1.64411	-0.03799
O	-2.69099	-3.66277	0.11388
Hf	-1.46615	1.99969	0.02794
O	-2.45861	0.37632	-0.94194
O	-1.22177	0.18120	1.09052
O	-2.15495	2.44652	2.16829
O	-2.03168	2.83176	-2.04434
O	-1.39053	4.28288	0.03648
O	-3.60733	2.85182	0.07853
Hf	1.58993	-2.06228	-0.02466
O	2.53011	-0.36593	-1.00005
O	1.32932	-0.19556	1.15936
O	2.23702	-2.47687	2.26498
O	1.59615	-2.84792	-2.22188
O	2.22695	-3.98473	0.19897
O	3.32273	-3.02890	-0.18686
Hf	2.11677	1.50508	-0.01957
O	0.37908	2.51490	0.93338
O	0.17070	1.36169	-1.16062
O	2.46062	2.20238	-2.30985
O	2.96274	1.68369	2.21992
O	4.04785	1.98366	-0.26893
O	3.24131	3.18086	0.15871
H	-2.15171	-1.71246	-2.83621
H	-2.36679	-1.19424	2.80918
H	-4.78882	-1.44087	-0.85221
H	-3.62929	-3.91599	0.04742
H	-2.20111	3.32049	2.59674
H	-2.03765	2.33256	-2.88040
H	-0.59228	4.74402	0.34996
H	-4.13835	2.88068	-0.73767
H	2.47112	-3.40047	2.01033
H	0.70458	-2.92309	-2.60503
H	2.18295	3.12195	-2.47500
H	3.43565	2.51927	2.00752
H	1.97345	-3.74593	-2.18009
H	3.42656	2.26707	-2.13383
H	2.43214	1.86096	3.01595
H	1.56279	-2.55182	2.96241
H	3.05896	-0.47559	-1.80500

H	1.73856	-0.27449	2.03624
H	-0.07650	-0.38191	-1.45176
H	-0.49578	-3.23613	1.59548
H	-0.26300	0.04057	1.36493
H	-3.15747	0.46226	-1.60907
H	0.23488	1.59808	-2.10025
H	0.40976	2.86512	1.83759
H	-1.92141	1.79106	2.84956
H	-4.18975	2.56537	0.80586
H	-1.74339	3.74097	-2.24788
H	-3.08420	-2.55821	2.48833
H	-4.75991	-1.21101	0.70092
H	-2.13801	-4.46274	0.07235
H	-2.84565	-3.00103	-2.30462
H	-2.16199	4.86692	0.15323

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Hf4_4_2_term_perox_conf2_diconf4.log Energy: -1267974.3182888

Hf	1.49076	1.92035	-0.06512
O	2.22896	0.26987	-1.13328
O	1.59364	0.25014	1.18801
O	2.15075	2.77252	2.02681
O	1.99904	2.80709	-2.16006
O	1.53828	4.21702	-0.04552
O	3.75115	2.09301	-0.16367
Hf	-2.02147	1.45564	0.05935
O	-0.31385	2.43822	0.95005
O	-0.24430	1.26683	-1.10704
O	-2.46846	2.26262	-2.04127
O	-2.69667	1.96623	2.19629
O	-4.31446	1.62390	-0.16841
O	-2.71412	3.67614	0.15126
Hf	2.01744	-1.61808	-0.01408
O	0.32970	-2.51416	0.96642
O	0.12600	-1.36414	-1.17480
O	2.74888	-2.45303	-1.66992
O	2.96704	-2.23076	2.03755
O	4.25930	-0.70922	0.21716
O	3.00132	-3.29415	-0.44166
Hf	-1.56425	-2.10869	-0.00367
O	-2.65608	-0.35277	-0.80142
O	-1.30207	-0.16910	1.14108
O	-2.22238	-2.47876	2.19648
O	-1.86482	-2.70586	-2.34454

O	-1.95808	-4.05848	0.04359
O	-3.21587	-3.28065	-0.24496
H	2.79790	2.35588	2.62352
H	1.36287	2.72685	-2.89425
H	0.69800	4.65888	0.18037
H	4.29182	2.67135	0.40304
H	-3.34118	2.18065	-2.46694
H	-2.45195	1.28871	2.85325
H	-4.90982	0.90664	0.11528
H	-2.36388	4.25238	0.85437
H	2.58392	-2.13056	2.92668
H	4.66429	-1.01203	1.05218
H	-2.60858	-1.71102	2.65254
H	-2.67795	-3.20483	-2.09924
H	3.34554	-3.12812	1.99714
H	-2.92111	-3.15647	2.13529
H	-2.14030	-2.02579	-2.98286
H	4.77932	-1.12071	-0.49960
H	0.35948	-3.02301	1.79078
H	0.20507	-1.77608	-2.05207
H	1.65673	0.32447	2.15371
H	2.23461	0.21184	-2.10067
H	-0.11829	0.32276	-1.41456
H	-0.30250	2.77886	1.86089
H	-0.43200	-0.07871	1.56902
H	-3.35596	-0.40147	-1.47079
H	-1.78219	2.06359	-2.70382
H	-2.58710	4.15061	-0.69198
H	-3.60475	2.24491	2.41419
H	2.89021	2.64326	-2.51966
H	1.84042	4.60156	-0.89084
H	4.12446	1.17717	-0.11385
H	2.32160	3.73200	2.05854
H	-4.76069	2.47265	0.00791

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Hf4_4_2_term_perox_conf2_diconf5.log Energy: -1267971.9777350

Hf	-1.55278	1.93811	0.01495
O	0.20136	2.57757	-0.85831
O	0.10647	1.40580	1.18034
O	-2.06972	2.62040	2.14619
O	-2.35646	2.36398	-2.11356
O	-3.80658	2.53433	0.09396
O	-1.81481	4.21596	-0.27136

Hf	-1.91930	-1.59074	-0.02397
O	-2.48677	0.22322	0.93419
O	-1.26045	0.12995	-1.09289
O	-2.75570	-1.84580	-2.14413
O	-2.65483	-2.29779	2.07196
O	-2.29957	-3.83181	-0.02026
O	-4.19152	-1.96569	0.00552
Hf	2.02789	1.65983	0.01989
O	2.36202	-0.25162	1.09464
O	1.41027	-0.05739	-1.19138
O	2.75410	2.42644	-1.69992
O	2.65616	2.44265	2.07897
O	2.94838	3.33822	-0.52463
O	4.32053	1.09222	-0.01367
Hf	1.66092	-1.92506	-0.02062
O	-0.24634	-2.48689	-0.99857
O	-0.19622	-1.44281	1.12939
O	1.78377	-2.79179	2.25202
O	2.42335	-2.31175	-2.29289
O	3.44728	-2.80327	0.24419
O	2.42697	-3.79948	-0.23734
H	-1.28612	2.64163	2.72633
H	-2.12720	1.72106	-2.80777
H	-4.41687	2.00202	0.63531
H	-2.58195	4.71290	0.06546
H	-3.02828	-2.68080	-2.56651
H	-2.54531	-1.83577	2.92195
H	-1.62108	-4.42493	-0.38963
H	-4.65364	-1.86165	0.85678
H	1.94205	2.58308	2.72658
H	4.59165	1.44619	-0.88221
H	1.29764	-3.62940	2.35925
H	2.66720	-3.23227	-2.03754
H	4.48063	0.13245	-0.02618
H	3.19692	3.25280	2.07075
H	2.71495	-3.06541	2.09724
H	1.85746	-2.37584	-3.08084
H	2.75302	-0.30774	1.97979
H	1.76529	-0.06766	-2.09523
H	0.06083	0.52474	1.59789
H	0.37819	3.01270	-1.70827
H	-0.31492	0.06002	-1.40216
H	-2.94500	0.31825	1.78485
H	-0.15413	-1.60717	2.08466

H	-0.29788	-2.77801	-1.92214
H	-2.39811	-1.26370	-2.83808
H	-4.73487	-1.54471	-0.68563
H	-2.53778	-3.24963	2.24897
H	-2.25666	3.25840	-2.48844
H	-4.19465	2.55885	-0.80180
H	-1.02426	4.77556	-0.16576
H	-2.62996	3.38139	2.38128
H	-3.17545	-4.24861	-0.11686

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Hf4_4_2_term_perox_conf2_diconf6.log Energy: -1267975.8684694

Hf	-1.57504	-2.00879	-0.02825
O	0.32036	-2.44429	1.00813
O	0.25915	-1.71232	-1.19555
O	-2.36797	-2.97836	-1.59612
O	-2.32651	-2.85039	2.01399
O	-3.96814	-1.69691	0.17197
O	-1.99620	-3.90044	-0.46281
Hf	-1.91874	1.54521	-0.03755
O	-2.07867	-0.23563	-1.17598
O	-1.68605	-0.13102	1.17859
O	-2.81165	2.21487	2.01926
O	-2.84519	2.29991	-2.05541
O	-2.38140	3.79056	-0.00967
O	-4.15215	1.06580	-0.13686
Hf	1.97358	-1.56934	-0.03590
O	2.44869	0.25873	-1.00118
O	1.46592	0.08941	1.10832
O	2.75877	-2.03533	2.10850
O	2.68302	-2.21348	-2.15935
O	2.44561	-3.79633	0.13634
O	4.26774	-1.55011	-0.19471
Hf	1.62611	2.01628	0.04374
O	-0.29640	2.39910	1.04807
O	-0.18249	1.69808	-1.18103
O	2.05164	2.66047	-2.23540
O	2.36693	2.33063	2.30895
O	3.37438	3.01718	-0.09399
O	2.22669	3.91996	0.28061
H	-2.14536	-2.56000	2.92450
H	-4.22570	-2.26047	-0.58782
H	-3.20988	3.10210	2.08159
H	-3.73787	1.97143	-2.26741

H	-1.62851	4.35679	0.24310
H	-4.27492	0.08349	-0.06045
H	3.22194	-1.35844	2.63355
H	2.19096	-2.81061	-2.74962
H	1.64727	-4.29866	0.38878
H	4.86996	-2.02463	0.40538
H	1.44083	3.32412	-2.60121
H	2.52395	3.29344	2.23151
H	4.63287	-0.65474	-0.32454
H	3.63426	-2.33621	-2.32945
H	2.86524	3.14139	-1.96271
H	1.86340	2.18545	3.12717
H	3.16196	-2.89789	2.31547
H	2.91028	-4.31157	-0.54713
H	2.67818	0.31811	-1.94300
H	1.04997	-0.00522	1.97701
H	0.18061	-1.39181	-2.10728
H	0.37864	-2.59815	1.96441
H	-1.42936	-0.03146	2.10831
H	-2.38586	-0.29207	-2.09349
H	-0.10740	1.23411	-2.02880
H	-0.41624	2.67651	1.96986
H	-3.29858	1.63119	2.62698
H	-4.80817	1.49169	0.44239
H	-2.36182	2.42493	-2.89132
H	-2.38063	-3.82284	2.02490
H	-4.33264	-2.11413	0.97521
H	-2.74166	4.13150	-0.84983

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Hf4_4_2_term_perox_conf2_diconf7.log Energy: -1267975.8455465

Hf	1.72618	-1.89894	-0.02244
O	2.06823	-0.09257	1.17385
O	1.64837	-0.03159	-1.16848
O	2.56402	-2.62798	-1.72138
O	2.41963	-2.78156	1.97538
O	2.60809	-3.59032	-0.57580
O	4.17048	-1.31100	-0.17442
Hf	-1.85163	-1.71079	0.02579
O	-0.12139	-2.41023	-1.01212
O	-0.16319	-1.72420	1.22667
O	-2.62330	-2.42354	2.10022
O	-2.72222	-2.32659	-2.06788
O	-4.14168	-1.80119	0.04691

O	-2.08953	-3.98341	-0.11643
Hf	1.79266	1.67447	0.02337
O	0.09460	2.41394	-1.02513
O	0.08013	1.75286	1.21474
O	2.70076	2.50070	2.01846
O	2.58063	2.37843	-2.07467
O	4.04657	1.38077	0.07515
O	2.07938	3.94328	-0.04018
Hf	-1.76887	1.89409	0.00010
O	-2.40678	0.07004	1.05291
O	-1.53273	-0.00484	-1.10656
O	-2.22926	2.21907	-2.38292
O	-2.24761	2.75727	2.17421
O	-2.65813	3.67407	-0.33506
O	-3.65318	2.58913	0.00007
H	2.89803	-3.62502	1.87484
H	4.13799	-1.76826	-1.05131
H	-3.54089	-2.70029	2.27218
H	-2.70592	-3.25807	-2.35167
H	-4.58019	-0.98233	0.34486
H	-1.25128	-4.44175	-0.31425
H	2.23395	2.63146	2.86254
H	3.16776	1.85689	-2.64964
H	4.26171	0.41138	-0.03418
H	2.41408	4.34507	0.78320
H	-2.93536	1.64640	-2.72968
H	-3.18894	2.96569	2.00694
H	1.26864	4.42069	-0.29960
H	2.87123	3.30687	-2.13664
H	-2.65309	3.07963	-2.16356
H	-2.20354	2.28922	3.02485
H	3.62155	2.25087	2.21530
H	4.66347	1.88815	-0.48049
H	0.09467	2.55075	-1.98656
H	0.08884	1.36156	2.10087
H	1.57983	-0.04351	-2.13605
H	2.47406	-0.11044	2.05399
H	-0.13174	-1.14502	2.00420
H	-0.05413	-2.66066	-1.94765
H	-0.99654	-0.01192	-1.91373
H	-2.76792	0.02528	1.95204
H	-2.04602	-2.86065	2.75028
H	-2.55571	-4.50883	0.55802
H	-2.68208	-1.77039	-2.86559

H	1.78670	-2.90554	2.70562
H	4.79486	-1.80934	0.38307
H	-4.51974	-2.02784	-0.82417

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Hf4_4_2_term_perox_conf2_diconf8.log Energy: -1267969.8192655

Hf	-0.02282	-2.56357	0.04234
O	1.78705	-1.76069	0.98995
O	1.10546	-1.08426	-1.14801
O	0.08276	-3.29375	-2.24411
O	-0.14369	-3.17760	2.34092
O	-0.78834	-4.42442	-0.10976
O	0.67048	-4.44342	0.26210
Hf	-2.50543	0.02241	-0.02099
O	-1.78339	-1.73212	-0.98036
O	-1.14083	-1.00443	1.16002
O	-3.45941	-0.05226	2.09806
O	-3.48356	0.23302	-2.13994
O	-4.31770	1.43105	0.05560
O	-4.31530	-1.37996	-0.25130
Hf	2.50371	-0.02612	-0.03490
O	1.77536	1.71803	-1.00513
O	1.15038	1.02096	1.14845
O	3.46170	0.09973	2.09033
O	3.35604	-0.14793	-2.20841
O	4.26595	-1.48034	0.10207
O	4.31984	1.36427	-0.28074
Hf	0.02759	2.56359	0.03786
O	-1.78052	1.76653	0.98531
O	-1.09803	1.05411	-1.13810
O	-0.10992	3.24999	-2.24720
O	0.35040	3.31324	2.30544
O	0.78129	4.42001	-0.14450
O	-0.67485	4.44274	0.23941
H	0.97163	-3.45641	-2.60695
H	-1.03311	-3.21574	2.73487
H	-4.34207	0.32405	2.26880
H	-4.10156	-0.43611	-2.48455
H	-4.08532	2.33542	0.33881
H	-4.05090	-2.31346	-0.35080
H	3.56540	0.94164	2.56915
H	3.38920	-0.97700	-2.71863
H	3.96841	-2.38989	0.29381
H	5.11195	1.37965	0.28604

H	-1.00630	3.33803	-2.61641
H	-0.08721	4.17309	2.12352
H	4.04443	2.28965	-0.42322
H	4.18215	0.33695	-2.38817
H	0.21238	4.15761	-2.06004
H	-0.07787	2.94635	3.09767
H	4.26888	-0.42266	2.25041
H	5.02374	-1.53751	-0.50702
H	1.86509	1.85992	-1.96208
H	1.08855	0.87928	2.10470
H	0.92047	-0.91452	-2.08373
H	1.89491	-1.87735	1.94832
H	-0.82646	-0.65132	2.00585
H	-1.90710	-1.94134	-1.92026
H	-0.75017	0.72713	-1.98048
H	-2.04711	1.94916	1.89970
H	-3.38512	-0.86887	2.62380
H	-5.12128	-1.36083	0.29514
H	-3.08150	0.69344	-2.89666
H	0.13800	-4.10334	2.17812
H	-0.28291	-4.17433	-2.00374
H	-4.76745	1.51438	-0.80673

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Hf4_4_2_term_perox_conf2_diconf9.log Energy: -1267976.1959101

Hf	1.50200	-2.07682	-0.03094
O	-0.39569	-2.44268	-0.98613
O	-0.33404	-1.68802	1.21643
O	2.21063	-2.97302	1.97212
O	2.26114	-2.88597	-1.72847
O	4.00209	-1.73115	-0.18676
O	2.22290	-3.84461	-0.57796
Hf	1.95975	1.48144	0.03491
O	2.03854	-0.30783	1.16139
O	1.57821	-0.19931	-1.18554
O	2.83593	2.11241	-2.05197
O	2.93455	2.18503	2.04498
O	2.51986	3.70077	0.00327
O	4.16432	0.94692	0.08973
Hf	-2.03668	-1.49751	0.01786
O	-2.51400	0.33666	0.94793
O	-1.30584	0.12659	-1.06445
O	-2.76796	-1.83542	-2.14979
O	-2.76397	-2.32767	2.08000

O	-2.70795	-3.67594	-0.18347
O	-4.35166	-1.50484	0.23002
Hf	-1.56574	2.06901	-0.02948
O	0.37764	2.42725	-1.01806
O	0.24241	1.71408	1.19975
O	-1.98908	2.71662	2.24437
O	-2.21396	2.31154	-2.29488
O	-3.28891	3.11929	0.09946
O	-2.11170	3.97676	-0.28469
H	1.62174	-2.98873	2.74815
H	4.55756	-2.29270	0.38340
H	3.22000	3.00783	-2.09064
H	3.82087	1.83464	2.24819
H	1.76958	4.28337	-0.21991
H	4.27736	-0.03950	-0.02727
H	-2.86472	-1.02460	-2.68078
H	-2.17341	-2.42399	2.84679
H	-2.05599	-4.25053	-0.62650
H	-4.91968	-2.16852	-0.20137
H	-1.37169	3.37076	2.61643
H	-2.30127	3.26941	-2.44914
H	-4.78166	-0.63869	0.10652
H	-3.66366	-2.14414	2.40438
H	-2.78679	3.21546	1.95220
H	-1.77778	1.91241	-3.06510
H	-3.47337	-2.45031	-2.41769
H	-2.90776	-4.08735	0.67934
H	-2.96109	0.44454	1.80275
H	-0.48909	-0.01726	-1.57283
H	-0.22287	-1.10595	1.98417
H	-0.39528	-2.67023	-1.93023
H	1.70694	-0.23298	-2.14765
H	2.42377	-0.36649	2.04903
H	0.16875	1.32300	2.08375
H	0.48175	2.63218	-1.96059
H	3.36019	1.55390	-2.65257
H	4.83397	1.39187	-0.45883
H	2.47639	2.36012	2.88593
H	3.93419	-2.18696	-1.06111
H	2.55667	-3.87902	1.87091
H	2.91680	4.02795	0.83242

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Hf4_4_2_term_perox_conf3_diconf10.log Energy: -1267989.3837871

Hf	1.40960	-2.07605	0.04991
O	2.06264	-0.38092	1.27293
O	2.04092	-0.35920	-1.16503
O	2.24137	-3.11393	-1.83086
O	1.70368	-3.54858	1.37283
O	0.77204	-3.99590	0.27795
O	3.84052	-2.09224	0.11434
Hf	-2.07293	-1.36391	-0.02688
O	-0.36377	-1.85257	-1.21319
O	-0.36816	-1.49958	1.15835
O	-2.82898	-1.98101	2.11223
O	-3.03182	-2.31034	-1.91761
O	-4.34225	-1.39798	0.08034
O	-1.87209	-3.63944	0.07995
Hf	2.05218	1.37298	0.05775
O	0.38387	1.62143	-1.21665
O	0.32467	1.82969	1.20108
O	2.98440	2.14135	1.98143
O	3.19596	2.11836	-1.79365
O	4.25804	0.71382	0.22694
O	1.81081	3.66821	-0.27542
Hf	-1.42464	2.08541	-0.06792
O	-2.39670	0.44230	1.02880
O	-2.03640	0.32710	-1.30056
O	-1.50685	3.43997	-1.58601
O	-2.04401	3.00290	1.97906
O	-0.84099	4.01232	-0.36624
O	-3.64122	2.74863	-0.20988
H	2.34980	-2.72460	-2.71652
H	4.17152	-2.56202	-0.67539
H	-3.72307	-2.34291	2.24674
H	-2.87187	-3.25943	-2.07127
H	-4.84401	-0.68434	0.51310
H	-0.90706	-3.87403	0.29879
H	2.70643	2.88199	2.54818
H	3.29569	1.59805	-2.61041
H	4.29164	-0.27494	0.22745
H	2.23050	4.33178	0.29862
H	-1.59302	3.85250	2.13900
H	-3.59316	3.36884	-0.96664
H	0.82432	3.90694	-0.35320
H	3.01352	3.04653	-2.03074
H	-4.33589	2.09859	-0.41443
H	-2.99701	3.21384	1.96806

H	3.94821	2.02386	2.07078
H	4.84474	1.02604	-0.48552
H	0.38169	2.16913	-2.02027
H	0.25392	1.69791	2.15970
H	1.43187	-0.21492	-1.90970
H	2.21800	-0.34367	2.23027
H	-0.23224	-0.92418	1.92571
H	-0.45801	-2.32530	-2.05465
H	-1.51386	0.22725	-2.11388
H	-2.53477	0.42029	1.98985
H	-2.22419	-2.46706	2.69997
H	-2.44027	-4.17005	0.66510
H	-3.13831	-1.87438	-2.78196
H	4.14144	-2.61936	0.87905
H	1.92668	-4.03043	-1.93630
H	-4.81266	-1.65405	-0.73399

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Hf4_4_2_term_perox_conf3_diconf1.log Energy: -1267973.4469354

Hf	-2.27742	-1.03832	-0.04273
O	-0.96067	-2.36257	0.96657
O	-0.69830	-1.62209	-1.23435
O	-3.16526	-1.44143	-2.14235
O	-3.23034	-1.15319	2.07814
O	-4.53539	-0.51712	-0.13482
O	-3.35930	-3.03128	0.18521
Hf	-0.95523	2.26434	0.01664
O	-2.21713	0.86804	-1.03207
O	-1.12982	0.39820	1.01243
O	-1.65128	2.70770	2.18119
O	-1.40884	3.38315	-1.98657
O	-0.54891	4.49003	0.24681
O	-2.96353	3.39984	0.07904
Hf	1.01680	-2.38659	-0.05579
O	1.89609	-0.79643	-1.16296
O	1.32901	-0.54853	1.19747
O	1.36777	-3.23462	2.11731
O	1.56725	-3.54177	-1.60312
O	0.97748	-4.33380	-0.46063
O	3.32939	-2.73212	0.37094
Hf	2.37984	0.98278	-0.05439
O	0.88488	2.29361	1.04498
O	0.63476	1.70257	-1.20185
O	3.56754	1.15459	-1.71881

O	3.48569	1.11781	1.95478
O	4.29620	0.66443	-0.50272
O	3.25663	3.15963	-0.14815
H	-2.71983	-2.08786	-2.71882
H	-2.87760	-0.64359	2.82851
H	-4.76496	0.37100	-0.46639
H	-4.07070	-3.37683	-0.38266
H	-1.59524	3.54833	2.66989
H	-1.40223	2.96778	-2.86716
H	0.21028	4.82041	0.75904
H	-3.46838	3.47838	-0.75035
H	2.33742	-3.29042	2.22351
H	3.49868	-3.37499	-0.34770
H	4.39707	1.42068	1.78557
H	3.69821	2.98575	-1.01156
H	3.88638	-1.95705	0.16068
H	2.62596	3.88363	-0.29565
H	3.17887	1.58734	2.75006
H	1.05741	-4.15649	2.18612
H	2.38945	-0.86202	-1.99594
H	1.59238	-0.62917	2.12905
H	-0.44632	-1.16165	-2.05132
H	-0.96581	-2.45317	1.93291
H	-0.24671	0.04484	1.32848
H	-2.64812	0.97926	-1.89605
H	0.55573	1.45155	-2.13525
H	0.89487	2.43913	2.00373
H	-1.59385	1.98328	2.82780
H	-3.58662	3.16450	0.79070
H	-0.90512	4.21365	-2.07696
H	-3.53805	-2.01226	2.42084
H	-4.94853	-0.58373	0.74774
H	-2.73516	-3.75957	0.36546
H	-4.12311	-1.50843	-2.30800
H	-1.28521	5.12122	0.35258

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Hf4_4_2_term_perox_conf3_diconf2.log Energy: -1267968.2786984

Hf	-1.74104	1.70995	-0.01877
O	-2.48471	0.06673	1.03825
O	-1.92960	0.05458	-1.24811
O	-2.56599	2.68060	-1.96015
O	-2.05930	2.54019	2.17545
O	-1.34581	3.95271	0.04137

O	-3.87533	2.43398	0.26103
Hf	1.80568	1.62948	-0.06082
O	0.04673	2.03529	-1.21517
O	0.03150	1.24658	1.02969
O	2.10473	2.55129	2.08142
O	2.68648	2.53605	-2.00676
O	4.00873	2.13469	0.16840
O	1.52494	3.97622	-0.00003
Hf	-1.88213	-1.82630	-0.04288
O	-0.04250	-2.02875	-1.09148
O	-0.03678	-1.37200	1.21152
O	-2.33902	-2.82645	1.97438
O	-2.56299	-2.78878	-1.70560
O	-4.24090	-1.71484	-0.05809
O	-2.43593	-3.67648	-0.50343
Hf	1.78710	-1.91531	-0.00150
O	2.48938	-0.01111	1.04181
O	1.95301	-0.07061	-1.22878
O	2.41238	-2.99176	-1.62364
O	2.27368	-2.81425	2.05454
O	2.22662	-3.81300	-0.38095
O	4.15074	-1.94339	-0.05056
H	-2.79513	2.20752	-2.77967
H	-1.43344	2.30256	2.88075
H	-0.39284	4.17929	-0.06656
H	-4.29495	2.76023	-0.55721
H	2.95378	2.69157	2.53661
H	2.21767	2.58691	-2.85898
H	4.59320	1.55552	0.68926
H	1.88703	4.48704	-0.75054
H	-2.97612	-3.54846	1.82014
H	-4.60623	-0.82239	-0.17719
H	2.87613	-3.56888	1.91864
H	4.14427	-2.43897	-0.90209
H	4.58023	-1.09106	-0.23047
H	2.60012	-2.33337	2.83523
H	-2.60754	-2.39071	2.80229
H	-4.30144	-2.16418	-0.93050
H	-0.04087	-2.52359	-1.92641
H	-0.04512	-1.70530	2.12424
H	-1.45022	0.00043	-2.09093
H	-2.63425	0.13653	1.99382
H	0.00809	0.28606	1.34468
H	-0.02354	2.43413	-2.09681

H	1.58953	-0.10116	-2.12869
H	2.57860	0.06958	2.00413
H	1.43089	2.36993	2.75923
H	1.84026	4.39804	0.82317
H	3.58886	2.23179	-2.21789
H	-2.89908	2.79064	2.59928
H	-1.64729	4.38887	0.86031
H	-4.53958	1.90771	0.74172
H	-2.40436	3.61632	-2.17870
H	4.47058	2.98454	0.04455

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Hf4_4_2_term_perox_conf3_diconf3.log Energy: -1267972.3923430

Hf	-2.46659	-0.29974	-0.03012
O	-1.71753	-2.11357	0.75701
O	-0.84910	-0.95044	-1.13243
O	-3.39525	-0.31479	-2.14328
O	-3.30174	-0.08500	2.08832
O	-4.50615	0.83808	-0.00577
O	-4.26196	-1.75117	0.10879
Hf	-0.24614	2.44361	0.07161
O	-1.97131	1.62018	-0.88384
O	-0.97991	0.74351	1.09587
O	-0.59029	3.16861	2.22059
O	-0.30479	3.49890	-1.99757
O	1.01757	4.33265	0.11789
O	-1.63825	4.27871	0.11094
Hf	0.29727	-2.55485	-0.01120
O	1.95141	-1.57056	-1.03725
O	1.01912	-0.84898	1.14577
O	0.52338	-3.22762	2.31002
O	-0.24285	-3.29863	-2.12880
O	-0.07656	-4.55709	0.23303
O	1.34539	-4.24056	-0.13733
Hf	2.62957	0.22784	-0.11757
O	1.60018	1.89214	0.97774
O	0.83222	1.12193	-1.16204
O	3.38269	1.09220	-1.72883
O	3.86069	-1.28441	1.16020
O	4.37692	0.14192	-1.14101
O	4.27518	1.34703	1.14768
H	-2.73171	-0.30809	-2.85781
H	-2.65636	0.09771	2.79455
H	-4.82410	1.31188	-0.79479

H	-5.18202	-1.44983	0.00154
H	-0.17196	3.93806	2.64687
H	-0.57936	3.08466	-2.83513
H	1.92156	4.29440	0.47682
H	-2.05499	4.58371	-0.71469
H	0.27183	-4.13998	2.02447
H	-1.02208	-2.85562	-2.50752
H	4.15069	-1.04719	2.05800
H	4.96088	1.22216	0.45265
H	-0.46193	-4.24251	-2.01118
H	4.17672	2.30521	1.28486
H	3.62577	-2.22757	1.16508
H	-0.13841	-2.94969	2.96640
H	2.35765	-1.92078	-1.84552
H	1.31192	-1.08662	2.04106
H	-0.25315	-0.23683	-1.46032
H	-2.16845	-2.63645	1.43781
H	-0.20908	0.12948	1.33606
H	-2.52390	2.06850	-1.54265
H	1.09640	1.37903	-2.06145
H	1.73582	2.02962	1.92996
H	-0.75994	2.49875	2.90646
H	-2.29680	4.34691	0.82589
H	0.41613	4.12179	-2.20444
H	-3.95957	-0.71393	2.43740
H	-4.66482	1.41456	0.76382
H	-4.22033	-2.70441	-0.08372
H	-4.02623	-1.02339	-2.36870
H	0.67220	5.23859	0.21652

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Hf4_4_2_term_perox_conf3_diconf4.log Energy: -1267974.5770172

Hf	-2.03944	1.40163	-0.00959
O	-2.26839	-0.34158	1.14260
O	-1.81133	-0.24953	-1.23063
O	-3.01541	2.35038	-1.85218
O	-3.12232	2.18565	1.87645
O	-1.87942	3.66232	0.17914
O	-4.25527	0.78053	-0.07564
Hf	1.48790	1.91638	-0.03893
O	-0.31257	2.05365	-1.19161
O	-0.20778	1.28520	1.05655
O	1.57586	2.85534	2.12106
O	2.22071	2.93725	-1.98745

O	3.57674	2.77191	0.19773
O	0.89601	4.20297	0.02975
Hf	-1.49676	-2.07876	0.06230
O	0.33583	-2.20220	-1.04269
O	0.26098	-1.40134	1.20903
O	-2.05188	-3.08549	1.70567
O	-2.21587	-3.05244	-1.95771
O	-3.89814	-2.02552	-0.16375
O	-1.65760	-3.99422	0.56299
Hf	2.12651	-1.60276	-0.02116
O	2.44773	0.41279	1.04734
O	1.85059	0.24491	-1.20338
O	2.92645	-2.41827	-1.70818
O	2.81460	-2.45198	1.99133
O	2.99833	-3.31879	-0.51095
O	4.44304	-1.10703	-0.06214
H	-3.17010	1.92923	-2.71651
H	-2.69507	2.27761	2.74788
H	-0.98775	4.06342	0.06435
H	-4.80913	1.12213	-0.80003
H	2.35146	3.11589	2.64867
H	1.74733	2.93437	-2.83844
H	4.22018	2.31659	0.76947
H	1.15326	4.76575	-0.72659
H	-2.01909	-2.71837	-2.85008
H	-4.16812	-2.53681	-0.95038
H	3.63541	-2.96483	1.87705
H	4.56673	-1.52771	-0.94162
H	-2.09443	-4.01847	-1.98260
H	4.66632	-0.16792	-0.16968
H	2.89054	-1.98431	2.84111
H	-4.20259	-2.52669	0.61812
H	0.50560	-2.60968	-1.90647
H	0.24048	-1.73277	2.12260
H	-1.24848	-0.15811	-2.01621
H	-2.42005	-0.37455	2.09899
H	-0.07789	0.36309	1.41228
H	-0.44777	2.44704	-2.06814
H	1.58050	0.18421	-2.13329
H	2.52291	0.49446	2.01099
H	0.87902	2.55652	2.73287
H	1.15354	4.66930	0.84889
H	3.16211	2.79791	-2.20113
H	-4.00186	1.78748	2.01581

H	-2.33300	4.10861	0.91666
H	-4.31452	-0.20743	-0.08161
H	-2.99973	3.31659	-1.97532
H	3.87655	3.69449	0.09725

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Hf4_4_2_term_perox_conf3_diconf5.log Energy: -1267981.1501601

Hf	-1.73227	-1.78070	-0.00138
O	-0.03903	-2.49579	0.98199
O	-0.10563	-1.85727	-1.25830
O	-2.77800	-2.58155	-1.90065
O	-2.53873	-2.24685	2.17407
O	-3.97391	-1.40322	0.17992
O	-2.16507	-4.00349	0.22215
Hf	-1.69018	1.76877	-0.04831
O	-2.13471	0.00719	-1.17427
O	-1.28506	-0.00245	1.05538
O	-2.51294	2.08616	2.13061
O	-2.70681	2.61026	-1.96487
O	-2.14349	3.99360	0.16270
O	-4.02173	1.49582	0.11145
Hf	1.82576	-1.84051	-0.00660
O	1.91102	-0.01198	-1.30895
O	1.39325	0.00365	1.16419
O	2.56708	-2.45275	1.75663
O	2.31822	-2.86930	-2.00703
O	2.75052	-3.46573	0.66864
O	4.00714	-1.24816	-0.30730
Hf	1.88285	1.74020	-0.08157
O	-0.00150	2.48142	0.94392
O	-0.03946	1.83503	-1.28875
O	3.72898	2.24809	-0.64819
O	2.47916	2.79318	1.90096
O	3.84221	1.21482	0.41355
O	1.73371	3.95847	-0.71979
H	-2.33410	-2.78743	-2.74222
H	-2.26734	-1.69258	2.92705
H	-4.22490	-0.45941	0.05599
H	-2.58160	-4.44632	-0.54023
H	-2.55009	2.92884	2.61672
H	-2.59853	2.22110	-2.85167
H	-1.43704	4.53755	0.55736
H	-4.54212	1.84426	-0.63908
H	1.56081	-3.32246	-2.41926

H	4.52096	-1.74535	0.35357
H	3.43307	2.56706	1.91537
H	2.55540	4.28357	-1.13036
H	4.10477	-0.25424	-0.09058
H	3.04053	-3.52043	-1.95367
H	1.00324	4.17805	-1.32543
H	2.40458	3.76390	1.94008
H	2.54208	-0.03399	-2.04641
H	1.76828	-0.03649	2.06035
H	-0.05869	-1.23884	-2.00597
H	0.07188	-2.68599	1.92737
H	-0.34288	-0.00760	1.39024
H	-2.60263	-0.06937	-2.02040
H	-0.03201	1.35126	-2.13018
H	0.01668	2.60352	1.90629
H	-2.30594	1.38284	2.77137
H	-4.42905	1.82463	0.93648
H	-2.57145	3.57015	-2.07570
H	-2.59548	-3.16552	2.49267
H	-4.32493	-1.67843	1.04855
H	-1.39040	-4.53542	0.48498
H	-3.73224	-2.48012	-2.06779
H	-2.98608	4.47117	0.27589

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Hf4_4_2_term_perox_conf3_diconf6.log Energy: -1267987.8622649

Hf	-0.22787	2.52920	-0.05292
O	-1.77294	1.45176	1.09759
O	-1.48321	1.12497	-1.20787
O	-0.35412	3.75870	-1.64765
O	-0.27064	3.73435	1.94429
O	1.67434	4.01248	0.03242
O	-1.26016	4.16049	-0.51419
Hf	2.42457	0.19089	-0.00694
O	1.32369	1.54372	-1.20604
O	1.24289	1.43136	1.22078
O	3.77803	0.30099	1.86634
O	3.81058	0.29870	-1.85739
O	3.98076	-1.51516	0.05570
O	3.69379	2.12782	-0.07266
Hf	-2.53949	-0.19454	0.00434
O	-1.51079	-1.68347	-1.08936
O	-1.29360	-1.32702	1.23351
O	-3.77476	-0.35439	1.99145

O	-3.76175	-0.23923	-2.00717
O	-4.30652	1.26960	0.02979
O	-4.03262	-1.93744	-0.04823
Hf	0.15496	-2.54781	-0.01653
O	1.50794	-1.29490	1.19470
O	1.42762	-1.21280	-1.20943
O	0.28906	-3.72029	-1.67200
O	0.19899	-3.68606	1.98689
O	-0.33856	-4.41159	-0.50268
O	2.33197	-3.68080	-0.07181
H	-0.10293	3.45118	2.85968
H	1.39797	4.51703	-0.76465
H	4.35486	-0.46823	2.02442
H	4.21357	1.17369	-2.00672
H	3.51630	-2.39142	-0.01804
H	3.09424	2.91791	-0.06812
H	-3.42145	-0.70152	2.82931
H	-3.45723	0.14120	-2.84963
H	-4.06887	2.18475	0.26915
H	-4.50459	-2.06606	0.79586
H	-0.07439	-4.61439	1.86855
H	2.04897	-4.07681	-0.93266
H	-3.64779	-2.79603	-0.30553
H	-4.32434	-1.00722	-2.21237
H	2.46633	-4.41415	0.55527
H	-0.26055	-3.36117	2.78156
H	-4.46462	0.29995	2.20111
H	-4.77773	1.30232	-0.82410
H	-1.62486	-1.93035	-2.02108
H	-0.90543	-0.90134	2.01401
H	-1.12918	0.86203	-2.07172
H	-1.96752	1.62870	2.03097
H	0.96639	1.06865	2.07618
H	1.47476	1.71974	-2.14754
H	1.17158	-1.04245	-2.12904
H	1.82948	-1.53003	2.07895
H	3.57731	0.72303	2.72013
H	4.31659	2.22872	0.66958
H	3.67918	-0.13391	-2.71954
H	-0.92251	4.45686	1.97184
H	1.62958	4.62039	0.79388
H	4.64137	-1.47262	-0.65876

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Hf4_4_2_term_perox_conf3_diconf7.log Energy: -1267981.2699391

Hf	1.92851	-1.71511	-0.07933
O	1.98932	0.09256	1.19545
O	1.78459	0.16450	-1.18912
O	2.81630	-2.33039	-1.79468
O	2.71819	-2.58177	1.90253
O	2.92406	-3.32599	-0.68269
O	4.25891	-0.92418	-0.13458
Hf	-1.61643	-1.83628	0.04226
O	0.10963	-2.30087	-1.08828
O	0.09522	-1.94283	1.25453
O	-2.31585	-2.67922	2.13757
O	-2.59260	-2.69460	-1.93043
O	-3.95436	-1.84698	0.06580
O	-1.56180	-4.13640	-0.04634
Hf	1.61010	1.84066	0.05466
O	-0.09844	2.29284	-1.07093
O	-0.11084	1.98336	1.25590
O	2.45376	2.74722	2.04958
O	2.42004	2.68954	-1.97603
O	3.90295	1.75822	0.15952
O	1.63595	4.13712	0.01936
Hf	-1.94720	1.73813	-0.07587
O	-2.02441	-0.12983	1.18232
O	-1.77871	-0.17121	-1.19282
O	-2.71693	2.36371	-1.83614
O	-2.76692	2.64695	1.86897
O	-2.86659	3.36768	-0.73474
O	-4.19943	1.09735	0.00047
H	3.28758	-3.36126	1.76469
H	4.33245	-1.33949	-1.02843
H	-3.11222	-3.14499	2.44792
H	-2.48683	-3.64658	-2.10888
H	-4.53885	-2.04331	0.82058
H	-0.68492	-4.46635	-0.31898
H	1.97268	2.79481	2.89412
H	2.99152	2.21155	-2.60125
H	4.19917	0.81595	0.03088
H	1.89734	4.52990	0.87331
H	-3.73781	2.59471	1.92849
H	-4.45190	1.45321	-0.87568
H	0.78438	4.53448	-0.24173
H	2.62854	3.63832	-2.04235
H	-4.29805	0.12470	-0.05706

H	-2.41393	2.51480	2.76520
H	3.39237	2.56810	2.23958
H	4.43750	2.31238	-0.43552
H	-0.11659	2.47484	-2.02396
H	-0.11746	1.46494	2.07577
H	1.51789	0.14929	-2.12142
H	2.37771	0.11242	2.08386
H	0.11030	-1.28401	1.96922
H	0.16720	-2.46359	-2.04385
H	-1.48168	-0.11372	-2.11416
H	-2.37796	-0.21644	2.08188
H	-1.58529	-2.94772	2.72317
H	-1.85127	-4.67620	0.71040
H	-2.65273	-2.23572	-2.78662
H	2.02949	-2.85535	2.53584
H	4.91474	-1.36084	0.43894
H	-4.30811	-2.32520	-0.71036

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Hf4_4_2_term_perox_conf3_diconf8.log Energy: -1267972.3901593

Hf	2.35622	-1.11057	0.00192
O	2.35893	0.83648	0.99235
O	1.48312	0.56337	-1.16484
O	3.07409	-1.26794	-2.25832
O	2.92382	-1.47641	2.33307
O	3.71984	-2.58596	-0.14475
O	4.35895	-1.27110	0.22201
Hf	-1.05533	-2.22237	-0.01747
O	0.81923	-2.28536	-1.04343
O	0.50381	-1.48070	1.14037
O	-1.37392	-3.12392	2.13360
O	-1.65933	-3.18438	-2.07899
O	-3.05163	-3.32988	0.11635
O	-0.41996	-4.42450	-0.13499
Hf	1.09084	2.23618	0.00186
O	-0.74935	2.25557	-1.03666
O	-0.45971	1.46735	1.14154
O	1.42261	3.10550	2.13944
O	1.72466	3.15226	-2.06649
O	3.12932	3.28347	0.13539
O	0.47138	4.44090	-0.12393
Hf	-2.35748	1.13180	-0.05792
O	-2.25020	-0.80883	1.02473
O	-1.50666	-0.57718	-1.19441

O	-3.27642	1.47245	-1.78942
O	-3.00357	2.09421	1.93091
O	-3.62567	2.51793	-0.77537
O	-4.64130	0.57539	0.57608
H	3.49454	-0.47209	-2.62899
H	2.70666	-2.35509	2.69176
H	-2.12468	-3.72373	2.29505
H	-1.24869	-4.02436	-2.35169
H	-3.81453	-2.83519	0.46538
H	0.53639	-4.51824	-0.30325
H	0.66760	3.32820	2.71165
H	1.90899	2.60758	-2.85142
H	3.83320	2.67281	0.42512
H	0.73763	5.12805	0.51254
H	-3.86390	1.76661	2.25151
H	-5.02819	1.25754	-0.01283
H	-0.48292	4.55222	-0.29228
H	1.33528	3.99185	-2.36972
H	-5.03065	-0.27792	0.32263
H	-2.40592	2.17290	2.69333
H	2.14124	3.73288	2.33616
H	3.41780	3.66940	-0.71352
H	-0.92529	2.50657	-1.95713
H	-0.27764	0.96383	1.94861
H	0.98591	0.38860	-1.97790
H	2.56123	0.90230	1.93976
H	0.42863	-1.25837	2.08038
H	0.92258	-2.42804	-1.99792
H	-1.35970	-0.48026	-2.14742
H	-2.42140	-0.92234	1.97365
H	-0.62867	-3.45581	2.66501
H	-0.68302	-5.12357	0.48946
H	-1.95697	-2.72376	-2.88248
H	3.87243	-1.51857	2.06972
H	3.78670	-1.91812	-2.08721
H	-3.32650	-3.71792	-0.73645

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Hf4_4_2_term_perox_conf3_diconf9.log Energy: -1267985.6458262

Hf	-1.14149	-2.25778	0.09698
O	0.75487	-2.17342	1.13591
O	0.64741	-1.94200	-1.22772
O	-1.59211	-3.34957	-1.88199
O	-1.80016	-3.11383	1.81754

O	-3.61587	-2.31717	0.12695
O	-1.55140	-4.09982	0.71859
Hf	-2.15153	1.18422	-0.08915
O	-1.81467	-0.58001	-1.19895
O	-1.68622	-0.42257	1.16726
O	-3.20668	1.60462	1.99296
O	-3.17529	1.69918	-2.14926
O	-3.21976	3.20057	-0.05891
O	-4.23748	0.28718	-0.25322
Hf	2.23091	-1.20030	-0.04023
O	1.67051	0.44364	-1.21976
O	1.70038	0.41903	1.21582
O	3.48232	-1.63251	1.82649
O	3.41570	-1.75119	-1.94386
O	2.86601	-3.42160	-0.00322
O	4.11666	0.12402	-0.24177
Hf	1.19923	2.18855	0.04440
O	-0.75572	2.25188	1.07605
O	-0.57935	2.00928	-1.25857
O	2.32143	2.93262	-1.50081
O	1.81300	3.05128	2.11831
O	3.15073	2.62732	-0.28886
O	0.91856	4.48208	0.04595
H	-0.81412	-3.40284	-2.46747
H	-4.06610	-2.98142	-0.42560
H	-3.83923	2.34110	2.07255
H	-3.98068	1.20329	-2.38285
H	-2.77763	3.97518	0.33319
H	-4.18171	-0.69669	-0.09570
H	3.54091	-1.08820	2.63073
H	2.97220	-1.97729	-2.78107
H	2.14230	-4.03498	0.21956
H	4.80137	0.03674	0.44447
H	1.69894	4.01802	2.15840
H	1.43737	4.68834	-0.76129
H	3.87310	1.10823	-0.31131
H	4.15689	-1.14957	-2.14381
H	0.03951	4.88586	-0.05788
H	1.58361	2.69902	2.99501
H	3.74991	-2.54323	2.04293
H	3.31288	-3.76109	-0.79962
H	2.16095	0.78669	-1.98764
H	1.26371	0.23682	2.06234
H	0.45128	-1.29359	-1.92628

H	0.77743	-2.37845	2.08462
H	-1.51131	-0.35750	2.11879
H	-2.12571	-0.69705	-2.11014
H	-0.37158	1.59022	-2.11005
H	-0.91190	2.34505	2.02938
H	-3.54361	0.88143	2.55035
H	-4.98645	0.62509	0.26816
H	-2.72752	1.96015	-2.97295
H	-3.52644	-2.70686	1.03254
H	-1.90257	-4.26476	-1.75377
H	-3.55054	3.46187	-0.93924

Optimized geometries of Hf tetramers with counterions, no explicit water

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Hf4_4_2_bridging_peroxide_conf1_deprot1_ion16.log Energy: -2423613.8364844

Hf	-2.53457	-0.89219	-0.25912
O	-1.77257	0.78537	-1.46012
O	-1.35260	0.52449	0.84809
O	-3.09446	-1.14255	1.95270
O	-3.28846	-1.13431	-2.49910
O	-4.02823	-2.20837	-0.30053
O	-4.16218	0.58480	-0.15572
Hf	0.99271	-2.24105	-0.37813
O	-1.04341	-2.33372	0.35695
O	-1.04110	-2.17270	-1.13773
O	1.20104	-3.01304	-2.59252
O	1.24925	-3.13112	1.72751
O	2.89938	-2.91560	-0.53449
O	0.36641	-4.49927	-0.48378
Hf	-1.07432	2.31006	-0.15971
O	1.04118	2.31979	0.45738
O	0.86998	2.23891	-1.03349
O	-1.36776	3.34572	-2.25627
O	-1.28452	3.00569	2.03207
O	-2.96311	3.03665	0.02886
O	-0.40777	4.55556	-0.10065
Hf	2.48787	0.95599	-0.43339
O	1.50840	-0.59961	-1.58573
O	1.50385	-0.56339	0.76192
O	3.49166	1.10656	1.60248
O	2.93188	1.32241	-2.74218
O	3.86096	2.39069	-0.69902

O	4.12108	-0.51509	-0.73692
Cl	-1.35936	0.54335	3.93319
Cl	2.59201	-1.14015	3.63231
Cl	-6.69869	-0.71093	0.84195
Cl	6.40070	0.30236	1.13399
H	-2.59614	-0.71708	2.69883
H	-3.95275	-1.81505	-2.25467
H	-4.88371	-2.01995	0.14215
H	-5.03452	0.31583	0.26530
H	2.06295	-3.47280	-2.57357
H	0.41316	-3.35562	2.17394
H	-0.54981	-4.61978	-0.17167
H	-1.02045	4.25479	-2.17445
H	-1.23514	2.31426	2.74898
H	-0.90620	5.13356	0.50444
H	3.21076	0.47534	2.31416
H	3.62341	2.00256	-2.59214
H	4.95196	-0.37676	-0.19915
H	0.51327	4.54918	0.22609
H	-2.20250	3.33971	2.05740
H	4.48284	0.96821	1.53477
H	4.33361	2.79898	0.04098
H	3.82667	-1.46999	-0.65776
H	2.21346	1.77919	-3.21515
H	-0.87976	2.94651	-2.99886
H	-3.36555	3.51374	-0.71491
H	-1.12612	0.41941	1.80127
H	-2.29914	0.99918	-2.24635
H	1.60986	-0.63410	1.73570
H	1.65095	-0.73143	-2.53545
H	0.53981	-3.69436	-2.81133
H	0.91409	-5.12972	0.01715
H	1.77446	-2.60227	2.39699
H	-2.67187	-1.55571	-3.12389
H	-3.92760	1.53483	0.02925
H	-3.33269	-2.04619	2.21836
H	3.30001	-3.47823	0.14650

64
Hf4_4_2_bridging_peroxide_conf1_deprot1_ion1.log Energy: -2423617.2317248

Hf	1.51249	-2.25693	0.20312
O	-0.21865	-2.14367	-1.19178
O	-0.25976	-1.44881	1.08495
O	1.64320	-2.66655	2.48468

O	2.22432	-2.79537	-1.99445
O	3.20356	-3.26376	0.37504
O	0.44807	-4.23766	0.36420
Hf	1.97600	1.53392	-0.28172
O	2.36696	-0.33961	0.81482
O	2.30706	-0.53097	-0.67063
O	2.46561	1.36091	-2.54800
O	2.97712	2.24795	1.66175
O	2.05080	3.50913	-0.75044
O	4.25773	1.45370	-0.55413
Hf	-1.99530	-1.67822	-0.02665
O	-2.36034	0.34779	0.79017
O	-2.34210	0.29391	-0.70813
O	-2.67855	-1.97478	-2.20398
O	-2.81000	-2.08431	2.07779
O	-2.14383	-3.71433	0.13539
O	-4.29488	-1.56056	-0.13082
Hf	-1.51456	2.13274	-0.09259
O	0.14677	1.46208	-1.32021
O	0.32103	1.84036	0.99384
O	-1.83976	2.92638	2.05709
O	-2.30716	2.41125	-2.31451
O	-3.21197	3.19139	0.02420
O	-0.49835	4.09662	-0.46535
Cl	4.71953	-0.75238	-2.76526
Cl	-4.71095	0.19853	-2.81197
Cl	-0.62923	-1.25736	4.13488
Cl	0.90760	3.72198	3.41682
H	0.93634	-2.29599	3.08029
H	3.12158	-2.39522	-2.10911
H	3.58312	-3.64140	1.18040
H	0.71518	-4.81179	1.10233
H	2.78795	2.21537	-2.88573
H	3.20796	1.49792	2.24065
H	4.56951	0.68400	-1.10471
H	-3.36239	-1.30379	-2.51044
H	-2.22450	-1.80242	2.83661
H	-4.64552	-1.26300	0.72835
H	-1.09833	3.36265	2.54647
H	-2.98418	1.71750	-2.52862
H	-0.88752	4.74997	-1.06978
H	-4.60338	-0.90431	-0.80904
H	-2.86347	-3.05869	2.11913
H	-2.55111	3.58126	1.91868

H	-3.65360	3.42493	-0.80600
H	0.49942	4.02846	-0.63955
H	-1.71126	2.46679	-3.08020
H	-1.93780	-1.87667	-2.82774
H	-2.55108	-4.24241	-0.56950
H	-0.29693	-1.04156	1.97903
H	-0.31510	-2.92181	-1.76489
H	0.47092	2.26500	1.86675
H	0.16222	1.16280	-2.24112
H	3.15454	0.67518	-2.77914
H	4.81668	1.50128	0.24010
H	2.43987	2.86470	2.23726
H	1.67717	-2.31624	-2.64238
H	-0.56383	-4.19113	0.34275
H	2.48990	-2.45444	2.91429
H	2.70317	4.12248	-0.37883

64
Hf4_4_2_bridging_peroxide_conf1_deprot1_ion6.log Energy: -2423617.7441741

Hf	-1.95757	-1.84075	-0.58130
O	-1.87455	0.14887	-1.45870
O	-1.52048	-0.27011	0.84141
O	-2.30749	-2.74818	1.50855
O	-2.65452	-1.97855	-2.82277
O	-2.76060	-3.63250	-0.98162
O	-4.06962	-1.09882	-0.22344
Hf	1.85406	-1.69676	-0.64163
O	-0.03302	-2.62324	-0.08544
O	-0.05609	-2.24655	-1.53960
O	2.41809	-1.84996	-2.89327
O	2.35026	-2.83861	1.28810
O	3.87285	-1.46942	-0.65929
O	2.23124	-3.94940	-1.10738
Hf	-1.91063	1.63104	0.09515
O	0.02188	2.10277	1.17725
O	0.02897	2.33873	-0.30347
O	-2.14205	2.93219	-1.78642
O	-2.69821	1.68636	2.24765
O	-3.92827	1.57670	-0.13798
O	-1.95522	3.86332	0.76977
Hf	1.95933	1.72383	0.19969
O	1.73929	0.27381	-1.44200
O	1.55142	-0.28196	0.84527
O	2.84226	1.39332	2.29665

O	2.17731	3.07247	-1.70398
O	2.66519	3.46616	0.87281
O	4.08597	1.14600	-0.28458
Cl	0.11782	-1.78731	3.24509
Cl	-0.20395	5.23916	-1.66555
Cl	-4.40165	-0.91771	2.87685
Cl	4.63248	-1.24491	2.53362
H	-2.99467	-2.25054	2.03345
H	-3.00903	-2.89273	-2.78713
H	-2.93286	-4.20895	-0.22095
H	-4.40020	-1.25105	0.69845
H	3.31930	-2.21464	-2.96972
H	1.59450	-2.78491	1.92796
H	1.43697	-4.40255	-1.44600
H	-1.45413	3.65218	-1.91554
H	-3.18889	0.84511	2.47225
H	-1.27375	3.86310	1.47306
H	3.42775	0.59319	2.39193
H	1.44965	3.75506	-1.69655
H	4.57822	1.67596	-0.93458
H	-1.56010	4.44821	0.07418
H	-3.36649	2.39111	2.33302
H	3.39260	2.18620	2.43998
H	2.89682	4.17278	0.25213
H	4.14082	0.17097	-0.55462
H	2.14856	2.68181	-2.59384
H	-2.35998	2.58843	-2.66811
H	-4.34335	2.01795	-0.89549
H	-1.07164	-0.45030	1.69251
H	-2.32609	0.27395	-2.30668
H	1.24649	-0.53069	1.74448
H	2.06757	0.34229	-2.35209
H	1.85184	-2.36071	-3.49901
H	2.41570	-4.35083	-0.23508
H	3.11587	-2.40726	1.77542
H	-1.94551	-1.98577	-3.49071
H	-4.13563	-0.09611	-0.30644
H	-1.48954	-2.66513	2.06438
H	4.37942	-1.67999	0.15112

64
Hf4_4_2_bridging_peroxide_conf1_deprot3_ion16.log Energy: -2423596.1359295

Hf	-2.74435	-0.48076	-0.11989
O	-2.52133	1.47678	-1.02625

O	-1.36484	0.81805	0.90644
O	-2.71949	-1.23272	2.05958
O	-3.83298	-0.83558	-1.77245
O	-4.30361	-2.16867	0.29069
O	-4.39113	0.71824	0.82798
Hf	0.65849	-2.36784	-0.65360
O	-1.44030	-2.15800	-0.33397
O	-1.04966	-1.07858	-1.31650
O	0.28892	-2.66395	-2.93983
O	0.96295	-3.52826	0.92819
O	2.31679	-3.76216	-1.51025
O	-0.31864	-4.53459	-1.03599
Hf	-0.92232	2.57104	-0.12505
O	1.17294	2.11782	0.37477
O	0.76980	1.65859	-1.00834
O	-1.04925	3.22325	-2.41159
O	-1.09243	3.56896	1.60061
O	-2.44040	4.29841	-0.41765
O	0.36535	4.53137	-0.57147
Hf	2.56876	0.62226	-0.32747
O	2.07868	-1.05694	-1.56558
O	1.17457	-0.77821	0.59108
O	3.35114	0.17319	1.75549
O	3.24071	1.35694	-2.07613
O	3.80343	2.48308	0.44692
O	4.71483	-0.10578	-0.63766
Cl	-0.15422	-0.36127	3.49977
Cl	3.43602	-2.68823	2.80278
Cl	-6.63683	-0.99305	1.87660
Cl	6.32963	1.18660	1.62920
H	-1.91653	-1.03147	2.61763
H	-3.51245	-0.57787	-2.64942
H	-5.10011	-1.92120	0.84563
H	-5.19622	0.25865	1.22216
H	0.25133	-3.59011	-3.23801
H	3.12065	-3.23936	-1.68645
H	-1.28914	-4.44603	-1.04989
H	-0.65068	4.11230	-2.46898
H	-2.67767	4.56914	0.49070
H	0.14977	5.13520	0.16384
H	3.29267	-0.77749	2.08405
H	4.71464	2.30527	0.80283
H	5.40887	0.18856	0.01507
H	1.28685	4.25251	-0.41009

H	-0.59822	3.30492	2.39089
H	4.27070	0.47064	1.96653
H	3.32954	2.95771	1.15168
H	4.93579	0.29823	-1.50052
H	2.59027	1.80543	-2.63726
H	-0.51024	2.66153	-2.99729
H	-3.27020	4.10661	-0.88910
H	-0.90181	0.58931	1.74710
H	-2.82956	1.66691	-1.92504
H	0.89851	-0.72560	1.53445
H	2.21831	-0.96743	-2.52092
H	-0.56607	-2.24673	-3.15835
H	-0.10084	-4.90119	-0.15371
H	1.65092	-3.27767	1.58736
H	-4.63504	-2.25453	-0.62671
H	-4.70818	1.44278	0.26179
H	-2.87626	-2.19037	2.12666
H	2.56188	-4.41599	-0.83028

64
Hf4_4_2_bridging_peroxide_conf1_deprot3_ion6.log Energy: -2423596.6095234

Hf	-2.57065	-0.74079	-0.53645
O	-2.42234	1.35362	-1.07710
O	-1.47645	0.46477	0.86778
O	-2.77001	-1.95550	1.39958
O	-3.36681	-0.86254	-2.37906
O	-4.09006	-2.51144	-0.70039
O	-4.47902	0.11571	0.28815
Hf	1.05451	-2.24552	-0.88197
O	-1.08596	-2.25319	-0.79502
O	-0.65612	-1.01181	-1.54336
O	1.13868	-2.07815	-3.21221
O	1.25170	-3.71348	0.45320
O	3.02209	-3.27227	-1.59350
O	0.37876	-4.31231	-1.86516
Hf	-1.04199	2.41017	0.17534
O	0.94912	1.91651	1.09895
O	0.85206	1.68588	-0.39480
O	-0.77323	3.24285	-2.00071
O	-1.62319	3.13789	1.94076
O	-2.66764	4.00915	-0.22347
O	0.10461	4.42372	0.22287
Hf	2.54997	0.68979	0.41510
O	2.44232	-0.64456	-1.25093

O	1.23045	-0.98226	0.75508
O	2.98215	-0.07774	2.48030
O	3.55334	1.93061	-0.82010
O	3.68306	2.33960	1.75069
O	4.75194	-0.04366	0.30640
Cl	-0.52681	-1.19703	3.37255
Cl	1.99300	4.53167	-2.20796
Cl	-5.50011	-1.35643	2.69954
Cl	3.33504	-3.02987	2.90979
H	-3.62964	-1.86580	1.89839
H	-2.96639	-0.34935	-3.09648
H	-3.75313	-3.36704	-0.38266
H	-4.92385	-0.31928	1.08253
H	1.22885	-2.92954	-3.67663
H	3.75464	-2.62894	-1.58501
H	-0.58671	-4.30035	-2.00101
H	0.13166	3.61750	-2.20763
H	-2.38741	4.65622	-0.89588
H	0.48903	4.52200	1.11111
H	3.07381	-1.07472	2.65159
H	3.99515	2.81216	0.94782
H	5.33905	-0.03834	1.08196
H	0.85225	4.52749	-0.43071
H	-1.37004	2.68887	2.76126
H	3.63030	0.38968	3.03389
H	3.05239	2.94222	2.18544
H	5.13935	0.56644	-0.35246
H	3.05371	2.57893	-1.35700
H	-0.94115	2.55749	-2.67023
H	-2.74587	4.48575	0.62515
H	-1.06469	0.09614	1.68151
H	-3.01191	1.75495	-1.73272
H	0.80714	-1.15746	1.62998
H	2.68151	-0.33296	-2.13749
H	0.30281	-1.67408	-3.51328
H	0.52659	-4.86372	-1.06831
H	1.77618	-3.53905	1.26578
H	-4.19900	-2.56664	-1.67086
H	-4.41617	1.06724	0.48047
H	-2.05142	-1.81302	2.07335
H	3.24630	-3.95862	-0.93831

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Hf4_4_2_bridging_peroxide_conf1_deprot4_ion16.log Energy: -2423606.1658338

Hf	2.68194	-0.09443	-0.25013
O	2.13781	-2.14089	-0.62570
O	1.27325	-0.89226	1.13612
O	3.85358	0.33995	1.28437
O	2.75511	-0.43752	-2.64246
O	3.78865	1.62434	-1.37522
O	4.67936	-1.01141	-0.84153
Hf	-0.35021	2.48890	-0.20608
O	1.62072	1.80119	0.15383
O	1.07186	1.05558	-1.03847
O	-0.01552	3.49533	-1.91261
O	-0.09431	2.89771	2.04863
O	-2.25712	3.64200	0.20952
O	0.38103	4.64431	0.22596
Hf	0.42864	-2.76625	0.53122
O	-1.55661	-2.08572	0.44744
O	-0.83918	-1.67536	-0.81946
O	0.38626	-4.23867	-0.82889
O	-0.11145	-2.63818	2.79696
O	2.14796	-3.78131	1.67446
O	-0.38573	-4.76259	1.44409
Hf	-2.52305	-0.32901	-0.57943
O	-1.79351	1.47189	-1.45945
O	-1.30902	0.79537	0.72235
O	-3.83729	-0.27908	0.89216
O	-2.33610	-0.75009	-2.92795
O	-3.61936	-2.28383	-1.20361
O	-4.37523	0.41202	-1.69739
Cl	-0.38579	0.28042	3.72592
Cl	-1.57654	5.59854	2.44024
Cl	6.77700	1.18426	-1.00596
Cl	-6.50999	-1.48676	-0.63073
H	3.57178	0.99956	1.93633
H	2.98546	0.44659	-2.98643
H	3.41072	2.44581	-1.01025
H	5.46294	-0.38718	-0.76280
H	0.10097	2.99365	-2.73329
H	-0.18460	2.14276	2.67946
H	-3.06021	3.09869	0.29029
H	-0.10508	5.20685	0.88166
H	-0.31999	-1.73184	3.14969
H	3.02074	-3.59356	1.28355
H	-1.14244	-4.69395	2.05188
H	-2.52824	-1.69884	-3.04868

H	-4.60503	-2.24283	-1.03764
H	-5.21905	-0.05158	-1.42516
H	-0.65501	-5.27984	0.66071
H	0.62596	-2.96384	3.34429
H	-4.73871	-0.63454	0.77019
H	-3.25290	-2.95914	-0.60092
H	-4.29381	0.30298	-2.66285
H	-1.45725	-0.59581	-3.31690
H	0.50236	-4.05591	-1.77265
H	2.06761	-4.75039	1.74203
H	0.95883	-0.37826	1.90563
H	2.45166	-2.67559	-1.36967
H	-1.21492	0.54070	1.66405
H	-2.05312	1.84954	-2.31228
H	0.32264	5.06397	-0.65405
H	-0.55823	3.67814	2.44274
H	1.90803	-0.67697	-3.05807
H	4.78103	1.65572	-1.23188
H	4.69009	-1.32596	-1.76365
H	-2.25990	4.30597	0.95686

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Hf4_4_2_bridging_peroxide_conf1_deprot4_ion1.log Energy: -2423600.9292672

Hf	1.99153	-1.53787	0.17736
O	0.40231	-2.77771	-0.65577
O	0.18945	-1.48899	1.22677
O	2.59066	-0.59906	1.92735
O	2.81767	-2.38451	-1.78625
O	4.24952	-1.89494	0.47021
O	2.37069	-3.55994	1.14506
Hf	1.47683	2.05089	-0.59544
O	2.69032	0.28034	-0.71914
O	1.30155	-0.03543	-1.20225
O	1.95147	2.64487	-2.44165
O	2.46478	1.99731	1.44797
O	1.13293	4.16326	0.12132
O	3.61287	2.98595	-0.63712
Hf	-1.50226	-2.27660	0.17851
O	-2.30879	-0.29998	0.66765
O	-1.78957	-0.43988	-0.75076
O	-1.99508	-3.10566	-1.61105
O	-2.12839	-2.45758	2.40810
O	-1.76387	-4.57983	0.53458
O	-3.79210	-2.59107	0.34293

Hf	-2.09002	1.65172	-0.17226
O	-0.52160	2.39763	-1.42284
O	-0.18673	1.57881	0.72956
O	-2.57226	2.55957	1.52407
O	-2.86248	1.37151	-2.41715
O	-4.38838	1.27946	-0.13411
O	-3.16693	3.56167	-0.95452
Cl	5.78168	-1.88083	-2.12956
Cl	-4.95340	-1.03537	-2.10787
Cl	-0.44544	-0.19344	3.86845
Cl	1.26847	4.28034	3.12568
H	2.06912	-0.74944	2.73428
H	3.79017	-2.24248	-2.00457
H	4.49032	-1.26322	1.17340
H	3.21870	-3.61487	1.62129
H	1.38630	2.46527	-3.20692
H	2.57846	1.04266	1.76270
H	0.28373	4.50923	-0.20657
H	3.87141	3.48431	0.15672
H	-1.68388	-1.79586	3.00471
H	-0.95708	-5.11289	0.65164
H	-4.10206	-2.15325	1.15613
H	-3.49176	0.60545	-2.46955
H	-4.86213	2.04069	-0.51584
H	-2.96659	4.38809	-0.48098
H	-4.26793	-2.14700	-0.41042
H	-2.03636	-3.32953	2.83023
H	-3.50372	2.56821	1.79452
H	-4.71115	0.47711	-0.62600
H	-3.15271	3.75096	-1.90933
H	-2.11639	1.11470	-2.98742
H	-2.72570	-2.67967	-2.09129
H	-2.06318	-4.73116	-0.39028
H	0.05180	-0.97187	2.05933
H	0.36541	-3.17873	-1.53833
H	-0.14056	1.27589	1.65473
H	-0.62770	2.86647	-2.26281
H	3.64591	3.58572	-1.40464
H	2.08667	2.55734	2.17649
H	2.32742	-2.01069	-2.54045
H	4.90274	-1.80940	-0.28593
H	1.67901	-3.93871	1.71500
H	1.12807	4.30294	1.12374

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Hf4_4_2_bridging_peroxide_conf1_deprot5_ion16.log Energy: -2423605.5287861

Hf	2.58158	0.75633	-0.34477
O	1.86885	-0.89747	-1.56302
O	1.29933	-0.62065	0.71193
O	3.25004	0.96000	1.80328
O	3.32537	1.04665	-2.58575
O	4.01095	2.16015	-0.47928
O	4.28113	-0.69640	-0.34036
Hf	-0.86747	2.58506	-0.37600
O	1.17916	2.37670	0.21117
O	0.97906	1.84893	-1.18631
O	-0.99768	3.63262	-2.09037
O	-1.00875	3.21281	1.85803
O	-3.05796	2.98414	0.02995
O	-0.58728	4.86456	-0.02182
Hf	0.84928	-2.34526	-0.36896
O	-1.22490	-2.22528	0.12135
O	-1.00686	-1.72413	-1.28499
O	1.05487	-3.26680	-2.52352
O	1.25589	-3.26602	1.37856
O	3.00406	-3.26649	-0.54868
O	0.19849	-4.62918	-0.43562
Hf	-2.55351	-0.52108	-0.38357
O	-1.78655	1.07667	-1.60282
O	-1.28876	0.73662	0.67504
O	-3.15338	-0.90921	1.74004
O	-3.35844	-0.87436	-2.56337
O	-3.92753	-2.35198	-0.48112
O	-4.23762	0.62424	-0.31771
Cl	1.77770	-0.99442	3.72481
Cl	-1.99462	1.08871	3.78198
Cl	6.17646	0.04880	1.89800
Cl	-5.93685	-2.21577	1.73143
H	2.80787	0.39417	2.49367
H	3.96891	1.75945	-2.38398
H	4.25012	2.69626	0.29128
H	5.00905	-0.55447	0.33705
H	-0.76205	3.21697	-2.93300
H	-0.19470	3.59025	2.23483
H	-3.62151	2.14455	-0.06948
H	-1.13234	5.36228	0.61211
H	0.83071	-4.21529	-2.55103
H	1.44984	-2.77463	2.20111

H	3.31236	-3.75643	-1.33387
H	0.39486	-4.77903	0.51681
H	-2.91960	-0.25111	2.44896
H	-3.92218	-1.67111	-2.52426
H	-4.70243	-2.36024	0.17184
H	-0.76300	-4.75514	-0.53493
H	-4.09318	-1.20887	1.88827
H	-3.40498	-3.15150	-0.28302
H	-4.76161	0.73091	-1.12850
H	-2.66903	-1.06588	-3.22478
H	0.50803	-2.84040	-3.20789
H	3.08959	-3.84799	0.23306
H	1.25458	-0.67615	1.69898
H	2.28148	-1.08333	-2.41962
H	-1.12142	0.64019	1.63371
H	-2.29306	1.37959	-2.37205
H	-0.75740	5.20891	-0.92287
H	-1.35027	2.55917	2.53869
H	2.64227	1.45675	-3.14612
H	4.04590	-1.64877	-0.35883
H	4.22975	0.79240	1.92430
H	-3.27673	3.37197	0.89529

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Hf4_4_2_bridging_peroxide_conf1_deprot5_ion1.log Energy: -2423598.2221726

Hf	2.38700	-1.21124	0.20894
O	0.89187	-2.43429	-0.88798
O	0.44632	-1.18066	1.09242
O	2.69320	-1.37936	2.49766
O	3.19827	-1.74535	-1.83056
O	4.35337	-1.01686	0.44061
O	2.87626	-3.40021	0.74607
Hf	1.07329	2.45431	-0.30635
O	2.39029	0.97430	0.51785
O	1.91354	0.56480	-0.85438
O	1.73229	3.19188	-2.05422
O	1.34253	3.20078	1.90985
O	-0.30207	4.26153	-0.15423
O	2.78050	3.96197	0.00991
Hf	-0.97751	-2.42491	0.15925
O	-2.34337	-0.76017	0.39295
O	-1.61155	-0.68947	-0.92595
O	-1.54874	-3.15988	-2.04736
O	-1.32035	-3.11509	1.99723

O	-0.55863	-4.68976	-0.02857
O	-3.09812	-3.39314	0.07363
Hf	-2.24608	1.25792	-0.38839
O	-0.55128	1.81684	-1.61184
O	-0.58048	1.63073	0.78987
O	-3.11441	1.62608	1.68648
O	-2.97273	0.98314	-2.59596
O	-4.50230	0.77847	-0.40900
O	-2.76794	3.21536	-0.60128
Cl	5.35527	-0.17184	-3.19826
Cl	-4.52959	-1.79287	-2.23972
Cl	0.16879	-1.03051	4.17578
Cl	-1.21014	3.06290	3.60217
H	1.95811	-1.24292	3.16315
H	3.99462	-1.21563	-2.16920
H	4.70522	-0.16595	0.74352
H	3.13955	-3.41168	1.68582
H	1.54042	2.73526	-2.88671
H	1.96415	2.66261	2.43058
H	-1.27080	4.00192	-0.28237
H	2.67833	4.62960	0.71049
H	-2.43741	-2.79698	-2.28509
H	-0.95592	-2.64237	2.77121
H	-1.03608	-5.10067	-0.77314
H	-3.39233	-3.33100	1.00134
H	-2.61855	2.20690	2.33025
H	-3.44353	0.11236	-2.67607
H	-5.06370	1.40282	-0.90333
H	-3.74706	-2.88551	-0.47615
H	-4.03544	1.93641	1.65509
H	-4.68922	-0.12114	-0.78713
H	-3.08562	3.58864	-1.43867
H	-2.20293	0.90524	-3.18796
H	-0.93922	-2.75881	-2.69244
H	-0.89050	-5.09913	0.79274
H	0.25540	-0.87108	2.00790
H	1.15675	-3.17026	-1.46069
H	-0.61893	1.67609	1.76560
H	-0.69277	2.47269	-2.31280
H	2.94972	4.39960	-0.84590
H	0.52604	3.29440	2.47771
H	2.54429	-1.70621	-2.54965
H	2.16795	-4.06157	0.64703
H	3.50714	-0.97818	2.84463

H	-0.11531	4.97205	-0.79290

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Hf4_4_2_bridging_peroxide_conf1_deprot5_ion6.log Energy: -2423613.0564964

Hf	-1.71890	-2.02564	-0.55881
O	-2.27192	-0.05541	-1.36946
O	-1.43901	-0.41983	0.81967
O	-1.91605	-2.98292	1.52954
O	-2.36757	-2.24579	-2.79651
O	-2.19776	-3.92892	-1.00080
O	-3.96078	-1.93254	-0.17267
Hf	2.18028	-1.62995	-0.69579
O	0.28757	-2.57765	-0.10393
O	0.21681	-1.98276	-1.48723
O	3.09414	-1.98995	-2.43671
O	2.69664	-2.59247	1.34329
O	4.21267	-0.66830	-0.19901
O	2.43656	-3.96042	-0.99181
Hf	-2.15033	1.44382	0.16118
O	-0.21378	2.11389	1.01093
O	-0.23817	2.08931	-0.49621
O	-2.38073	2.67031	-1.95690
O	-3.09274	1.54543	1.90756
O	-4.34698	1.67691	-0.51931
O	-2.51390	3.68176	0.51590
Hf	1.75591	1.79375	0.05194
O	1.91341	0.34368	-1.53733
O	1.60112	-0.15090	0.74669
O	2.45347	1.83761	2.22925
O	1.80064	3.13477	-1.90093
O	1.77802	4.00216	0.66979
O	3.76530	2.00453	-0.18909
Cl	0.34569	-1.68913	3.24095
Cl	-0.44130	5.28414	-1.17633
Cl	-4.35520	-1.43806	2.78513
Cl	4.49467	-0.53147	2.86734
H	-2.68347	-2.59885	2.03363
H	-2.36811	-3.21906	-2.89714
H	-2.15192	-4.55700	-0.26330
H	-4.33294	-2.82047	-0.32289
H	3.78241	-1.41816	-2.80647
H	1.88482	-2.59340	1.91303
H	4.16903	0.32477	-0.34205
H	2.78302	-4.39318	-0.19062

H	-1.81963	3.48009	-1.92998
H	-3.39141	0.70234	2.30728
H	-4.40769	2.37470	-1.19915
H	-2.57332	3.80764	1.48019
H	3.11188	1.12413	2.45516
H	1.08417	3.81871	-1.83829
H	2.57412	4.48398	0.37980
H	-1.82009	4.30153	0.16800
H	2.85891	2.68436	2.48617
H	1.00324	4.51597	0.31753
H	4.09377	2.42029	-1.00254
H	1.62903	2.66922	-2.73767
H	-2.00780	2.12574	-2.67268
H	-4.86526	1.97266	0.25141
H	-1.00951	-0.53780	1.69027
H	-3.03543	-0.07733	-1.96833
H	1.23461	-0.41665	1.61878
H	2.32903	0.49551	-2.39887
H	3.13457	-3.99894	-1.67323
H	3.34538	-2.07270	1.89199
H	-1.77238	-1.88167	-3.47520
H	-4.23883	-1.66453	0.75532
H	-1.12821	-2.76643	2.09342
H	4.48492	-0.72069	0.75548

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Hf4_4_2_bridging_peroxide_conf1_deprot6_ion16.log Energy: -2423605.8265833

Hf	-2.64787	-0.94796	-0.44230
O	-2.51520	1.10012	-1.18019
O	-1.58245	0.40095	0.85496
O	-2.98614	-1.87061	1.59117
O	-3.38039	-0.88330	-2.68922
O	-3.79621	-2.53562	-0.90074
O	-4.62241	-0.01197	0.08718
Hf	1.08238	-2.18043	-0.73724
O	-0.97905	-2.32389	-0.25626
O	-0.83800	-1.43025	-1.46288
O	1.34328	-2.93761	-2.57297
O	1.10160	-3.08490	1.44308
O	3.29744	-2.49454	-0.32234
O	1.05513	-4.48058	-0.67336
Hf	-1.39834	2.36723	0.12610
O	0.69261	2.22106	0.71808
O	0.51158	2.06787	-0.77687

O	-1.53610	3.46520	-1.99044
O	-1.88362	2.97351	1.96746
O	-3.20392	3.77027	-0.02126
O	-0.47367	4.56841	0.18364
Hf	2.33774	1.12858	-0.25115
O	1.91551	-0.42740	-1.68068
O	1.32016	-0.51293	0.60341
O	3.31054	0.83125	1.74965
O	2.98166	1.92594	-2.37255
O	3.34072	2.86115	-0.10438
O	4.38789	0.13937	-0.72735
Cl	-0.48834	-1.11603	3.33800
Cl	3.77528	-2.18832	2.69424
Cl	-5.85492	-1.32430	2.49375
Cl	6.33453	1.11247	1.34679
H	-2.29258	-1.69992	2.27695
H	-3.82290	-1.75920	-2.68206
H	-3.85629	-3.25659	-0.25618
H	-5.16210	-0.40897	0.84035
H	1.17610	-2.41027	-3.36764
H	0.40218	-2.67478	2.00834
H	3.80620	-1.73556	-0.68902
H	1.40501	-4.92908	0.11561
H	-1.18301	4.36418	-1.84804
H	-3.68315	3.82463	0.82552
H	-0.87875	4.97366	0.97321
H	3.30245	-0.09448	2.11019
H	3.29545	2.80871	-2.08076
H	5.13965	0.43044	-0.11220
H	0.45259	4.38179	0.43641
H	-1.46960	2.59554	2.75726
H	4.27300	1.10218	1.77792
H	3.40133	3.35423	0.72696
H	4.66866	0.37617	-1.63118
H	2.29470	2.07475	-3.04633
H	-0.96720	3.06917	-2.67447
H	-3.84570	3.77866	-0.75172
H	-1.22387	0.12690	1.72871
H	-2.91524	1.36816	-2.02083
H	0.90958	-0.52027	1.49026
H	2.30598	-0.49393	-2.56385
H	1.47756	-4.84067	-1.47406
H	1.93668	-2.88769	1.94834
H	-2.65400	-0.94970	-3.33483

H	-4.61706	0.95149	0.21346
H	-3.88094	-1.74341	2.01947
H	3.56532	-2.50728	0.64072

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Hf4_4_2_bridging_peroxide_conf1_deprot6_ion1.log Energy: -2423601.6499430

Hf	-2.68404	-0.28764	0.21801
O	-2.14710	1.66082	-0.62276
O	-1.21901	0.77771	1.36933
O	-2.88846	-0.99626	2.39870
O	-3.66873	-0.05295	-1.81635
O	-4.33031	-1.40907	0.40586
O	-4.21864	1.18681	1.10225
Hf	0.50949	-2.47732	-0.60672
O	-1.43744	-2.03090	0.13728
O	-1.13325	-1.12231	-1.03298
O	0.31067	-3.17159	-2.47406
O	0.63118	-3.48775	1.52456
O	2.40100	-3.71825	-0.55849
O	-0.38290	-4.62004	-0.55413
Hf	-0.60804	2.62280	0.54153
O	1.41147	1.74905	0.99491
O	1.00550	1.68700	-0.46050
O	-0.60712	3.52789	-1.65486
O	-0.77361	3.24664	2.42327
O	-1.97327	4.45507	0.32183
O	0.94430	4.35348	0.50454
Hf	2.62840	0.40129	-0.25422
O	1.85667	-1.08719	-1.61127
O	1.34724	-1.01919	0.68874
O	3.67815	-0.30877	1.62721
O	2.84980	1.32532	-2.38886
O	4.07427	1.78393	-0.04000
O	4.59796	-0.52962	-1.06984
Cl	-5.67543	-2.17677	-2.44698
Cl	2.23026	4.45518	-2.34152
Cl	-0.06184	-1.22245	3.61337
Cl	3.73396	-3.38339	2.13139
H	-2.05898	-1.22388	2.89457
H	-4.33436	-0.75121	-2.12093
H	-4.83863	-1.73944	-0.36298
H	-4.91912	0.63585	1.49839
H	0.22399	-2.58161	-3.23696
H	0.19636	-2.92091	2.20986

H	2.94803	-3.63415	-1.35841
H	-0.01613	-5.18925	0.14480
H	0.27629	3.81424	-2.02126
H	-2.75806	4.56876	0.88463
H	1.64173	3.98692	1.08155
H	3.68274	-1.28954	1.81466
H	2.80398	2.31514	-2.31048
H	5.19736	0.24282	-1.05849
H	1.40653	4.48754	-0.36908
H	-0.57429	4.17389	2.62734
H	4.59769	0.00348	1.68538
H	4.01924	2.39762	0.70754
H	4.62402	-0.89529	-1.97090
H	2.12688	1.09513	-2.99855
H	-0.92542	2.82050	-2.24301
H	-2.19496	4.72739	-0.58632
H	-0.76068	0.41084	2.15325
H	-2.86988	2.13579	-1.06154
H	1.04319	-0.91824	1.61421
H	2.09940	-1.26378	-2.53139
H	-0.19419	-5.02306	-1.42153
H	1.56866	-3.54513	1.84479
H	-3.04926	0.09360	-2.55206
H	-3.89983	1.79017	1.79724
H	-3.45533	-1.78765	2.34108
H	3.00976	-3.62537	0.23322

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Hf4_4_2_bridging_peroxide_conf1_deprot6_ion6.log Energy: -2423604.9048158

Hf	-2.46673	-1.01526	-0.60379
O	-2.39984	1.11015	-1.10652
O	-1.60787	0.22404	0.92049
O	-2.86015	-2.22524	1.26835
O	-3.05572	-0.72154	-2.87349
O	-3.53783	-2.56541	-1.31398
O	-4.49780	-0.21259	-0.05122
Hf	1.32202	-2.18784	-0.83740
O	-0.76397	-2.31439	-0.47109
O	-0.54022	-1.26653	-1.53528
O	1.71834	-2.62555	-2.75108
O	1.26014	-3.43399	1.17020
O	3.40431	-2.97051	-0.44098
O	0.99987	-4.45705	-1.19339
Hf	-1.35367	2.25280	0.37348
O	0.69061	1.83810	1.26590

O	0.63087	1.86295	-0.24409
O	-1.07081	3.33988	-1.72377
O	-2.08297	2.59161	2.19168
O	-2.97779	3.82307	-0.06543
O	-0.28313	4.26376	0.86128
Hf	2.47400	1.03114	0.25956
O	2.45290	-0.39687	-1.35712
O	1.44391	-0.76820	0.72953
O	3.20352	0.34858	2.30314
O	2.88881	2.27366	-1.67013
O	3.39881	2.68751	0.92238
O	4.74800	0.71498	-0.10129
Cl	-0.46370	-1.69781	3.19684
Cl	1.42630	5.11048	-1.60257
Cl	-5.77349	-1.84115	2.13138
Cl	4.02408	-2.65141	2.49869
H	-3.76438	-2.15551	1.68752
H	-3.44901	-1.61003	-3.00928
H	-3.62547	-3.34687	-0.74781
H	-5.04938	-0.72681	0.61760
H	1.65026	-1.97032	-3.46077
H	0.55539	-3.08674	1.77202
H	4.06642	-2.70200	-1.10098
H	1.33335	-5.02512	-0.47671
H	-0.26671	3.92708	-1.80687
H	-3.84977	3.75029	0.35948
H	0.40584	3.89462	1.45158
H	3.43421	-0.61943	2.39217
H	2.55468	3.20021	-1.53820
H	5.11877	1.60184	0.07381
H	0.24198	4.66933	0.11782
H	-2.08309	3.50161	2.52830
H	3.97380	0.85486	2.61498
H	3.06937	3.13495	1.71561
H	5.08212	0.42858	-0.96838
H	2.41321	1.95214	-2.45603
H	-0.96900	2.67001	-2.42201
H	-3.10717	4.06116	-1.00069
H	-1.23506	-0.11523	1.76062
H	-2.91273	1.43426	-1.86205
H	0.91641	-0.86890	1.54889
H	2.94232	-0.39136	-2.19237
H	1.46908	-4.68197	-2.01784
H	2.08993	-3.30743	1.69880

H	-2.29294	-0.65857	-3.47600
H	-4.49603	0.71457	0.24178
H	-2.18247	-2.13307	1.98635
H	3.80074	-2.82207	0.46816

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Hf4_8_2_bridging_peroxide_conf1.log Energy: -3580319.4395593

Hf	2.36130	-0.30176	0.58723
O	1.69596	1.63978	1.14288
O	1.45392	0.73759	-1.01762
O	3.91699	-0.15404	-0.96317
O	1.94264	-0.48333	2.78337
O	3.72309	-2.03518	1.09335
O	4.16157	0.56175	1.65171
Hf	-0.45953	-2.71802	-0.35304
O	1.53694	-1.97989	-0.65416
O	1.14404	-2.03588	0.79739
O	-0.57408	-3.96429	1.50181
O	-0.28060	-3.10889	-2.55873
O	-2.24335	-3.98493	-0.76069
O	0.50746	-4.72462	-0.70571
Hf	0.56889	2.52150	-0.44121
O	-1.36732	1.82563	-0.95639
O	-1.03881	1.48551	0.47813
O	0.04127	3.82270	1.32834
O	1.00966	2.70389	-2.62663
O	2.34917	3.85335	-0.50712
O	-0.36290	4.42005	-1.27092
Hf	-2.52876	0.14693	-0.03367
O	-1.84444	-1.63480	0.86156
O	-1.16320	-0.94666	-1.23024
O	-3.49339	0.07568	-2.03679
O	-2.69734	0.42733	2.22423
O	-3.91051	1.87834	0.03428
O	-4.51341	-0.73799	0.47631
Cl	-0.12906	1.75091	3.68032
Cl	0.77537	-0.55563	-3.72084
Cl	0.97626	-3.13356	3.91010
Cl	-2.80775	4.76671	0.42672
Cl	4.06561	2.49431	-2.59394
Cl	-3.38302	-2.76395	-3.24870
Cl	6.49751	-0.99291	0.45843
Cl	-5.68448	1.18776	2.44047
H	3.95289	0.68422	-1.51052

H	1.71160	-1.40237	3.13039
H	3.44088	-2.89152	0.72433
H	5.06770	0.21153	1.41687
H	-1.39993	-4.39491	1.78479
H	0.22242	-2.37975	-3.03648
H	-2.82896	-3.64461	-1.51133
H	1.03346	-4.86689	-1.51335
H	-0.85333	4.24758	1.20556
H	1.95804	2.55321	-2.90029
H	2.78156	4.03298	0.34844
H	0.16677	5.23339	-1.17098
H	-3.49323	-0.82523	-2.48481
H	-3.56261	0.75806	2.58161
H	-4.60724	1.86795	0.74931
H	-5.08826	-0.27301	1.16080
H	-1.27700	4.62468	-0.90206
H	0.68834	3.51763	-3.05595
H	-4.40018	0.43039	-2.08273
H	-3.49790	2.79100	0.06259
H	-4.54583	-1.69586	0.65209
H	-1.96236	0.91468	2.67844
H	-0.04366	3.30637	2.17538
H	3.06790	3.53673	-1.14099
H	1.32984	0.32377	-1.91968
H	1.41769	1.81883	2.06764
H	-0.79907	-0.62526	-2.08951
H	-2.01881	-1.80051	1.80231
H	-0.05465	-3.69259	2.33614
H	0.91266	-5.21062	0.03472
H	-1.17373	-3.11422	-2.99335
H	1.26217	0.12086	3.17981
H	4.70779	-1.94496	0.94678
H	4.06276	0.48792	2.61984
H	4.85448	-0.41498	-0.74459
H	-2.07399	-4.92808	-0.94642

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Hf4_8_2_bridging_peroxide_conf2.log Energy: -3580314.4394948

Hf	2.65282	-0.02040	0.16469
O	1.63698	1.84007	0.76456
O	1.44466	1.50320	-0.69652
O	3.40255	0.23080	-1.91953
O	3.32688	-0.00149	2.29261
O	4.46784	-1.34422	0.15153

O	4.36266	1.44973	0.31478
Hf	0.02509	-2.35693	0.32301
O	1.79988	-1.68815	-0.77672
O	0.97879	-0.76272	1.24065
O	0.01127	-2.75396	2.59243
O	-0.01749	-3.66863	-1.52916
O	-1.31219	-4.17972	0.78568
O	1.47898	-4.02170	0.74499
Hf	-0.07872	2.77716	-0.03056
O	-1.63938	1.65549	-1.02866
O	-1.49012	1.35410	0.44549
O	-0.26381	3.17454	2.12335
O	0.21089	3.61728	-2.03111
O	1.19501	4.59774	0.23909
O	-1.71249	4.28286	0.09474
Hf	-2.63693	-0.20757	-0.42466
O	-1.80468	-1.49269	1.00081
O	-0.83441	-1.03472	-1.09545
O	-3.03205	-0.88464	-2.55056
O	-3.75645	0.47344	1.40829
O	-4.28850	1.05387	-1.29925
O	-4.33548	-1.60550	-0.15576
Cl	0.87594	0.95524	3.86841
Cl	0.74961	-1.73956	-3.71391
Cl	3.03578	-3.00427	3.17286
Cl	-3.30871	3.41383	2.48557
Cl	2.48170	2.61716	-3.62169
Cl	-3.20875	-4.01216	-1.75741
Cl	6.47484	0.19093	-1.48214
Cl	-6.68552	0.21526	0.31638
H	3.07126	1.01450	-2.45595
H	3.42272	-0.93850	2.62958
H	4.31714	-2.24729	-0.18211
H	5.17423	1.27811	-0.24286
H	-0.44764	-3.56892	2.86668
H	0.29389	-3.19228	-2.35804
H	-2.10908	-4.24643	0.19706
H	1.98147	-4.31524	-0.03724
H	-1.20385	3.27771	2.44963
H	1.02528	3.27707	-2.56956
H	1.25380	4.98323	1.13325
H	-2.20736	4.58621	-0.68756
H	-3.02382	-1.87023	-2.64966
H	-3.55168	1.38921	1.74711

H	-5.19977	0.96087	-0.88158
H	-5.28093	-1.28768	-0.11033
H	-2.39330	4.10394	0.82115
H	-0.51974	3.69596	-2.67070
H	-3.87385	-0.55570	-2.91761
H	-4.08312	2.00447	-1.37319
H	-4.26357	-2.47665	-0.62740
H	-4.74537	0.40548	1.36323
H	0.16212	2.48377	2.72124
H	1.12959	5.32970	-0.40154
H	0.71263	-0.35148	2.10142
H	1.81620	-1.70047	-1.76578
H	-0.47899	-0.99038	-2.01891
H	-2.20331	-1.64387	1.87342
H	0.91609	-2.77037	3.01332
H	2.14079	-3.82907	1.47607
H	-0.94759	-3.93975	-1.74035
H	2.65288	0.41669	2.90532
H	5.29086	-0.99388	-0.30927
H	4.66623	1.55665	1.23591
H	4.38082	0.16698	-2.07393
H	-0.84570	-5.03409	0.71359

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Hf4_4_2_bridging_peroxide_conf1_deprot4_ion6.log Energy: -2423585.0532839

Hf	-0.19648	-2.49494	-0.16542
O	-1.73246	-1.15141	-1.01124
O	-0.87464	-1.03560	1.18005
O	0.53493	-3.29512	1.52543
O	-0.50587	-3.24590	-2.38432
O	0.45396	-4.73618	-0.46329
O	-2.10579	-3.54616	0.18256
Hf	2.75498	-0.21239	-0.81851
O	1.87148	-2.16061	-0.84219
O	0.92105	-1.14166	-1.40773
O	3.23738	-0.16810	-2.76227
O	3.61511	-1.15426	1.13195
O	4.28243	1.36139	-0.32750
O	4.77323	-1.28976	-1.17679
Hf	-2.59513	0.09326	0.47918
O	-1.17003	1.75903	1.20505
O	-1.26407	1.65654	-0.30320
O	-3.96344	0.30740	-0.94398
O	-2.97352	0.02227	2.79042

O	-3.61519	-1.72180	1.00272
O	-3.72223	2.04238	1.19441
Hf	0.60816	2.40712	0.30936
O	1.65300	1.60119	-1.37720
O	1.64200	0.70776	0.83644
O	0.88866	3.52464	1.93724
O	-1.94378	3.98257	-2.55921
O	0.07508	4.10362	-0.98511
O	2.72222	3.57391	0.25029
Cl	1.48828	-0.84524	3.50550
Cl	-4.78950	3.48598	-1.28607
Cl	-6.69754	-1.79196	-0.78187
Cl	6.54872	-0.13220	1.09875
H	0.79156	-2.72788	2.27602
H	-0.30886	-2.49595	-2.97434
H	0.63835	-4.98107	0.46597
H	-2.05377	-4.24943	0.85254
H	2.55228	0.05420	-3.41035
H	3.05692	-1.12067	1.94640
H	3.90622	2.19731	0.03274
H	5.54396	-1.05651	-0.59777
H	-3.45144	-0.83613	2.76817
H	-7.50001	-2.74957	-0.45406
H	-2.96647	2.59539	1.47765
H	-2.80927	3.83663	-2.09769
H	-0.75454	4.05085	-1.60267
H	2.64648	4.07309	1.09103
H	-4.16005	2.55289	0.45507
H	-3.62748	0.69201	3.06239
H	0.20561	3.58390	2.62260
H	0.14811	5.01625	-0.65778
H	2.89799	4.22011	-0.45776
H	-1.83605	3.20324	-3.12976
H	-4.30234	1.18685	-1.20190
H	-4.47056	-1.78515	0.54298
H	-0.44236	-0.90112	2.04547
H	-2.35443	-1.33553	-1.73034
H	1.56497	0.30725	1.73816
H	1.88396	2.07093	-2.19181
H	4.98705	-1.03399	-2.09452
H	4.53328	-0.89175	1.39243
H	-1.37740	-3.58858	-2.64870
H	-0.10952	-5.42056	-0.86223
H	-2.80880	-2.82037	0.54432

H	5.08059	1.10258	0.20808

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Hf4_4_2_term_perox_conf1_ion10_diconf5.log Energy: -2423606.7121560

Hf	1.98008	1.45110	0.32590
O	0.30605	2.38667	1.08174
O	0.52318	1.72530	-1.14499
O	3.12228	2.48401	-1.37526
O	2.28309	1.40616	2.68532
O	4.14941	0.84132	0.71203
O	3.00511	3.37718	1.10175
Hf	1.43427	-1.95931	-0.44058
O	2.48291	-0.21948	-1.03400
O	1.29737	-0.41183	0.97893
O	2.08211	-2.88427	1.57055
O	2.06854	-2.30100	-2.71288
O	1.09925	-4.13686	-1.02089
O	3.51508	-2.95953	-0.68663
Hf	-1.46321	2.21574	-0.27484
O	-2.02642	0.53963	-1.58711
O	-1.68941	0.43121	0.85169
O	-2.20651	3.25619	1.34236
O	-1.64224	3.29327	-2.31589
O	-1.88841	4.12692	0.16287
O	-3.80754	2.22904	-0.40577
Hf	-2.08328	-1.30588	-0.36539
Cl	-0.35428	-0.24899	3.62458
Cl	1.98307	0.70338	-3.88008
Cl	4.14104	-1.08411	3.07167
Cl	-5.63893	-1.71223	2.33286
O	-0.39627	-2.50578	0.46523
O	-0.21625	-1.36427	-1.53776
O	-3.17860	-1.96796	-1.94180
O	-2.63011	-2.00644	1.80123
O	-4.30671	-0.47837	-0.10331
O	-3.08177	-2.98391	-0.83412
H	2.96191	2.16474	-2.29487
H	2.89878	0.68188	2.97915
H	4.36692	0.30005	-0.07173
H	2.56981	4.21447	0.85761
H	2.36319	-3.81124	1.66419
H	2.02831	-1.50241	-3.29546
H	0.30584	-4.53174	-0.61559
H	3.88264	-2.78084	-1.57288

H	-1.80008	2.80236	-3.14010
H	-3.84964	2.69219	0.46238
H	-3.59525	-1.99366	2.05432
H	-4.59712	-0.96155	-0.90926
H	-4.12653	1.30526	-0.25530
H	-2.31963	3.99083	-2.26389
H	-4.84367	-0.83181	0.66760
H	-2.15484	-1.52295	2.51007
H	-2.71044	0.60294	-2.26947
H	-1.39697	0.40913	1.78609
H	0.65325	1.43376	-2.06949
H	0.05571	2.76457	1.93927
H	0.75548	-0.50657	1.80311
H	2.55503	0.00458	-1.99096
H	-0.21619	-0.71240	-2.25815
H	-0.44120	-2.85514	1.36863
H	2.70764	-2.32766	2.11931
H	4.22077	-2.78975	-0.03712
H	1.50683	-2.97639	-3.13435
H	1.43115	1.16539	3.12398
H	4.30031	0.22258	1.48731
H	2.98782	3.32566	2.07776
H	4.06674	2.70505	-1.29106
H	1.80837	-4.80441	-1.03802

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Hf4_4_2_term_perox_conf1_ion10_diconf9.log Energy: -2423612.4005106

Hf	-1.21239	2.33117	-0.32469
O	0.83538	2.27111	-1.13785
O	0.40037	1.68790	1.06957
O	-1.54359	3.69021	1.53447
O	-1.51205	3.05186	-2.18182
O	-3.54557	2.75257	-0.40770
O	-1.38070	4.14921	-1.16404
Hf	-2.10639	-1.05462	0.35278
O	-2.24432	0.92679	1.07595
O	-1.64633	0.38601	-1.14780
O	-3.37034	-2.12553	-1.21622
O	-2.51769	-1.15085	2.74621
O	-2.10410	-3.23428	1.13978
O	-4.30799	-1.14373	0.93035
Hf	2.18635	1.20404	0.14545
O	2.37311	-0.65975	1.11520
O	1.57390	-0.36790	-1.09064

O	3.47578	1.63382	-1.73144
O	2.63259	1.78024	2.44740
O	2.81245	3.41036	0.39068
O	4.45297	1.20039	0.68557
Hf	1.20391	-2.21367	0.02305
Cl	-0.10713	-0.85316	-3.75369
Cl	0.10501	0.36521	3.92793
Cl	-6.10240	-0.88643	-1.47956
Cl	5.46764	-0.73941	-1.41535
O	-0.76421	-2.13167	-0.94642
O	-0.25341	-1.21631	1.23270
O	1.54207	-3.44381	1.58627
O	1.44935	-3.10983	-2.11933
O	3.39632	-2.84827	-0.41812
O	0.45764	-3.98839	0.69823
H	-0.83744	3.65641	2.20449
H	-3.99466	2.80968	0.45282
H	-2.89486	-2.44689	-2.00017
H	-1.80440	-0.75766	3.30229
H	-1.14788	-3.57759	1.07308
H	-4.51336	-0.65355	1.74466
H	4.13191	0.89823	-1.88281
H	1.97332	1.46084	3.10724
H	2.65430	3.67755	1.31664
H	4.88381	2.03980	0.43802
H	2.38634	-3.27582	-2.32482
H	3.74780	-3.26178	0.39041
H	4.93677	0.48671	0.17709
H	3.51374	1.49884	2.75206
H	4.05255	-2.14928	-0.69437
H	1.08113	-2.55200	-2.84734
H	3.02015	1.76710	-2.58033
H	2.23425	3.96061	-0.17065
H	2.62721	-0.77037	2.04314
H	1.13209	-0.21578	-1.95274
H	0.16387	1.29613	1.93928
H	0.81414	2.46325	-2.08790
H	-1.32601	0.14341	-2.04142
H	-2.44753	1.13749	1.99926
H	-0.01397	-0.86207	2.11657
H	-0.70739	-1.82205	-1.87506
H	-4.26732	-1.77384	-1.50248
H	-5.02891	-0.96631	0.25270
H	-2.52222	-2.10632	2.94519

H	-3.56735	3.64468	-0.80207
H	-1.64328	4.62786	1.28935
H	-2.64849	-3.82252	0.58687

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Hf4_4_2_term_perox_conf1_ion11_diconf5.log Energy: -2423605.7538048

Hf	-0.49606	2.18827	-0.20105
O	1.13237	1.66692	-1.39157
O	0.94871	1.24037	0.90598
O	-0.41757	3.42690	1.75469
O	-1.17864	2.86277	-2.31997
O	-2.48415	3.30751	-0.03505
O	0.39492	4.26287	-0.58129
Hf	-2.31025	-0.75980	0.50138
O	-1.78114	1.14140	1.27938
O	-1.40219	0.45983	-0.96150
O	-3.69117	-0.76206	-1.35789
O	-2.76786	-0.91129	2.82162
O	-3.50733	-2.65316	0.91216
O	-4.45051	-0.05608	1.11909
Hf	2.58534	0.36921	-0.32343
O	2.26143	-1.39524	0.89577
O	1.41378	-1.13828	-1.30710
O	3.47754	0.54586	-2.11631
O	3.44136	1.31980	1.62185
O	4.01690	1.57472	-1.16504
O	4.87710	-0.38490	0.18190
Hf	0.67185	-2.65082	0.03785
Cl	-0.71492	-1.13603	-3.66426
Cl	-0.14269	0.29572	3.90485
Cl	-4.18698	2.18508	-2.32839
Cl	2.50467	4.36241	1.68901
O	-1.43313	-2.27293	-0.68304
O	-0.56032	-1.47688	1.35579
O	1.18323	-3.89842	1.57583
O	0.43119	-3.65396	-2.07730
O	2.64351	-3.87961	-0.55911
O	0.15596	-4.49125	0.65066
H	0.52379	3.68565	1.97145
H	-2.13688	2.65236	-2.50856
H	-2.87227	2.92032	0.77492
H	1.20179	4.43324	-0.01714
H	-4.54434	-1.22880	-1.38096
H	-2.02080	-0.56793	3.38423

H	-3.24313	-3.37859	0.31617
H	-4.44631	0.21773	2.05534
H	3.19574	2.27800	1.70670
H	5.13261	0.33422	-0.45187
H	1.30764	-4.01471	-2.30273
H	2.55457	-4.27132	0.34861
H	5.19514	-1.22199	-0.19503
H	4.41103	1.26415	1.67503
H	3.39566	-3.26628	-0.49864
H	0.19185	-3.01177	-2.78856
H	2.61641	-1.52915	1.78667
H	0.98893	-0.94549	-2.16666
H	0.81383	0.95696	1.83456
H	1.46190	1.88058	-2.27765
H	-1.18159	0.08072	-1.84863
H	-1.46321	1.21964	2.20383
H	-0.20916	-1.10262	2.19530
H	-1.57581	-2.19667	-1.64702
H	-3.83878	0.13853	-1.76287
H	-4.89862	0.64270	0.60919
H	-2.90119	-1.83899	3.08874
H	-0.68373	2.48072	-3.06537
H	-3.15143	3.09390	-0.75017
H	0.64409	4.44982	-1.50348
H	-0.91424	4.26497	1.72094
H	-4.47007	-2.69482	1.05453

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Hf4_4_2_term_perox_conf1_ion11_diconf7.log Energy: -2423603.0372410

Hf	0.14140	-2.35772	-0.00141
O	1.42315	-1.25772	1.37723
O	1.37626	-0.85849	-0.99179
O	0.58964	-3.55988	-1.59835
O	-0.48536	-3.33421	2.01615
O	-0.21407	-4.25027	-0.53518
O	2.35143	-3.53109	0.26203
Hf	-2.49472	-0.00827	-0.45352
O	-1.35340	-1.57545	-1.34303
O	-1.30940	-0.95361	0.92436
O	-3.76628	-0.27004	1.51026
O	-3.04801	-0.05799	-2.72758
O	-4.38762	1.23024	-0.86039
O	-4.04985	-1.65126	-0.76647
Hf	2.32735	0.37849	0.37589

O	1.64482	2.07844	-0.70330
O	0.77924	1.43803	1.37199
O	3.02249	0.44289	2.66417
O	3.54879	0.52658	-1.64428
O	3.93463	-1.19928	0.51316
O	4.12167	1.78025	0.78940
Hf	-0.32592	2.76116	0.01531
Cl	-0.03241	-0.42347	3.91349
Cl	-0.13738	-0.20364	-3.92592
Cl	-3.67711	-3.37229	1.77945
Cl	5.34616	-1.84788	-2.11241
O	-2.19115	1.76678	0.66409
O	-1.04335	1.24239	-1.30519
O	-0.16107	4.08381	-1.52406
O	-0.89733	3.68560	2.11340
O	1.08109	4.63073	0.66297
O	-1.36332	4.33420	-0.65251
H	-1.46742	-3.49276	1.97728
H	2.10924	-3.87966	-0.63614
H	-4.70257	-0.00441	1.50894
H	-2.25113	-0.07544	-3.32068
H	-4.46255	2.08606	-0.40228
H	-3.84441	-2.10474	-1.60478
H	3.33186	1.32586	2.93330
H	4.04535	-0.29129	-1.94912
H	3.45195	-2.04399	0.68487
H	5.00832	1.41526	0.96508
H	-0.36221	4.50303	2.13587
H	0.96230	4.92943	-0.27435
H	4.24407	2.63673	0.34462
H	4.20305	1.24155	-1.72457
H	2.02795	4.44665	0.77657
H	-0.65571	3.19636	2.91957
H	2.33563	0.18745	3.31627
H	4.51428	-1.40236	-0.27820
H	1.90023	2.20114	-1.63107
H	0.41148	1.05111	2.19368
H	1.28078	-0.66064	-1.94527
H	1.04819	-1.09289	2.27142
H	-1.23719	-0.67440	1.85895
H	-1.03877	-1.53655	-2.26943
H	-0.58057	0.96564	-2.13046
H	-2.55057	1.84678	1.56118
H	-3.74923	-1.21630	1.82231

H	-4.00407	-2.34889	-0.04973
H	-3.57506	0.71545	-2.99729
H	-0.36738	-2.74638	2.79160
H	2.28287	-4.28034	0.87868
H	-5.28434	0.87781	-1.00354

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Hf4_4_2_term_perox_conf1_ion11_diconf9.log Energy: -2423609.5979027

Hf	-0.19258	-2.42199	-0.50270
O	-1.61120	-1.13433	-1.54820
O	-1.41813	-0.99596	0.76763
O	-1.09443	-3.65503	1.23924
O	-0.05979	-3.18868	-2.35916
O	1.50499	-3.99970	-0.18305
O	-0.94384	-4.00658	-1.46238
Hf	2.29399	-0.07558	0.44922
O	1.20273	-1.77464	1.11676
O	1.42942	-1.09710	-1.16808
O	4.05175	0.40897	-0.94290
O	2.75955	-0.31435	2.77591
O	3.38034	1.78577	1.36874
O	3.98837	-1.48421	0.80469
Hf	-2.53341	0.32836	-0.31584
O	-1.87827	1.97356	0.90007
O	-1.13381	1.53468	-1.28389
O	-3.50164	0.59428	-2.46876
O	-3.56157	0.06151	1.78985
O	-4.30666	-1.07288	-0.55446
O	-4.40574	1.71626	-0.31881
Hf	0.09189	2.64759	0.15002
Cl	0.82525	1.12727	-3.72269
Cl	-0.18497	-0.64612	3.81125
Cl	6.25931	-1.63644	-1.14439
Cl	-4.11676	-2.97560	1.83205
O	1.72935	1.58332	-0.79376
O	0.72749	0.98037	1.31464
O	0.33351	3.72998	1.87438
O	0.54625	3.75976	-1.85412
O	-1.15893	4.65323	-0.05740
O	1.56108	3.76225	1.01148
H	-2.02219	-3.37718	1.47178
H	1.87649	-3.95890	0.71480
H	3.87365	1.00201	-1.69137
H	1.94985	-0.41769	3.33779

H	2.73422	2.56792	1.34611
H	4.10834	-1.76824	1.72686
H	-4.08967	1.37234	-2.46477
H	-3.70082	-0.89751	2.02265
H	-4.33960	-1.48149	-1.43809
H	-5.30393	1.34119	-0.26968
H	-0.13294	4.42691	-2.05671
H	-0.86300	4.92167	0.84543
H	-4.39998	2.54566	0.19022
H	-4.40224	0.50908	1.98681
H	-2.12161	4.52356	0.00311
H	0.62677	3.17236	-2.64250
H	-2.89949	0.72482	-3.22206
H	-4.33505	-1.81631	0.11867
H	-2.09405	1.96077	1.84650
H	-0.70258	1.22619	-2.11349
H	-1.20763	-0.86125	1.71638
H	-1.67987	-1.34550	-2.49160
H	1.39294	-0.73061	-2.07242
H	0.82376	-1.75127	2.01756
H	0.33140	0.71829	2.17588
H	1.58539	1.40810	-1.75171
H	4.81354	-0.19887	-1.18086
H	4.82554	-1.64722	0.27228
H	3.17917	0.52652	3.03964
H	1.26217	-4.91991	-0.38077
H	-1.16776	-4.59270	0.98774
H	4.13262	2.03499	0.80275

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Hf4_4_2_term_perox_conf1_ion12_diconf5.log Energy: -2423603.9388340

Hf	2.47777	-0.12516	-0.54878
O	1.34437	-1.61614	-1.46811
O	1.36074	-1.13642	0.82739
O	3.82198	-0.36480	1.33944
O	3.10190	-0.01353	-2.82144
O	4.15838	1.39665	-0.90057
O	4.15561	-1.59972	-0.95028
Hf	0.27121	2.56756	0.05565
O	2.05388	1.56779	0.71773
O	1.01389	1.18767	-1.35125
O	0.05803	3.58788	-2.08841
O	0.85423	3.58988	2.06741
O	-1.06212	4.39823	0.43338

O	1.84568	4.16202	-0.31963
Hf	-0.17411	-2.48355	-0.10573
O	-1.24775	-1.37933	1.46919
O	-1.40702	-0.94077	-0.92474
O	-0.59840	-3.49611	-1.82521
O	0.74604	-3.63481	1.69580
O	0.25397	-4.28421	-0.87626
O	-2.11611	-3.67155	0.36844
Hf	-2.38081	0.24860	0.59684
Cl	-1.16212	1.06095	-3.60254
Cl	1.36783	1.07989	3.76873
Cl	-6.31960	-1.16316	-1.14201
Cl	3.93027	-3.44009	1.50950
O	-1.63718	1.99537	-0.59837
O	-0.70150	1.38381	1.44101
O	-3.28508	0.26191	2.42590
O	-3.77696	0.54615	-1.26543
O	-3.92229	-1.59450	0.68838
O	-3.89543	1.24035	1.45822
H	3.84172	-1.31653	1.63752
H	3.48434	0.85228	-3.05437
H	4.06573	2.17965	-0.32607
H	4.17640	-2.35111	-0.28729
H	-0.57369	4.32549	-2.16049
H	1.08746	2.92390	2.77507
H	-1.98983	4.25215	0.17194
H	2.20789	4.64892	0.44219
H	1.73340	-3.52067	1.70227
H	-2.22012	-4.05658	-0.52490
H	-4.64944	0.06192	-1.28513
H	-4.13910	-1.30777	1.60736
H	-2.85376	-3.02233	0.49420
H	0.59940	-4.58880	1.56613
H	-4.76504	-1.54301	0.14983
H	-3.36817	0.40425	-2.14002
H	-1.43698	-1.70390	2.36091
H	-1.33098	-0.69046	-1.86242
H	1.15210	-0.76679	1.70445
H	1.32691	-2.03899	-2.34009
H	0.45189	0.93669	-2.12426
H	2.19807	1.40637	1.67735
H	-0.26989	1.11774	2.28464
H	-1.81207	1.94513	-1.55822
H	-0.21360	2.94280	-2.78896

H	1.82304	4.74598	-1.09785
H	0.10522	4.10188	2.42336
H	2.44333	-0.21042	-3.51044
H	5.10663	1.23091	-1.04980
H	4.13788	-1.99357	-1.84078
H	4.75108	-0.07872	1.29831
H	-0.87212	5.35219	0.38714

64
Hf4_4_2_term_perox_conf1_ion12_diconf7.log Energy: -2423606.6589683

Hf	-0.15555	-2.50656	0.49875
O	1.35699	-1.22437	1.41992
O	0.94608	-1.31652	-0.93799
O	-0.05766	-4.04317	-0.85275
O	-0.13851	-3.09142	2.73899
O	-0.70388	-4.43296	0.44612
O	1.99388	-3.74542	0.64271
Hf	-2.74243	-0.14254	-0.07733
O	-1.80900	-1.88969	-0.77308
O	-1.55422	-1.00731	1.38978
O	-4.07201	-0.00937	1.90246
O	-3.57474	-0.50503	-2.25911
O	-4.41469	1.36755	-0.58272
O	-4.48987	-1.59821	-0.03661
Hf	2.15447	0.12074	-0.01731
O	1.33805	1.61188	-1.26076
O	0.77968	1.38661	1.01682
O	3.27131	0.63571	2.00849
O	2.96639	-0.16671	-2.23430
O	3.68041	-1.55079	0.13279
O	4.19911	1.19794	-0.40632
Hf	-0.42224	2.56989	-0.35312
Cl	0.07955	-0.04851	3.94894
Cl	-0.88101	-1.08728	-3.71046
Cl	3.98510	3.61584	1.38518
Cl	4.49986	-2.76689	-2.55003
O	-2.16671	1.72042	0.77179
O	-1.40014	0.87743	-1.28456
O	-0.46850	3.61303	-2.06316
O	-0.80077	3.80985	1.65588
O	1.22123	4.18785	0.07025
O	-1.57117	4.02467	-1.11624
H	-0.78706	-3.76510	3.00838
H	1.60535	-4.28045	-0.09738

H	-4.51530	0.80549	2.19622
H	-2.85343	-0.70988	-2.91329
H	-4.18137	2.24633	-0.22874
H	-4.83289	-1.88384	-0.90272
H	3.46754	1.60916	2.05506
H	3.34359	-1.05915	-2.48440
H	3.19697	-2.30954	0.54025
H	4.93319	0.67766	-0.02943
H	-1.61885	4.32900	1.55327
H	1.35677	4.61850	-0.79314
H	4.24847	2.09662	0.03776
H	3.71412	0.45218	-2.32974
H	2.11799	3.93814	0.42370
H	-0.07913	4.46792	1.62004
H	2.77492	0.42505	2.82082
H	4.06306	-1.93625	-0.70968
H	1.48949	1.57249	-2.21771
H	0.51449	1.18351	1.93487
H	0.69665	-1.28302	-1.88436
H	1.12029	-0.88317	2.31029
H	-1.25972	-0.55542	2.21224
H	-1.63824	-2.05965	-1.72145
H	-1.06755	0.45915	-2.11114
H	-2.21069	1.89099	1.72471
H	-3.71149	-0.43744	2.69885
H	-5.23388	-1.44842	0.57274
H	-4.00982	0.30420	-2.58387
H	-0.18761	-2.35634	3.39211
H	1.99243	-4.31191	1.43389
H	-5.38348	1.27376	-0.55814

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Hf4_4_2_term_perox_conf1_ion12_diconf9.log Energy: -2423612.0092019

Hf	-1.14301	2.20003	-0.77074
O	0.87715	1.82336	-1.49442
O	0.35480	1.59740	0.76965
O	-1.13877	3.88994	0.78231
O	-1.40406	2.56576	-2.73319
O	-3.42151	2.78142	-0.88267
O	-1.17709	3.82603	-1.95207
Hf	-2.42577	-0.94939	0.27000
O	-2.32957	1.09183	0.80102
O	-1.65135	0.16469	-1.30543
O	-3.57985	-1.62307	-1.69556

O	-3.24162	-0.81641	2.47684
O	-3.38492	-2.94310	0.93141
O	-4.68266	-0.50317	0.32129
Hf	2.10728	0.87101	-0.01457
O	2.06049	-0.82278	1.21826
O	1.31670	-0.82791	-1.01181
O	3.43751	0.86796	-1.93399
O	2.52927	1.66245	2.17129
O	3.05727	2.96431	-0.16811
O	4.34064	0.66590	0.59620
Hf	0.81100	-2.44515	0.39523
Cl	-1.01280	-1.88994	-3.61446
Cl	-0.99552	0.91880	3.70853
Cl	5.29260	-1.51532	-1.27301
Cl	1.64847	4.63791	1.98789
O	-1.21814	-2.51421	-0.50791
O	-0.72318	-1.28014	1.42221
O	1.34848	-3.35983	2.10394
O	0.90766	-3.62415	-1.65198
O	2.95851	-3.24847	-0.08972
O	0.53187	-4.25454	1.20354
H	-0.25733	4.05384	1.22094
H	-3.85148	2.93177	-0.02370
H	-4.14038	-2.41827	-1.66709
H	-2.64214	-0.28757	3.06976
H	-2.89908	-3.68896	0.53288
H	-4.90466	0.07725	1.07209
H	4.06916	0.09352	-1.91525
H	2.21648	2.59058	2.33776
H	2.95593	3.31122	-1.07258
H	4.83361	1.45305	0.29584
H	1.83985	-3.85175	-1.81625
H	3.21013	-3.55797	0.80135
H	4.79583	-0.11903	0.17480
H	3.47355	1.63256	2.40596
H	3.67321	-2.63234	-0.39941
H	0.55937	-3.18211	-2.45894
H	2.96157	0.79151	-2.77877
H	2.63227	3.63809	0.43909
H	2.31172	-0.77325	2.15294
H	0.85160	-0.71417	-1.85650
H	0.10303	1.43040	1.70265
H	0.92044	1.93257	-2.45661
H	-1.42552	-0.23912	-2.17202

H	-2.13766	1.32900	1.73070
H	-0.53951	-0.74150	2.22162
H	-1.26333	-2.67396	-1.46982
H	-2.98964	-1.73585	-2.48085
H	-5.04720	-0.09592	-0.48554
H	-3.29435	-1.70628	2.86994
H	-3.44898	3.61745	-1.38277
H	-1.39350	4.74272	0.38758
H	-4.33483	-3.15587	0.94486

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Hf4_4_2_term_perox_conf1_ion13_diconf5.log Energy: -2423604.3615307

Hf	-0.04592	2.39106	-0.24074
O	-1.88972	1.95198	0.67623
O	-1.18415	1.11118	-1.38394
O	0.12237	3.31644	-2.42474
O	0.00585	3.50308	1.78772
O	1.83678	3.70755	-0.23117
O	-1.23856	4.34574	-0.45910
Hf	2.23246	-0.26858	0.03886
O	1.56044	1.30782	-1.21827
O	0.88676	1.05756	1.04576
O	3.16433	0.30062	2.06338
O	3.21643	-0.63680	-2.05291
O	3.78729	-1.82802	0.41023
O	4.09413	1.07867	-0.30762
Hf	-2.87480	0.18307	-0.19908
O	-2.04368	-1.64823	-1.00221
O	-1.60608	-0.82007	1.19361
O	-4.09684	0.32761	1.37308
O	-3.63795	0.69683	-2.36332
O	-4.67120	1.08490	0.21508
O	-4.88427	-1.11980	-0.98735
Hf	-0.52955	-2.48488	0.35909
Cl	-0.09304	-0.12733	3.86902
Cl	0.60961	0.16618	-3.87393
Cl	2.95088	3.38935	2.64685
Cl	5.04696	-3.04222	-2.00109
O	1.31040	-1.65106	1.33973
O	0.81327	-1.42363	-0.96340
O	-0.60586	-4.05960	-0.94111
O	-0.60536	-3.02418	2.64777
O	-2.42885	-3.85690	0.88929
O	0.29208	-4.31090	0.24022

H	0.05531	2.65683	-3.14694
H	0.87980	3.45559	2.26891
H	2.47492	3.18094	-0.75441
H	-1.25397	4.67900	-1.37628
H	3.99692	-0.08996	2.38007
H	2.61456	-0.56606	-2.82733
H	3.35125	-2.51494	0.95075
H	4.36597	0.95505	-1.23803
H	-2.98480	0.77809	-3.07772
H	-5.36097	-0.39766	-0.49882
H	-1.45201	-3.48228	2.79647
H	-2.14702	-4.39489	0.10538
H	-5.13391	-1.96433	-0.57852
H	-4.29618	0.03233	-2.64134
H	-3.25554	-3.41921	0.62572
H	-0.58800	-2.24115	3.24927
H	-2.30025	-2.09168	-1.82369
H	-1.40974	-0.44952	2.07754
H	-0.78082	0.62478	-2.13458
H	-2.08309	2.17485	1.60046
H	0.57145	0.83809	1.95785
H	1.43079	1.09269	-2.17157
H	0.58938	-1.28815	-1.90481
H	1.21976	-1.35664	2.26828
H	3.13930	1.26193	2.32922
H	4.89598	1.01436	0.23950
H	3.78388	-1.45406	-2.19030
H	-0.24759	4.44347	1.76185
H	2.26994	3.79174	0.66582
H	-2.16732	4.20724	-0.19319
H	0.88091	3.88659	-2.64753
H	4.29810	-2.29961	-0.32773

64
Hf4_4_2_term_perox_conf1_ion13_diconf7.log Energy: -2423607.0298139

Hf	-0.48556	2.40159	-0.25712
O	-2.12143	1.31561	0.73857
O	-1.30737	0.80764	-1.47628
O	-0.45001	3.55400	-1.98334
O	-0.55278	3.41430	1.81944
O	-0.13317	4.31241	-0.73075
O	-2.74570	3.36445	-0.99496
Hf	2.34037	0.22473	-0.03145
O	1.35920	1.70495	-1.16424

O	0.73757	1.11467	0.98061
O	3.24140	1.05892	1.88511
O	3.04058	-0.03549	-2.27892
O	4.17599	-1.04502	0.20260
O	4.07805	1.66562	-0.61230
Hf	-2.60568	-0.40680	-0.40143
O	-1.44166	-2.09243	-0.87998
O	-1.88360	-1.34965	1.31702
O	-4.47011	-0.23791	1.08496
O	-3.04408	-0.73746	-2.75327
O	-4.16367	1.08753	-1.15512
O	-4.25486	-1.97882	-0.77575
Hf	0.08071	-2.42531	0.72385
Cl	-1.02486	0.61686	3.67994
Cl	0.06299	-0.87751	-3.73331
Cl	2.39742	3.90966	2.58795
Cl	5.31230	-2.04881	-2.37649
O	1.86719	-1.30012	1.42615
O	1.16830	-1.31116	-0.79963
O	0.32519	-4.13344	-0.30844
O	0.07485	-2.39905	3.07988
O	-1.46869	-4.03870	1.60497
O	1.19073	-4.07287	0.92213
H	0.37670	3.71572	2.04734
H	-2.11320	3.68325	-1.71054
H	4.17440	0.93724	2.12993
H	2.29854	-0.20881	-2.89858
H	3.87520	-1.79945	0.74627
H	4.23386	1.59476	-1.57355
H	-4.36694	-0.33067	2.04792
H	-2.24541	-0.77050	-3.32970
H	-3.74958	1.99936	-1.11700
H	-4.93150	-1.96072	-0.07257
H	-0.54665	-3.09361	3.36582
H	-1.24913	-4.70917	0.92420
H	-3.95090	-2.89913	-0.87388
H	-3.60805	-1.48975	-3.00383
H	-2.38598	-3.75776	1.44796
H	-0.22672	-1.55885	3.49864
H	-4.96852	0.58380	0.92483
H	-4.32273	0.90352	-2.10053
H	-1.17913	-2.28749	-1.79585
H	-1.83231	-0.83797	2.15163
H	-0.81136	0.48941	-2.26495

H	-2.07417	1.21513	1.70991
H	0.43309	0.83010	1.86574
H	1.58713	2.08513	-2.02649
H	0.82930	-1.28542	-1.72192
H	2.01006	-1.13034	2.36983
H	2.97271	2.00035	2.13222
H	4.94719	1.58384	-0.18204
H	3.73320	-0.73827	-2.46065
H	-0.77192	2.78922	2.54409
H	-3.03527	4.14080	-0.48608
H	4.66127	-1.42416	-0.60058

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Hf4_4_2_term_perox_conf1_ion13_diconf9.log Energy: -2423605.4853813

Hf	0.26900	2.58768	0.12560
O	2.01632	1.78931	-0.88836
O	1.42612	1.09478	1.24875
O	0.18798	3.64819	2.16807
O	0.34954	3.85655	-1.50223
O	-1.81563	3.91025	-0.18040
O	0.92165	4.44366	-0.24790
Hf	-2.16383	0.01408	0.01494
O	-1.26647	1.54005	1.29839
O	-0.93430	1.31428	-1.12772
O	-3.55106	-0.19493	-1.76432
O	-3.12784	-0.11176	2.09017
O	-3.17929	-2.09351	0.15017
O	-3.57073	1.80354	0.03214
Hf	2.81567	0.08683	0.09994
O	2.06827	-1.76553	0.86787
O	1.71012	-0.93834	-1.31959
O	4.12938	0.35926	-1.85418
O	3.58784	0.06251	2.35002
O	4.57087	1.49939	0.47689
O	4.66768	-1.28581	0.10168
Hf	0.36321	-2.40855	-0.39650
Cl	0.21792	-0.12353	-3.92129
Cl	0.93533	-0.71619	3.75893
Cl	-6.12150	1.37685	-1.57263
Cl	-4.77109	-2.53843	2.75960
O	-1.23493	-1.33198	-1.37625
O	-0.63344	-1.06908	0.93442
O	-0.01434	-3.86104	1.00372
O	0.39170	-3.06883	-2.64432

O	1.83837	-4.23266	-0.76317
O	-1.03438	-3.84377	-0.09830
H	0.32980	3.15331	2.99403
H	-1.89349	4.68206	0.40775
H	-3.69083	-1.15178	-1.88916
H	-2.55513	0.19697	2.81203
H	-2.45697	-2.78566	0.11708
H	-3.10998	2.64623	-0.19900
H	4.70295	-0.41548	-2.00043
H	2.85073	-0.10237	2.99785
H	4.72068	2.21087	-0.17081
H	5.57399	-0.97836	0.28619
H	1.14996	-3.64865	-2.83431
H	1.42564	-4.67160	0.02260
H	4.56042	-2.16549	0.50435
H	4.30834	-0.53712	2.61117
H	2.76943	-4.07791	-0.52918
H	0.41859	-2.32531	-3.29219
H	3.66410	0.49943	-2.69754
H	4.58249	1.89145	1.36941
H	1.93617	-1.85462	1.83209
H	1.42297	-0.52326	-2.16810
H	1.04662	0.68383	2.05925
H	2.21140	2.23007	-1.72964
H	-0.62817	1.07741	-2.02811
H	-1.91798	2.12189	1.72089
H	-0.36365	-0.99142	1.87392
H	-1.06396	-0.99784	-2.28097
H	-4.45276	0.24874	-1.79526
H	-4.45749	1.79185	-0.42808
H	-3.66074	-0.89475	2.42876
H	-1.29250	4.20897	-0.98079
H	0.71018	4.46788	2.22809
H	-3.75113	-2.32650	0.93000

64
Hf4_4_2_term_perox_conf1_ion14_diconf5.log Energy: -2423604.6258628

Hf	-1.58851	-2.10520	0.19598
O	0.27854	-2.73597	0.83840
O	-0.14371	-1.84710	-1.27448
O	-2.58348	-2.93985	-1.75919
O	-1.85050	-2.73725	2.49018
O	-3.80984	-1.96563	0.85693
O	-2.27632	-4.27100	0.45881

Hf	-1.83075	1.40758	0.28517
O	-2.40775	-0.36828	-0.76129
O	-1.31031	-0.35259	1.28671
O	-2.35694	1.72848	2.57957
O	-3.05697	2.06604	-1.54995
O	-2.25670	3.58852	0.60708
O	-4.09020	1.07833	0.75018
Hf	1.92458	-1.95653	-0.43320
O	1.93826	-0.06861	-1.56607
O	1.78737	-0.25871	0.88376
O	2.97478	-2.87454	1.06112
O	2.21612	-2.81327	-2.56217
O	2.84966	-3.71151	-0.17726
O	4.16852	-1.36861	-0.73073
Hf	1.68204	1.62010	-0.23408
Cl	-0.36587	-0.36326	4.09144
Cl	-1.65978	-0.18962	-3.67462
Cl	5.42791	3.23598	1.61304
Cl	-3.57469	5.03559	-1.63575
O	-0.02110	2.15780	1.08668
O	-0.32274	1.50100	-1.12995
O	2.32833	2.66259	-1.86371
O	2.55507	2.24635	1.84164
O	4.07598	1.37758	-0.41371
O	2.11287	3.52920	-0.65115
H	-2.29841	-2.45227	-2.56250
H	-2.78422	-2.57140	2.71997
H	-4.18225	-1.07873	0.66614
H	-2.13145	-4.88915	-0.28077
H	-2.37438	2.64373	2.91118
H	-2.81214	1.63277	-2.39585
H	-1.40766	4.02564	0.80853
H	-4.66871	1.36665	0.01869
H	2.05793	-2.30233	-3.37422
H	4.46068	-1.81639	0.09095
H	3.41709	2.75310	1.80873
H	4.00181	1.91482	-1.23998
H	4.28258	-0.39561	-0.59428
H	3.09111	-3.23026	-2.65352
H	4.62929	1.92062	0.21975
H	2.75490	1.47644	2.40213
H	2.38738	0.08995	-2.40875
H	1.48723	-0.41907	1.79320
H	-0.29326	-1.25752	-2.04067

H	0.56248	-3.16583	1.65966
H	-0.87536	-0.35048	2.18349
H	-2.41127	-0.35097	-1.74674
H	-0.42165	1.10711	-2.01987
H	0.18032	2.25440	2.03011
H	-1.87318	1.18218	3.24632
H	-4.41974	1.47537	1.57759
H	-3.22247	3.03760	-1.74597
H	-1.33226	-2.18954	3.13175
H	-4.50141	-2.63129	0.69712
H	-1.96567	-4.69995	1.27732
H	-3.55400	-3.00242	-1.81837
H	-2.73332	4.17318	-0.07065

64
Hf4_4_2_term_perox_conf1_ion14_diconf7.log Energy: -2423611.2169524

Hf	-0.07624	2.68322	-0.25391
O	1.83119	1.74261	-0.82720
O	0.69088	1.35834	1.25964
O	-0.52626	4.05551	1.22650
O	0.35030	3.43421	-2.38145
O	-0.75211	4.56126	-0.16673
O	1.90595	4.07440	0.58115
Hf	-2.47149	0.03633	-0.36542
O	-1.95486	1.88359	0.50486
O	-1.00622	1.09655	-1.44396
O	-3.27896	0.12247	-2.56234
O	-3.44774	0.11389	1.76298
O	-4.05129	-1.56162	-0.49543
O	-4.46609	1.23782	-0.39970
Hf	2.30297	0.21699	0.61994
O	1.46267	-1.58926	1.27314
O	1.47379	-0.88911	-0.96755
O	4.10699	0.19435	-0.83288
O	2.34225	0.35020	3.06325
O	3.50398	2.01062	1.35263
O	4.16523	-0.76696	1.61953
Hf	0.11124	-2.44493	-0.26919
Cl	1.09378	0.56364	-3.74920
Cl	-0.82637	0.18457	3.72067
Cl	4.93032	-2.76213	-0.53732
Cl	-5.47317	-2.13508	2.06303
O	-1.57376	-1.60661	-1.41621
O	-1.18681	-1.07555	0.81875

O	-0.11826	-3.89625	1.10163
O	0.40950	-2.99217	-2.57714
O	1.98354	-3.80072	-0.62612
O	-0.81903	-4.21628	-0.19739
H	-0.25379	4.10806	-2.73952
H	1.16136	4.42492	1.15121
H	-4.12551	-0.29015	-2.80961
H	-2.78666	0.16592	2.49308
H	-3.58871	-2.36135	-0.81220
H	-4.68532	1.48939	0.51753
H	4.44053	-0.73105	-0.99595
H	1.46933	0.29592	3.51905
H	3.05354	2.83849	1.02651
H	4.94087	-0.17498	1.61711
H	1.14648	-3.63192	-2.55333
H	1.87283	-4.43600	0.10668
H	4.45578	-1.57269	1.09873
H	2.92584	-0.31766	3.46467
H	2.89680	-3.41602	-0.54439
H	0.69754	-2.27306	-3.17173
H	4.01213	0.62439	-1.69959
H	3.39297	2.02197	2.32380
H	1.44938	-1.91053	2.18628
H	1.42045	-0.49461	-1.86454
H	0.16318	1.15179	2.06595
H	1.89766	1.52461	-1.77723
H	-0.53736	0.71896	-2.21863
H	-2.27690	2.28742	1.32548
H	-0.99552	-0.85445	1.75704
H	-1.64085	-1.67827	-2.38006
H	-3.23754	0.98856	-3.00509
H	-5.27178	0.83206	-0.76676
H	-4.08797	-0.61646	2.01119
H	0.46999	2.74284	-3.07396
H	2.16612	4.78193	-0.03298
H	-4.60801	-1.83188	0.30699

64
Hf4_4_2_term_perox_conf1_ion14_diconf9.log Energy: -2423611.9089510

Hf	-0.62989	2.55373	-0.27480
O	1.40596	2.21299	-0.96610
O	0.71849	1.61665	1.18123
O	-0.96874	3.91119	1.55301
O	-0.81330	3.42464	-2.12668

O	-3.04735	3.14633	-0.90372
O	-0.58514	4.40980	-1.02365
Hf	-2.34280	-0.55124	-0.11920
O	-1.97911	1.30057	0.88646
O	-1.20582	0.75010	-1.28455
O	-3.08056	-0.76231	-2.44321
O	-3.44174	-0.67473	1.89912
O	-3.97919	-2.13856	-0.41149
O	-4.19850	0.69932	-0.52192
Hf	2.40781	0.78891	0.33642
O	1.99696	-1.02337	1.29774
O	1.50753	-0.58246	-0.96885
O	3.86253	0.97583	-1.45716
O	2.87669	1.23746	2.65204
O	3.52385	2.78319	0.67439
O	4.57604	0.22911	0.98700
Hf	0.71307	-2.36440	0.09486
Cl	-0.17913	-0.69251	-3.86183
Cl	0.21874	0.22012	3.90944
Cl	5.38546	-1.69226	-1.20615
Cl	-6.19841	-1.87648	1.58982
O	-1.24640	-2.14817	-0.92781
O	-0.81322	-1.22977	1.17037
O	1.03795	-3.59393	1.64814
O	0.86357	-3.14264	-2.12394
O	2.81575	-3.27295	-0.37869
O	0.24799	-4.25709	0.54663
H	-0.47442	3.73691	2.37344
H	-3.36501	3.97406	-0.50384
H	-3.59584	-1.57418	-2.59500
H	-2.96757	-1.24282	2.53245
H	-3.60118	-3.03607	-0.36965
H	-3.89967	1.64648	-0.60508
H	4.38540	0.13427	-1.58876
H	2.12096	1.01669	3.25775
H	3.15188	3.46757	0.08729
H	5.18009	0.98237	0.84506
H	1.75351	-3.51677	-2.25153
H	2.99501	-3.73189	0.46348
H	4.95930	-0.52241	0.44785
H	3.64920	0.73111	2.96119
H	3.60860	-2.71179	-0.58519
H	0.71705	-2.46780	-2.83106
H	3.50173	1.20437	-2.33073

H	3.36649	3.07130	1.59411
H	1.98758	-1.12584	2.26317
H	1.21739	-0.35275	-1.87153
H	0.36897	1.24224	2.02515
H	1.51422	2.41699	-1.90822
H	-0.85249	0.47495	-2.16179
H	-2.40538	1.47652	1.73830
H	-0.55829	-0.76476	1.99759
H	-1.31519	-2.41061	-1.85749
H	-2.36815	-0.73502	-3.12487
H	-4.56578	0.46720	-1.39555
H	-4.39842	-0.98402	1.91150
H	-2.56311	3.39714	-1.73820
H	-0.86813	4.85928	1.35434
H	-4.79549	-2.13646	0.18335

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Hf4_4_2_term_perox_conf1_ion15_diconf5.log Energy: -2423603.5606278

Hf	1.07472	-2.02009	0.43641
O	2.49062	-0.56429	0.97018
O	1.30755	-0.60662	-1.02286
O	1.46304	-3.31250	-1.43495
O	1.48711	-2.25883	2.77602
O	0.21061	-4.03094	1.13725
O	2.88908	-3.36926	0.84799
Hf	-2.27887	-0.88871	0.20691
O	-0.83009	-2.24383	-0.60880
O	-0.56242	-1.14035	1.42424
O	-3.07236	-1.23647	2.39561
O	-3.08812	-1.54314	-1.83464
O	-4.44199	-0.28665	0.27179
O	-3.22166	-3.00413	0.37744
Hf	2.42384	1.21772	-0.31835
O	0.78196	2.22173	-1.30594
O	0.78844	1.64342	1.01287
O	3.46574	2.10127	1.14184
O	3.48222	0.28124	-2.17361
O	4.41317	1.48807	0.16046
O	3.45375	2.94113	-1.65059
Hf	-0.95023	2.40175	0.04306
Cl	0.25998	0.49029	3.93686
Cl	-0.66453	-0.85702	-3.63380
Cl	4.42580	-2.75431	-1.77613
Cl	-5.98375	-0.71808	-2.23706

O	-2.28019	1.00347	1.15600
O	-1.56444	0.61455	-1.03065
O	-1.58544	3.67584	-1.40813
O	-1.17877	3.12789	2.31879
O	0.08698	4.53499	0.42116
O	-2.50182	3.65107	-0.21354
H	2.39861	-3.18435	-1.77019
H	0.92296	-2.96387	3.14382
H	-0.66117	-4.23650	0.75117
H	3.59570	-3.24606	0.15364
H	-4.03061	-1.18670	2.56105
H	-2.47174	-1.34558	-2.58918
H	-4.46507	0.65649	0.52194
H	-3.26561	-3.36954	-0.52697
H	3.70066	-0.68022	-2.06991
H	4.23806	2.84043	-1.05077
H	-0.74143	3.99884	2.33765
H	-0.32732	4.84253	-0.41961
H	3.13948	3.85811	-1.58245
H	4.32122	0.72069	-2.39493
H	1.04552	4.50482	0.26169
H	-0.70191	2.56734	2.96830
H	0.77810	2.60865	-2.19321
H	0.85565	1.35238	1.94315
H	0.78508	-0.61420	-1.85311
H	3.00942	-0.50284	1.78622
H	-0.43988	-0.58905	2.23759
H	-0.75886	-2.38018	-1.57219
H	-1.22543	0.41045	-1.93304
H	-2.38553	1.06188	2.11799
H	-2.71513	-1.95585	2.94500
H	-4.09581	-3.15421	0.78012
H	-4.01039	-1.27216	-2.11846
H	1.25674	-1.44474	3.29150
H	0.72277	-4.85720	1.19785
H	3.28817	-3.16306	1.71295
H	1.32656	-4.27433	-1.37169
H	-5.07057	-0.40580	-0.51532

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Hf4_4_2_term_perox_conf1_ion15_diconf7.log Energy: -2423601.6649468

Hf	-1.05628	-2.26893	-0.30617
O	-2.07755	-0.59565	-1.25885
O	-1.47625	-0.61372	1.05103

O	-1.58050	-3.52186	1.22815
O	-1.59553	-2.97314	-2.45906
O	-1.28305	-4.23989	-0.05718
O	-3.53164	-2.58737	-0.14294
Hf	2.26888	-0.99041	-0.21416
O	0.83789	-2.25200	0.74161
O	0.65530	-1.44972	-1.46126
O	3.18078	-1.36766	-2.36898
O	3.09685	-1.49655	1.87146
O	4.45023	-0.38768	-0.25926
O	3.09429	-3.14028	-0.35321
Hf	-2.19178	1.05522	0.03805
O	-0.78050	2.30385	1.02473
O	-0.62214	1.70873	-1.24076
O	-3.27982	1.67044	-2.01835
O	-2.85842	1.29744	2.28913
O	-4.23247	0.11511	0.16495
O	-3.42292	3.01040	0.13987
Hf	1.11818	2.37784	-0.09162
Cl	-0.90874	-0.06020	-4.00220
Cl	0.54229	-0.80466	3.61600
Cl	-5.29154	-0.33869	2.98617
Cl	5.98567	-0.62412	2.28087
O	2.28123	0.88889	-1.21700
O	1.45844	0.53483	0.94683
O	1.76684	3.43392	1.52641
O	1.57193	3.32926	-2.20398
O	0.38985	4.67382	-0.25862
O	2.77690	3.37312	0.41020
H	-1.28824	-3.86372	-2.70377
H	-3.28832	-3.16106	0.62900
H	4.15378	-1.41792	-2.39063
H	2.47715	-1.28302	2.61189
H	4.48183	0.53406	-0.57796
H	2.67166	-3.62695	0.37954
H	-3.24746	2.63166	-2.17012
H	-3.55572	0.66652	2.64167
H	-4.11880	-0.81474	-0.15124
H	-4.39745	3.00069	0.12959
H	1.44011	4.28526	-2.05426
H	0.78785	4.78027	0.64280
H	-3.14476	3.77736	0.66909
H	-3.17498	2.17407	2.56712
H	-0.56406	4.82998	-0.16029

H	0.97806	3.10210	-2.94130
H	-2.91015	1.26217	-2.82685
H	-4.69552	0.02186	1.04876
H	-0.77491	2.36510	1.99297
H	-0.56319	1.30684	-2.13190
H	-1.13514	-0.59854	1.97093
H	-1.85629	-0.44792	-2.20582
H	0.49394	-0.98682	-2.30881
H	0.73306	-2.26192	1.71344
H	1.10599	0.33816	1.84715
H	2.46524	0.95523	-2.16650
H	2.84981	-2.17854	-2.79469
H	4.04798	-3.33539	-0.31092
H	4.01135	-1.20900	2.15490
H	-1.36699	-2.37235	-3.20179
H	-3.81783	-3.18207	-0.85786
H	5.06602	-0.44254	0.54423

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Hf4_4_2_term_perox_conf1_ion15_diconf9.log Energy: -2423609.6988752

Hf	-1.04725	-2.23647	-0.51891
O	-2.26543	-0.65085	-1.31883
O	-1.53265	-0.58612	0.89969
O	-1.98085	-3.26520	1.31310
O	-1.29275	-3.07624	-2.37479
O	0.50320	-4.23548	-0.96284
O	-2.19041	-3.66568	-1.33241
Hf	2.17493	-0.87390	-0.07670
O	0.68597	-2.13118	0.79675
O	0.64706	-1.26846	-1.44182
O	3.24774	-1.18217	-2.30199
O	2.96097	-1.48413	1.97721
O	4.35027	-0.26375	-0.04409
O	2.91744	-2.99559	-0.47922
Hf	-2.37064	1.04804	0.01272
O	-1.06537	2.32625	1.04565
O	-0.72999	1.62176	-1.18024
O	-3.47229	1.70510	-1.94462
O	-3.04029	0.97860	2.28070
O	-4.49759	0.19983	0.10282
O	-3.89396	2.80173	0.38769
Hf	0.91959	2.45246	0.04197
Cl	1.05498	0.66618	-3.91975
Cl	0.30907	-0.82546	3.66147

Cl	-4.46562	-1.75051	2.46896
Cl	5.84445	-0.65610	2.50619
O	2.23758	1.04490	-1.01059
O	1.33926	0.63860	1.12039
O	1.38357	3.58305	1.66498
O	1.37031	3.33615	-2.08600
O	-0.01999	4.64198	-0.26944
O	2.47029	3.56854	0.62078
H	-2.72687	-2.75113	1.73153
H	0.20890	-5.07419	-0.56806
H	4.14656	-0.80837	-2.32831
H	2.32581	-1.32895	2.71611
H	4.36247	0.67915	-0.29702
H	2.11064	-3.57245	-0.54308
H	-3.93357	2.55392	-1.80771
H	-3.40736	0.09143	2.54629
H	-4.72950	-0.22928	-0.74074
H	-4.81946	2.56326	0.57824
H	0.86112	4.15993	-2.18889
H	0.35086	4.86342	0.61955
H	-3.69924	3.64533	0.83169
H	-3.66113	1.64057	2.62997
H	-0.98564	4.64054	-0.15419
H	1.17049	2.76405	-2.86108
H	-2.93259	1.81870	-2.74684
H	-4.61747	-0.49955	0.81247
H	-1.15386	2.45359	2.00361
H	-0.52227	1.17372	-2.02175
H	-1.10722	-0.54262	1.78317
H	-2.53585	-0.72958	-2.24654
H	0.61586	-0.86472	-2.33620
H	0.52746	-2.07897	1.76110
H	0.98855	0.43209	2.01765
H	2.18716	1.05736	-1.98636
H	2.76136	-0.79568	-3.06451
H	3.30663	-2.99319	-1.37529
H	3.86940	-1.21955	2.29924
H	0.03964	-4.15347	-1.84048
H	-2.36001	-4.12920	1.07207
H	4.95677	-0.36890	0.75963

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Hf4_4_2_term_perox_conf1_ion1_diconf5.log Energy: -2423598.6990923

Hf	2.18121	1.15274	0.43014

O	0.60103	2.16904	1.34234
O	0.59527	1.42743	-0.85843
O	3.05318	2.07428	-1.42996
O	2.94578	1.00660	2.62606
O	4.48743	0.94820	0.50445
O	3.05961	3.18727	1.18300
Hf	1.22985	-2.21493	-0.05364
O	2.52685	-0.61187	-0.76912
O	1.33321	-0.60540	1.26115
O	1.60280	-3.18526	2.06072
O	1.95584	-3.02646	-2.10943
O	0.78718	-4.45701	-0.22191
O	3.35361	-3.08505	0.15960
Hf	-1.28024	2.05857	0.17002
O	-1.98819	0.69564	-1.41164
O	-1.78680	0.16779	0.97789
O	-1.89464	2.78296	1.97046
O	-1.25469	3.42787	-1.67225
O	-1.77859	3.86471	0.94104
O	-3.75454	2.35233	0.09014
Hf	-2.19601	-1.32175	-0.63185
Cl	1.30878	-1.05038	4.27960
Cl	-4.80628	0.23556	2.43686
Cl	1.41528	3.97074	-3.09458
Cl	1.49071	-0.52576	-3.81703
O	-0.75160	-2.51242	0.66438
O	-0.13593	-1.49325	-1.37934
O	-2.70372	-1.81040	-2.51199
O	-3.46088	-2.21255	1.12681
O	-4.32266	-0.37155	-0.59439
O	-2.83267	-2.97405	-1.55861
H	2.49213	2.70742	-1.98814
H	2.51153	0.38387	3.27356
H	4.86158	0.27444	-0.09129
H	3.82676	3.59496	0.74385
H	1.18060	-4.03446	2.27896
H	2.87618	-3.34476	-2.13590
H	-0.17355	-4.54315	-0.06008
H	4.06056	-2.43541	-0.00488
H	-0.38061	3.53848	-2.15231
H	-3.59671	3.28674	0.35056
H	-3.88061	-1.60766	1.78982
H	-4.12406	0.52583	-0.93251
H	-4.03854	1.92552	0.93158

H	-1.54226	4.32932	-1.44509
H	-4.69519	-0.22163	0.31045
H	-3.22456	-3.04335	1.56921
H	-1.95440	0.90167	-2.35705
H	-2.27974	0.17429	1.81672
H	0.58000	1.02210	-1.74298
H	0.39823	2.35238	2.27392
H	0.96357	-0.61863	2.17517
H	2.54998	-0.45601	-1.73923
H	0.10398	-1.15967	-2.27502
H	-0.91148	-2.42593	1.61640
H	1.55200	-2.60724	2.87461
H	3.47752	-3.42953	1.06554
H	1.85621	-2.36912	-2.85517
H	3.09309	1.85766	3.07537
H	4.76734	0.71311	1.41016
H	2.35133	3.85710	1.20023
H	3.98661	2.32378	-1.53689
H	0.96655	-4.82890	-1.10594

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Hf4_4_2_term_perox_conf1_ion1_diconf7.log Energy: -2423605.5202834

Hf	-1.58841	1.95836	-0.30108
O	0.28552	1.80334	-1.46155
O	0.17691	1.94076	0.94724
O	-2.31173	3.24550	1.13212
O	-2.28053	2.44778	-2.46685
O	-3.19476	3.12741	-0.07273
O	-0.68007	4.26603	-0.54662
Hf	-2.07051	-1.53914	0.05218
O	-2.32901	0.37704	0.98633
O	-1.80098	-0.00499	-1.27162
O	-3.02076	-2.30139	-1.97024
O	-3.06931	-2.12041	2.08950
O	-2.53026	-3.79641	0.19317
O	-4.35582	-1.17987	-0.02690
Hf	1.87935	1.37590	-0.12185
O	1.96408	-0.20944	1.32911
O	1.77085	-0.49414	-1.03713
O	2.94502	1.77692	-2.17737
O	2.90374	2.39316	1.65070
O	1.98823	3.64303	-0.49527
O	4.17665	0.90232	-0.06080
Hf	1.42615	-2.15234	0.39772

Cl	-2.25447	-0.23443	-4.24443
Cl	4.58343	-1.00841	-2.50298
Cl	0.88489	3.28842	3.65413
Cl	-1.49065	-0.41110	4.02797
O	-0.38993	-2.51879	-0.83230
O	-0.47056	-1.63538	1.34059
O	1.85653	-3.04175	2.14497
O	2.18717	-3.14198	-1.60321
O	3.77176	-2.07339	0.37898
O	1.55071	-4.03034	1.04102
H	-2.37161	1.72562	-3.13876
H	-1.23923	4.41036	0.26658
H	-3.04791	-3.25335	-2.16649
H	-4.02043	-1.91233	2.11761
H	-1.70436	-4.27510	-0.01345
H	-4.54389	-0.24177	0.16621
H	3.38800	1.03157	-2.64358
H	2.29943	2.76058	2.37944
H	1.06246	4.00367	-0.53027
H	4.77616	1.67102	-0.07665
H	2.49686	-4.05266	-1.45035
H	3.98354	-1.35543	1.00426
H	4.45169	0.34104	-0.83636
H	3.54080	1.80712	2.09718
H	4.17563	-1.80124	-0.47968
H	2.92003	-2.67190	-2.06383
H	2.48443	2.32439	-2.83547
H	2.46596	4.13800	0.19358
H	1.64000	-0.02685	2.22444
H	1.74094	-0.60535	-1.99855
H	0.19701	2.30974	1.86622
H	0.23701	1.31253	-2.29497
H	-1.77068	-0.12362	-2.25349
H	-2.16966	0.46640	1.94984
H	-0.52844	-1.25596	2.24906
H	-0.27385	-2.62313	-1.78910
H	-2.84702	-1.81369	-2.81793
H	-4.70447	-1.37624	-0.91707
H	-2.65103	-1.66211	2.87759
H	-3.12802	2.92632	-2.44603
H	-1.07618	4.78349	-1.26913
H	-2.77973	-4.02739	1.10848

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Hf4_4_2_term_perox_conf1_ion1_diconf9.log Energy: -2423616.7780229

Hf	-1.31073	2.09191	-0.67831
O	0.66925	1.92436	-1.48972
O	0.27464	1.60307	0.79612
O	-1.48888	3.71348	0.92191
O	-1.84234	2.53365	-2.60939
O	-3.85835	2.09680	-1.06803
O	-1.70339	3.74230	-1.73749
Hf	-2.32182	-1.14288	0.25202
O	-2.31070	0.90037	0.85413
O	-1.69423	0.05238	-1.31683
O	-3.40100	-2.08651	-1.69468
O	-3.29033	-1.12783	2.40098
O	-3.26322	-3.16497	0.79581
O	-4.46608	-0.37844	-0.00960
Hf	2.05382	1.03786	-0.04893
O	2.13417	-0.62301	1.22064
O	1.35034	-0.71021	-0.99617
O	3.28158	1.10752	-2.02443
O	2.47997	1.88710	2.11388
O	2.79731	3.20743	-0.24516
O	4.30974	1.04129	0.45923
Hf	1.01539	-2.35918	0.43924
Cl	-0.76610	-1.90990	-3.59113
Cl	5.34030	-1.10847	-1.39717
Cl	1.28680	4.75149	1.94360
Cl	-1.09996	0.68926	3.76683
O	-0.97452	-2.58530	-0.50857
O	-0.65123	-1.36433	1.46902
O	1.61690	-3.19621	2.16315
O	1.23378	-3.55704	-1.59408
O	3.22593	-2.97724	-0.03451
O	0.88412	-4.17016	1.27207
H	-0.61442	3.99894	1.31170
H	-4.30692	2.91445	-0.79170
H	-3.71411	-3.00218	-1.58372
H	-4.14167	-0.65236	2.37908
H	-2.59178	-3.85977	0.65248
H	-4.37356	0.56518	-0.31567
H	3.97761	0.38920	-2.01643
H	2.08406	2.78296	2.28446
H	2.64905	3.54825	-1.14555
H	4.72013	1.86648	0.13772
H	2.18114	-3.73496	-1.73124

H	3.53212	-3.22901	0.85694
H	4.81901	0.29179	0.03370
H	3.42921	1.94844	2.32139
H	3.87673	-2.31987	-0.39694
H	0.88468	-3.14724	-2.41657
H	2.79057	0.97791	-2.85404
H	2.32424	3.83951	0.37222
H	2.37825	-0.52714	2.15392
H	0.88285	-0.67170	-1.84800
H	0.06272	1.38127	1.72541
H	0.71929	2.07664	-2.44608
H	-1.42611	-0.31549	-2.18887
H	-2.11372	1.10493	1.79185
H	-0.53313	-0.82573	2.28423
H	-0.97723	-2.72059	-1.47594
H	-2.83427	-2.08619	-2.50244
H	-4.90880	-0.84980	-0.74016
H	-2.72121	-0.64511	3.05714
H	-3.52104	2.25623	-1.99103
H	-1.89123	4.52137	0.55575
H	-3.52756	-3.20015	1.73510

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Hf4_4_2_term_perox_conf1_ion2_diconf5.log Energy: -2423607.4992663

Hf	2.20851	1.11059	0.19299
O	0.74343	2.05872	1.32948
O	0.58845	1.61272	-0.99604
O	3.14312	2.18660	-1.59408
O	2.98096	0.78123	2.38045
O	4.47530	0.66180	0.10737
O	3.38180	2.99468	0.88234
Hf	1.11016	-2.20146	-0.47841
O	2.38587	-0.58347	-1.13428
O	1.27423	-0.65502	0.90158
O	1.71151	-3.14200	1.53762
O	1.42156	-2.61374	-2.74762
O	0.83819	-4.49297	-0.61533
O	3.18797	-3.22512	-0.75297
Hf	-1.18608	2.30082	0.22246
O	-2.06080	0.95496	-1.25960
O	-1.61702	0.36590	1.07395
O	-1.68985	3.07834	2.04834
O	-1.26209	3.69057	-1.61065
O	-1.35022	4.12391	1.02959

O	-3.52027	2.61933	0.25274
Hf	-2.26950	-1.04082	-0.45671
Cl	0.28096	-0.03392	3.76913
Cl	4.64418	-2.00956	1.74278
Cl	-6.14548	-1.85484	1.62032
Cl	1.06807	3.10527	-3.65673
O	-0.78376	-2.55699	0.28504
O	-0.33473	-1.07976	-1.51611
O	-3.33800	-1.30574	-2.16391
O	-3.10410	-2.00566	1.49365
O	-4.41746	-0.02362	-0.11918
O	-3.32916	-2.52872	-1.28607
H	2.60580	2.52164	-2.36815
H	3.54228	-0.02948	2.41450
H	4.72148	-0.24344	0.43199
H	3.37846	3.70243	0.21193
H	1.75908	-4.11502	1.54697
H	0.68055	-2.14536	-3.18061
H	-0.03428	-4.85330	-0.85435
H	3.63214	-2.97403	-1.58332
H	-0.56739	3.63838	-2.31759
H	-3.50539	2.86745	1.20208
H	-4.09791	-2.11533	1.54132
H	-4.63945	-0.25113	-1.05144
H	-3.95112	1.73436	0.18315
H	-1.32866	4.62227	-1.33863
H	-5.07110	-0.52305	0.45100
H	-2.87059	-1.51200	2.29852
H	-2.48370	1.22455	-2.08666
H	-1.25270	0.19274	1.96424
H	0.67243	1.89689	-1.93660
H	0.57371	1.91778	2.28015
H	0.83430	-0.66105	1.78809
H	2.71432	-0.50619	-2.04366
H	-0.09886	-0.14085	-1.67011
H	-1.01856	-3.11276	1.04474
H	2.57194	-2.80235	1.89397
H	3.80823	-2.93403	-0.02867
H	1.45141	-3.50584	-3.13775
H	2.22991	0.58603	3.00155
H	4.99445	1.29676	0.63574
H	3.05265	3.38220	1.71331
H	4.01879	1.90272	-1.90919
H	1.52442	-5.08372	-0.97396

64
Hf4_4_2_term_perox_conf1_ion2_diconf7.log Energy: -2423610.7539571

Hf	-1.54954	-1.99793	-0.14417
O	0.30037	-2.22186	0.99923
O	0.19705	-1.53261	-1.30379
O	-2.23531	-2.96680	-1.83239
O	-2.42575	-2.49105	1.94629
O	-3.09772	-3.17608	-0.62540
O	-0.57879	-4.34034	-0.49258
Hf	-2.04357	1.53418	-0.21233
O	-2.36400	-0.30966	-1.22056
O	-1.55177	-0.08623	0.94926
O	-2.92814	1.91188	1.93019
O	-2.79388	2.12119	-2.37143
O	-2.70270	3.73665	-0.31057
O	-4.33609	1.44446	-0.27428
Hf	1.90482	-1.37397	-0.14143
O	2.30552	0.44676	-1.10991
O	1.49400	0.28112	1.11451
O	2.86348	-1.99667	1.89856
O	2.57824	-1.96389	-2.43693
O	2.06375	-3.63220	-0.48413
O	4.17197	-1.79140	-0.41299
Hf	1.45399	2.16603	-0.01056
Cl	-0.00943	-0.86367	3.72361
Cl	-4.90182	-0.47055	2.09569
Cl	5.36214	-0.10442	1.77691
Cl	0.62684	0.02656	-3.94840
O	-0.54876	2.57987	0.85053
O	-0.24878	1.65359	-1.27514
O	2.29889	3.20266	-1.51002
O	1.74983	3.00999	2.20026
O	3.71240	2.29690	0.61940
O	1.70663	4.10024	-0.45091
H	-3.27678	-1.98209	2.03008
H	-1.15457	-4.23554	-1.30349
H	-3.45480	2.71514	2.08671
H	-2.33605	1.72788	-3.13587
H	-2.11362	4.37633	0.12828
H	-4.66634	1.18121	-1.15224
H	3.64676	-1.42225	2.11240
H	2.06685	-1.49922	-3.14376
H	1.15059	-4.01383	-0.37945

H	4.40913	-2.70077	-0.15125
H	2.68255	3.29801	2.17326
H	4.11062	2.58953	-0.22154
H	4.73295	-1.19328	0.16748
H	3.51883	-1.75515	-2.57777
H	4.21009	1.49266	0.92461
H	1.70095	2.38148	2.94234
H	2.26368	-1.92398	2.66770
H	2.27621	-3.73249	-1.43355
H	2.30797	0.51087	-2.08140
H	1.10782	0.11811	2.00006
H	0.14332	-1.14168	-2.20762
H	0.23981	-1.96778	1.94679
H	-1.15552	-0.00898	1.84068
H	-2.73058	-0.53555	-2.08914
H	-0.07070	1.19047	-2.12467
H	-0.66747	2.79059	1.78960
H	-3.50450	1.14808	2.21194
H	-4.69549	0.77999	0.38187
H	-2.75362	3.08632	-2.50467
H	-1.86835	-2.15804	2.68354
H	-0.99511	-5.01546	0.07003
H	-3.62016	4.05461	-0.23062

64
Hf4_4_2_term_perox_conf1_ion2_diconf9.log Energy: -2423616.5357227

Hf	-0.92441	2.34550	-0.42336
O	0.95319	1.89376	-1.43827
O	0.71197	1.59779	0.89235
O	-1.02633	3.84191	1.28706
O	-1.40415	2.98427	-2.31895
O	-3.37205	2.77886	-0.72590
O	-1.04282	4.09566	-1.38358
Hf	-2.27075	-0.80974	0.52588
O	-1.98661	1.21977	1.12454
O	-1.62298	0.38523	-1.08610
O	-3.73241	-2.29493	-0.35369
O	-3.50764	-0.58115	2.44999
O	-2.28458	-2.75119	1.88091
O	-4.24924	0.29529	0.06775
Hf	2.36865	0.90063	-0.14039
O	2.34950	-0.74688	1.17904
O	1.43677	-0.76019	-0.99366
O	3.43350	0.74446	-2.20410

O	3.17712	1.91387	1.84702
O	3.25199	2.99832	-0.51769
O	4.63749	0.68544	0.15457
Hf	0.92491	-2.29723	0.44641
Cl	-0.32396	-1.43151	-3.49029
Cl	-6.08834	-1.23932	-1.84870
Cl	5.18045	-1.74697	-1.55403
Cl	0.87779	3.02402	3.60978
O	-1.08658	-2.23624	-0.52991
O	-0.41364	-0.92867	1.48755
O	1.25440	-3.23309	2.20060
O	0.97780	-3.59960	-1.49807
O	3.00108	-3.27991	0.06552
O	0.08266	-3.83521	1.48155
H	-0.45559	3.72523	2.09565
H	-3.68884	3.61252	-0.33740
H	-3.23632	-2.97011	-0.85163
H	-4.40202	-0.23932	2.26430
H	-1.36827	-3.19496	1.87539
H	-4.03406	1.22057	-0.20970
H	3.97619	-0.09177	-2.23700
H	2.59781	2.25722	2.57712
H	2.66508	3.52392	-1.09245
H	5.13237	1.40618	-0.27872
H	1.86979	-3.94901	-1.67072
H	3.36329	-3.51586	0.93808
H	4.99004	-0.16525	-0.24327
H	4.00498	1.57573	2.22867
H	3.70487	-2.75752	-0.41037
H	0.67662	-3.14035	-2.31797
H	2.88896	0.73818	-3.01003
H	3.35230	3.48123	0.32439
H	2.59536	-0.67831	2.11417
H	0.98187	-0.73407	-1.86531
H	0.74289	1.93177	1.82328
H	0.87409	1.95275	-2.40359
H	-1.30944	-0.00158	-1.93104
H	-2.26076	1.54315	1.99515
H	-0.02761	-0.04138	1.62586
H	-1.03650	-2.12325	-1.50364
H	-4.55171	-2.05127	-0.89526
H	-4.90793	-0.06314	-0.58902
H	-3.58464	-1.41707	2.94590
H	-3.06491	2.98206	-1.65183

H	-0.95507	4.77173	1.00853
H	-2.90639	-3.41478	1.53436

64
Hf4_4_2_term_perox_conf1_ion3_diconf5.log Energy: -2423606.4494429

Hf	-2.06525	1.40440	-0.22054
O	-0.48978	2.36673	-1.16100
O	-0.53654	1.85108	1.11625
O	-3.21874	2.18096	1.70883
O	-2.78662	1.45003	-2.46996
O	-4.31761	1.12349	-0.42619
O	-2.91522	3.52083	-0.52217
Hf	-1.34976	-1.99291	0.31072
O	-2.34306	-0.26940	1.08630
O	-1.41129	-0.41195	-1.07139
O	-1.92486	-2.96910	-1.71857
O	-1.95836	-2.67182	2.49121
O	-1.04494	-4.24672	0.53389
O	-3.59606	-2.55311	0.30359
Hf	1.38688	2.27901	0.06732
O	1.96384	0.69051	1.46712
O	1.63399	0.42462	-0.92350
O	2.02942	3.16945	-1.65943
O	1.61009	3.47353	2.05934
O	1.75133	4.14887	-0.55691
O	3.70542	2.37136	0.22779
Hf	2.12236	-1.20490	0.41489
Cl	0.49702	-0.82401	-3.55684
Cl	-4.53517	-1.25790	-2.41542
Cl	5.96095	-1.58766	-1.94876
Cl	-1.38899	0.22907	3.89774
O	0.49543	-2.37590	-0.61228
O	0.22354	-1.43427	1.52320
O	3.13677	-1.75953	2.09446
O	2.92261	-1.96757	-1.63539
O	4.33302	-0.31525	0.27512
O	3.07259	-2.84954	1.05785
H	-2.83925	1.90190	2.56912
H	-3.27594	0.62202	-2.70485
H	-4.72483	1.00950	0.45247
H	-3.73141	3.54874	-1.05618
H	-2.17330	-3.91100	-1.70358
H	-2.82022	-3.06700	2.71473
H	-0.14489	-4.44108	0.20607

H	-4.05982	-2.00421	0.96276
H	0.78855	3.62456	2.55929
H	3.83764	2.72584	-0.67551
H	3.89844	-1.90590	-1.82583
H	4.53101	-0.73420	1.14581
H	4.06053	1.44712	0.23645
H	1.96906	4.35534	1.85155
H	4.96962	-0.69479	-0.40086
H	2.45369	-1.60433	-2.41783
H	2.41835	0.84425	2.30755
H	1.36759	0.28553	-1.85583
H	-0.50096	1.41030	1.98913
H	-0.26653	2.65094	-2.06162
H	-0.88109	-0.46857	-1.91016
H	-2.25835	-0.12467	2.06042
H	0.11900	-0.90168	2.33625
H	0.50608	-2.39757	-1.58807
H	-2.62999	-2.48800	-2.21780
H	-4.04013	-2.32185	-0.55528
H	-1.77262	-1.99939	3.18897
H	-2.09169	1.54012	-3.14566
H	-4.61923	0.36666	-0.99848
H	-2.27305	4.11488	-0.95280
H	-3.25671	3.15488	1.72282
H	-1.09793	-4.59123	1.44469

64
Hf4_4_2_term_perox_conf1_ion3_diconf7.log Energy: -2423610.9358470

Hf	-1.58670	-1.95869	-0.13417
O	0.29613	-2.20754	0.94409
O	0.15479	-1.54106	-1.37361
O	-2.32908	-2.94498	-1.78262
O	-2.38594	-2.48602	1.99324
O	-3.20678	-3.04024	-0.57223
O	-0.71564	-4.32519	-0.41221
Hf	-1.95662	1.58450	-0.11972
O	-2.29695	-0.23538	-1.22356
O	-1.57083	-0.06960	1.02364
O	-2.86373	2.11450	1.95119
O	-2.69649	2.29435	-2.25469
O	-2.51773	3.81788	-0.13946
O	-4.22200	1.15173	-0.19926
Hf	1.88951	-1.42243	-0.23302
O	2.31919	0.39394	-1.18740

O	1.55106	0.22674	1.04574
O	2.88327	-2.10219	1.77872
O	2.53141	-2.07350	-2.54086
O	1.95755	-3.68601	-0.54871
O	4.14103	-1.91312	-0.57634
Hf	1.56039	2.13381	-0.03996
Cl	0.07187	-0.91842	3.69788
Cl	-4.72830	-0.29075	2.49826
Cl	5.42223	-0.26462	1.59316
Cl	-0.81522	0.31348	-3.94730
O	-0.38964	2.52386	0.95211
O	-0.20816	1.71205	-1.23466
O	2.35762	3.17370	-1.56141
O	1.98131	2.92644	2.16760
O	3.84394	2.19426	0.49471
O	1.83391	4.06666	-0.46172
H	-3.19943	-1.94013	2.15879
H	-1.31336	-4.25547	-1.21039
H	-3.41532	2.91719	1.98053
H	-3.64132	2.19713	-2.47289
H	-1.76876	4.32669	0.22583
H	-4.20406	0.38728	-0.81290
H	3.68458	-1.54713	1.97545
H	2.00419	-1.88589	-3.33602
H	1.04135	-4.04350	-0.39995
H	4.35550	-2.83088	-0.32457
H	2.91800	3.19537	2.10661
H	4.23645	2.49356	-0.34601
H	4.73240	-1.33594	-0.00482
H	3.46673	-1.92626	-2.76630
H	4.33021	1.37537	0.78184
H	1.95162	2.27967	2.89493
H	2.30345	-2.01325	2.56112
H	2.14746	-3.82782	-1.49693
H	2.62215	0.48432	-2.10288
H	1.11909	0.07279	1.91121
H	0.02238	-1.10304	-2.24064
H	0.26881	-1.95998	1.89579
H	-1.21469	-0.04308	1.93574
H	-2.12305	-0.28375	-2.18681
H	-0.13889	1.31131	-2.13185
H	-0.47495	2.68971	1.90345
H	-3.41267	1.37564	2.33888
H	-4.57233	0.76145	0.65209

H	-2.19567	1.85452	-2.98815
H	-1.77204	-2.21961	2.71298
H	-1.11020	-4.97420	0.19544
H	-2.66623	4.14597	-1.04682

64
Hf4_4_2_term_perox_conf1_ion3_diconf9.log Energy: -2423614.4276171

Hf	-0.99441	2.37543	-0.35336
O	0.99644	2.18251	-1.22926
O	0.61667	1.74276	1.02554
O	-1.38521	3.82542	1.41703
O	-1.44918	3.10947	-2.20686
O	-3.45653	2.66600	-0.60499
O	-1.18990	4.18277	-1.19358
Hf	-2.17614	-0.89365	0.31759
O	-1.98870	1.09592	1.11094
O	-1.64177	0.48601	-1.18524
O	-3.45537	-1.93665	-1.22300
O	-2.98805	-1.01448	2.53650
O	-2.31622	-3.12536	1.05267
O	-4.23759	0.10443	0.35297
Hf	2.32102	1.07251	0.10081
O	2.33670	-0.73298	1.17443
O	1.56767	-0.49196	-1.04665
O	3.63034	1.26408	-1.80776
O	2.83964	1.76086	2.38784
O	3.11797	3.22630	0.19162
O	4.56716	0.92722	0.66616
Hf	1.06444	-2.25240	0.15601
Cl	-0.11010	-0.93059	-3.70279
Cl	-6.40655	-1.37426	-1.19549
Cl	5.45296	-1.19438	-1.30393
Cl	-0.28234	0.76576	3.83807
O	-0.86975	-2.08359	-0.85715
O	-0.38256	-1.16333	1.33147
O	1.32709	-3.44706	1.76147
O	1.26778	-3.23623	-1.96269
O	3.20197	-3.06904	-0.23659
O	0.27377	-3.99484	0.83627
H	-0.91184	3.73373	2.26313
H	-3.76846	3.48414	-0.18019
H	-3.20828	-2.87568	-1.28886
H	-3.78658	-0.45472	2.57998
H	-1.38091	-3.50209	1.07176

H	-4.10997	1.04724	0.09062
H	4.22100	0.46099	-1.87122
H	2.16824	1.62957	3.08692
H	3.01211	3.57232	1.09881
H	5.06570	1.71725	0.38442
H	2.18947	-3.49107	-2.14391
H	3.49895	-3.47473	0.59770
H	5.00786	0.15265	0.20860
H	3.68802	1.42976	2.73219
H	3.92041	-2.44335	-0.53089
H	0.96372	-2.67281	-2.71469
H	3.18925	1.33729	-2.67154
H	2.58315	3.79245	-0.39648
H	2.63161	-0.82172	2.09271
H	1.12562	-0.35712	-1.91357
H	0.37203	1.43408	1.92878
H	0.99319	2.29935	-2.19197
H	-1.36857	0.20416	-2.08402
H	-1.73288	1.18156	2.04840
H	-0.15154	-0.72607	2.17801
H	-0.83835	-1.87445	-1.81421
H	-4.45788	-1.87011	-1.27783
H	-5.03072	-0.25539	-0.13724
H	-2.37106	-0.67453	3.21963
H	-3.22151	2.91152	-1.53483
H	-1.29873	4.75676	1.14530
H	-2.64294	-3.14353	1.96990

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Hf4_4_2_term_perox_conf1_ion4_diconf5.log Energy: -2423604.3496708

Hf	-2.42820	0.61889	-0.57845
O	-1.07379	1.95974	-1.40901
O	-0.97329	1.15160	0.78756
O	-3.63760	1.22361	1.22337
O	-2.97419	0.36868	-2.90598
O	-4.55082	-0.20857	-0.88101
O	-3.78500	2.33871	-1.41042
Hf	-0.75403	-2.40583	0.12029
O	-2.41888	-1.16057	0.73661
O	-1.46206	-1.06493	-1.35136
O	-0.64021	-3.80044	-1.76775
O	-1.25812	-3.35631	2.13592
O	0.82110	-3.97868	0.63532
O	-2.56971	-3.80735	-0.10590

Hf	0.62961	2.47647	-0.04518
O	1.67197	1.13684	1.41638
O	1.72221	0.91432	-1.02167
O	1.09393	3.58777	-1.68615
O	0.12109	3.52318	1.92098
O	0.38140	4.37374	-0.62501
O	2.76779	3.30922	0.38868
Hf	2.30085	-0.62935	0.38532
Cl	-0.44525	-1.63983	-4.07226
Cl	5.96221	0.62316	-1.98194
Cl	-2.71012	3.37844	3.08306
Cl	-0.21270	-1.68675	4.37640
O	1.02799	-1.84773	-0.87967
O	0.38104	-1.24373	1.37818
O	3.20862	-1.40301	2.01485
O	3.61992	-1.22704	-1.40905
O	4.20655	0.81423	0.48184
O	3.01192	-2.46908	0.96969
H	-3.27351	1.94238	1.84173
H	-2.37471	-0.13796	-3.49679
H	-4.81922	-0.94605	-0.30435
H	-4.73451	2.34939	-1.19391
H	0.17583	-4.33286	-1.72394
H	-2.13177	-3.76306	2.26533
H	1.67576	-3.46946	0.86599
H	-3.44256	-3.38505	-0.02121
H	-0.79969	3.40478	2.29935
H	2.92945	3.69423	-0.49519
H	4.39019	-0.66393	-1.71316
H	4.68880	0.58169	1.29630
H	3.35126	2.51847	0.47691
H	0.24819	4.48280	1.82053
H	4.87928	0.80053	-0.26382
H	3.99447	-2.08916	-1.14979
H	1.48144	1.19004	2.36383
H	1.73751	0.85997	-1.98784
H	-0.61269	0.44794	1.36085
H	-1.03899	2.39174	-2.27662
H	-1.04238	-1.08188	-2.25411
H	-2.64299	-1.01553	1.67002
H	0.34852	-1.30942	2.37010
H	1.05173	-1.68182	-1.83755
H	-0.60239	-3.29822	-2.62689
H	-2.54794	-4.28802	-0.95501

H	-0.99764	-2.87638	2.98770
H	-3.23480	1.18046	-3.37565
H	-4.67348	-0.49924	-1.80560
H	-3.44837	3.23799	-1.24313
H	-4.60201	1.34300	1.18651
H	0.55921	-4.46912	1.43594

64
Hf4_4_2_term_perox_conf1_ion4_diconf7.log Energy: -2423611.8260884

Hf	-1.20980	2.14262	-0.59961
O	0.73089	1.52903	-1.40772
O	0.30399	1.92845	0.92474
O	-1.98337	3.66776	0.53433
O	-1.21581	2.67509	-2.90070
O	-2.68600	3.47487	-0.78182
O	0.07480	4.21607	-0.87591
Hf	-2.38366	-1.12425	-0.12370
O	-2.38862	0.83982	0.69183
O	-1.99457	0.31114	-1.59079
O	-3.54632	-2.27035	-1.77815
O	-3.63186	-1.48144	1.79054
O	-2.54161	-3.40786	0.36652
O	-4.56550	-0.29135	-0.36970
Hf	2.05083	1.02752	0.15211
O	1.74997	-0.61187	1.48725
O	1.91730	-0.82681	-0.86757
O	3.51733	1.22519	-1.68851
O	2.75499	1.97715	2.12475
O	2.56108	3.24399	-0.20380
O	4.24765	0.53544	0.70352
Hf	0.88912	-2.29988	0.36044
Cl	0.07924	-0.31378	-3.83337
Cl	5.23000	-1.50216	-1.28249
Cl	0.64348	3.35144	3.71066
Cl	-1.96905	-0.05786	3.84230
O	-0.74433	-2.06339	-1.09627
O	-0.85751	-1.35236	1.22866
O	0.81265	-3.50792	1.96993
O	1.41516	-3.52911	-1.59674
O	3.06119	-3.07616	0.36604
O	0.01023	-4.08131	0.83136
H	-2.08949	2.96768	-3.21455
H	-0.59707	4.58970	-0.24458
H	-3.34912	-3.21845	-1.65019

H	-4.51808	-1.08478	1.70522
H	-1.61381	-3.72230	0.64067
H	-4.52206	0.67937	-0.28377
H	3.99955	0.39205	-1.90681
H	2.11528	2.42930	2.76409
H	1.72866	3.71805	-0.46526
H	4.86202	1.28121	0.57381
H	0.64468	-4.06991	-1.84545
H	3.41430	-3.28502	1.24738
H	4.63753	-0.20990	0.15184
H	3.38429	1.44560	2.64149
H	3.75366	-2.55468	-0.12618
H	2.12803	-4.15644	-1.37655
H	3.16176	1.59271	-2.51550
H	2.86771	3.65818	0.62305
H	1.50431	-0.43917	2.40907
H	1.82369	-0.86478	-1.83520
H	0.23326	2.33944	1.82066
H	0.70872	0.97189	-2.21807
H	-1.53905	0.06617	-2.42834
H	-2.25810	0.93259	1.65852
H	-0.91929	-0.98338	2.14041
H	-0.48411	-1.74572	-1.98506
H	-3.41863	-2.07352	-2.72333
H	-5.03351	-0.49488	-1.19861
H	-3.20611	-1.07856	2.60970
H	-0.90308	1.98575	-3.52501
H	-0.10023	4.59183	-1.75705
H	-3.09909	-3.48477	1.16299

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Hf4_4_2_term_perox_conf1_ion4_diconf9.log Energy: -2423616.7789453

Hf	-1.31149	2.09152	-0.67793
O	0.66850	1.92506	-1.48956
O	0.27408	1.60302	0.79621
O	-1.48991	3.71243	0.92319
O	-1.84390	2.53374	-2.60883
O	-3.86020	2.09467	-1.06909
O	-1.70578	3.74202	-1.73630
Hf	-2.32139	-1.14372	0.25155
O	-2.31129	0.89956	0.85392
O	-1.69432	0.05210	-1.31710
O	-3.40003	-2.08791	-1.69552
O	-3.29050	-1.12926	2.40018

O	-3.26186	-3.16633	0.79489
O	-4.46590	-0.38031	-0.01052
Hf	2.05349	1.03851	-0.04897
O	2.13429	-0.62218	1.22080
O	1.35045	-0.70966	-0.99608
O	3.28109	1.10831	-2.02449
O	2.47939	1.88800	2.11379
O	2.79645	3.20827	-0.24530
O	4.30938	1.04269	0.45906
Hf	1.01615	-2.35876	0.43945
Cl	-0.76277	-1.90906	-3.59095
Cl	5.34040	-1.10703	-1.39717
Cl	1.28573	4.75207	1.94343
Cl	-1.10135	0.68841	3.76686
O	-0.97333	-2.58519	-0.50921
O	-0.65107	-1.36460	1.46893
O	1.61730	-3.19543	2.16367
O	1.23566	-3.55691	-1.59352
O	3.22707	-2.97612	-0.03352
O	0.88495	-4.16963	1.27250
H	-0.61538	3.99850	1.31234
H	-4.30886	2.91236	-0.79309
H	-3.71228	-3.00388	-1.58464
H	-4.14216	-0.65438	2.37784
H	-2.59012	-3.86086	0.65171
H	-4.37380	0.56333	-0.31684
H	3.97724	0.39010	-2.01639
H	2.08318	2.78375	2.28429
H	2.64803	3.54902	-1.14570
H	4.71955	1.86794	0.13739
H	2.18312	-3.73466	-1.73026
H	3.53335	-3.22739	0.85803
H	4.81888	0.29324	0.03371
H	3.42862	1.94970	2.32122
H	3.87762	-2.31866	-0.39625
H	0.88678	-3.14736	-2.41623
H	2.79021	0.97863	-2.85416
H	2.32329	3.84028	0.37209
H	2.37803	-0.52603	2.15413
H	0.88324	-0.67182	-1.84812
H	0.06221	1.38094	1.72544
H	0.71852	2.07718	-2.44595
H	-1.42569	-0.31545	-2.18912
H	-2.11442	1.10408	1.79169

H	-0.53350	-0.82633	2.28444
H	-0.97545	-2.71927	-1.47679
H	-2.83383	-2.08691	-2.50355
H	-4.90820	-0.85207	-0.74108
H	-2.72195	-0.64599	3.05645
H	-3.52078	2.25463	-1.99135
H	-1.89338	4.52011	0.55781
H	-3.52657	-3.20175	1.73406

64
Hf4_4_2_term_perox_conf1_ion5_diconf7.log Energy: -2423609.5479529

Hf	0.68852	-2.27084	0.07380
O	-0.85936	-1.68967	-1.36189
O	-1.12573	-1.59708	1.02500
O	0.76237	-3.53427	1.68092
O	1.56564	-3.06966	-1.94662
O	1.81377	-3.81591	0.64988
O	-0.86478	-4.19135	-0.22353
Hf	2.29702	0.92440	0.27535
O	1.71148	-0.85151	1.34686
O	1.52982	-0.48014	-0.99759
O	3.55855	1.14786	-1.65364
O	3.24027	1.29130	2.37789
O	3.51514	2.88408	0.36672
O	4.16236	-0.42347	0.49192
Hf	-2.32560	-0.60250	-0.35302
O	-2.05044	1.04376	0.95555
O	-1.54711	1.03894	-1.40152
O	-3.14735	-0.84574	-2.61665
O	-3.90346	-1.00349	1.26426
O	-3.22259	-2.71191	-0.66784
O	-4.28751	0.65075	-0.84681
Hf	-0.81119	2.58990	0.00233
Cl	-0.18686	-0.27758	-3.96585
Cl	4.48789	-1.76510	-2.25630
Cl	-2.72174	-2.57702	3.49333
Cl	0.93961	0.45947	4.17081
O	1.17897	2.31661	-0.90448
O	0.71376	1.76580	1.33019
O	-1.40985	3.74220	1.55048
O	-0.85419	3.63568	-2.12321
O	-3.01508	3.26862	-0.55506
O	-0.59195	4.50080	0.53431
H	2.51154	-2.77346	-2.03669

H	-0.52964	-4.44212	0.67692
H	4.33828	1.72806	-1.58870
H	4.07392	0.82432	2.56668
H	2.98962	3.60278	-0.03298
H	3.80894	-1.13087	1.06878
H	-2.45077	-0.68018	-3.29459
H	-3.59714	-1.60237	2.02916
H	-2.47657	-3.35781	-0.55912
H	-4.40992	0.51248	-1.80965
H	-0.45309	4.52063	-2.04565
H	-3.17587	3.73496	0.29110
H	-5.14017	0.42440	-0.43075
H	-4.23542	-0.20310	1.70961
H	-3.60787	2.48637	-0.56949
H	-1.80698	3.80434	-2.25731
H	-3.42373	-1.77486	-2.72724
H	-3.94196	-2.98959	-0.07327
H	-1.96017	0.90906	1.91126
H	-1.10635	0.90750	-2.26924
H	-1.41812	-1.88878	1.92482
H	-0.60971	-1.35234	-2.25445
H	1.30192	-0.29397	-1.92833
H	1.41335	-0.77778	2.27934
H	0.52249	1.46794	2.25060
H	1.30069	2.35254	-1.86629
H	3.86451	0.28415	-2.04608
H	4.42250	-0.89606	-0.35152
H	2.60908	1.07638	3.12852
H	1.12933	-2.73452	-2.75180
H	-0.54195	-4.86841	-0.84414
H	3.68702	3.12832	1.29597

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Hf4_4_2_term_perox_conf1_ion5_diconf9.log Energy: -2423613.2886122

Hf	-0.06547	-2.37791	-0.47240
O	-1.62389	-1.32704	-1.52488
O	-1.38815	-1.05841	0.78222
O	-0.86374	-3.71039	1.22779
O	0.31546	-3.22930	-2.29858
O	2.15096	-3.67762	-0.54595
O	-0.46267	-4.11868	-1.38186
Hf	2.30119	0.08097	0.42931
O	1.23401	-1.67629	1.10419
O	1.39131	-0.91932	-1.17126

O	4.01318	0.56193	-0.95301
O	2.91711	-0.20178	2.67001
O	3.24865	2.03261	1.29845
O	3.76205	-1.67075	0.53934
Hf	-2.58859	0.17920	-0.30721
O	-2.03162	1.87546	0.86201
O	-1.18214	1.36925	-1.27398
O	-3.54429	0.37896	-2.45031
O	-3.55835	-0.12690	1.82055
O	-4.27532	-1.33263	-0.50566
O	-4.56544	1.41395	-0.29348
Hf	-0.07923	2.64125	0.13492
Cl	0.77271	1.12857	-3.71674
Cl	6.43772	-1.20320	-0.85096
Cl	-3.89961	-3.19521	1.89431
Cl	0.00321	-0.61623	3.84376
O	1.68076	1.74415	-0.76342
O	0.65992	1.02185	1.30814
O	0.05162	3.74872	1.85696
O	0.26894	3.73447	-1.89526
O	-1.45871	4.56546	-0.09522
O	1.26515	3.89929	0.98679
H	-1.80362	-3.50569	1.49064
H	2.08742	-4.57783	-0.18351
H	4.19169	1.51839	-0.97018
H	3.41683	-1.03948	2.70620
H	2.56241	2.76971	1.27640
H	3.27996	-2.47604	0.22301
H	-4.21551	1.08661	-2.44731
H	-3.63471	-1.09015	2.06573
H	-4.27840	-1.76571	-1.37833
H	-5.43025	0.97040	-0.22352
H	-0.44773	4.36074	-2.09856
H	-1.18319	4.83642	0.81488
H	-4.62602	2.27023	0.16508
H	-4.41738	0.27581	2.03541
H	-2.40781	4.35816	-0.03430
H	0.37534	3.13901	-2.67523
H	-2.95002	0.58142	-3.19421
H	-4.23857	-2.06342	0.18158
H	-2.26850	1.88853	1.80340
H	-0.72409	1.08895	-2.09993
H	-1.17065	-0.88219	1.72040
H	-1.69112	-1.50477	-2.47550

H	1.32411	-0.53419	-2.06910
H	0.87105	-1.66176	2.01242
H	0.29723	0.74255	2.17944
H	1.65350	1.60018	-1.73346
H	4.89384	0.07440	-0.97770
H	4.66287	-1.65765	0.10749
H	2.13191	-0.31516	3.26760
H	1.85799	-3.73778	-1.49443
H	-0.86570	-4.64526	0.95490
H	3.48172	1.89059	2.23347

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Hf4_4_2_term_perox_conf1_ion6_diconf5.log Energy: -2423615.5529613

Hf	1.28670	-1.96822	0.32086
O	1.55276	-0.14425	1.27389
O	1.66603	-0.46928	-1.08041
O	2.14894	-3.10265	-1.42536
O	1.92128	-2.74224	2.40515
O	0.71363	-4.23054	0.49132
O	3.58840	-1.74709	0.54604
Hf	-2.04564	-1.14516	0.20495
O	-0.47834	-2.16354	-0.85758
O	-0.55224	-1.91552	1.49204
O	-3.36166	-1.58219	2.10017
O	-2.94712	-1.76748	-1.84089
O	-3.99900	0.00965	0.13187
O	-2.82079	-3.31628	0.24469
Hf	2.15881	1.43812	-0.09822
O	0.52736	2.37241	-1.27311
O	0.75431	2.55431	1.09996
O	3.49993	1.81876	1.39036
O	3.10939	1.33306	-2.24260
O	4.06332	0.86706	0.37944
O	3.19942	3.47223	-0.61150
Hf	-1.16144	2.27697	0.10042
Cl	-0.47240	-0.78337	-3.66153
Cl	0.30803	-0.62197	4.13014
Cl	4.57710	-1.61637	-2.48722
Cl	-5.82293	-0.88589	-2.13137
O	-1.68501	0.59666	1.39630
O	-1.43765	0.43127	-0.97309
O	-2.43965	3.00314	-1.33552
O	-1.65206	3.17891	2.23701
O	-1.06874	4.65172	0.08384

O	-3.17036	2.58090	-0.09430
H	2.92652	-2.69803	-1.91632
H	1.52536	-2.22357	3.15477
H	-0.22168	-4.29719	0.21839
H	4.07097	-1.92132	-0.29895
H	-4.00967	-0.85281	2.14018
H	-2.38355	-1.52808	-2.61473
H	-3.77451	0.98503	-0.02962
H	-3.14886	-3.58304	-0.63475
H	3.57429	0.46292	-2.33977
H	3.69442	3.51690	0.23630
H	-2.57379	2.97493	2.47649
H	-1.69706	4.66098	-0.67897
H	2.62076	4.25274	-0.64992
H	3.79286	2.02217	-2.32125
H	-0.23148	5.03285	-0.23150
H	-1.62206	4.14692	2.11372
H	0.42882	2.16228	-2.21500
H	0.82696	2.56911	2.06656
H	1.28048	-0.48949	-1.97905
H	1.36886	-0.00220	2.22610
H	-0.44737	-1.54233	2.40266
H	-0.38276	-1.97540	-1.82015
H	-1.20465	0.31391	-1.92166
H	-1.29826	0.53185	2.28798
H	-2.98723	-1.69184	2.99215
H	-3.52138	-3.49747	0.89783
H	-3.88763	-1.48927	-2.06260
H	2.89112	-2.66269	2.48694
H	0.75252	-4.52054	1.42161
H	3.78977	-0.76468	0.70395
H	2.29238	-4.06106	-1.33493
H	-4.69439	-0.23701	-0.54546

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Hf4_4_2_term_perox_conf1_ion6_diconf7.log Energy: -2423610.1083063

Hf	0.73944	-2.38487	-0.07258
O	1.84785	-1.02031	1.23161
O	1.60702	-0.66017	-1.12284
O	1.23310	-3.43256	-1.78348
O	0.90494	-3.54388	1.91983
O	0.71221	-4.28970	-0.67055
O	3.16136	-3.02464	-0.20079
Hf	-2.38235	-0.69611	-0.05790

O	-0.98999	-1.80699	-1.23240
O	-0.93186	-1.61318	1.08621
O	-3.48207	-1.45202	1.89712
O	-3.22781	-0.76710	-2.25757
O	-4.39986	0.31413	0.08025
O	-3.60786	-2.57802	-0.39938
Hf	2.35803	0.75211	0.19569
O	1.04087	2.04602	-0.85499
O	0.90420	1.49218	1.52309
O	3.66837	0.95189	2.15530
O	3.59117	1.54102	-1.56316
O	4.25354	-0.52929	0.10774
O	3.14118	3.00779	0.62596
Hf	-0.75520	2.44562	0.39313
Cl	-0.23339	0.18374	-3.64524
Cl	-1.29295	-2.46640	3.96958
Cl	6.16109	0.15926	-2.15707
Cl	-5.84524	0.75465	-2.50007
O	-2.12095	0.96460	1.29744
O	-1.50695	0.95731	-0.96038
O	-1.16265	3.87264	-0.97401
O	-1.10367	3.07263	2.65510
O	0.65449	4.23470	0.98733
O	-2.16928	3.83412	0.15072
H	0.25904	-3.33689	2.64640
H	2.83048	-3.38908	-1.07346
H	-4.21307	-0.91527	2.24807
H	-2.56840	-0.51443	-2.93763
H	-4.23760	1.16792	0.52476
H	-3.96891	-2.68471	-1.29822
H	3.31790	1.00502	3.06181
H	4.44957	1.12117	-1.89461
H	3.96835	-1.47549	0.00384
H	3.76410	2.99953	1.37827
H	-1.92783	3.59171	2.69751
H	0.41119	4.82186	0.24337
H	3.65514	3.28335	-0.15746
H	3.15362	1.96394	-2.32092
H	1.59519	3.97288	0.85312
H	-0.39223	3.72300	2.81211
H	4.38147	0.28640	2.14070
H	4.97014	-0.37247	-0.57436
H	0.85938	1.93943	-1.80479
H	0.66807	0.92627	2.27456

H	1.21428	-0.41641	-1.99136
H	2.17100	-1.28351	2.10572
H	-0.94442	-1.66068	2.07200
H	-0.80842	-1.60400	-2.17008
H	-1.14094	0.87281	-1.87365
H	-2.14118	0.86042	2.26081
H	-2.95242	-1.79309	2.66414
H	-4.30586	-2.76146	0.25431
H	-4.05951	-0.24961	-2.47049
H	0.86704	-4.50579	1.77341
H	3.42976	-3.78010	0.35024
H	-4.97921	0.50144	-0.72657

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Hf4_4_2_term_perox_conf1_ion6_diconf9.log Energy: -2423610.0882009

Hf	-1.03019	-2.25524	-0.49438
O	-2.15509	-0.62857	-1.37558
O	-1.62979	-0.64383	0.93671
O	-1.97512	-3.29304	1.33301
O	-1.31400	-3.11893	-2.33391
O	0.46068	-4.23502	-0.86865
O	-2.23886	-3.64314	-1.27971
Hf	2.19423	-0.86544	-0.11075
O	0.70462	-2.08605	0.81108
O	0.65732	-1.30210	-1.45635
O	3.23778	-1.16393	-2.34859
O	3.04742	-1.53891	1.91990
O	4.35249	-0.20505	-0.11376
O	2.92291	-2.99299	-0.53109
Hf	-2.37364	1.01732	0.01137
O	-0.93982	1.99971	1.20204
O	-0.85247	1.76485	-1.18508
O	-3.71745	1.80056	-1.72113
O	-3.39996	1.15980	2.07556
O	-4.38039	-0.19318	-0.08060
O	-2.99261	3.32502	0.24920
Hf	0.89534	2.43661	0.07390
Cl	0.33385	-0.80005	3.64118
Cl	0.90472	0.71876	-3.90207
Cl	-4.41037	-1.67916	2.62832
Cl	5.89525	-0.55835	2.41082
O	2.17569	1.05044	-1.05821
O	1.49593	0.64473	1.14450
O	1.34397	3.54559	1.69540

O	1.30443	3.39112	-2.05943
O	-0.35185	4.41579	-0.25399
O	2.35885	3.68589	0.58703
H	-2.67620	-2.75219	1.78744
H	0.21212	-5.06291	-0.42147
H	4.12840	-0.77293	-2.39530
H	2.42947	-1.37813	2.66839
H	4.34282	0.73486	-0.37712
H	2.11901	-3.57426	-0.55209
H	-3.36669	2.07592	-2.58659
H	-3.64348	0.25749	2.43922
H	-4.15634	-0.88202	-0.73752
H	-3.77495	3.60456	-0.26326
H	0.70961	4.16052	-2.12142
H	-0.11170	4.85557	0.58607
H	-3.07534	3.70816	1.14166
H	-4.19998	1.70450	2.18543
H	-1.30771	4.20048	-0.19341
H	1.11720	2.82299	-2.83979
H	-4.57188	1.35779	-1.87272
H	-4.57452	-0.69935	0.75863
H	-1.00068	2.04351	2.16855
H	-0.64679	1.37181	-2.05623
H	-1.15000	-0.58176	1.79125
H	-2.24641	-0.63349	-2.34125
H	0.57975	-0.85576	-2.32745
H	0.56020	-2.00921	1.77774
H	1.12208	0.42873	2.02962
H	2.07058	1.05975	-2.03078
H	2.73147	-0.79585	-3.10450
H	3.26990	-2.99070	-1.44451
H	3.95136	-1.23709	2.22076
H	0.00594	-4.23084	-1.75375
H	-2.40695	-4.12621	1.07315
H	4.97010	-0.28822	0.68453

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Hf4_4_2_term_perox_conf1_ion7_diconf7.log Energy: -2423610.8527334

Hf	-0.41048	-2.52847	-0.62720
O	-1.67078	-0.94564	-1.42616
O	-1.23758	-1.20097	0.88263
O	-0.73369	-3.99117	0.77957
O	-0.73687	-3.23197	-2.81606
O	-0.26248	-4.52184	-0.53887

O	-2.80397	-3.34161	-0.55586
Hf	2.53921	-0.55211	-0.35521
O	1.40553	-2.20126	0.47470
O	1.18588	-1.43050	-1.73576
O	3.91301	-0.32943	-2.18452
O	3.51161	-1.08627	1.63759
O	4.02054	1.17158	0.00675
O	3.67991	-2.58531	-0.77884
Hf	-2.29787	0.41926	0.10583
O	-1.06915	1.74205	1.23521
O	-1.10365	1.67276	-1.12948
O	-3.53581	0.95043	-1.82122
O	-2.91805	0.23286	2.35809
O	-4.06151	-0.97359	0.02358
O	-3.87741	1.99606	0.69663
Hf	0.61234	2.40822	-0.01392
Cl	0.87473	-1.15805	3.42839
Cl	-3.62429	4.11397	-1.40637
Cl	-5.21721	-1.70056	2.72394
Cl	6.01426	0.50565	2.22642
O	1.73276	1.13595	-1.40042
O	1.34646	0.58339	0.87382
O	1.41405	3.44877	1.50447
O	1.05932	3.68379	-1.96144
O	-0.75121	4.28976	-0.11332
O	2.41241	3.30296	0.38714
H	-0.67082	-4.20399	-2.85204
H	-2.41763	-3.89133	0.18150
H	4.61420	0.32456	-2.00132
H	2.87521	-1.10920	2.39434
H	3.48872	1.98635	0.27675
H	3.04551	-3.18078	-0.32738
H	-3.60219	1.93159	-1.94951
H	-3.57416	-0.48095	2.61665
H	-3.71656	-1.85817	-0.27525
H	-4.81089	1.71534	0.70176
H	1.86110	4.16016	-1.66734
H	-0.82771	4.74394	0.74320
H	-3.84836	2.81605	0.11116
H	-3.33229	1.06753	2.64388
H	-1.67047	4.20124	-0.48451
H	0.38390	4.37733	-2.07561
H	-4.44468	0.59971	-1.80776
H	-4.57140	-1.18198	0.86562

H	-1.01597	1.64110	2.19830
H	-0.98327	1.35376	-2.03733
H	-0.89581	-1.21053	1.80082
H	-2.09590	-0.93221	-2.29721
H	0.90946	-0.78724	-2.40878
H	1.29785	-2.28858	1.44453
H	1.05541	0.23397	1.74807
H	2.15360	1.50830	-2.19025
H	4.33780	-1.13742	-2.52473
H	4.52283	-2.69291	-0.30028
H	4.33446	-0.59981	1.94650
H	-0.13569	-2.89073	-3.50194
H	-3.08039	-3.95256	-1.26049
H	4.74181	1.05692	0.68832

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Hf4_4_2_term_perox_conf1_ion7_diconf9.log Energy: -2423613.1417498

Hf	-0.56483	-2.43247	-0.76171
O	-2.06751	-0.97229	-1.29324
O	-1.25110	-1.09738	0.90240
O	-1.06932	-3.80407	1.02329
O	-0.90858	-3.14765	-2.65671
O	1.21792	-4.06990	-1.55663
O	-1.57211	-3.95069	-1.58279
Hf	2.37211	-0.50019	-0.41715
O	1.22388	-2.10523	0.42836
O	0.96773	-1.27341	-1.79035
O	3.71159	-0.22298	-2.27979
O	3.53143	-1.22384	1.41884
O	3.92089	1.19130	0.00694
O	3.44489	-2.49697	-1.08804
Hf	-2.41533	0.47331	0.31166
O	-1.19298	1.81000	1.42517
O	-1.11854	1.52218	-0.92994
O	-3.78302	1.39628	-1.34223
O	-2.93062	0.04383	2.55631
O	-4.26429	-0.86630	0.32861
O	-4.00473	1.95961	1.17006
Hf	0.52520	2.47012	0.13441
Cl	0.93696	-1.23350	3.41726
Cl	-2.59635	4.08950	-2.39068
Cl	-3.70806	-2.93516	2.53613
Cl	5.95245	0.41067	2.17141
O	1.64854	1.27875	-1.30937

O	1.29595	0.62566	0.94161
O	1.38960	3.41579	1.68710
O	0.50737	3.60630	-1.92765
O	-0.87619	4.31540	0.20915
O	2.28527	3.40978	0.47119
H	-1.85636	-3.49035	1.54855
H	1.15142	-4.98393	-1.23067
H	4.34788	0.49204	-2.08447
H	2.94482	-1.33996	2.20342
H	3.40680	2.01444	0.25720
H	2.70786	-3.12944	-1.30630
H	-3.38140	2.20402	-1.78046
H	-3.06958	-0.92171	2.75799
H	-4.29460	-1.36823	-0.50737
H	-4.59471	2.24334	0.44571
H	-0.41254	3.77838	-2.26177
H	-1.30850	4.38450	1.07745
H	-3.63951	2.76836	1.57142
H	-3.73396	0.50442	2.85903
H	-1.59702	4.30722	-0.47703
H	0.94729	4.47385	-1.88627
H	-4.33837	0.94548	-2.00059
H	-4.21547	-1.57462	1.03854
H	-1.15145	1.70611	2.38918
H	-0.96763	1.16979	-1.81974
H	-0.76445	-1.09289	1.75414
H	-2.31863	-0.92694	-2.22883
H	0.81212	-0.84192	-2.64405
H	1.11464	-2.13261	1.40226
H	1.08791	0.27901	1.83865
H	1.87537	1.63749	-2.17962
H	4.22612	-1.03848	-2.43253
H	3.87653	-2.86246	-0.29369
H	4.34936	-0.73371	1.74147
H	0.64351	-4.00813	-2.36854
H	-1.30773	-4.69335	0.70547
H	4.63171	1.06608	0.69389

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Hf4_4_2_term_perox_conf1_ion8_diconf5.log Energy: -2423606.2198121

Hf	2.46855	0.16237	0.37374
O	1.31267	1.54511	1.48162
O	1.24662	1.23558	-0.85298
O	3.75752	0.52721	-1.50366

O	3.27741	-0.18022	2.55490
O	4.33809	-1.18004	0.42360
O	3.85424	1.94886	0.78300
Hf	0.28029	-2.54422	-0.21697
O	1.99293	-1.46953	-0.96235
O	1.13742	-1.24306	1.19222
O	0.39909	-3.70736	1.81379
O	0.66059	-3.30827	-2.41165
O	-1.01780	-4.37564	-0.63584
O	1.72326	-4.31848	-0.30016
Hf	-0.26179	2.48656	0.26075
O	-1.45112	1.44345	-1.25500
O	-1.46423	0.91428	1.12759
O	-0.57808	3.44148	2.03579
O	0.42274	3.71365	-1.59088
O	0.21752	4.25823	1.06117
O	-2.26568	3.66047	0.00459
Hf	-2.46666	-0.25922	-0.40217
Cl	1.00503	-0.54946	-3.82305
Cl	1.09998	-1.74400	4.16267
Cl	-6.53446	0.58490	1.24752
Cl	3.63768	3.57080	-1.84254
O	-1.58339	-2.04901	0.63527
O	-0.80498	-1.24679	-1.39059
O	-3.47596	-0.23084	-2.17465
O	-3.75229	-0.64266	1.50155
O	-4.08224	1.54451	-0.34236
O	-3.98226	-1.28140	-1.22196
H	3.72390	1.46473	-1.84526
H	2.68259	-0.66301	3.19509
H	4.22242	-2.00946	-0.07572
H	3.94187	2.54216	-0.02005
H	-0.21549	-4.42387	2.04778
H	0.77385	-2.56509	-3.06296
H	-1.93373	-4.34445	-0.30633
H	2.34655	-4.33548	-1.04814
H	1.40333	3.62587	-1.72547
H	-2.29266	3.97656	0.93097
H	-4.72417	-0.42734	1.40049
H	-4.27867	1.29324	-1.27756
H	-2.99794	3.00458	-0.10300
H	0.26985	4.65925	-1.41451
H	-4.92243	1.36834	0.16928
H	-3.46693	-0.09899	2.25614

H	-1.63902	1.77063	-2.14594
H	-1.23220	0.62836	2.02257
H	1.05196	0.95756	-1.76953
H	1.20572	1.65261	2.43872
H	0.86861	-1.21553	2.14387
H	2.04806	-1.23598	-1.91523
H	-0.43159	-0.86127	-2.21674
H	-1.86451	-2.26603	1.53706
H	0.60584	-3.21185	2.65225
H	2.19909	-4.55577	0.51582
H	-0.09415	-3.83507	-2.73112
H	3.75286	0.50153	3.06083
H	4.57630	-1.41453	1.34053
H	3.36027	2.49975	1.42031
H	4.69774	0.28477	-1.42787
H	-0.70117	-5.29576	-0.59461

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Hf4_4_2_term_perox_conf1_ion8_diconf7.log Energy: -2423607.3722521

Hf	-0.37557	-2.52352	0.19057
O	1.10449	-1.42273	1.29857
O	1.00832	-1.37716	-1.07274
O	-0.25862	-3.95465	-1.28938
O	-0.66705	-3.30722	2.34367
O	-1.02168	-4.39638	-0.07671
O	1.73716	-3.93667	0.29502
Hf	-2.69083	0.12495	-0.23398
O	-1.83217	-1.61055	-1.12366
O	-1.66304	-1.00811	1.12157
O	-3.99186	0.20289	1.74646
O	-3.53437	0.00887	-2.46559
O	-4.19978	1.83419	-0.64318
O	-4.54498	-1.17164	-0.34551
Hf	2.21420	-0.10092	0.05856
O	1.48531	1.41076	-1.29768
O	0.99058	1.25994	1.05272
O	3.04523	0.00499	2.29463
O	3.52388	-0.20467	-1.80296
O	3.58507	-1.85862	0.37376
O	3.86539	1.55208	0.21640
Hf	-0.10802	2.60739	-0.31041
Cl	-0.70809	-0.59962	-3.88988
Cl	-2.35849	-1.20790	4.05954
Cl	3.13766	3.18242	2.76316

Cl	5.80815	-2.13938	-1.67775
O	-1.91220	1.85749	0.75710
O	-1.28148	1.12493	-1.36407
O	-0.17552	3.72212	-1.97585
O	-0.09778	3.63726	1.81209
O	1.88510	3.81191	-0.07199
O	-1.05412	4.26934	-0.87087
H	-1.19926	-2.76993	2.98708
H	1.29814	-4.30245	-0.52485
H	-4.40537	1.03100	2.04466
H	-2.82875	-0.19448	-3.12816
H	-3.85475	2.66157	-0.25706
H	-4.94581	-1.31716	-1.22136
H	3.10504	0.91606	2.67363
H	4.31595	-0.82068	-1.89730
H	3.02939	-2.68115	0.38194
H	4.79803	1.31546	0.06682
H	0.74363	3.50631	2.30553
H	2.48455	3.35334	-0.69121
H	3.84019	2.09199	1.05202
H	3.75787	0.64162	-2.22053
H	2.32715	3.74247	0.80975
H	-0.25223	4.59810	1.78009
H	3.90975	-0.42381	2.42243
H	4.37263	-2.03847	-0.21911
H	1.44077	1.25561	-2.25387
H	0.59912	0.93810	1.87908
H	0.78080	-1.20211	-2.00760
H	1.36486	-1.53310	2.22509
H	-1.68469	-0.87776	2.09935
H	-1.58054	-1.62999	-2.07075
H	-0.97453	0.74797	-2.22120
H	-1.98503	2.03241	1.70756
H	-3.60717	-0.23050	2.55627
H	-5.24399	-1.05365	0.32181
H	-3.88693	0.88297	-2.71363
H	-1.04243	-4.20546	2.34357
H	1.71635	-4.64056	0.96585
H	-5.17028	1.84582	-0.56712

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Hf4_4_2_term_perox_conf1_ion8_diconf9.log Energy: -2423612.0093212

Hf	-1.14303	2.20009	-0.77056
O	0.87694	1.82320	-1.49468

O	0.35508	1.59742	0.76953
O	-1.13843	3.89002	0.78247
O	-1.40444	2.56586	-2.73297
O	-3.42155	2.78153	-0.88209
O	-1.17723	3.82610	-1.95187
Hf	-2.42574	-0.94926	0.27047
O	-2.32930	1.09196	0.80146
O	-1.65163	0.16480	-1.30515
O	-3.58034	-1.62287	-1.69477
O	-3.24116	-0.81623	2.47750
O	-3.38474	-2.94294	0.93208
O	-4.68260	-0.50289	0.32231
Hf	2.10734	0.87090	-0.01503
O	2.06070	-0.82283	1.21788
O	1.31650	-0.82803	-1.01206
O	3.43717	0.86776	-1.93471
O	2.52986	1.66238	2.17073
O	3.05734	2.96417	-0.16880
O	4.34083	0.66569	0.59527
Hf	0.81095	-2.44515	0.39516
Cl	-0.99476	0.91898	3.70871
Cl	-1.01418	-1.89025	-3.61418
Cl	5.29226	-1.51562	-1.27413
Cl	1.64909	4.63783	1.98753
O	-1.21828	-2.51405	-0.50774
O	-0.72298	-1.28006	1.42240
O	1.34866	-3.35982	2.10380
O	0.90729	-3.62444	-1.65198
O	2.95837	-3.24860	-0.09013
O	0.53192	-4.25453	1.20351
H	-0.25691	4.05389	1.22095
H	-3.85133	2.93192	-0.02303
H	-4.14098	-2.41798	-1.66597
H	-2.64160	-0.28731	3.07027
H	-2.89907	-3.68884	0.53339
H	-4.90435	0.07743	1.07326
H	4.06883	0.09333	-1.91603
H	2.21725	2.59058	2.33720
H	2.95584	3.31107	-1.07326
H	4.83379	1.45281	0.29483
H	1.83949	-3.85229	-1.81594
H	3.21016	-3.55809	0.80089
H	4.79590	-0.11927	0.17381
H	3.47418	1.63236	2.40521

H	3.67304	-2.63255	-0.40002
H	0.55935	-3.18253	-2.45914
H	2.96104	0.79122	-2.77938
H	2.63249	3.63798	0.43848
H	2.31218	-0.77332	2.15250
H	0.85109	-0.71417	-1.85656
H	0.10349	1.43045	1.70258
H	0.92007	1.93244	-2.45687
H	-1.42624	-0.23893	-2.17189
H	-2.13715	1.32913	1.73109
H	-0.53914	-0.74149	2.22182
H	-1.26338	-2.67346	-1.46972
H	-2.99019	-1.73604	-2.48007
H	-5.04730	-0.09546	-0.48435
H	-3.29373	-1.70608	2.87066
H	-3.44910	3.61755	-1.38221
H	-1.39318	4.74281	0.38775
H	-4.33464	-3.15570	0.94595

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Hf4_4_2_term_perox_conf1_ion9_diconf5.log Energy: -2423607.2923199

Hf	-1.65562	-2.00779	0.10903
O	0.14577	-2.67146	0.91610
O	-0.13708	-1.98429	-1.30143
O	-2.74636	-2.72844	-1.88464
O	-2.34644	-2.72970	2.24062
O	-3.94243	-1.83404	0.36838
O	-1.95962	-4.26864	0.04414
Hf	-1.75527	1.48729	0.24943
O	-2.23784	-0.23393	-0.90022
O	-1.46773	-0.30983	1.31698
O	-2.49291	1.89857	2.43624
O	-2.91340	2.20956	-1.62984
O	-2.05642	3.69361	0.50826
O	-4.06657	1.11975	0.51130
Hf	1.88006	-2.04085	-0.32417
O	1.97216	-0.15325	-1.45937
O	1.80770	-0.31731	0.96841
O	2.82900	-2.96868	1.22613
O	2.34981	-2.88030	-2.43450
O	2.71643	-3.82871	0.00194
O	4.15045	-1.53631	-0.54953
Hf	1.77867	1.55853	-0.15112
Cl	-1.39265	-0.20216	-3.75695

Cl	-1.64461	-0.48175	4.31596
Cl	5.54998	3.05802	1.72198
Cl	-3.15764	5.20520	-1.80519
O	0.04713	2.11737	1.14284
O	-0.19064	1.58425	-1.11329
O	2.50446	2.56045	-1.77562
O	2.63630	2.18176	1.92361
O	4.16501	1.21228	-0.29698
O	2.30481	3.44216	-0.57190
H	-2.41353	-2.29320	-2.69991
H	-2.16510	-2.14797	3.02833
H	-4.18715	-0.88011	0.35852
H	-2.28070	-4.55993	-0.83109
H	-2.47404	2.80696	2.78364
H	-2.69110	1.75110	-2.46516
H	-1.20271	4.07809	0.78291
H	-4.54763	1.47393	-0.26207
H	2.28630	-2.35566	-3.25079
H	4.40555	-1.96468	0.29385
H	3.51646	2.65655	1.88838
H	4.11287	1.74290	-1.13038
H	4.29123	-0.56262	-0.44129
H	3.24189	-3.27077	-2.42152
H	4.72871	1.74578	0.33481
H	2.80287	1.42088	2.50672
H	2.36466	-0.01130	-2.33252
H	1.48951	-0.45900	1.87147
H	-0.22428	-1.44939	-2.11784
H	0.36530	-2.93200	1.82356
H	-1.27926	-0.34971	2.29052
H	-2.09798	-0.21310	-1.88110
H	-0.25189	1.17197	-1.99741
H	0.20090	2.20280	2.09623
H	-2.29063	1.27218	3.18110
H	-4.44159	1.52408	1.31656
H	-2.99939	3.18786	-1.84631
H	-2.22141	-3.65325	2.51911
H	-4.20927	-2.18958	1.23741
H	-1.14009	-4.76383	0.23020
H	-3.70028	-2.52887	-1.84169
H	-2.44187	4.30580	-0.20263

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Hf4_4_2_term_perox_conf1_ion9_diconf9.log Energy: -2423609.8047172

Hf	0.22651	2.69191	0.26106
O	-1.75664	2.03025	0.83237
O	-0.88163	1.57585	-1.28784
O	0.50011	4.04282	-1.58981
O	0.16895	3.63472	2.08093
O	2.46424	3.65958	0.92434
O	-0.16003	4.53703	0.93277
Hf	2.36113	-0.14044	0.23187
O	1.78693	1.61125	-0.82589
O	1.09407	1.06601	1.38560
O	3.28777	-0.30807	2.45974
O	3.71998	-0.01041	-1.60855
O	3.78969	-1.90949	0.36474
O	4.02464	1.41772	0.66006
Hf	-2.45504	0.48400	-0.52803
O	-1.70503	-1.24154	-1.46884
O	-1.45643	-0.70317	0.84442
O	-4.01869	0.25906	1.14780
O	-2.88844	0.93064	-2.85500
O	-3.87917	2.26389	-0.80457
O	-4.43825	-0.46445	-1.30955
Hf	-0.36890	-2.39725	-0.08055
Cl	-0.03328	0.12702	-3.91082
Cl	0.50435	-0.66573	3.99146
Cl	-3.97351	-2.46808	2.51932
Cl	5.09623	-2.61630	-2.25385
O	1.31177	-1.74171	1.17829
O	1.11389	-1.11622	-1.10395
O	-0.22581	-3.68533	-1.60756
O	-0.83686	-3.10104	2.17637
O	-2.37258	-3.52311	0.10535
O	0.56883	-4.12705	-0.39933
H	0.01314	3.80877	-2.40020
H	2.68209	4.50397	0.49278
H	3.84477	-1.10286	2.54719
H	4.43669	0.62694	-1.43220
H	3.20516	-2.63592	0.66020
H	3.57249	2.30170	0.72395
H	-3.97570	-0.58141	1.69964
H	-2.09228	0.81098	-3.43151
H	-3.50867	3.02943	-0.32527
H	-5.09692	-0.46086	-0.58888
H	-1.80005	-3.04180	2.38747
H	-2.75365	-3.67859	-0.77435

H	-4.35219	-1.38730	-1.60966
H	-3.60724	0.41059	-3.25507
H	-3.08724	-3.17882	0.70297
H	-0.41190	-2.56806	2.88287
H	-4.36025	0.97728	1.70674
H	-3.90522	2.50351	-1.75132
H	-1.41918	-1.19543	-2.40186
H	-1.34597	-0.43734	1.77161
H	-0.42246	1.22128	-2.08639
H	-1.97407	2.14787	1.77034
H	0.78768	0.79216	2.27764
H	2.03416	1.71690	-1.75683
H	0.93822	-0.79121	-2.01328
H	1.13215	-1.58781	2.12907
H	2.61222	-0.35994	3.17944
H	4.39207	1.24165	1.54686
H	4.16010	-0.83588	-1.97611
H	1.94880	3.88113	1.74585
H	0.28703	4.97295	-1.39304
H	4.29486	-2.24138	-0.44139

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Hf4_4_2_term_perox_conf4_ion10_diconf9.log Energy: -2423601.5180719

Hf	-1.14371	2.30511	-0.08841
O	0.81074	2.26655	-1.01646
O	0.53692	1.71749	1.25693
O	-1.67552	3.49932	1.82020
O	-1.71919	3.19658	-1.84065
O	-3.64210	2.45412	-0.30375
O	-1.48489	4.17234	-0.72754
Hf	-2.17608	-1.06853	0.17978
O	-2.04198	0.78309	1.18575
O	-1.56088	0.45658	-1.12421
O	-3.18836	-1.69081	-1.80724
O	-2.99742	-1.43687	2.37586
O	-2.92482	-3.26267	0.57101
O	-4.26039	-0.22307	0.15822
Hf	2.22857	1.14431	0.20310
O	2.26008	-0.66681	1.22805
O	1.46142	-0.41184	-0.96874
O	3.34221	1.44203	-1.79646
O	2.83056	1.71844	2.44251
O	2.78120	3.41868	0.20670
O	4.51577	1.02729	0.61621

Hf	1.21281	-2.27902	0.05043
Cl	1.03720	0.86439	-3.81919
Cl	-0.75606	0.34946	3.94150
Cl	-6.17450	-1.32333	-1.93445
Cl	5.43319	-0.92737	-1.45059
O	-0.80534	-2.31927	-0.85054
O	-0.45720	-1.53995	1.30547
O	1.45504	-3.39640	2.06234
O	1.55375	-3.10846	-1.75674
O	3.50041	-2.83468	0.18622
O	1.41082	-4.14895	-0.68428
H	-1.27537	3.28899	2.68324
H	-3.99616	3.17431	0.24626
H	-2.90905	-2.51284	-2.24236
H	-2.47854	-0.97186	3.07305
H	-2.29909	-3.84078	0.09456
H	-4.18598	0.75987	0.07407
H	4.03331	0.73802	-1.90862
H	2.52212	2.60725	2.69226
H	2.03559	3.69649	-0.37110
H	5.07775	1.80940	0.46986
H	0.61788	-3.56215	2.53125
H	3.45051	-3.63062	-0.37853
H	4.94949	0.29958	0.06989
H	3.79054	1.69966	2.60482
H	1.91816	-4.25082	2.00539
H	4.11447	-2.21087	-0.27759
H	2.73518	1.33911	-2.57937
H	3.58665	3.71271	-0.25611
H	2.57479	-0.75771	2.14011
H	1.20300	-0.24474	-1.90380
H	0.37421	1.33390	2.14554
H	0.76625	2.11474	-1.98749
H	-1.43881	0.32572	-2.07879
H	-1.79502	0.77891	2.13687
H	-0.28852	-1.05835	2.14208
H	-0.68792	-2.49664	-1.79722
H	-4.17775	-1.60604	-1.96578
H	-4.98594	-0.52365	-0.46011
H	-2.92662	-2.38715	2.57739
H	-3.40710	2.85315	-1.18217
H	-1.61445	4.46399	1.70286
H	-3.82156	-3.55179	0.32239

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Hf4_4_2_term_perox_conf4_ion12_diconf6.log Energy: -2423608.3151353

Hf	-1.07383	2.24970	-0.44107
O	0.89323	1.88129	-1.33832
O	0.43619	1.60074	0.96341
O	-1.62588	3.78557	0.77308
O	-1.40849	2.72243	-2.72152
O	-3.42205	2.73623	-0.81860
O	-0.86255	4.23767	-0.44636
Hf	-2.53480	-0.89741	0.13256
O	-2.24804	1.03737	0.92730
O	-1.72052	0.33912	-1.33875
O	-3.70937	-1.46763	-1.95268
O	-3.47131	-0.92416	2.28465
O	-3.81822	-2.77254	0.49680
O	-4.51741	0.21127	-0.15252
Hf	2.09070	0.72737	0.04079
O	1.88062	-0.98239	1.22113
O	1.16010	-0.86750	-1.01085
O	3.24572	0.61285	-2.00562
O	2.72842	1.33776	2.21535
O	3.12611	2.74589	-0.15838
O	4.33470	0.33117	0.42416
Hf	0.63939	-2.55446	0.21750
Cl	0.32056	0.24174	-3.91656
Cl	-1.10643	0.61903	3.77982
Cl	4.98647	-1.93986	-1.43243
Cl	2.88432	4.37267	2.37348
O	-1.37071	-2.41724	-0.69900
O	-0.91363	-1.40128	1.33647
O	0.73550	-3.39181	2.37657
O	0.83028	-3.69459	-1.43708
O	2.83200	-3.37523	0.40867
O	0.52727	-4.51273	-0.21244
H	-1.02082	2.08059	-3.36116
H	-3.32511	3.46841	-0.16176
H	-3.96408	-2.37281	-2.20098
H	-2.89357	-0.47296	2.95023
H	-3.45078	-3.61659	0.17937
H	-4.30325	1.17235	-0.24948
H	3.80868	-0.20692	-2.04000
H	2.69241	2.31475	2.43312
H	2.66024	3.17397	-0.90210

H	4.86318	1.08225	0.09368
H	-0.12118	-3.38354	2.83989
H	2.70613	-4.21563	-0.07148
H	4.69269	-0.48344	-0.04091
H	3.65333	1.06812	2.36298
H	1.06933	-4.30523	2.42854
H	3.51153	-2.87331	-0.10930
H	2.66453	0.56146	-2.79262
H	3.07219	3.38599	0.61913
H	2.09642	-0.98301	2.16591
H	0.91912	-0.79133	-1.95656
H	0.21423	1.41715	1.89984
H	0.83563	1.56471	-2.26467
H	-1.25410	0.01057	-2.13409
H	-2.04794	1.15602	1.88139
H	-0.71171	-0.85723	2.12936
H	-1.37438	-2.80757	-1.58686
H	-3.36659	-1.04704	-2.76045
H	-4.93897	-0.06934	-0.98665
H	-3.58340	-1.83681	2.60529
H	-1.05237	3.59902	-2.95228
H	-3.58731	3.13980	-1.68987
H	-4.78801	-2.85558	0.53146

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Hf4_4_2_term_perox_conf4_ion10_diconf10.log Energy: -2423608.4317642

Hf	-1.37559	2.12222	-0.03699
O	0.51044	2.12573	-1.12227
O	0.31834	1.59851	1.23246
O	-1.87620	3.07644	2.07271
O	-2.05286	3.24196	-1.59114
O	-3.05497	3.11779	-0.46988
O	-0.40176	4.33372	0.14969
Hf	-2.10097	-1.34674	0.12484
O	-2.40098	0.52631	1.06475
O	-1.63770	0.27055	-1.13599
O	-2.93424	-1.91668	-1.97282
O	-2.87889	-1.76691	2.35745
O	-2.66315	-3.56194	0.43509
O	-4.36090	-1.36699	0.23517
Hf	2.03877	1.28195	0.10180
O	2.30400	-0.46698	1.20629
O	1.53656	-0.41812	-1.02435
O	3.08333	1.61855	-1.96284

O	2.72548	2.08720	2.35868
O	2.30287	3.55918	0.22037
O	4.29071	1.62056	0.42080
Hf	1.40759	-2.22503	0.10686
Cl	0.58033	0.58226	-3.81081
Cl	-1.04702	0.44876	3.89380
Cl	-5.48852	-0.32074	-2.34832
Cl	5.45730	-0.42671	-1.42344
O	-0.57123	-2.40787	-0.84357
O	-0.36142	-1.53069	1.28757
O	1.68800	-3.16330	2.20415
O	1.87177	-3.19349	-1.60258
O	3.73945	-2.51832	0.26504
O	1.74055	-4.12858	-0.43320
H	-1.67363	2.53545	2.86864
H	-0.78019	4.82930	0.89848
H	-3.20370	-2.84208	-2.10769
H	-2.39953	-1.26570	3.05742
H	-2.06132	-4.21555	0.03682
H	-4.66906	-0.94832	1.05869
H	3.83171	0.97415	-2.05755
H	2.18916	2.00752	3.16536
H	1.42437	3.96999	0.02517
H	4.59261	2.47899	0.06932
H	0.85679	-3.34313	2.67848
H	3.82113	-3.29927	-0.31415
H	4.84021	0.92471	-0.05829
H	3.64623	1.88045	2.59585
H	2.18700	-3.99950	2.19171
H	4.26538	-1.80621	-0.17937
H	2.47608	1.42688	-2.71646
H	2.49831	3.76953	1.15478
H	2.63141	-0.51611	2.11619
H	1.21433	-0.33493	-1.95098
H	0.17314	1.22495	2.12663
H	0.45161	1.87068	-2.07023
H	-1.22841	0.14555	-2.01446
H	-2.31725	0.58214	2.03696
H	-0.27642	-1.02223	2.11728
H	-0.54732	-2.66956	-1.77660
H	-3.71522	-1.36484	-2.27906
H	-4.87550	-0.96212	-0.53187
H	-2.76042	-2.71023	2.56933
H	-0.90175	4.58880	-0.66192

H	-2.81227	3.33628	2.13951
H	-3.57619	-3.89262	0.36039

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Hf4_4_2_term_perox_conf4_ion10_diconf2.log Energy: -2423601.3368535

Hf	1.55038	-1.80483	0.01491
O	-0.24153	-2.27987	-0.93307
O	-0.00040	-1.65977	1.37373
O	2.43251	-2.65987	2.05055
O	2.18949	-2.39273	-2.17955
O	3.84115	-2.16740	-0.11137
O	1.53048	-4.08549	0.08821
Hf	1.81409	1.72347	0.05531
O	2.35529	-0.10301	1.02267
O	1.41914	-0.00827	-1.09295
O	2.59000	2.08913	-2.11585
O	2.63583	2.30593	2.20562
O	2.25488	3.95339	0.14178
O	4.11373	1.92529	0.07482
Hf	-1.95913	-1.59130	0.36736
O	-2.14412	0.29950	1.36281
O	-1.62532	0.13525	-0.95871
O	-3.08068	-2.15998	-1.56855
O	-2.72147	-2.21314	2.18297
O	-1.71270	-3.95661	0.59551
O	-3.74001	-2.15006	1.08280
Hf	-1.76732	1.99428	0.02349
Cl	-0.25055	-1.00278	-3.72716
Cl	1.39303	-0.17749	3.91619
Cl	4.82253	-0.13661	-2.18263
Cl	-5.50306	-0.29102	-1.65845
O	0.17608	2.55941	-0.91481
O	0.12771	1.72599	1.25260
O	-2.17177	3.15068	2.00045
O	-2.37184	2.75252	-1.75296
O	-4.10191	1.82490	0.19018
O	-2.46635	3.76196	-0.64537
H	2.12456	-2.19962	2.86490
H	2.98218	-1.87974	-2.45151
H	4.31853	-1.45117	-0.62103
H	2.03258	-4.55133	0.78197
H	3.01008	2.93848	-2.33891
H	2.28913	1.74195	2.93812
H	1.62476	4.55387	-0.29501

H	4.45156	1.73925	0.97040
H	-3.92057	-1.60903	-1.61857
H	-0.76579	-4.18320	0.63096
H	-1.36531	3.27629	2.53164
H	-4.30956	2.63793	-0.30937
H	-2.53547	4.03944	1.83902
H	-4.50552	1.08386	-0.34008
H	-2.59990	-1.96210	-2.39439
H	-2.02511	-3.84352	1.52672
H	-2.73175	0.27798	2.13209
H	-1.38888	0.04570	-1.89985
H	0.11063	-1.29565	2.27607
H	-0.33115	-2.05262	-1.88535
H	0.94552	0.01532	-1.95242
H	2.34955	-0.14458	2.00599
H	0.05774	1.13288	2.02311
H	0.10246	2.78226	-1.85610
H	3.22979	1.38173	-2.39024
H	4.57730	1.30673	-0.54917
H	2.40601	3.22403	2.43739
H	1.50265	-2.15942	-2.85280
H	4.15408	-3.00666	-0.49684
H	1.55934	-4.61414	-0.73014
H	3.40304	-2.55904	2.03415
H	3.15066	4.32922	0.06488

64
Hf4_4_2_term_perox_conf4_ion13_diconf9.log Energy: -2423602.1285822

Hf	0.43352	-2.51686	0.35690
O	-1.32127	-2.17709	-0.85899
O	-1.20877	-1.38481	1.35147
O	0.61749	-3.22291	2.56131
O	0.83616	-3.93211	-1.07506
O	2.79058	-3.26662	0.42645
O	0.27681	-4.50669	0.19374
Hf	2.12750	0.55592	-0.00828
O	1.62170	-0.98663	1.36565
O	1.31618	-1.08426	-1.02615
O	3.18753	0.69103	-2.06880
O	3.09102	1.22157	2.03141
O	3.39489	2.52523	-0.18047
O	3.98197	-0.72227	0.19615
Hf	-2.60110	-0.72544	-0.01894
O	-2.38031	1.23458	0.81672

O	-1.63179	0.56067	-1.30395
O	-3.50200	-1.26842	-2.15282
O	-3.76602	-0.91577	2.06768
O	-3.91834	-2.57746	0.10573
O	-4.66834	0.25299	-0.32615
Hf	-0.93884	2.41847	-0.39941
Cl	-0.80806	-1.20113	-3.78676
Cl	0.04922	-0.32231	3.95863
Cl	5.63270	-1.06267	-2.34924
Cl	2.30107	4.25176	2.12359
O	0.94415	1.78589	-1.26476
O	0.50297	1.44084	0.96861
O	-0.69883	3.71899	1.46815
O	-1.26037	3.10437	-2.25297
O	-2.88117	3.94676	-0.09686
O	-0.72441	4.20294	-1.38589
H	0.39384	-2.55668	3.25236
H	2.92699	-3.85875	1.18662
H	3.52551	1.59781	-2.18410
H	2.98567	0.62431	2.79195
H	2.99436	3.24886	0.38283
H	3.66841	-1.63259	0.41950
H	-4.11126	-0.57031	-2.45346
H	-3.24494	-1.17204	2.84830
H	-4.27059	-2.92984	-0.73126
H	-5.54161	-0.17770	-0.32679
H	0.24919	3.90592	1.71734
H	-2.36425	4.50636	-0.73328
H	-4.77581	1.13849	0.06241
H	-4.47598	-0.33033	2.38290
H	-1.17340	4.56773	1.46491
H	-3.69456	3.69121	-0.56276
H	-2.79497	-1.32219	-2.84840
H	-4.58944	-2.66443	0.80471
H	-2.56028	1.46137	1.74182
H	-1.26702	0.23874	-2.15965
H	-1.00026	-0.94036	2.20812
H	-1.13465	-2.21137	-1.82218
H	1.04904	-1.04795	-1.96427
H	1.29447	-0.72914	2.25555
H	0.25178	1.19334	1.87712
H	1.06417	1.88886	-2.22054
H	3.95432	0.08447	-2.29609
H	4.61841	-0.83817	-0.56703

H	2.79867	2.12528	2.32234
H	2.50522	-3.83366	-0.33906
H	0.12955	-4.03771	2.77390
H	4.30010	2.42692	0.16995

64
Hf4_4_2_term_perox_conf4_ion8_diconf9.log Energy: -2423605.5673215

Hf	-1.35720	2.12596	-0.68016
O	0.66363	1.90767	-1.49382
O	0.22921	1.55519	0.77821
O	-1.48549	3.70061	0.99067
O	-1.68943	2.60098	-2.60998
O	-3.67702	2.49035	-0.70507
O	-1.54032	3.81829	-1.74410
Hf	-2.32309	-1.16175	0.24520
O	-2.39944	0.84948	0.87597
O	-1.74323	0.10184	-1.30086
O	-3.45513	-1.90167	-1.68235
O	-3.13868	-1.18028	2.49279
O	-3.00469	-3.28524	0.86378
O	-4.61387	-0.99800	0.39469
Hf	2.01840	1.03825	-0.08021
O	2.14559	-0.63986	1.15265
O	1.37524	-0.74291	-1.07041
O	3.27769	1.12834	-2.04388
O	2.44260	1.84678	2.10654
O	2.71330	3.23700	-0.24229
O	4.28340	1.13603	0.43656
Hf	1.04423	-2.39303	0.29507
Cl	-0.97316	0.67882	3.73993
Cl	-1.18390	-1.67989	-3.76597
Cl	5.40916	-1.00598	-1.35305
Cl	1.28208	4.71541	2.04698
O	-0.93613	-2.48992	-0.64231
O	-0.61276	-1.44421	1.41437
O	1.50396	-3.17603	2.43035
O	1.41097	-3.67568	-1.25269
O	3.37407	-2.90214	0.25782
O	1.15566	-4.37158	0.05299
H	-0.60307	3.95255	1.38246
H	-4.09757	2.46772	0.17113
H	-3.86487	-2.78391	-1.66580
H	-2.57074	-0.63225	3.09547
H	-2.43519	-3.95823	0.44746

H	-4.88670	-0.47297	1.16885
H	3.98710	0.42405	-2.02179
H	2.03349	2.73094	2.30510
H	2.44411	3.57458	-1.11580
H	4.64766	1.97383	0.09314
H	1.45545	-2.63562	3.23739
H	3.22959	-3.51969	-0.49226
H	4.82443	0.40353	0.01856
H	3.39664	1.93019	2.28370
H	2.38623	-3.59018	2.42083
H	3.96953	-2.20338	-0.10377
H	2.79528	0.98210	-2.87553
H	2.27481	3.83990	0.42646
H	2.40728	-0.49972	2.07509
H	0.88550	-0.71393	-1.90926
H	0.02302	1.33258	1.71048
H	0.65234	2.02562	-2.45612
H	-1.51566	-0.24928	-2.19425
H	-2.20384	1.06497	1.80988
H	-0.49276	-0.89801	2.22239
H	-0.89711	-2.64807	-1.60628
H	-2.87331	-1.88653	-2.49272
H	-5.07347	-0.64628	-0.38886
H	-3.10957	-2.08557	2.85095
H	-3.85026	3.36158	-1.10395
H	-1.86015	4.53354	0.65281
H	-3.92036	-3.61629	0.86989

64
Hf4_4_2_term_perox_conf4_ion9_diconf9.log Energy: -2423606.0211426

Hf	1.01628	-2.59115	-0.24279
O	-1.07838	-2.42370	-0.91393
O	-0.39357	-1.59078	1.14975
O	1.19152	-3.81857	1.72237
O	1.16031	-3.49447	-2.03300
O	3.29010	-3.18583	-0.29783
O	0.99976	-4.48253	-0.91429
Hf	2.29323	0.72795	-0.01965
O	2.25310	-1.13208	0.99696
O	1.55318	-0.79873	-1.27037
O	3.57095	0.91342	-1.93986
O	2.90535	1.24862	2.25678
O	3.33008	2.78553	0.01836
O	4.57883	0.45204	0.40402

Hf	-2.19878	-1.06566	0.32790
O	-2.11189	0.89273	1.01193
O	-1.51086	0.25644	-1.17495
O	-3.70120	-1.53703	-1.37545
O	-2.44440	-1.32994	2.74156
O	-2.99673	-3.14814	0.91196
O	-4.36731	-0.79751	1.11079
Hf	-0.95566	2.22016	-0.41493
Cl	0.48806	-0.22789	3.80555
Cl	1.56417	0.36068	-4.15720
Cl	-5.50767	0.95196	-1.07836
Cl	1.99842	4.31807	2.28521
O	1.03166	1.89749	-1.26284
O	0.57813	1.34736	0.94028
O	-0.91424	3.58651	1.41757
O	-1.30134	2.87354	-2.28836
O	-3.18023	2.97517	-0.27471
O	-0.97169	3.99812	-1.34648
H	0.49425	-3.64080	2.37873
H	3.74858	-3.05060	0.54890
H	3.90674	1.82334	-2.03856
H	2.32830	0.77910	2.90444
H	2.85538	3.46681	0.57701
H	4.73146	0.08916	1.29489
H	-4.33362	-0.77016	-1.48624
H	-1.68509	-1.03020	3.29092
H	-2.52652	-3.82252	0.38669
H	-4.87862	-1.62644	1.05454
H	0.00926	3.80531	1.72816
H	-3.17779	3.60429	-1.01981
H	-4.87789	-0.12369	0.57283
H	-3.24607	-0.91057	3.10094
H	-1.35143	4.43850	1.24305
H	-3.88194	2.30770	-0.48085
H	-3.31810	-1.68702	-2.25685
H	-2.77698	-3.30728	1.85051
H	-2.46762	1.22147	1.85035
H	-1.04973	-0.10235	-1.94863
H	-0.05176	-1.14024	1.95553
H	-1.19054	-2.76793	-1.81346
H	1.43334	-0.63827	-2.23665
H	2.20168	-1.18712	1.96565
H	0.35457	1.07986	1.85351
H	1.05959	1.86008	-2.23749

H	3.05639	0.71910	-2.77812
H	5.04760	-0.11835	-0.23163
H	2.70031	2.20584	2.41852
H	3.31157	-4.13894	-0.49947
H	1.18186	-4.77920	1.56134
H	4.22846	2.71848	0.39298

Optimized geometries of Hf tetramers with counterions and explicit water

109
Hf4_4_2_bridging_peroxide_conf1_deprot1_ion16.log Energy: -3143075.0549975

Hf	2.69249	0.41722	0.24931
O	1.92972	-1.17858	-1.15107
O	1.15764	-0.90542	1.10468
O	3.16072	0.26512	2.45516
O	3.51211	0.68649	-1.90482
O	4.06272	1.83562	0.40630
O	4.30509	-1.11250	0.35766
Hf	-0.59618	2.66401	0.16796
O	1.26862	1.90032	0.93271
O	1.25847	1.78042	-0.56816
O	-0.29288	3.79981	-1.81082
O	-0.62654	2.96330	2.55067
O	-2.12649	3.93820	0.42341
O	0.66420	4.53310	0.56434
Hf	0.55174	-2.44341	-0.15112
O	-1.54543	-1.85598	0.03090
O	-0.97982	-1.36086	-1.27360
O	0.77565	-3.29050	-2.42309
O	-0.08363	-3.13876	1.92684
O	1.93635	-3.85470	0.14847
O	-0.77097	-4.31583	-0.63314
Hf	-2.62391	-0.14488	-0.63705
O	-1.63285	1.59679	-1.38299
O	-1.56331	0.92529	0.86756
O	-3.80284	-0.47912	1.22459
O	-2.77047	-0.28240	-3.13201
O	-3.95490	-1.59559	-1.32956
O	-4.35017	1.15472	-0.95642
Cl	1.63532	-1.84359	4.20329
Cl	-2.50965	0.83775	3.81139
O	-3.35849	-4.53878	0.27293
O	4.32045	-2.32992	-2.04455

O	-4.43008	3.08242	-2.82623
O	-2.58954	4.99543	-2.01819
O	3.54790	2.64439	3.79206
O	-4.90339	-2.85041	1.73514
O	5.10157	2.46117	-3.08590
O	-6.39052	-0.43298	-1.29084
O	3.18245	-4.76607	-2.20375
O	-1.01116	5.72095	2.30637
Cl	8.32184	-0.29844	-1.22413
Cl	-7.76686	-2.03981	1.11683
O	5.88621	-0.28994	-3.16427
O	-3.80603	1.61355	-4.95324
O	-1.18962	-5.58955	1.67092
O	3.77506	-3.07821	2.01701
H	2.66161	-0.33011	3.07047
H	3.94408	1.54509	-2.19392
H	3.81181	2.72076	0.74031
H	4.16702	-1.81105	1.08490
H	-1.15463	4.30238	-2.04144
H	0.22981	2.68647	2.92347
H	1.57245	4.39705	0.96110
H	0.02355	-3.91509	-2.46163
H	0.48009	-2.90442	2.70645
H	-0.57230	-5.07192	-0.03515
H	-3.50923	-0.08717	2.08392
H	-3.37471	-1.04448	-2.92018
H	-5.24466	0.67035	-0.99709
H	-3.96652	-3.97533	0.82096
H	4.19814	-3.29386	-2.20477
H	4.95272	-1.96023	-2.69728
H	-4.22945	2.61047	-3.68977
H	-5.33400	3.42917	-2.91129
H	-3.24247	4.38107	-2.43154
H	-2.63886	4.75904	-1.05644
H	4.45679	2.75406	4.12208
H	2.98248	2.69414	4.58243
H	-4.87296	-3.04721	2.68733
H	-5.87228	-2.68771	1.52340
H	5.61621	1.67549	-3.37865
H	-6.87303	-0.76253	-0.49711
H	3.39119	-5.65534	-2.53252
H	2.38734	-4.46580	-2.68719
H	-0.90193	4.99653	2.95132
H	-0.98749	6.55267	2.80624

H	5.15964	-0.06464	-2.55173
H	-3.43459	0.86185	-4.44075
H	-1.18127	-6.37083	2.24606
H	3.10818	-3.47477	1.39582
H	-3.92500	-5.18432	-0.18104
H	-1.73411	-4.14779	-0.47217
H	-0.41025	-4.07164	2.02604
H	-2.12789	-5.40865	1.42884
H	-5.65722	-1.08954	-1.39881
H	-3.04328	1.99840	-5.41541
H	6.69091	-0.32191	-2.57917
H	4.68745	2.80119	-3.89633
H	3.23528	-2.75892	2.77161
H	-4.20154	-1.37831	1.41762
H	-3.78396	-2.50122	-1.02072
H	-4.35390	1.88971	-1.63795
H	-1.95018	-0.69250	-3.46257
H	0.60836	-2.60682	-3.09644
H	2.42558	-4.29859	-0.57711
H	0.79857	-0.78891	2.00046
H	2.64836	-1.62728	-1.65223
H	-1.65355	0.72981	1.82626
H	-1.49038	1.80702	-2.31707
H	0.36487	4.48705	-1.59618
H	0.17991	5.17083	1.15246
H	-1.30375	2.41146	3.03309
H	2.86571	0.43582	-2.58791
H	4.44364	-1.62891	-0.48426
H	3.35321	1.11099	2.93269
H	-2.07533	4.63308	1.10752
O	3.14360	4.26753	1.59576
H	3.66308	5.08636	1.65055
H	3.20841	3.83945	2.48277

109
Hf4_4_2_bridging_peroxide_conf1_deprot1_ion1.log Energy: -3143100.5123978

Hf	-2.69067	0.95778	-0.16972
O	-2.32887	-0.87950	0.87195
O	-1.61724	-0.53402	-1.33755
O	-3.40863	1.17135	-2.31068
O	-3.28998	1.17448	2.06139
O	-3.75490	2.72155	-0.09382
O	-4.73088	-0.01969	-0.20280
Hf	0.94975	2.59327	-0.00565

O	-1.09473	2.26992	-0.76384
O	-0.96690	1.83601	0.67495
O	0.78345	3.35282	2.16840
O	1.07813	3.35793	-2.19139
O	2.70942	3.56784	0.14100
O	-0.00531	4.66280	-0.03038
Hf	-1.20910	-2.28942	-0.24308
O	0.90753	-1.89978	-0.82634
O	0.61548	-1.51619	0.59904
O	-1.28296	-2.89895	2.10315
O	-1.09560	-3.02898	-2.39015
O	-2.90774	-3.34353	-0.40420
O	-0.18126	-4.31335	0.03072
Hf	2.44916	-0.64846	-0.02579
O	1.97477	1.08463	1.18077
O	1.42771	0.88223	-1.11991
O	3.24276	-0.68236	-2.13501
O	2.70389	-1.25530	2.30267
O	3.59355	-2.34140	0.03384
O	4.48008	0.29493	0.18949
Cl	-1.30399	2.43361	4.28202
Cl	1.48617	-4.15401	2.73593
Cl	-2.43353	-0.99392	-4.38964
Cl	1.58322	0.98787	-4.23131
O	3.46286	-4.44787	-1.88286
O	-4.72408	-1.58223	2.07315
O	5.50204	1.23546	2.48111
O	3.41924	2.98592	2.66582
O	-3.57490	3.83000	-2.42740
O	5.04416	-2.53324	-2.94629
O	-1.97719	-0.63902	3.72522
O	6.03981	-1.78751	-0.58775
O	-3.77825	-4.14020	2.11640
O	2.12433	6.36898	0.01634
O	-4.48920	-1.01275	4.80310
O	5.10606	-1.04050	3.77989
O	0.87465	-4.82190	-2.38923
O	-4.65118	-1.96124	-1.99239
H	-3.06661	0.60526	-3.04606
H	-2.92889	1.99834	2.45218
H	-4.62946	2.66228	0.32136
H	-4.77725	-0.69610	-0.96006
H	1.62515	3.22537	2.66324
H	0.27189	3.84982	-2.49524

H	-0.52041	4.86831	-0.85676
H	-0.43718	-3.31358	2.42569
H	-1.41178	-2.46021	-3.13530
H	0.26657	-4.62427	-0.80668
H	2.81920	-0.17233	-2.86946
H	2.37928	-2.19713	2.37101
H	5.20611	-0.29821	-0.14033
H	4.07656	-3.91812	-2.45043
H	-4.63453	-2.56371	2.10818
H	-4.78165	-1.29470	3.01261
H	5.45775	0.41900	3.06443
H	6.43895	1.47905	2.40338
H	4.25078	2.47262	2.78795
H	3.43324	3.31973	1.73056
H	-3.73799	3.59517	-1.45436
H	-4.34754	4.32847	-2.73961
H	5.51552	-2.42300	-3.78788
H	5.68387	-2.32603	-2.21391
H	-2.72272	-0.82128	4.34131
H	5.18820	-2.18738	-0.21119
H	-4.00628	-4.97809	2.54916
H	-2.86309	-3.90924	2.39199
H	2.14090	7.01994	-0.70460
H	2.32965	6.87100	0.82233
H	-4.89860	-0.22502	5.19855
H	4.25209	-1.21982	3.32565
H	0.72219	-5.68618	-2.80426
H	-4.05697	-2.54628	-1.44693
H	3.94540	-5.25243	-1.63295
H	0.50492	-4.31573	0.74467
H	-0.30028	-3.55340	-2.66009
H	1.86232	-4.69666	-2.32766
H	6.77986	-2.11408	-0.05071
H	4.86721	-0.89839	4.71061
H	-4.75551	-1.75385	5.37256
H	-1.50308	0.14031	4.09451
H	-4.09198	-1.69206	-2.75070
H	3.85705	-1.36318	-2.51919
H	3.34994	-3.10422	-0.53079
H	4.83053	0.70576	1.03322
H	2.05189	-0.72328	2.79537
H	-1.40427	-2.07448	2.64203
H	-3.34441	-3.76512	0.36441
H	-1.31454	-0.40296	-2.25216

H	-3.08637	-1.21947	1.40640
H	1.13884	0.76656	-2.04853
H	2.55146	1.51048	1.85372
H	0.05461	3.00534	2.74931
H	0.66093	5.38787	0.08232
H	1.28663	2.68623	-2.88795
H	-2.83678	0.46664	2.59691
H	-4.91575	-0.53947	0.61993
H	-3.51849	2.10766	-2.62540
H	2.75355	4.51245	-0.10045
O	-1.11601	4.90898	-2.46655
H	-1.10494	5.76002	-2.93279
H	-2.04862	4.55637	-2.51529

109
Hf4_4_2_bridging_peroxide_conf1_deprot1_ion6.log Energy: -3143092.4042162

Hf	-2.34732	-1.72620	-0.43622
O	-2.32525	0.25060	-1.25364
O	-1.81667	-0.27375	1.03323
O	-3.34630	-2.45253	1.42777
O	-2.28927	-2.06442	-2.99003
O	-2.74927	-3.64747	-1.01642
O	-4.49559	-1.44127	-0.98510
Hf	1.63781	-2.14401	-0.39505
O	-0.44041	-2.64700	0.20528
O	-0.37836	-1.96138	-1.13162
O	1.73580	-2.53052	-2.69397
O	1.98351	-3.06167	1.69928
O	3.61181	-2.54237	-0.49201
O	1.40771	-4.37784	-0.75281
Hf	-2.00352	1.70510	0.31565
O	0.10852	1.87510	1.14919
O	-0.00245	1.78015	-0.34528
O	-2.04335	2.88759	-1.75762
O	-2.44703	1.94490	2.50344
O	-3.98103	2.06113	0.23713
O	-1.70952	3.93249	0.75208
Hf	1.99042	1.37437	0.17089
O	2.10693	-0.23806	-1.29728
O	1.45585	-0.54709	0.94459
O	2.78315	1.22220	2.26956
O	1.88171	2.44044	-2.04483
O	2.51660	3.29808	0.43887
O	4.18362	1.18511	-0.22886

Cl	-0.12808	-1.63254	3.56592
Cl	-0.00574	5.18175	-1.60540
Cl	-4.17819	-0.39390	3.67108
Cl	4.17683	-1.42626	3.20997
O	1.71244	4.66385	2.79325
O	-4.45425	0.41004	-3.02440
O	5.12108	0.38918	-2.66029
O	4.30425	-2.24713	-3.08779
O	-1.73125	-4.18824	2.67472
O	3.99408	3.33867	3.53606
O	-0.41602	1.75422	-3.61674
O	5.03288	3.67053	-0.41543
O	-4.72614	3.01135	-2.30579
O	3.93071	-5.35812	-0.38172
O	-2.30289	0.06010	-4.72235
O	4.39175	2.95220	-3.08964
O	-0.84531	3.95047	3.30694
O	-5.64998	0.02086	0.83115
H	-3.51211	-1.78290	2.14549
H	-2.65466	-2.95628	-2.76658
H	-2.05343	-4.27973	-0.77768
H	-5.01426	-0.96103	-0.24091
H	2.68914	-2.44771	-3.02834
H	1.25901	-2.77384	2.31181
H	0.85167	-4.80680	-0.02838
H	-1.51936	3.73550	-1.72114
H	-2.91438	1.21432	2.98861
H	-1.39386	4.06652	1.69131
H	3.21043	0.36100	2.53525
H	1.47458	3.30758	-1.79385
H	4.66396	2.07598	-0.20989
H	2.50776	4.30711	3.25602
H	-4.73801	1.34906	-2.90485
H	-3.87830	0.38305	-3.82239
H	4.93398	1.29120	-3.03598
H	6.08904	0.33304	-2.58870
H	4.57106	-1.30748	-3.19186
H	4.30157	-2.37348	-2.10250
H	-2.10090	-4.70491	3.41139
H	-1.21184	-3.45452	3.09356
H	4.25174	3.13312	4.45091
H	4.77938	3.74102	3.12739
H	-0.95022	1.02870	-4.03358
H	4.10622	3.81791	-0.08684

H	-5.19512	3.77769	-2.67257
H	-3.76316	3.21190	-2.34850
H	4.01452	-5.96894	0.36920
H	4.40302	-5.78355	-1.11648
H	-2.29847	-0.85025	-4.34865
H	3.43035	2.84560	-2.89020
H	-1.21101	4.62361	3.90371
H	-5.08926	0.82510	0.64196
H	1.80748	5.63040	2.79915
H	-1.04399	4.37874	0.16872
H	-1.80281	2.41921	3.07975
H	0.12726	4.14468	3.22913
H	4.94178	3.67302	-1.39380
H	4.44518	3.43456	-3.93085
H	-2.29889	-0.04068	-5.68863
H	-0.35710	2.43859	-4.30565
H	-5.37298	-0.22381	1.74194
H	3.32409	1.95833	2.64747
H	2.13322	3.82430	1.17211
H	4.50655	0.72665	-1.04954
H	1.19406	2.00949	-2.61022
H	-1.52305	2.36239	-2.43245
H	-4.40050	2.46769	-0.54896
H	-1.38169	-0.52063	1.87598
H	-3.02828	0.43583	-1.92101
H	0.98470	-0.64868	1.79645
H	2.56353	-0.18946	-2.14931
H	1.47137	-3.45914	-2.82042
H	2.28214	-4.84650	-0.71478
H	2.78988	-2.62331	2.09871
H	-1.32412	-2.22081	-2.96485
H	-4.60968	-0.86442	-1.78475
H	-2.86970	-3.21680	1.86176
H	3.94013	-3.42576	-0.23375
O	0.29486	-5.59375	1.33236
H	1.02337	-5.33245	1.92180
H	-0.49040	-5.14248	1.72285

109
Hf4_4_2_bridging_peroxide_conf1_deprot2_ion16.log Energy: -3143068.4525625

Hf	2.66851	-0.27392	-0.40399
O	1.48488	-1.39420	-1.80866
O	1.11601	-1.39640	0.50490
O	3.32370	-0.48824	1.73866

O	3.44417	0.44829	-2.56701
O	4.26819	1.25810	-0.08364
O	4.15608	-1.57081	-0.69787
Hf	0.11060	2.80060	-0.10239
O	1.76985	1.55047	0.45997
O	1.48552	1.43348	-1.01380
O	0.22511	3.76782	-2.21137
O	0.25784	3.34330	2.10531
O	-1.55423	4.22200	0.18355
O	1.46426	4.30040	-0.11368
Hf	-0.07253	-2.53039	-0.85132
O	-1.77540	-1.57253	-0.01528
O	-1.46543	-1.01537	-1.38022
O	-0.25368	-2.85471	-3.24056
O	-0.16010	-3.69143	1.05108
O	1.46952	-4.11576	-1.17089
O	-1.39685	-4.05207	-1.34622
Hf	-2.60116	0.47376	-0.22120
O	-1.47327	1.91274	-1.32548
O	-1.03805	1.26330	0.90481
O	-3.20638	-0.03930	1.89731
O	-3.52772	0.43021	-2.51922
O	-4.35524	-0.99385	-0.51226
O	-4.02748	1.82121	-0.00141
Cl	1.37856	-2.34569	3.46495
Cl	-1.19462	1.22547	3.99928
O	-3.95441	-3.75500	0.19924
O	3.71303	-3.64711	-2.63107
O	-3.75029	4.35520	-1.53854
O	-1.64193	5.53042	-2.93471
O	4.27413	1.63586	3.07463
O	-4.04612	-2.50586	2.57344
O	6.36003	1.22731	-1.60336
O	-6.74826	-0.57570	0.46872
O	0.05730	-6.29302	-1.48481
O	-1.23173	6.64973	1.23090
Cl	7.17570	0.75088	2.59831
Cl	-6.97043	-2.01758	3.23730
O	6.79780	-0.97690	-0.16910
O	-4.55780	2.84784	-3.55536
O	-2.04846	-5.52005	1.37469
O	3.03217	-4.46356	1.36078
H	2.82101	-1.05453	2.37051
H	2.88690	1.16177	-2.92581

H	3.86473	2.12818	0.07887
H	-0.49993	4.40948	-2.48983
H	1.20071	3.52438	2.38232
H	-2.34043	4.21888	-0.40992
H	2.11366	4.31138	0.61480
H	-0.97803	-3.50379	-3.07206
H	0.19314	-3.35899	1.91014
H	2.21500	-3.95912	-1.80963
H	-2.68935	0.35162	2.64445
H	-4.23101	-0.20833	-2.26444
H	-5.27094	-0.81901	-0.10571
H	-4.02503	-3.37579	1.12055
H	4.32744	-4.39968	-2.58344
H	3.64534	-3.43093	-3.57642
H	-4.08402	3.81769	-2.32515
H	-4.47625	4.94845	-1.28128
H	-2.46395	5.25682	-2.46454
H	-1.39592	6.38012	-2.53344
H	5.24854	1.47632	2.90361
H	4.16090	1.49183	4.03013
H	-3.57708	-2.93038	3.31177
H	-4.99640	-2.38506	2.87300
H	6.67028	0.38138	-1.15599
H	-6.84304	-1.01547	1.35329
H	-0.69288	-5.63900	-1.43022
H	0.07565	-6.57462	-2.41466
H	-1.83663	6.76728	1.98242
H	-1.50787	7.32327	0.58697
H	5.85384	-1.26531	-0.25857
H	-4.24196	1.95341	-3.29894
H	-2.31151	-5.61401	2.30523
H	2.51566	-4.30318	0.54987
H	-4.80078	-4.20331	0.02897
H	-2.27491	-3.97191	-0.92816
H	-0.86904	-4.38738	1.21653
H	-2.81096	-5.08155	0.93615
H	-7.38173	-1.03876	-0.10395
H	-4.04866	3.07521	-4.35086
H	6.85869	-0.55201	0.71630
H	5.98116	0.93808	-2.45025
H	2.59545	-3.89823	2.02443
H	-3.44599	-0.97188	2.15558
H	-4.14332	-1.95116	-0.39177
H	-4.00546	2.65130	-0.51226

H	-2.93828	-0.07291	-3.11058
H	-0.66824	-2.11523	-3.71878
H	1.08751	-5.04497	-1.31472
H	1.00231	-1.43798	1.47752
H	1.57912	-1.37903	-2.77018
H	-0.91270	1.05355	1.85576
H	-1.51137	2.03938	-2.28328
H	0.99980	4.32821	-1.99669
H	-0.15459	2.75025	2.77958
H	3.62005	-0.16879	-3.29718
H	5.06276	1.34706	-0.71815
H	4.11258	-2.22610	-1.42354
H	3.63291	0.32571	2.23068
H	-1.43864	5.13337	0.58506
O	2.86148	3.89866	2.38616
H	3.12127	4.61225	2.99067
H	3.42740	3.12014	2.62200

109
Hf4_4_2_bridging_peroxide_conf1_deprot3_ion16.log Energy: -3143081.7026885

Hf	2.63893	0.90489	0.36316
O	2.58939	-0.80250	-1.00669
O	1.24475	-0.59915	0.91154
O	2.35283	1.26739	2.59564
O	3.92561	1.53543	-1.10665
O	4.05536	2.64518	1.13985
O	4.15149	-0.36589	1.37267
Hf	-0.83340	2.50818	-0.32537
O	1.25469	2.50783	0.31409
O	1.07924	1.70364	-0.94747
O	-0.63911	3.22855	-2.55329
O	-1.23563	3.20472	1.53828
O	-2.87424	3.35534	-0.66648
O	-0.15788	4.72900	-0.46735
Hf	1.25335	-2.32381	-0.29696
O	-0.95005	-2.22756	0.08373
O	-0.51878	-1.67016	-1.24903
O	1.38407	-2.47173	-2.86673
O	1.40466	-3.29310	1.44642
O	3.05131	-3.50570	-0.83444
O	0.39527	-4.36644	-1.03429
Hf	-2.35977	-0.75295	-0.58732
O	-1.80830	1.05041	-1.59979
O	-1.36097	0.70438	0.63593

O	-3.13841	-0.97364	1.52466
O	-2.89879	-1.07373	-2.56744
O	-3.59738	-2.67418	-0.61398
O	-4.33531	0.33043	-0.49788
Cl	0.06407	-0.33911	3.81471
Cl	-3.68712	1.62347	3.14958
O	-3.08168	-4.74246	1.08723
O	5.34342	-2.40834	0.01213
O	-4.61435	2.25656	-2.52590
O	-2.79930	3.94926	-3.94929
O	2.61483	3.93464	3.03934
O	-4.21010	-3.08055	2.84440
O	6.48573	1.89264	1.66684
O	-6.08727	-1.71435	-0.32944
O	2.53181	-5.05949	-2.90895
O	-2.61797	6.03635	-0.52035
Cl	7.32688	-1.54352	-2.10601
Cl	-7.21113	-2.71896	2.34279
O	6.68135	1.38127	-0.92950
O	-4.22297	0.40761	-4.28427
O	-0.44502	-5.40594	1.22875
O	2.98628	-1.91125	3.19783
H	1.57366	0.84276	3.04455
H	3.64323	1.32503	-2.01077
H	4.22539	3.05979	0.27136
H	3.73333	-0.89948	2.13171
H	-1.44977	3.52762	-3.06856
H	-3.45744	3.00531	-1.38080
H	0.20637	4.99872	0.44227
H	0.48520	-2.29756	-3.20135
H	3.96968	-3.21787	-0.57711
H	0.08422	-4.88613	-0.22278
H	-3.37552	-0.14388	2.02615
H	-4.57815	-2.51522	-0.53980
H	-5.12212	-0.27254	-0.40758
H	-3.49361	-4.30326	1.88055
H	5.83211	-2.95085	0.65489
H	6.01379	-2.15382	-0.69255
H	-4.51081	1.56889	-3.27904
H	-5.53160	2.57888	-2.55534
H	-3.56074	3.48329	-3.54080
H	-2.99617	4.89465	-3.84679
H	3.30511	3.81889	2.34667
H	3.07689	4.23817	3.83844

H	-4.01904	-3.06985	3.79729
H	-5.20419	-3.01498	2.75526
H	6.69153	1.62634	0.71814
H	-6.51354	-1.99521	0.52990
H	1.74692	-5.36712	-2.41636
H	2.18317	-4.26910	-3.36778
H	-2.83011	6.49811	0.30852
H	-2.95268	6.60581	-1.23336
H	5.70673	1.41829	-1.09276
H	-3.68505	-0.20483	-3.68809
H	-0.34584	-6.35718	1.39619
H	2.45743	-2.51380	2.60944
H	-3.64656	-5.50563	0.87793
H	-0.41881	-4.19743	-1.54251
H	0.80495	-4.03026	1.67541
H	-1.41928	-5.20890	1.26108
H	-6.75129	-1.85523	-1.02452
H	-3.60818	0.70886	-4.97298
H	6.94506	0.48023	-1.22352
H	7.02133	2.68763	1.82555
H	2.28650	-1.38978	3.63976
H	-3.54088	-1.74864	2.00005
H	-3.35684	-3.44122	-0.02581
H	-4.50911	0.96740	-1.23492
H	-3.17738	-1.99622	-2.68369
H	1.90192	-1.69063	-3.13209
H	3.04815	-4.13292	-1.61660
H	0.70100	-0.60489	1.73144
H	3.40946	-1.02037	-1.47397
H	-1.30899	0.61091	1.60357
H	-1.68735	1.01453	-2.55975
H	-0.01668	3.97642	-2.57004
H	-0.92539	5.33443	-0.60342
H	-1.98227	2.79897	2.02629
H	4.98468	2.33235	1.45066
H	4.64828	-1.03663	0.82992
H	2.37725	2.21583	2.89073
H	-3.00582	4.33322	-0.57543
O	0.35032	5.26775	2.04475
H	-0.29755	4.51811	2.13599
H	1.19242	4.89856	2.39211

109
Hf4_4_2_bridging_peroxide_conf1_deprot3_ion1.log Energy: -3143079.5200223

Hf	2.59907	-0.82690	0.27663
O	1.39502	-1.98379	-1.15303
O	0.72777	-1.52630	1.01483
O	2.90244	-0.86509	2.57422
O	3.78701	-1.05722	-1.38173
O	4.53419	0.25228	0.83084
O	3.40293	-2.82955	0.81402
Hf	0.50909	2.52696	0.02845
O	1.99633	1.18218	0.82347
O	1.73446	0.87621	-0.63240
O	0.95048	2.84339	-2.23083
O	0.67265	3.48485	1.82526
O	-0.61271	4.42247	-0.40158
O	2.41549	3.80555	-0.19473
Hf	-0.40372	-2.72091	-0.34173
O	-2.02696	-1.35719	0.64043
O	-1.56831	-1.02992	-0.75936
O	-0.74926	-2.46960	-2.80675
O	-0.49636	-3.92755	1.26366
O	0.41840	-4.61255	-1.27751
O	-2.25774	-3.81101	-0.94757
Hf	-2.57980	0.62892	0.01879
O	-1.19530	1.84201	-1.09237
O	-0.90558	1.40215	1.14408
O	-3.34947	0.85973	2.17097
O	-3.47745	0.69659	-1.83197
O	-4.59290	-0.51697	0.24371
O	-3.60137	2.64923	0.19231
Cl	3.76847	1.69722	-3.39517
Cl	-3.79316	-2.36699	-3.24476
Cl	0.31902	-1.37920	4.23623
Cl	-1.81492	2.90953	3.90419
O	-4.53718	-2.53268	2.16273
O	3.17152	-4.86392	-1.02645
O	-2.82644	4.33209	-1.99517
O	-0.42771	4.64827	-3.70719
O	4.08517	1.47951	3.48460
O	-2.80376	-1.23358	3.80953
O	6.02359	1.14537	-1.12380
O	-6.16925	1.76488	0.45968
O	0.02556	-4.88356	-3.90171
O	1.30736	6.32959	-0.60849
O	6.41596	-1.50801	-1.66869
O	-3.56131	2.52026	-3.69120

O	-3.25297	-4.77544	1.28170
O	1.84411	-3.98430	2.63816
H	2.08674	-0.96125	3.12780
H	3.71960	-0.30557	-2.00867
H	4.36461	1.00801	1.42209
H	2.85840	-3.25882	1.55900
H	0.57101	3.56738	-2.79812
H	-1.35478	4.42421	-1.05430
H	2.85919	3.90125	0.70623
H	-1.71281	-2.30755	-3.02314
H	1.38634	-4.75620	-1.13776
H	-2.76356	-4.21876	-0.18029
H	-2.97910	1.64388	2.65957
H	-5.32944	0.12217	0.38615
H	-4.58482	2.54235	0.26302
H	-3.89948	-2.18796	2.83946
H	3.50108	-5.70093	-0.65582
H	3.59884	-4.78154	-1.89653
H	-3.12832	3.67438	-2.71750
H	-3.40088	5.11369	-2.06279
H	-1.27665	4.71565	-3.22458
H	-0.09257	5.55807	-3.75269
H	4.98703	1.42496	3.84752
H	3.52157	1.68596	4.25150
H	-1.82318	-1.35901	3.87763
H	-3.10995	-1.07949	4.71931
H	6.35484	0.25470	-1.41363
H	-6.61945	1.97755	1.29475
H	-0.76104	-5.42171	-4.09101
H	-0.30114	-3.95842	-3.88561
H	1.46165	6.94661	0.12683
H	1.39727	6.85917	-1.41831
H	5.42400	-1.49338	-1.55508
H	-3.53145	1.74720	-3.03671
H	-3.82759	-5.55734	1.25449
H	0.98309	-4.06892	2.14380
H	-5.37272	-2.67799	2.63820
H	-2.89999	-3.34989	-1.54810
H	-1.28724	-4.47171	1.43768
H	-3.79981	-4.03065	1.64660
H	-6.82012	1.94352	-0.24015
H	-2.86215	2.34269	-4.34121
H	6.74657	-1.85900	-0.82582
H	5.38727	1.40641	-1.82971

H	1.62366	-3.31430	3.31424
H	-3.16232	0.08990	2.77468
H	-4.62173	-1.19735	0.96474
H	-3.40602	3.24943	-0.57050
H	-3.71972	-0.19401	-2.15573
H	-0.28103	-1.65503	-3.06211
H	0.24856	-4.79093	-2.25028
H	0.35029	-1.34824	1.89849
H	1.90700	-2.24351	-1.93335
H	-0.92936	1.51273	2.11237
H	-1.13826	1.75116	-2.05413
H	1.84750	2.58670	-2.55599
H	2.19675	4.72496	-0.47438
H	-0.08807	3.46481	2.43871
H	5.09455	0.61183	0.05578
H	3.42174	-3.49585	0.08319
H	3.40145	-0.10474	2.95763
H	-0.09810	5.26500	-0.46168
O	3.19122	4.04921	2.32800
H	2.21360	3.85254	2.40292
H	3.62761	3.22980	2.63146

109
Hf4_4_2_bridging_peroxide_conf1_deprot3_ion6.log Energy: -3143072.8943256

Hf	2.56182	0.90740	-0.38633
O	2.31350	-0.99416	-1.32917
O	1.51672	-0.56120	0.78631
O	3.35192	1.31595	1.74479
O	3.04182	1.27928	-2.36688
O	3.78069	2.82549	-0.28692
O	4.65883	0.04022	-0.29641
Hf	-1.08870	2.44367	-0.09152
O	1.03635	2.24632	0.41613
O	0.76559	1.84821	-1.01505
O	-1.16609	3.16955	-2.32648
O	-1.43023	3.24966	1.73803
O	-3.17870	3.28825	-0.29818
O	-0.25123	4.60015	-0.27747
Hf	1.18860	-2.43289	-0.17184
O	-0.90797	-2.16745	0.58471
O	-0.69552	-1.71877	-0.84229
O	0.91538	-2.86669	-2.64570
O	1.65763	-3.24085	1.57345
O	3.01442	-3.63710	-0.79446

O	0.23230	-4.47115	-0.50567
Hf	-2.47730	-0.86973	-0.10330
O	-2.17306	0.95860	-1.20126
O	-1.38830	0.65273	0.94774
O	-3.11618	-0.90922	2.08989
O	-3.13079	-1.36426	-2.00363
O	-3.60006	-2.81508	0.18471
O	-4.53329	0.12275	-0.03324
Cl	0.24836	0.14476	3.72292
Cl	-1.70009	-4.46254	-2.98878
Cl	4.94611	-0.91784	3.32173
Cl	-3.77783	1.75143	3.56575
O	-3.09402	-4.63768	2.12450
O	5.03572	-2.48789	0.63813
O	-4.92038	2.03550	-2.10361
O	-3.40284	3.97918	-3.54553
O	1.88874	2.74782	3.44197
O	-4.34973	-2.81996	3.68326
O	5.76858	3.31151	-1.92512
O	-6.21342	-2.03748	-0.08187
O	3.54304	-2.71005	-3.27418
O	-2.68631	5.95536	-0.12971
O	5.59418	0.84711	-2.97168
O	-4.33843	0.12956	-3.76759
O	-0.40739	-5.19409	1.98691
O	6.44553	1.09462	1.36751
H	3.73809	0.56246	2.25819
H	2.70442	2.12660	-2.69617
H	4.15858	2.89090	0.60866
H	5.34186	0.50112	0.28456
H	-1.98568	3.54558	-2.76688
H	-3.78474	2.94895	-0.99543
H	0.22138	4.78690	0.59651
H	0.11027	-3.42092	-2.85366
H	3.74885	-3.40647	-0.16915
H	-0.09247	-4.84355	0.36412
H	-3.30339	-0.02866	2.52158
H	-4.57766	-2.76871	0.05894
H	-5.28646	-0.51941	-0.03622
H	-3.51982	-4.15424	2.87615
H	4.98613	-2.17730	1.58095
H	5.94879	-2.79615	0.50931
H	-4.73528	1.32788	-2.81684
H	-5.87203	2.23330	-2.13943

H	-4.08776	3.39535	-3.15166
H	-3.68121	4.88235	-3.32250
H	2.36251	2.89819	4.27752
H	1.23406	2.02481	3.63578
H	-4.09340	-2.62876	4.60174
H	-5.31798	-2.90903	3.69723
H	5.84418	2.42240	-2.38032
H	-6.84517	-2.20116	0.63866
H	4.16642	-3.08080	-3.91928
H	2.64494	-2.98195	-3.55357
H	-2.83588	6.38089	0.73157
H	-2.99611	6.59322	-0.79442
H	4.60461	0.98147	-2.89436
H	-3.84901	-0.51427	-3.15727
H	-0.28744	-6.12931	2.21774
H	7.32719	0.76530	1.12467
H	-3.61798	-5.44567	1.99106
H	-0.51872	-4.51244	-1.15086
H	1.03182	-3.87395	1.97539
H	-1.36297	-4.99198	2.14614
H	-6.70133	-2.20719	-0.90541
H	-3.70099	0.39203	-4.45099
H	5.75907	0.33792	-2.15757
H	5.46562	3.92022	-2.61880
H	6.17483	0.54228	2.13839
H	-3.67073	-1.57882	2.55245
H	-3.39208	-3.49303	0.88350
H	-4.69392	0.77646	-0.75738
H	-2.80834	-2.24171	-2.28663
H	0.66766	-1.97720	-2.95547
H	3.35124	-3.39743	-1.70014
H	1.14598	-0.36369	1.67338
H	2.81066	-1.17321	-2.14728
H	-1.01985	0.51158	1.84807
H	-2.23163	0.93565	-2.16659
H	-0.44776	3.80990	-2.46368
H	-1.00910	5.23396	-0.29418
H	-2.10013	2.80179	2.29667
H	4.52724	3.02483	-0.94779
H	4.75420	-0.92925	-0.08879
H	2.80058	1.85653	2.38347
H	-3.25399	4.27155	-0.22281
O	0.51236	4.94806	2.24643
H	-0.31182	4.39229	2.31114

H	1.18683	4.31224	2.56641

109
Hf4_4_2_bridging_peroxide_conf1_deprot4_ion16.log Energy: -3143073.7411559

Hf	2.50159	0.80723	0.14447
O	2.43986	-0.97847	-1.19024
O	1.60372	-0.88799	1.01497
O	2.17963	1.47175	2.08716
O	3.51348	1.46926	-1.92648
O	3.98956	2.60048	0.25671
O	4.42515	-0.04767	0.70139
Hf	-0.85283	2.47595	-0.26710
O	1.31281	2.53285	-0.35318
O	0.81750	1.30814	-1.06743
O	-1.09982	3.38334	-2.02581
O	-0.24697	2.67404	1.97693
O	-2.77936	3.15844	0.59997
O	-0.39827	4.71402	0.16860
Hf	1.02980	-2.47663	-0.28134
O	-1.09159	-2.33517	-0.55704
O	-0.35118	-1.25263	-1.29619
O	1.40694	-3.43081	-2.05761
O	0.32376	-2.99612	1.83817
O	2.90634	-3.51351	0.42615
O	0.42575	-4.72420	-0.17986
Hf	-2.50556	-0.71288	-0.59082
O	-2.14077	1.20431	-1.42089
O	-1.35412	0.53939	0.68828
O	-3.33279	-1.12164	1.14933
O	-2.37234	-1.15601	-2.91962
O	-3.73158	-2.64452	-1.25052
O	-4.48597	0.00243	-1.32917
Cl	1.78857	-1.23223	4.09440
Cl	-1.90579	1.14362	3.99166
O	-3.67025	-4.69564	0.55685
O	4.88683	-2.13739	-0.77835
O	-4.88488	2.64547	-0.95335
O	-2.21033	5.93051	-2.76445
O	3.20145	3.89702	2.48183
O	-5.17702	-3.09342	2.03115
O	6.58576	2.13126	0.20232
O	-6.33746	-1.90952	-1.30536
O	3.06507	-5.47069	-1.35166
O	-2.79486	5.84039	0.98969

Cl	7.45377	-2.01752	-2.42744
Cl	-8.08398	-2.75365	1.06780
O	6.45537	1.01105	-2.25270
O	-4.40623	4.20548	-3.04818
O	-1.32272	-5.09867	1.76982
O	4.79347	-0.51972	3.26637
H	2.10392	0.82749	2.81885
H	3.72666	2.39314	-1.67322
H	3.78671	3.25152	0.97875
H	4.60291	-0.20462	1.68669
H	-1.08191	4.35288	-2.09878
H	0.64492	2.23096	2.08574
H	-3.58756	2.92054	0.05366
H	0.15149	4.92015	0.98648
H	0.75913	-2.68168	2.66250
H	3.74209	-3.04253	0.17654
H	-0.25092	-5.02543	0.49087
H	-2.83275	-2.01560	-2.98519
H	-4.71804	-2.53130	-1.29606
H	-5.31761	-0.52872	-1.22604
H	-4.31092	-4.23613	1.17455
H	5.73694	-2.19911	-1.30069
H	4.18646	-1.80359	-1.38032
H	-4.73102	3.23735	-1.75676
H	-5.74267	2.90485	-0.57706
H	-2.40926	6.77358	-2.32440
H	-1.94280	6.18170	-3.66446
H	3.87444	4.02048	3.17168
H	2.83424	2.97709	2.60227
H	-5.15479	-3.19703	2.99658
H	-6.13859	-3.01295	1.78355
H	6.62418	1.67272	-0.68495
H	-6.94330	-2.17122	-0.55584
H	2.47464	-6.19218	-1.07867
H	2.46818	-4.84051	-1.83553
H	-2.75935	6.20394	1.89049
H	-3.49592	6.33338	0.53177
H	5.48953	0.95133	-2.36773
H	-4.10198	3.62651	-3.76584
H	-1.31699	-5.88147	2.34360
H	5.36963	-1.29603	3.36578
H	-4.10927	-5.50811	0.25352
H	0.07708	-4.92307	-1.06649
H	-0.32880	-3.71054	2.05016

H	-2.24235	-5.00336	1.39108
H	-6.84675	-2.02303	-2.12450
H	-3.64657	4.81710	-2.88914
H	6.77693	0.07938	-2.30053
H	7.01957	2.98752	0.05325
H	3.91363	-0.81282	3.60363
H	-4.04303	-1.75710	1.37098
H	-3.58015	-3.44114	-0.67647
H	-4.68156	0.97406	-1.21926
H	-1.41494	-1.35765	-2.97509
H	1.68722	-2.92338	-2.83284
H	2.98558	-4.38240	-0.08093
H	1.47626	-0.92893	1.98774
H	2.23097	-0.77101	-2.11463
H	-1.57901	0.47753	1.63820
H	-2.27248	1.48688	-2.33860
H	-1.18481	5.29687	0.25810
H	-0.84815	2.22062	2.64105
H	2.87943	1.52906	-2.66458
H	4.97927	2.38603	0.32432
H	4.73992	-0.85762	0.19325
H	-2.88242	4.11131	0.85450
O	0.78022	5.24343	2.49641
H	0.29478	4.45561	2.80904
H	1.71776	4.93555	2.50850

109
Hf4_4_2_bridging_peroxide_conf1_deprot4_ion6.log Energy: -3143072.8012659

Hf	-1.77716	-1.93246	-0.18171
O	-2.55709	-0.21742	-1.27940
O	-1.58370	-0.09907	0.83417
O	-1.64580	-2.65982	1.71030
O	-2.20255	-2.67876	-2.45555
O	-2.20385	-4.19995	-0.46548
O	-3.95052	-2.05444	0.06369
Hf	2.04915	-1.66001	-0.56037
O	0.19479	-2.72775	-0.49623
O	0.01540	-1.48462	-1.32871
O	2.55909	-2.00001	-2.44535
O	2.15122	-2.43731	1.76572
O	4.21431	-1.37958	-0.01719
O	2.75489	-3.83336	-0.45836
Hf	-2.02313	1.64226	-0.35721
O	-0.11080	2.36560	0.64637

O	-0.00626	1.94393	-0.79948
O	-2.11785	2.00958	-2.40974
O	-2.69589	2.19916	1.73052
O	-4.28915	1.92243	-0.54459
O	-2.26071	3.89116	-0.49243
Hf	1.91782	1.86597	0.13770
O	2.50120	0.36695	-1.23087
O	1.43887	-0.07062	0.78881
O	2.60497	2.02252	2.04585
O	2.12914	3.11895	-1.95157
O	1.98152	4.22819	0.50845
O	4.07974	2.43960	-0.24010
Cl	0.01372	-0.66537	3.63978
Cl	-0.35558	4.79573	-2.80952
Cl	-5.09373	0.84545	3.12936
Cl	4.52877	-2.10665	3.62507
O	0.33460	4.70305	2.69024
O	-5.69874	-0.40871	-1.47182
O	5.49108	0.52833	-1.77790
O	5.40695	-2.10745	-2.97377
O	-0.85540	-5.15860	1.63990
O	0.71449	2.38159	4.09448
O	-4.72411	-4.93882	-0.75929
O	4.35857	3.91812	1.87974
O	-4.47101	3.11613	-2.87425
O	5.46990	-3.59426	-0.74972
O	-5.09551	-3.09543	-2.74509
O	3.65336	1.42463	-3.51762
O	-2.24511	4.83039	1.99108
O	-5.11726	-2.17916	2.37915
H	-1.29477	-2.08711	2.41933
H	-1.96532	-3.62318	-2.34608
H	-1.73097	-4.75896	0.20831
H	-4.39017	-2.16195	0.97937
H	3.47827	-2.11991	-2.75453
H	1.45714	-2.04854	2.34177
H	4.63480	-0.65372	-0.52900
H	2.44358	-4.42185	0.29717
H	-3.51335	1.77070	2.11055
H	-4.76417	1.07464	-0.69740
H	-2.20184	4.41810	0.35016
H	2.69639	3.87382	-1.71220
H	2.83269	4.44564	0.95620
H	4.53478	2.92716	0.50015

H	0.39929	3.87737	3.23728
H	-6.63495	-0.36669	-1.20756
H	-5.66960	-0.05587	-2.37877
H	4.98252	0.92607	-2.53693
H	6.40638	0.85184	-1.84393
H	5.62102	-1.20041	-2.66450
H	5.85295	-2.21555	-3.82930
H	-1.33141	-5.73244	2.26262
H	-1.09497	-4.21055	1.88536
H	0.28794	1.49580	4.02659
H	1.05539	2.44215	5.00191
H	-4.96195	-4.29134	-1.47674
H	3.78081	3.18854	2.25917
H	-4.35266	4.07393	-2.76282
H	-3.53508	2.74779	-2.89463
H	6.27229	-4.01016	-0.39672
H	5.67900	-3.23151	-1.64864
H	-4.15377	-2.87374	-2.88287
H	3.13266	2.20951	-3.23394
H	-2.76518	5.56506	2.35281
H	-6.05656	-2.38805	2.24302
H	0.70109	5.41504	3.24166
H	-1.63740	4.28920	-1.15779
H	-2.69175	3.15447	1.99628
H	-1.31234	4.91184	2.33090
H	5.01701	4.17479	2.54353
H	3.58850	1.36194	-4.48340
H	-5.45695	-2.30271	-2.30599
H	-4.72866	-5.80607	-1.19676
H	-5.11116	-1.22895	2.67108
H	1.99115	2.06064	2.81022
H	1.29653	4.41475	1.20404
H	4.67712	1.75893	-0.62966
H	1.26250	3.53969	-2.22050
H	-1.45370	2.66346	-2.70386
H	-4.48696	2.47904	-1.36653
H	-1.20287	-0.00440	1.72924
H	-2.53527	-0.08065	-2.24068
H	1.14066	-0.17429	1.71247
H	2.74530	0.49338	-2.16919
H	3.71479	-4.00152	-0.60175
H	3.00588	-2.26994	2.27578
H	-1.53034	-2.29461	-3.04850
H	-3.17097	-4.49850	-0.49272

H	-4.46364	-1.39169	-0.44511
H	4.81649	-2.17349	-0.08515
O	1.92146	-5.20756	1.66295
H	2.01363	-4.33928	2.10518
H	0.94128	-5.31864	1.61092

109
Hf4_4_2_bridging_peroxide_conf1_deprot5_ion1.log Energy: -3143078.0391063

Hf	2.58226	0.49423	0.51481
O	2.16458	-1.15588	-0.88916
O	1.01867	-0.79662	1.12786
O	2.52527	0.73575	2.76828
O	3.86373	0.70748	-1.48844
O	4.01732	1.88811	0.94044
O	4.00054	-1.04555	1.29771
Hf	-0.64966	2.57864	-0.30218
O	1.22124	2.15784	0.66820
O	1.25765	1.62115	-0.73924
O	-0.55143	3.16498	-2.21830
O	-1.01800	3.52992	1.76381
O	-2.67001	3.57851	-0.27472
O	0.32716	4.67822	-0.20947
Hf	0.71987	-2.53957	-0.10644
O	-1.34343	-2.06940	0.62610
O	-1.04329	-1.63989	-0.78100
O	0.60498	-2.60134	-2.64370
O	0.95549	-3.59931	1.59774
O	2.37133	-3.94123	-0.74999
O	-0.34460	-4.37340	-0.81638
Hf	-2.64731	-0.41878	-0.07634
O	-1.79428	1.07586	-1.34275
O	-1.46275	0.98030	0.94772
O	-3.40755	-0.60345	2.04021
O	-3.18626	-1.00676	-2.36600
O	-3.96605	-2.24910	-0.14131
O	-4.39388	0.59932	-0.18513
Cl	5.58475	3.12944	-1.66997
Cl	-2.21402	-3.81464	-3.28138
Cl	0.35767	-0.87670	4.32613
Cl	-2.89003	1.97008	3.71701
O	-3.33054	-4.16319	1.74552
O	4.91120	-2.96355	-0.40858
O	-4.49859	2.98798	-2.24671
O	-2.66116	4.81321	-3.27824

O	3.22550	3.30984	2.95209
O	-2.24809	-2.44528	3.62637
O	7.00436	0.98527	-3.90499
O	-6.37204	-1.16840	0.11816
O	2.18441	-4.81197	-3.24857
O	-1.94983	6.05109	-0.99542
O	6.07456	-1.03867	-1.94008
O	-5.06801	0.74919	-3.56630
O	-1.45826	-6.00213	0.92861
O	2.95454	-2.57646	3.16631
H	1.78012	0.36263	3.29935
H	4.39956	1.56384	-1.58942
H	4.54958	2.33918	0.25674
H	3.62039	-1.56682	2.08507
H	-1.22483	3.71075	-2.66922
H	-0.26305	3.96824	2.23503
H	-3.30822	3.28470	-0.97160
H	0.67689	4.95772	0.67482
H	-0.30838	-2.86073	-2.94384
H	0.24257	-3.51620	2.25120
H	3.31248	-3.64618	-0.65334
H	-0.71460	-5.00446	-0.11778
H	-3.41490	0.24909	2.55126
H	-3.16482	-1.99640	-2.46081
H	-4.93569	-2.01111	-0.01194
H	-2.85459	-3.65101	2.44389
H	5.55649	-3.56374	0.00127
H	5.41054	-2.42747	-1.08207
H	-4.67837	2.17822	-2.81669
H	-5.36929	3.37806	-2.05850
H	-3.44099	4.23588	-3.10055
H	-2.74415	5.12538	-4.19306
H	3.65905	2.93756	2.11407
H	3.94232	3.58739	3.54566
H	-1.36418	-2.04830	3.83887
H	-2.70116	-2.53882	4.48197
H	6.76944	0.17103	-3.42429
H	-5.81531	-0.34582	0.03577
H	1.57812	-5.56717	-3.32868
H	1.62253	-4.02482	-3.41230
H	-2.33663	6.90324	-0.73830
H	-2.23026	5.86519	-1.92844
H	5.32048	-0.41753	-1.82085
H	-4.53015	0.03193	-3.16526

H	-1.90018	-6.70062	0.41838
H	2.30307	-3.05227	2.58493
H	-4.11289	-4.53832	2.18480
H	-1.05944	-4.24529	-1.48965
H	-2.19037	-5.42365	1.25896
H	-6.64229	-1.19122	1.05095
H	-4.79145	0.77786	-4.49701
H	6.74962	-0.71676	-1.31693
H	6.68252	1.69020	-3.31236
H	2.36449	-2.03789	3.73259
H	-2.98061	-1.27375	2.64370
H	-3.73334	-2.95983	0.51328
H	-4.48723	1.31884	-0.83184
H	-2.45271	-0.73061	-2.94345
H	0.74838	-1.70081	-2.98490
H	2.29462	-4.38174	-1.64940
H	0.50158	-0.73698	1.95259
H	2.78363	-1.45727	-1.56887
H	-1.50719	1.08028	1.91566
H	-1.77083	1.27823	-2.28964
H	-0.31048	5.36441	-0.52114
H	-1.62787	3.11519	2.42455
H	3.26190	0.69315	-2.25546
H	4.36719	-1.74039	0.68904
H	2.70540	1.66459	3.07761
H	-2.58063	4.56760	-0.35575
O	1.15975	4.93299	2.36847
H	1.15488	5.72149	2.93369
H	1.97131	4.40382	2.60405

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Hf4_4_2_bridging_peroxide_conf1_deprot6_ion1.log Energy: -3143070.0525046

Hf	2.62911	0.40794	0.64263
O	2.37156	-1.27751	-0.72351
O	1.09014	-0.89899	1.23850
O	2.27601	0.91444	2.81977
O	3.74600	0.91258	-1.40101
O	4.23616	1.59524	1.13575
O	3.90181	-1.09285	1.80187
Hf	-0.51880	2.50945	-0.24375
O	1.53955	2.21700	0.38013
O	1.16784	1.27513	-0.73492
O	-0.35325	3.17733	-2.12037
O	-0.74775	3.06221	1.98448

O	-2.50793	3.58656	-0.15432
O	0.24740	4.68470	0.02434
Hf	0.82634	-2.60943	-0.00721
O	-1.26793	-2.09914	0.49876
O	-0.84716	-1.63899	-0.87274
O	0.90136	-2.80598	-2.50910
O	0.85860	-3.61858	1.72643
O	2.57895	-3.99117	-0.46277
O	-0.25918	-4.47041	-0.68513
Hf	-2.53820	-0.51118	-0.24203
O	-1.80786	1.16749	-1.36579
O	-1.34229	0.84107	0.88238
O	-3.34135	-0.49112	1.85040
O	-2.84180	-0.94451	-2.63253
O	-3.91784	-1.99276	-0.44064
O	-4.35895	0.76102	-0.47645
Cl	5.21094	3.39687	-2.24346
Cl	-1.90636	-3.90012	-3.30945
Cl	-0.09976	-0.45545	4.13804
Cl	-3.41322	2.20114	3.44833
O	-3.93761	-4.26278	1.28635
O	5.02913	-2.84141	0.03149
O	-4.27490	2.97055	-2.26523
O	-2.40621	4.96110	-3.11071
O	3.30163	3.40523	2.84480
O	-4.99339	-2.37620	2.98048
O	6.45580	0.82793	-4.02221
O	-6.32804	-0.93780	-0.68338
O	2.63117	-4.94006	-2.95053
O	-1.95327	6.11992	-0.74474
O	5.92586	-0.84716	-1.61868
O	-4.41693	0.98605	-4.00639
O	-1.43298	-5.26213	1.56286
O	2.48749	-2.48396	3.55917
H	1.45748	0.64337	3.31263
H	4.21539	1.80218	-1.51321
H	4.83463	1.13585	1.74800
H	3.37107	-1.60380	2.50178
H	-0.92358	3.85605	-2.52946
H	-0.24539	3.78468	2.43182
H	-3.12164	3.31094	-0.87258
H	0.59157	4.94753	0.91763
H	-0.00085	-3.04240	-2.86413
H	3.48713	-3.63783	-0.28289

H	-0.75595	-4.87430	0.08902
H	-3.40052	0.37314	2.34394
H	-2.92263	-1.92953	-2.69774
H	-5.23678	0.26255	-0.54726
H	-4.34433	-3.74068	2.01912
H	5.74369	-3.42207	0.34185
H	5.43309	-2.22776	-0.64022
H	-4.31423	2.28107	-3.00242
H	-5.16159	3.36928	-2.21892
H	-3.16251	4.34367	-2.98998
H	-2.49464	5.33701	-4.00112
H	3.77296	2.93286	2.09406
H	3.97774	3.61604	3.50952
H	-4.80553	-2.40778	3.93440
H	-5.95905	-2.28351	2.91135
H	6.40228	0.13034	-3.34449
H	-6.79846	-1.01551	0.16289
H	2.10872	-5.75413	-3.04223
H	2.00694	-4.21612	-3.16996
H	-2.38429	6.93974	-0.45557
H	-2.17527	5.97445	-1.70087
H	5.16462	-0.22142	-1.56811
H	-3.98004	0.21095	-3.58955
H	-1.48901	-6.21267	1.75092
H	1.90115	-2.99801	2.93807
H	-4.59790	-4.92991	1.03649
H	-0.91396	-4.34560	-1.42010
H	0.08483	-4.16311	1.97417
H	-2.36708	-4.92079	1.54855
H	-5.53378	-1.54420	-0.59581
H	-3.92898	1.13738	-4.83236
H	6.61645	-0.42794	-1.07608
H	6.14490	1.62456	-3.54878
H	1.85832	-1.85378	3.96683
H	-4.03999	-1.10283	2.18713
H	-3.83608	-2.80898	0.09673
H	-4.36622	1.53387	-1.08437
H	-1.99693	-0.77177	-3.08638
H	1.09966	-1.92257	-2.86823
H	2.61598	-4.44719	-1.35532
H	0.56910	-0.87463	2.07009
H	3.04380	-1.58656	-1.34588
H	-1.13545	0.71870	1.82403
H	-1.76893	1.40113	-2.30435

H	-0.38837	5.38127	-0.26650
H	-1.60581	2.89154	2.45395
H	3.07460	0.88634	-2.10753
H	4.36171	-1.76842	1.23786
H	2.52113	1.84502	3.06132
H	-2.45676	4.58177	-0.19316
O	1.08334	4.94241	2.56478
H	1.10648	5.75361	3.09613
H	1.95660	4.48380	2.67967

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Hf4_4_2_bridging_peroxide_conf1_deprot6_ion6.log Energy: -3143069.4060192

Hf	-2.41256	-1.42539	-0.41414
O	-2.46863	0.57875	-1.20444
O	-1.72990	0.10885	0.95202
O	-3.07667	-2.22710	1.59603
O	-2.54329	-1.52077	-2.75747
O	-3.20641	-3.21384	-0.89060
O	-4.60368	-0.79999	-0.28416
Hf	1.49836	-2.21484	-0.40904
O	-0.57212	-2.45181	0.20870
O	-0.46249	-1.81669	-1.15620
O	1.81374	-2.83460	-2.28023
O	1.88526	-2.80602	1.93512
O	3.69566	-2.63571	-0.07171
O	1.34642	-4.46719	-0.19398
Hf	-1.62547	2.07862	0.12736
O	0.44192	2.12032	0.78551
O	0.33283	1.81348	-0.68880
O	-1.60968	2.80456	-2.36709
O	-2.09630	2.65956	1.96289
O	-3.66189	2.99090	-0.25621
O	-1.08830	4.28153	-0.11800
Hf	2.28583	1.30510	-0.00687
O	2.36846	-0.42531	-1.29515
O	1.48111	-0.45420	0.83729
O	2.87272	1.31697	2.16264
O	2.51475	2.09033	-2.29610
O	2.99514	3.20261	0.08949
O	4.46932	0.87309	-0.16468
Cl	-0.11690	-0.97822	3.64563
Cl	0.77316	4.77878	-2.65188
Cl	-4.97300	-0.59884	3.49510
Cl	4.19449	-1.21254	3.38071

O	2.20217	5.07909	2.08106
O	-5.35555	1.38101	1.14881
O	5.35189	-1.21267	-1.88728
O	4.45592	-3.66355	-3.06847
O	-1.43089	-3.74545	3.10765
O	3.90653	3.48889	3.51767
O	-4.85111	-1.87521	-3.99040
O	5.62085	3.20913	-0.26982
O	-4.31588	2.70389	-2.86794
O	3.94264	-5.15006	-0.89140
O	-5.84778	0.26279	-2.70919
O	4.52951	0.60163	-3.64683
O	-0.49307	5.02580	2.36589
O	-6.25635	-2.33878	1.11767
H	-3.55041	-1.64010	2.23955
H	-3.43444	-1.71732	-3.19657
H	-3.46864	-3.74419	-0.12235
H	-5.22099	-1.47645	0.14105
H	2.67201	-3.11316	-2.65319
H	1.21944	-2.33639	2.49538
H	4.29323	-2.10489	-0.64560
H	1.09210	-4.85672	0.69873
H	-0.94000	3.52056	-2.55026
H	-4.31855	2.57525	0.35863
H	-0.84052	4.68218	0.76703
H	3.28023	0.48308	2.53325
H	2.25585	3.04761	-2.25496
H	5.08880	1.67206	-0.20045
H	2.79569	4.65273	2.74530
H	-5.22118	0.94310	2.03121
H	-6.31677	1.49638	1.05688
H	5.09830	-0.58677	-2.63029
H	6.32287	-1.19566	-1.82469
H	4.96419	-2.86990	-2.79161
H	4.75519	-3.88641	-3.96439
H	-1.91887	-4.12859	3.85717
H	-0.97155	-2.94585	3.47183
H	3.77627	3.33913	4.46991
H	4.84324	3.73117	3.42095
H	-5.30900	-1.05947	-3.64237
H	6.06660	3.41986	0.56709
H	-4.81989	3.42649	-3.27847
H	-3.36799	2.88237	-3.06399
H	4.57269	-5.81010	-0.56047

H	4.25385	-4.85985	-1.78631
H	-5.31378	1.06717	-2.87872
H	3.96124	1.29449	-3.24806
H	-0.80530	5.90004	2.64940
H	-7.16873	-2.04779	0.95199
H	2.55998	5.97028	1.93542
H	-0.35475	4.48084	-0.74994
H	-1.58740	3.39457	2.35567
H	0.49967	5.06520	2.38254
H	4.66013	3.45092	-0.12232
H	4.08675	0.33315	-4.46805
H	-5.52739	-0.06985	-1.84629
H	-4.67076	-1.68453	-4.92553
H	-6.01645	-1.92603	1.98005
H	3.35613	2.08334	2.55540
H	2.62115	3.86127	0.71211
H	4.81992	0.14719	-0.72735
H	1.80428	1.69472	-2.83280
H	-1.21896	2.02197	-2.79432
H	-4.03346	2.90755	-1.17466
H	-1.35029	-0.10483	1.82806
H	-2.85088	0.70388	-2.08302
H	0.98616	-0.42159	1.67901
H	2.68266	-0.51724	-2.20582
H	2.14012	-4.94878	-0.52283
H	2.73886	-2.38573	2.22899
H	-1.98288	-2.28881	-2.96335
H	-4.80819	0.05476	0.19017
H	-2.47363	-2.82403	2.11990
H	3.93762	-3.59631	-0.21019
O	0.77783	-5.32273	2.26796
H	1.41788	-4.63845	2.54847
H	-0.08409	-4.91685	2.51811

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Hf4_8_2_bridging_peroxide_conf1.log Energy: -4299802.5860394

Hf	2.44390	0.55334	0.15823
O	1.57973	-1.01760	-0.98627
O	1.24713	-0.79885	1.28880
O	3.26516	0.53292	2.18246
O	3.11433	0.96390	-1.97143
O	3.76331	2.25218	0.23041
O	4.17439	-0.84520	0.00453
Hf	-0.98368	2.38731	-0.00223

O	0.97184	2.02118	0.88453
O	0.93470	1.82183	-0.60692
O	-0.74397	3.15065	-2.11102
O	-1.41220	2.94998	2.13410
O	-2.71387	3.66473	-0.25027
O	-0.04215	4.44436	0.24468
Hf	0.69228	-2.50776	0.22626
O	-1.37397	-2.20067	0.76747
O	-1.14724	-2.05821	-0.71395
O	0.94154	-3.46583	-1.92545
O	0.82117	-3.08221	2.38821
O	2.74627	-3.27498	0.32854
O	0.03588	-4.63244	0.25400
Hf	-2.71481	-0.73436	-0.15955
O	-2.16833	1.05637	-1.18125
O	-1.42959	0.53727	0.92209
O	-3.61678	-0.73033	1.84228
O	-3.02258	-1.19413	-2.39419
O	-3.91589	-2.63189	-0.14738
O	-4.69308	0.06308	-0.69321
Cl	2.57916	-1.54098	-3.87902
Cl	-0.16060	0.67017	3.83397
Cl	2.12303	3.51102	-3.35498
Cl	-1.67913	-3.81663	-3.54325
Cl	3.20350	-1.95475	3.96653
Cl	-4.27797	2.12317	2.99174
O	-2.43341	-4.83406	-0.74027
O	5.32904	-1.14853	-2.38714
O	-5.03694	2.57290	0.02245
O	-1.91898	5.50251	-2.93550
O	4.06116	2.92708	2.83405
O	-5.70239	-2.26370	2.22163
O	4.94289	3.41302	-1.67326
O	-5.50323	-2.42070	-2.27981
O	2.95861	-5.31400	-1.26395
O	-1.96181	6.18719	-0.32613
Cl	8.39236	0.92317	-0.04933
Cl	-7.44690	-1.18518	-0.20896
O	6.54459	1.46605	-2.58617
O	-7.24620	3.84837	-0.77831
O	0.31792	-5.72449	2.69643
O	6.19478	-0.52064	1.57887
H	3.25610	-0.25929	2.79600
H	2.75221	1.80539	-2.38090

H	3.92809	2.72352	1.08574
H	4.95410	-0.70255	0.66657
H	-1.24253	3.94709	-2.43140
H	-0.93678	2.34671	2.76971
H	-3.66578	3.30765	-0.21340
H	0.38927	4.53706	1.11199
H	0.07962	-3.63541	-2.40615
H	1.62013	-2.72968	2.88390
H	3.42645	-2.56684	0.21310
H	0.10285	-5.17009	1.08704
H	-3.78914	0.16253	2.25021
H	-3.96600	-1.40681	-2.59230
H	-4.57275	-2.69955	-0.90260
H	-5.56737	-0.36517	-0.45736
H	-2.87248	-5.70052	-0.68246
H	5.99881	-1.85353	-2.39226
H	4.62113	-1.43768	-3.01069
H	-5.87061	3.05369	-0.26252
H	-5.04136	2.49428	1.01146
H	-2.78528	5.42119	-3.37085
H	-1.34328	5.94029	-3.58650
H	4.86786	3.17619	3.31257
H	3.27661	3.14566	3.42077
H	-5.35643	-3.07442	1.80950
H	-6.36337	-1.94188	1.56205
H	5.51719	2.69647	-2.08296
H	-6.33301	-2.09015	-1.85420
H	2.72362	-6.12566	-0.78313
H	2.13079	-5.03086	-1.70636
H	-2.20915	7.03947	0.06727
H	-1.98972	6.27186	-1.31043
H	6.06424	0.61317	-2.63404
H	-7.11689	4.13088	-1.69921
H	1.03554	-6.35539	2.87634
H	6.91307	-0.06221	1.06131
H	-2.29651	-4.64834	-1.70986
H	-0.89013	-4.78048	-0.11009
H	0.67673	-4.01272	2.69117
H	-0.45997	-6.04725	3.18240
H	-5.74001	-3.21742	-2.78330
H	-7.33709	4.67912	-0.28227
H	7.16117	1.33795	-1.82616
H	4.23060	3.59736	-2.32183
H	6.56065	-1.39488	1.79376

H	-4.43871	-1.31079	2.01123
H	-3.35305	-3.45498	-0.21337
H	-4.82473	1.04803	-0.50372
H	-2.50570	-1.96649	-2.74980
H	1.48690	-2.96517	-2.58374
H	2.97560	-4.08341	-0.24715
H	0.96315	-0.54842	2.19702
H	1.77287	-1.14186	-1.94100
H	-1.11583	0.34808	1.83581
H	-2.37133	1.21004	-2.11781
H	0.18966	3.24510	-2.44554
H	-0.61762	5.24988	0.10972
H	-2.37614	2.82660	2.37427
H	3.00148	0.27313	-2.66742
H	4.25610	2.73772	-0.56023
H	4.60528	-0.96461	-0.89836
H	3.74302	1.30963	2.59062
H	-2.69331	4.64939	-0.11619
O	1.90030	3.20232	4.35919
H	1.33701	3.95216	4.10796
H	1.34534	2.40813	4.19601

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Hf4_8_2_bridging_peroxide_conf2.log Energy: -4299796.4134484

Hf	2.45681	0.94141	0.02720
O	1.93655	-1.13646	-0.62947
O	1.69038	-0.87509	0.83670
O	3.12790	0.86713	2.16143
O	3.09820	1.04880	-2.17244
O	3.81628	2.63245	0.07931
O	4.35836	-0.12091	-0.09240
Hf	-0.70897	2.49832	-0.05651
O	1.13920	2.30800	0.97801
O	0.66390	1.23833	-1.03586
O	-0.58386	3.28457	-2.17280
O	-1.33036	3.18062	2.03164
O	-2.53296	3.74621	-0.32265
O	0.09837	4.64516	0.19209
Hf	0.71399	-2.62557	0.23236
O	-1.18805	-2.02804	0.98934
O	-1.07255	-1.85357	-0.50044
O	0.69246	-3.20055	-1.98807
O	1.11152	-2.98713	2.37812
O	2.52495	-3.87571	0.09498

O	-0.08823	-4.66212	0.35068
Hf	-2.63353	-0.51118	-0.10344
O	-2.08669	1.23193	-1.15711
O	-1.31106	0.72105	0.97032
O	-3.62371	-0.32536	1.80328
O	-2.57960	-1.07351	-2.43983
O	-3.78129	-2.34666	-0.07812
O	-4.62685	0.11457	-0.79559
Cl	0.49613	-0.52727	-3.59990
Cl	-0.39145	1.08507	4.09764
Cl	2.25452	3.73842	-3.27626
Cl	-2.04807	-4.07147	-3.19020
Cl	3.73471	-1.83814	3.53992
Cl	-4.28423	2.52076	2.90076
O	-2.64014	-4.79002	-0.29889
O	4.63596	-2.63801	-1.01490
O	-4.97848	2.68359	-0.05878
O	-1.78099	5.67927	-2.90398
O	4.13011	3.25241	2.69013
O	-5.54455	-1.86866	2.56825
O	6.13524	2.73892	-0.99639
O	-6.13715	-2.70315	-1.07998
O	2.19867	-5.68868	-1.77875
O	-1.90863	6.31459	-0.28927
Cl	7.56764	-1.89586	-0.61619
Cl	-8.09669	-1.30399	0.88347
O	6.15534	0.51140	-2.46721
O	-5.03812	-0.12920	-3.38799
O	0.72288	-5.64789	2.70427
O	6.10789	-0.42616	1.80450
H	3.30595	-0.00208	2.61624
H	2.89715	1.96473	-2.55697
H	3.95101	3.07074	0.96215
H	5.01587	-0.15343	0.68607
H	-1.06226	4.11643	-2.42370
H	-0.97030	2.59350	2.75383
H	-3.46242	3.37832	-0.32467
H	0.89298	4.82918	-0.34011
H	-0.18232	-3.55429	-2.32342
H	1.96756	-2.60267	2.73294
H	3.36353	-3.41642	-0.19553
H	0.15288	-5.20889	1.14826
H	-3.76078	0.56953	2.22023
H	-2.55203	-2.05774	-2.60309

H	-4.72117	-2.45444	-0.47480
H	-4.86106	0.02740	-1.77788
H	-3.16490	-5.57510	-0.06416
H	5.62320	-2.64447	-0.87010
H	4.50932	-2.71423	-1.97636
H	-5.76134	3.18422	-0.34652
H	-4.97360	2.69453	0.93823
H	-2.63251	5.56315	-3.35994
H	-1.21421	6.15548	-3.53535
H	4.90571	3.60507	3.15447
H	3.31727	3.54702	3.16874
H	-5.29643	-2.75882	2.26799
H	-6.38219	-1.66566	2.07176
H	6.25283	1.91947	-1.56253
H	-6.79941	-2.23544	-0.50376
H	1.53365	-6.34389	-1.50692
H	1.69965	-5.04402	-2.31632
H	-2.18022	7.14883	0.12588
H	-1.93545	6.42332	-1.27078
H	5.19171	0.40976	-2.35439
H	-4.12886	-0.47255	-3.50641
H	1.48070	-6.25604	2.74875
H	6.71501	-0.97992	1.25881
H	-2.57133	-4.76712	-1.29328
H	-1.07419	-4.78434	0.17535
H	1.05462	-3.92414	2.69845
H	0.06754	-5.98334	3.33995
H	-6.35720	-3.64563	-0.99077
H	-5.03714	0.74556	-3.81211
H	6.55201	-0.19762	-1.91372
H	6.15767	3.48558	-1.61772
H	5.62934	-1.04451	2.39801
H	-4.40750	-0.93372	2.06981
H	-3.35030	-3.24311	-0.04357
H	-4.85891	1.05015	-0.53052
H	-1.73154	-0.75991	-2.84163
H	0.82250	-2.37835	-2.53938
H	2.42546	-4.66081	-0.53778
H	0.44774	0.71337	-1.84315
H	1.31245	2.79107	1.82628
H	-1.02457	0.54199	1.89335
H	-2.38829	1.52095	-2.03185
H	0.33297	3.35205	-2.56927
H	-0.52234	5.41791	0.07190

H	-2.31153	3.12231	2.18022
H	2.53217	0.44473	-2.70990
H	4.73762	2.64626	-0.39580
H	4.33854	-1.03796	-0.48423
H	3.69809	1.58097	2.54773
H	-2.55704	4.72108	-0.14051
O	1.56367	3.46511	3.42484
H	1.06539	4.28026	3.60273
H	1.09622	2.74545	3.91567

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Hf4_4_2_term_perox_conf1_ion10_diconf5.log Energy: -3143082.5504915

Hf	-2.15403	-1.10721	0.12301
O	-0.49132	-2.18686	0.80121
O	-0.65913	-1.30021	-1.32862
O	-3.20610	-1.62901	-1.90573
O	-2.43286	-1.19347	2.52460
O	-4.32359	-0.77567	0.63354
O	-2.92694	-3.16745	0.39217
Hf	-1.22010	2.30767	-0.19233
O	-2.55008	0.77890	-0.83789
O	-1.19289	0.56963	1.00776
O	-1.55910	3.11937	1.93544
O	-1.88056	2.76856	-2.39568
O	-0.67544	4.47978	-0.47666
O	-3.26228	3.28725	-0.09522
Hf	1.22728	-2.17013	-0.62663
O	2.05157	-0.43969	-1.68405
O	1.76367	-0.62254	0.71994
O	1.88047	-3.42447	0.86469
O	0.63705	-3.09169	-2.72981
O	1.20558	-4.22207	-0.19089
O	3.12930	-2.84877	-1.77126
Hf	2.22168	1.24568	-0.27731
O	0.71678	2.45231	0.73911
O	0.34258	1.56659	-1.35943
O	3.18864	2.21043	-1.76173
O	2.81289	1.52273	2.11398
O	4.35492	0.38204	0.02912
O	3.35611	2.93901	-0.45627
Cl	0.47422	-0.15495	3.62516
Cl	-1.32707	0.14709	-4.02643
Cl	-3.55149	1.44680	3.66198
Cl	5.00524	-0.50958	3.01308

O	5.46716	-3.24647	-0.74808
O	-1.23994	-5.17655	0.39953
O	1.83975	5.10048	-0.52142
O	-2.63526	5.51932	1.26405
O	-5.82321	-1.38145	-1.51433
O	6.37508	-0.78683	-1.55209
O	-5.68044	-2.51753	2.15625
O	6.09043	2.00058	1.15488
O	4.50447	-3.50412	1.75930
O	-1.23017	5.32184	-3.01613
O	-3.69501	-3.43671	3.63831
O	4.42630	3.81011	2.37861
O	2.09730	-5.30129	-2.40467
O	-5.55285	-3.70861	-0.22575
H	-2.79336	-1.13029	-2.64714
H	-2.90765	-0.36601	2.84620
H	-4.96744	-0.70689	-0.11664
H	-3.80363	-3.47047	0.04225
H	-1.95054	4.02865	1.94792
H	-1.69626	2.01262	-3.01079
H	0.33531	4.66946	-0.42179
H	-3.88516	3.09988	-0.84314
H	-0.32945	-3.09871	-2.83035
H	2.98576	-3.73893	-2.16589
H	3.52836	0.90456	2.42903
H	4.98805	1.11441	0.35092
H	5.94170	-2.39823	-0.92911
H	-0.32512	-4.80010	0.24073
H	-1.20456	-5.55878	1.29167
H	2.41514	4.26950	-0.50172
H	1.98918	5.48754	-1.39983
H	-1.85359	5.80585	0.75630
H	-2.97595	6.29512	1.73772
H	-6.01453	-2.30273	-1.20295
H	-6.56838	-1.07578	-2.05504
H	7.15431	-0.45742	-1.07539
H	5.61996	-0.32563	-1.12568
H	-5.03994	-2.93541	2.80956
H	5.57004	2.75007	1.54832
H	4.57164	-2.63054	2.19826
H	3.57151	-3.55797	1.43707
H	-0.44543	5.60092	-3.51721
H	-1.94429	5.92988	-3.27079
H	-3.13253	-2.68528	3.34070

H	3.70426	3.14449	2.36152
H	1.89646	-5.26780	-1.43442
H	-5.82752	-3.46687	0.69688
H	5.27175	-3.28993	0.22679
H	4.04116	-2.94202	-1.31170
H	0.96061	-4.01985	-2.85095
H	2.28827	-6.21884	-2.65284
H	6.20579	1.37834	1.90024
H	4.68840	3.86043	3.31261
H	-3.36214	-4.19379	3.12848
H	-6.44882	-2.20390	2.66044
H	-5.88740	-4.60309	-0.40175
H	4.39078	-0.27687	0.75851
H	2.03942	1.25537	2.66513
H	2.78825	-0.65788	-2.27444
H	1.44500	-0.69445	1.64264
H	-0.71341	-0.81561	-2.18322
H	-0.34499	-2.67981	1.62123
H	-0.53904	0.46672	1.73163
H	-3.30445	1.00179	-1.41963
H	0.22521	1.09624	-2.20328
H	0.76819	2.85165	1.61943
H	-2.17491	2.54385	2.47398
H	-3.35104	4.21242	0.23172
H	-1.60496	3.60398	-2.84298
H	-1.53378	-1.07342	2.91879
H	-4.78601	-1.35275	1.31089
H	-2.27238	-3.94495	0.38508
H	-4.19150	-1.52297	-1.99005
H	-0.95764	4.91054	-1.32288
O	-4.68896	2.13700	-2.06175
H	-4.46997	2.45690	-2.95247
H	-5.65127	2.00465	-2.04841

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Hf4_4_2_term_perox_conf1_ion10_diconf7.log Energy: -3143083.6448366

Hf	-2.41125	0.40841	-0.15632
O	-1.53068	-1.27529	0.93708
O	-1.24359	-0.92406	-1.41193
O	-3.55030	0.87069	-1.80470
O	-3.28454	0.70570	1.99156
O	-4.06255	1.50701	-0.54636
O	-3.86168	-1.42098	-0.15516
Hf	0.50126	2.53826	-0.18764

O	-1.30653	2.07474	-1.13018
O	-0.72039	1.26438	0.95205
O	0.34321	3.50452	1.86032
O	0.84766	3.07208	-2.61763
O	2.40266	3.74462	-0.43358
O	-0.23500	4.66998	-0.46524
Hf	-0.19204	-2.34262	-0.26280
O	1.54449	-1.68197	-1.27378
O	1.20405	-1.47826	1.08923
O	-0.46621	-3.61195	1.83464
O	-0.29274	-3.24048	-2.43843
O	-2.13276	-3.49880	-0.59849
O	1.05334	-4.23659	-0.18060
Hf	2.66359	-0.29316	0.04336
O	1.93804	1.44044	1.03271
O	1.38692	0.93809	-1.16231
O	3.96664	-0.03578	-1.57483
O	3.69130	-0.30798	2.28908
O	3.80073	-2.31203	0.38421
O	4.55354	0.41653	-0.28055
Cl	-1.84530	-1.54573	3.96525
Cl	0.21921	0.25416	-3.98433
Cl	-2.59094	3.52797	2.95634
Cl	2.54269	-3.14663	3.27404
O	3.18090	-4.52325	-1.72070
O	-4.33383	-2.64292	2.23196
O	3.59661	4.48986	1.84750
O	1.29395	5.96990	1.53607
O	-5.96177	0.51126	-3.05068
O	4.41190	-2.43517	-2.84712
O	-6.67359	2.19313	-0.98910
O	6.05371	-1.09656	1.22458
O	-2.90557	-4.98240	1.48687
O	3.52808	2.47883	-2.48332
O	-6.03412	-0.31331	2.31297
O	3.24863	2.23089	3.35237
O	0.87696	-5.63894	-2.54143
O	-6.10253	-1.65587	-1.51420
H	-3.11672	1.65337	2.29039
H	-4.72576	-1.43176	-0.68796
H	0.59832	4.46404	1.93556
H	0.45437	2.32732	-3.13846
H	2.94240	3.93148	0.38550
H	-0.32804	5.04589	-1.39736

H	0.41508	-3.92292	2.13667
H	-1.24083	-3.39803	-2.59536
H	-2.82626	-2.77938	-0.56833
H	0.65726	-5.05417	-0.54550
H	4.65263	-0.51971	2.14630
H	4.75069	-2.16512	0.61406
H	3.62045	-3.70128	-2.09818
H	-4.07402	-3.57247	2.04850
H	-3.65794	-2.33267	2.87565
H	3.57967	3.73798	2.49169
H	4.52030	4.78300	1.78411
H	2.22264	5.70796	1.74217
H	1.05749	6.68613	2.14740
H	-5.02104	0.62690	-2.76487
H	-6.42104	1.15586	-2.45779
H	5.36242	-2.63216	-2.86729
H	4.33307	-1.60900	-2.30638
H	-5.74191	1.97822	-0.73121
H	5.87514	-0.45641	0.48808
H	-3.11091	-5.93108	1.44054
H	-2.03062	-4.90483	1.91869
H	3.69929	1.52054	-2.23862
H	4.32392	2.81280	-2.92715
H	-5.19133	0.17347	2.25879
H	3.62646	1.33360	3.21406
H	0.70820	-6.23548	-3.28794
H	-5.95407	-2.42820	-2.08385
H	3.87789	-5.00108	-1.24254
H	1.93251	-4.16866	-0.67863
H	0.14687	-4.12980	-2.58752
H	1.84317	-5.43863	-2.53662
H	7.00804	-1.11543	1.39756
H	2.79620	2.21297	4.21099
H	-5.73852	-1.24020	2.36409
H	-6.63047	3.11740	-1.28278
H	-6.13629	-0.87379	-2.14514
H	3.42254	-2.79983	1.15359
H	3.35008	-1.05958	2.83442
H	-0.81969	-3.07246	2.58468
H	-2.42408	-4.16700	0.08425
H	1.46629	-1.53599	-2.23271
H	1.37248	-1.86021	1.97898
H	-0.93275	-0.64321	-2.30356
H	-1.47610	-1.28957	1.91634

H	-0.23458	0.69833	1.57184
H	-1.73452	2.39616	-1.93820
H	1.06505	0.63086	-2.03972
H	2.21660	1.76393	1.91627
H	-0.58744	3.42395	2.21694
H	0.28814	5.32216	0.05434
H	1.82167	2.95544	-2.77323
H	-2.85356	0.15191	2.68430
H	-4.06407	-1.79842	0.74931
H	3.01012	3.31119	-1.10041
O	-0.32842	5.51959	-2.96306
H	0.13700	4.68960	-3.20956
H	-1.22193	5.42817	-3.33423

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Hf4_4_2_term_perox_conf1_ion10_diconf9.log Energy: -3143083.2703138

Hf	0.95762	2.30414	0.29617
O	-0.94101	1.77053	1.23181
O	-0.60837	1.60515	-1.07929
O	0.93506	3.68942	-1.55830
O	1.21637	3.14008	2.20063
O	3.09749	3.11599	0.13158
O	0.77032	4.14380	1.18874
Hf	2.37034	-0.90749	-0.32786
O	2.07744	1.04974	-1.10008
O	1.63763	0.43479	1.15151
O	3.23647	-1.64366	1.69592
O	3.37534	-0.64413	-2.56170
O	3.30239	-2.83293	-0.88485
O	4.49976	-0.19494	-0.13213
Hf	-2.30983	0.88115	-0.11416
O	-2.08110	-0.74390	-1.45340
O	-1.52131	-0.82230	0.83802
O	-3.46386	0.59991	2.06098
O	-2.92676	1.81057	-2.25109
O	-3.27274	2.88155	0.28422
O	-4.49084	0.52628	-0.40974
Hf	-0.91170	-2.36169	-0.54109
O	1.00739	-2.28776	0.51844
O	0.71926	-1.34017	-1.58290
O	-1.23365	-3.33415	-2.31564
O	-1.03097	-3.55956	1.57735
O	-3.11449	-3.03566	-0.23751
O	-0.82466	-4.26235	-1.20505

Cl	-0.08957	-1.23365	3.56999
Cl	0.84198	0.98440	-3.93568
Cl	5.18935	0.52743	2.82332
Cl	-5.07372	-2.09884	2.00650
O	-5.56928	-1.62579	-1.38476
O	-1.88650	4.70377	1.64531
O	2.99006	-5.17053	0.31425
O	4.78998	-3.81196	1.84580
O	2.12074	6.04765	-1.72375
O	-3.57822	-2.34216	-3.12292
O	3.89693	3.50702	2.60162
O	-3.39527	-4.79470	1.85481
O	-5.28691	2.70457	2.02838
O	4.94715	-2.80897	-3.03623
O	-0.99970	3.00845	3.66487
O	0.74735	-5.70967	1.61357
O	-5.53360	2.54957	-1.91538
O	-0.62134	6.12881	-1.57846
H	0.91194	3.24523	-2.42830
H	3.68679	2.63956	-0.48809
H	3.83651	-2.45191	1.71268
H	2.70263	-0.43551	-3.24516
H	3.06353	-3.71562	-0.47434
H	4.74674	0.55938	-0.73473
H	-3.98148	-0.25223	2.01742
H	-2.29095	2.52506	-2.42686
H	-2.67815	3.56395	0.74078
H	-5.00903	1.25144	-0.83759
H	-1.88782	-4.02831	1.78959
H	-3.17411	-3.97953	0.00984
H	-4.90990	-2.03155	-2.00267
H	-1.91116	4.31133	2.54214
H	-0.92801	4.58497	1.41028
H	2.12955	-5.37388	0.79593
H	3.19178	-5.94428	-0.23658
H	4.23968	-4.47770	1.36583
H	4.77168	-4.09126	2.77574
H	1.18722	6.37510	-1.69885
H	2.42186	6.22159	-2.63081
H	-2.84093	-2.93721	-2.80603
H	-3.62641	-2.44048	-4.08657
H	2.91478	3.42063	2.70318
H	-3.47077	-5.58292	2.41677
H	-6.12344	2.39433	1.64437

H	-4.83636	1.89004	2.33826
H	4.78814	-3.43958	-3.75864
H	5.91203	-2.71548	-2.96494
H	-0.06289	3.11323	3.33242
H	0.15597	-4.92024	1.58812
H	-5.76673	3.41106	-1.53101
H	-1.03080	6.33879	-2.43402
H	-5.59674	-2.20440	-0.60145
H	-4.86606	-0.34378	-0.79272
H	-3.82153	2.22851	-2.27090
H	-6.21526	2.35625	-2.58069
H	-4.04065	-4.13705	2.19926
H	0.96999	-5.82430	2.55190
H	-0.94987	2.48964	4.48326
H	4.25310	2.61445	2.80927
H	-0.48160	5.16180	-1.60539
H	-3.62448	-2.57065	0.47131
H	-0.84767	-2.94909	2.33464
H	-2.83290	0.46330	2.79148
H	-4.10468	2.86933	0.84481
H	-2.64995	-0.96393	-2.22051
H	-1.07246	-0.73686	1.70908
H	-0.37629	1.27096	-1.96984
H	-1.11791	2.08607	2.14807
H	1.26671	0.08706	1.98818
H	1.84932	1.13038	-2.04974
H	0.51913	-0.84214	-2.39796
H	1.08244	-2.36345	1.48517
H	3.70838	-0.95372	2.22430
H	4.81589	0.04933	0.77928
H	3.95100	-1.36122	-2.92681
H	3.57906	3.30755	0.99370
H	1.58876	4.45470	-1.61498
H	3.98806	-2.97321	-1.58086
O	4.81737	1.83344	-1.83092
H	4.35042	1.29608	-2.49987
H	5.69342	2.03568	-2.19992

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Hf4_4_2_term_perox_conf1_ion11_diconf5.log Energy: -3143078.5478847

Hf	-2.21839	-0.43676	0.37922
O	-0.82300	-1.71908	1.23605
O	-0.87814	-1.24449	-1.04072
O	-3.48727	-1.06283	-1.35323

O	-2.32185	-0.11108	2.82465
O	-4.13016	0.60467	0.75308
O	-3.51982	-2.14255	1.21744
Hf	-0.47866	2.51807	-0.55335
O	-2.18361	1.30300	-0.94572
O	-0.90310	1.10192	0.96571
O	-0.92254	3.77638	1.31292
O	-0.99165	2.87225	-2.80809
O	0.58144	4.37793	-1.07272
O	-2.17296	4.15888	-0.89626
Hf	0.76373	-2.37484	-0.16253
O	1.95460	-1.15916	-1.52472
O	1.73548	-0.80061	0.86574
O	1.09026	-3.46660	1.57413
O	0.09439	-3.56311	-2.06808
O	0.21372	-4.24261	0.65917
O	2.56319	-3.64398	-0.90301
Hf	2.62846	0.67185	-0.48188
O	1.41874	2.32153	0.43656
O	0.80017	1.25031	-1.54847
O	3.61577	1.13884	-2.17795
O	3.52715	1.28239	1.69556
O	4.44986	-0.70755	-0.17436
O	4.08791	1.95322	-0.99636
Cl	0.93239	0.63821	3.57717
Cl	-0.59752	0.05926	-4.17844
Cl	-2.93247	2.82279	3.59757
Cl	-3.03045	-3.90816	-2.58272
O	4.55858	-3.21444	0.75644
O	-2.16483	-4.31361	1.88436
O	2.47942	5.50302	0.39674
O	0.46353	5.82397	2.19720
O	-6.15039	-1.08761	-1.49626
O	6.97357	-4.29619	0.08608
O	-5.46083	0.90636	2.91184
O	6.11237	0.46494	1.69829
O	3.29409	-4.37826	2.78744
O	-0.27207	5.43884	-3.40123
O	-4.54656	-1.47585	3.83889
O	4.25313	3.99605	1.66372
O	1.15956	-5.91287	-1.11730
O	-5.26799	-3.43674	-0.43225
H	-3.25073	-1.90696	-1.81626
H	-2.54354	0.84243	3.03015

H	-4.14884	1.44642	0.26731
H	-4.20630	-2.53592	0.61145
H	-0.38665	4.55869	1.67212
H	-0.72138	2.13639	-3.40828
H	1.37665	4.73619	-0.58042
H	-2.34537	4.46828	0.01389
H	-0.88690	-3.56597	-2.20107
H	2.33823	-4.60292	-0.97629
H	4.43413	0.92596	1.88178
H	5.21979	-0.25191	0.22706
H	5.43579	-3.62592	0.53928
H	-1.27256	-4.32531	1.42523
H	-1.97889	-4.43182	2.82962
H	3.17313	4.91932	0.83438
H	2.95268	6.25377	0.00210
H	1.25541	5.84304	1.60155
H	0.81538	5.61080	3.07709
H	-6.14213	-2.00935	-1.14781
H	-6.41149	-1.17196	-2.42813
H	7.65173	-3.62198	0.25773
H	6.97666	-4.39466	-0.88049
H	-5.26764	0.04710	3.38000
H	6.72855	1.21550	1.66074
H	3.29996	-3.84275	3.59736
H	2.41974	-4.16743	2.35560
H	0.36870	5.69405	-4.08589
H	-0.99921	6.08086	-3.45981
H	-3.64715	-1.09139	3.87966
H	3.94541	3.06071	1.64444
H	0.79254	-5.60623	-0.24541
H	-5.70513	-4.20310	-0.02523
H	4.21941	-3.62042	1.60630
H	3.36717	-3.56696	-0.30201
H	0.35359	-4.51239	-1.99955
H	1.22431	-6.88011	-1.10492
H	6.48464	-0.15059	2.35155
H	4.20583	4.25333	2.59910
H	-4.50749	-1.88796	2.95217
H	-4.88604	1.57484	3.34600
H	-4.65089	-3.79566	-1.11852
H	4.39606	-1.58974	0.28334
H	2.93812	1.02359	2.44222
H	2.59096	-1.65172	-2.06328
H	1.44487	-0.59498	1.77709

H	-0.82237	-0.90196	-1.95613
H	-0.81706	-2.21416	2.06792
H	-0.26433	0.97939	1.70046
H	-2.66384	1.27636	-1.81651
H	0.57991	0.74832	-2.36046
H	1.48262	2.51745	1.38314
H	-1.44058	3.37521	2.05531
H	-3.00776	3.80100	-1.24243
H	-0.73424	3.73261	-3.21984
H	-1.40067	-0.19228	3.15594
H	-4.69724	0.70980	1.61438
H	-2.96309	-2.93751	1.51192
H	-4.48350	-0.94659	-1.41393
H	0.32696	4.97987	-1.81279
O	-3.46558	1.26199	-3.37683
H	-3.29159	2.15604	-3.71557
H	-2.74455	0.72758	-3.77758

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Hf4_4_2_term_perox_conf1_ion11_diconf7_b.log Energy: -3143085.2471193

Hf	-1.85882	-1.48825	0.17311
O	-1.95855	0.22154	-1.24807
O	-1.56178	0.46958	1.10830
O	-2.64887	-2.29706	1.89811
O	-2.23200	-2.55248	-1.91782
O	-2.52649	-3.29481	0.78492
O	-4.04322	-1.01540	-0.02367
Hf	1.70928	-1.85224	0.50944
O	-0.12266	-2.03625	1.45415
O	0.07890	-1.64530	-0.81500
O	2.21167	-3.18723	-1.27126
O	2.15612	-1.68732	2.99447
O	3.92546	-1.95573	0.92124
O	1.98689	-3.98931	1.26089
Hf	-1.26384	1.97119	-0.33641
O	0.56197	2.50529	0.61942
O	0.46010	1.55224	-1.53345
O	-1.80634	2.51081	-2.74567
O	-1.85382	3.12576	1.61491
O	-3.44806	2.53304	-0.46779
O	-1.13193	4.19153	-0.84015
Hf	2.28483	1.54359	-0.35190
O	2.50269	-0.48158	-0.97553
O	1.67490	0.13017	1.11689

O	3.45350	2.23507	1.25234
O	3.38754	1.58814	-2.54517
O	2.38957	3.67617	-1.17385
O	4.27402	1.83450	0.07382
Cl	-0.60275	-0.31802	-3.94887
Cl	0.19983	0.66336	3.80919
Cl	-0.25936	-4.86364	-2.23123
Cl	-3.75799	2.24460	3.91365
O	1.01154	5.46914	0.23238
O	-5.48585	-0.43558	-2.14741
O	5.54361	-2.52723	-1.13196
O	4.15271	-4.80394	-0.42607
O	-5.41978	-2.67152	2.31535
O	2.69258	4.71809	2.13271
O	-4.99507	-4.29833	0.01905
O	5.01025	3.55316	-1.74915
O	-4.50530	2.06619	-2.91443
O	4.23678	0.05532	2.63229
O	-4.89893	-3.06832	-2.60471
O	4.30422	-1.01837	-3.03886
O	-3.21229	5.24028	0.47044
O	-4.93579	1.19460	1.31691
H	-1.64509	-3.37364	-1.95520
H	-4.39143	-0.39670	0.66075
H	2.90095	-3.89199	-1.12719
H	1.42793	-1.12341	3.36071
H	4.56271	-2.04941	0.15780
H	1.99800	-4.16924	2.25385
H	-1.39709	3.38885	-2.86253
H	-2.36580	2.69344	2.35281
H	-4.01772	2.07672	0.22393
H	-1.92690	4.71815	-0.55778
H	4.09506	2.29161	-2.49085
H	3.29348	4.00799	-1.37662
H	1.53906	5.25528	1.06204
H	-5.09235	0.28385	-2.68129
H	-5.35022	-1.28818	-2.61825
H	5.23712	-2.00900	-1.91841
H	6.48420	-2.31931	-1.00859
H	4.87687	-4.19538	-0.70504
H	4.30350	-5.64841	-0.88117
H	-4.46569	-2.44554	2.25349
H	-5.53093	-3.21081	1.50432
H	3.07760	3.87687	1.77174

H	2.34560	4.48268	3.00824
H	-4.10856	-3.95194	0.28401
H	5.07420	3.04840	-0.89458
H	-5.13080	2.73905	-3.23110
H	-3.63197	2.30038	-3.29216
H	3.93136	0.91159	2.20434
H	5.08648	0.23273	3.06604
H	-3.92903	-2.98144	-2.46099
H	4.24220	-0.04030	-3.09206
H	-4.01909	4.81489	0.13282
H	-5.88686	1.39097	1.27284
H	1.16598	6.40564	0.02568
H	-0.35250	4.63776	-0.40714
H	-2.34182	3.96280	1.42920
H	-3.43744	6.16339	0.67199
H	5.89100	3.88281	-1.98682
H	4.00539	-1.36093	-3.89663
H	-4.99887	-3.64875	-3.37658
H	-5.14362	-3.88326	-0.85499
H	-4.63652	1.47534	2.22862
H	1.88764	4.40114	-0.70790
H	2.77806	1.88228	-3.24577
H	-1.34525	1.89731	-3.36134
H	-3.88954	2.34354	-1.34437
H	0.51323	2.76176	1.55415
H	0.35815	0.96063	-2.30730
H	-1.16686	0.52538	2.00976
H	-1.72400	0.07204	-2.18766
H	0.24452	-1.28068	-1.70169
H	-0.42944	-2.41093	2.29379
H	1.19007	0.41689	1.92531
H	3.00571	-0.80738	-1.75168
H	1.39261	-3.66153	-1.59272
H	2.79060	-4.41694	0.88901
H	2.95358	-1.10558	3.09240
H	-1.88096	-1.99799	-2.65120
H	-4.49135	-0.72576	-0.87917
H	4.21991	-1.16717	1.46409
O	2.12316	-4.26464	3.88292
H	2.18705	-3.28332	3.91869
H	1.25727	-4.47520	4.27062

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Hf4_4_2_term_perox_conf1_ion11_diconf7.log Energy: -3143085.2468996

Hf	-1.85906	-1.48779	0.17329
O	-1.95843	0.22171	-1.24810
O	-1.56160	0.47003	1.10827
O	-2.64899	-2.29672	1.89835
O	-2.23290	-2.55213	-1.91758
O	-2.52664	-3.29436	0.78505
O	-4.04335	-1.01456	-0.02318
Hf	1.70891	-1.85254	0.50942
O	-0.12290	-2.03590	1.45435
O	0.07849	-1.64560	-0.81503
O	2.21093	-3.18780	-1.27115
O	2.15567	-1.68746	2.99470
O	3.92500	-1.95636	0.92134
O	1.98612	-3.98959	1.26103
Hf	-1.26345	1.97139	-0.33661
O	0.56245	2.50508	0.61920
O	0.46046	1.55204	-1.53362
O	-1.80661	2.51084	-2.74578
O	-1.85317	3.12643	1.61454
O	-3.44770	2.53345	-0.46787
O	-1.13106	4.19162	-0.84048
Hf	2.28517	1.54313	-0.35210
O	2.50249	-0.48215	-0.97570
O	1.67512	0.12991	1.11675
O	3.45393	2.23453	1.25209
O	3.38799	1.58736	-2.54518
O	2.39033	3.67565	-1.17402
O	4.27442	1.83363	0.07367
Cl	-0.60364	-0.31796	-3.94935
Cl	0.20031	0.66468	3.80898
Cl	-0.26053	-4.86355	-2.23166
Cl	-3.75692	2.24589	3.91400
O	1.01262	5.46884	0.23223
O	-5.48662	-0.43524	-2.14662
O	5.54319	-2.52817	-1.13162
O	4.15175	-4.80457	-0.42594
O	-5.41970	-2.67106	2.31593
O	2.69364	4.71776	2.13267
O	-4.99531	-4.29808	0.01976
O	5.01102	3.55219	-1.74931
O	-4.50549	2.06633	-2.91413
O	4.23655	0.05475	2.63233
O	-4.89999	-3.06806	-2.60387
O	4.30391	-1.01958	-3.03855

O	-3.21156	5.24062	0.46946
O	-4.93513	1.19561	1.31761
H	-1.64603	-3.37333	-1.95522
H	-4.39126	-0.39576	0.66131
H	2.90016	-3.89262	-1.12707
H	1.42749	-1.12353	3.36081
H	4.56235	-2.05016	0.15797
H	1.99742	-4.16942	2.25399
H	-1.39736	3.38883	-2.86297
H	-2.36496	2.69436	2.35274
H	-4.01718	2.07737	0.22412
H	-1.92602	4.71841	-0.55837
H	4.09565	2.29069	-2.49097
H	3.29429	4.00728	-1.37683
H	1.54007	5.25486	1.06191
H	-5.09344	0.28408	-2.68088
H	-5.35119	-1.28796	-2.61731
H	5.23692	-2.00978	-1.91807
H	6.48383	-2.32059	-1.00811
H	4.87598	-4.19604	-0.70481
H	4.30256	-5.64906	-0.88098
H	-4.46564	-2.44497	2.25380
H	-5.53091	-3.21060	1.50507
H	3.07854	3.87650	1.77165
H	2.34647	4.48226	3.00810
H	-4.10877	-3.95162	0.28449
H	5.07479	3.04738	-0.89475
H	-5.13094	2.73930	-3.23068
H	-3.63219	2.30039	-3.29201
H	3.93133	0.91107	2.20430
H	5.08641	0.23193	3.06586
H	-3.93004	-2.98116	-2.46048
H	4.24284	-0.04146	-3.09187
H	-4.01827	4.81508	0.13181
H	-5.88617	1.39225	1.27388
H	1.16729	6.40533	0.02562
H	-0.35165	4.63773	-0.40732
H	-2.34126	3.96338	1.42865
H	-3.43690	6.16367	0.67110
H	5.89185	3.88171	-1.98685
H	4.00699	-1.36190	-3.89708
H	-5.00021	-3.64864	-3.37559
H	-5.14418	-3.88292	-0.85420
H	-4.63556	1.47628	2.22925

H	1.88855	4.40074	-0.70810
H	2.77869	1.88133	-3.24600
H	-1.34572	1.89713	-3.36143
H	-3.88937	2.34373	-1.34433
H	0.51378	2.76130	1.55401
H	0.35837	0.96048	-2.30749
H	-1.16679	0.52595	2.00977
H	-1.72402	0.07215	-2.18772
H	0.24406	-1.28109	-1.70176
H	-0.42979	-2.41065	2.29392
H	1.19046	0.41684	1.92518
H	3.00492	-0.80809	-1.75218
H	1.39180	-3.66189	-1.59270
H	2.78962	-4.41746	0.88899
H	2.95313	-1.10570	3.09272
H	-1.88200	-1.99761	-2.65098
H	-4.49165	-0.72505	-0.87860
H	4.21949	-1.16785	1.46423
O	2.12230	-4.26469	3.88311
H	2.18636	-3.28337	3.91887
H	1.25637	-4.47510	4.27078

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Hf4_4_2_term_perox_conf1_ion11_diconf9.log Energy: -3143091.3245485

Hf	1.01702	-2.18162	0.29631
O	1.92135	-0.51028	1.32961
O	1.54947	-0.43824	-0.96660
O	2.17590	-2.98989	-1.44039
O	1.21832	-2.95472	2.23262
O	0.14457	-4.27932	-0.04633
O	2.35718	-3.33283	1.34549
Hf	-2.30746	-1.00046	-0.43137
O	-0.62818	-2.07709	-1.21873
O	-0.90384	-1.53789	1.05911
O	-3.51425	-1.41634	1.50215
O	-2.69038	-1.46027	-2.79311
O	-4.34743	-0.28691	-0.93317
O	-3.22219	-3.04379	-0.59471
Hf	2.16598	1.19241	0.15210
O	0.82401	2.33070	-1.08936
O	0.36059	1.66904	1.11811
O	2.72091	2.05399	2.42133
O	3.27285	1.34703	-1.88476
O	4.29945	0.56637	0.57089

O	3.18139	3.24294	0.13698
Hf	-1.16832	2.40401	-0.17425
O	-2.42715	0.83126	0.66359
O	-1.42225	0.64409	-1.40510
O	-1.72078	3.48684	-1.82441
O	-2.03235	3.11549	2.00735
O	-0.19171	4.39608	0.52424
O	-2.74611	3.58639	-0.73708
Cl	0.20469	1.41146	4.19916
Cl	0.05498	-0.45435	-3.94701
Cl	-3.37746	-4.44811	2.17879
Cl	4.35161	-1.34143	-3.05625
O	1.81901	5.22743	-1.05306
O	4.50263	-1.69888	2.03245
O	-5.82567	1.30344	0.60162
O	-6.18275	-1.24409	1.49415
O	3.76118	-5.10464	-1.24012
O	-0.02934	5.27469	-2.92045
O	-0.24345	-5.23133	2.35073
O	-2.54260	5.54557	1.02226
O	5.52845	1.88941	2.52949
O	-5.19886	-0.67906	-3.46517
O	2.35495	-1.17365	3.92201
O	-4.67308	2.42872	2.72337
O	5.41951	3.00903	-1.34858
O	5.84466	-3.37378	-1.11095
H	2.77866	-2.36908	-1.92069
H	-0.68435	-4.12441	-0.53042
H	-4.51927	-1.34853	1.45945
H	-1.94863	-1.09104	-3.33728
H	-4.80955	0.42457	-0.40381
H	-3.04351	-3.62556	-1.39313
H	2.70842	3.01259	2.24023
H	3.55273	0.45446	-2.22627
H	4.32709	-0.33202	1.03521
H	4.10542	3.28117	-0.22160
H	-2.22195	4.09190	1.94082
H	-0.82556	5.13583	0.65665
H	1.23315	5.24791	-1.87469
H	4.13238	-1.38417	2.88051
H	3.79759	-2.32930	1.72720
H	-5.39386	1.76965	1.37666
H	-6.45028	1.92919	0.20110
H	-6.30507	-0.30826	1.20480

H	-6.46507	-1.25960	2.42334
H	4.60107	-4.57268	-1.17385
H	3.80022	-5.51943	-2.11737
H	-0.73390	4.72720	-2.47464
H	0.16715	4.80296	-3.74602
H	0.28496	-4.41581	2.55901
H	-2.83703	5.04482	0.21184
H	5.87141	2.78077	2.35155
H	4.63776	2.03236	2.90949
H	-5.38389	0.10034	-4.01572
H	-5.83669	-1.36147	-3.73428
H	1.85982	-1.94313	3.53167
H	-3.72766	2.63741	2.55741
H	6.25784	2.62681	-1.03925
H	6.64691	-3.69773	-1.55186
H	2.12587	6.13548	-0.89600
H	2.67200	3.93906	-0.36965
H	4.10244	1.88084	-1.85485
H	5.66118	3.75279	-1.92592
H	-3.17829	6.25578	1.20066
H	-4.67753	1.81592	3.47649
H	1.67609	-0.57004	4.28704
H	-1.18340	-4.97200	2.47790
H	5.48456	-2.68879	-1.72191
H	0.56025	4.74140	-0.02775
H	-1.37659	2.98170	2.72405
H	2.00549	1.89751	3.09469
H	4.85303	1.14255	1.17685
H	1.02524	2.43392	-2.03141
H	0.20607	1.34381	2.03217
H	1.21748	-0.34961	-1.88325
H	2.15146	-0.60559	2.28560
H	-1.02034	-1.27437	1.98436
H	-0.34479	-1.91560	-2.13854
H	-0.90847	0.53597	-2.23414
H	-2.74661	0.81006	1.57652
H	-3.34940	-2.31267	1.89264
H	-3.33028	-3.61375	0.21209
H	-3.53407	-1.15171	-3.21130
H	-0.06491	-4.78770	0.80523
H	2.68942	-3.85096	-1.32885
H	-4.83275	-0.41799	-1.78281
O	-2.80730	-4.26218	-2.90553
H	-2.64518	-3.35389	-3.23665

H	-1.96264	-4.72811	-3.01912

109
Hf4_4_2_term_perox_conf1_ion12_diconf5.log Energy: -3143082.0801857

Hf	-2.31291	-0.56107	0.55207
O	-0.74231	-1.75474	1.23343
O	-1.11866	-1.23889	-1.01144
O	-3.75307	-0.95085	-1.16254
O	-2.53396	-0.55081	2.99254
O	-4.17479	0.47449	1.20823
O	-3.34526	-2.49598	1.09161
Hf	-0.71688	2.55124	-0.09963
O	-2.37311	1.26722	-0.62824
O	-1.11107	1.02913	1.33047
O	-0.50479	3.50052	2.04982
O	-1.57359	3.26892	-2.25648
O	0.13303	4.55504	-0.50973
O	-2.50665	3.87461	0.38706
Hf	0.72421	-2.26400	-0.34239
O	1.59446	-0.91205	-1.80992
O	1.77659	-0.67017	0.62008
O	1.43973	-3.32383	1.25827
O	-0.15657	-3.44024	-2.14646
O	0.51607	-4.18652	0.48016
O	2.44197	-3.39140	-1.48409
Hf	2.38021	0.88101	-0.79379
O	1.26172	2.22160	0.53708
O	0.37150	1.46763	-1.46878
O	3.00935	1.52381	-2.61092
O	3.86312	1.52370	1.06480
O	4.23431	-0.44212	-0.93836
O	3.60835	2.31917	-1.47626
Cl	0.47480	-0.27691	3.77997
Cl	-1.60285	0.57154	-3.78092
Cl	5.17196	-0.53221	2.94643
Cl	-3.22066	-3.51418	-2.94279
O	4.71894	-2.96796	-0.24758
O	-1.82332	-4.51030	1.75396
O	1.56943	5.80603	1.31659
O	-1.17058	6.04971	1.84142
O	-6.37740	-1.33579	-0.99424
O	7.36070	-2.57253	-0.66546
O	-6.17501	-0.33187	2.60695
O	6.68289	-0.01448	0.23352

O	4.00606	-3.53035	2.24657
O	-0.08087	5.39727	-3.05284
O	-4.68698	-2.32577	3.61457
O	2.75953	3.64174	2.47696
O	1.15699	-5.75547	-1.50620
O	-5.13372	-3.72133	-0.52849
H	-3.50178	-1.68255	-1.78215
H	-2.91865	0.32691	3.17184
H	-4.41308	1.20120	0.60812
H	-4.01477	-2.91663	0.48070
H	-0.80327	4.44803	2.15637
H	-1.56081	2.49573	-2.88445
H	0.79898	4.99498	0.09740
H	-3.22221	3.97662	-0.31594
H	-1.13310	-3.40165	-2.30438
H	2.23391	-4.35184	-1.58160
H	4.64199	1.83133	0.56485
H	5.11455	-0.05754	-0.72885
H	5.69508	-2.98133	-0.44618
H	-0.93551	-4.35663	1.31163
H	-1.63953	-4.43032	2.70451
H	2.07449	5.11300	1.81485
H	2.22343	6.45057	0.99993
H	-0.22476	6.29447	1.71943
H	-1.47584	6.52353	2.63281
H	-6.22986	-2.29774	-0.83739
H	-6.74554	-1.27973	-1.89163
H	7.29206	-1.63737	-0.35921
H	7.51729	-2.50294	-1.62127
H	-5.75192	-1.10679	3.07840
H	7.35500	0.68511	0.28496
H	4.15954	-2.63177	2.60865
H	3.05507	-3.55305	1.97799
H	0.67538	5.28281	-3.65306
H	-0.49539	6.24347	-3.29230
H	-3.94497	-1.76968	3.91947
H	3.38925	2.98807	2.09645
H	0.98996	-5.49640	-0.56163
H	-5.42314	-4.59326	-0.21177
H	4.58070	-3.22501	0.71135
H	3.34952	-3.33358	-1.06740
H	0.09964	-4.39129	-2.15519
H	1.33101	-6.70860	-1.54075
H	6.38573	-0.18249	1.16377

H	2.61615	3.38011	3.40031
H	-4.35377	-2.58621	2.72992
H	-6.34464	0.32876	3.29934
H	-4.59792	-3.87816	-1.34919
H	4.28631	-1.37362	-0.57905
H	4.20352	0.81232	1.68057
H	2.15365	-1.34892	-2.46935
H	1.62362	-0.52250	1.57188
H	-1.19314	-0.87182	-1.91670
H	-0.34302	-1.71291	2.12297
H	-0.41893	0.78814	1.98620
H	-2.60889	1.08835	-1.55827
H	-0.00561	1.03123	-2.26032
H	1.61544	2.67532	1.32886
H	-1.06490	2.96208	2.63522
H	-2.26213	4.77227	0.69715
H	-1.08967	4.00122	-2.71599
H	-1.63551	-0.52094	3.42031
H	-5.00683	0.16867	1.73466
H	-2.69424	-3.24442	1.35422
H	-4.75558	-0.97778	-1.07721
H	0.15237	5.00208	-1.39269
O	-4.15812	4.11777	-1.65166
H	-3.40616	3.80726	-2.20074
H	-4.80729	3.39529	-1.68165

109
Hf4_4_2_term_perox_conf1_ion12_diconf7.log Energy: -3143084.9460779

Hf	1.98293	-1.63906	0.12826
O	1.74754	0.19578	1.31581
O	2.04250	0.14892	-1.04812
O	3.00446	-2.54835	-1.41373
O	2.56407	-2.51180	2.27338
O	2.67474	-3.53684	-0.34347
O	4.13325	-1.11738	0.61918
Hf	-1.55986	-2.21481	-0.18870
O	0.30851	-2.13062	-1.15295
O	0.09836	-2.11836	1.20724
O	-2.22141	-3.04826	1.90482
O	-1.91561	-3.15943	-2.32179
O	-3.70197	-2.84287	-0.33014
O	-1.10898	-4.44268	-0.07399
Hf	1.29659	1.81060	0.02734
O	-0.33327	1.82048	-1.32511

O	-0.56142	1.60246	1.01135
O	1.38169	2.90433	2.31678
O	2.18715	2.69117	-1.86977
O	3.45390	2.29086	0.58433
O	0.87527	4.04567	0.02857
Hf	-2.19938	1.28401	-0.34566
O	-2.36174	-0.55464	0.83298
O	-1.90326	-0.53633	-1.44417
O	-3.11178	1.90390	-2.07596
O	-3.37663	1.91343	1.72042
O	-2.17070	3.62216	-0.03808
O	-4.11098	1.56691	-1.01275
Cl	-0.04037	0.15142	3.85673
Cl	-0.29917	-1.29554	-4.16091
Cl	-1.51207	4.14477	2.99939
Cl	3.58261	0.71029	-3.76257
O	-0.43299	5.39372	-1.87096
O	4.40720	0.75008	2.58106
O	-5.41527	-2.14830	1.60454
O	-4.37503	-4.53555	2.39515
O	5.74564	-3.11687	-1.18118
O	-2.52950	4.32947	-3.15030
O	4.52705	-4.10470	1.47396
O	-4.87589	3.66692	0.32866
O	3.58716	4.60257	1.82643
O	-4.60169	-3.02220	-2.85900
O	3.05475	-0.62705	4.39588
O	-4.01895	-0.37100	3.04313
O	2.26264	5.35227	-1.88571
O	5.25785	0.66317	-1.03083
H	3.35222	-3.13253	2.14419
H	4.58977	-0.60896	-0.11631
H	-3.00514	-3.66518	2.05145
H	-1.39015	-2.68092	-3.01773
H	-4.34526	-2.49833	0.35737
H	-0.33773	-4.73874	-0.68175
H	0.50275	3.35655	2.41372
H	2.71986	2.16579	-2.52299
H	3.72766	1.75168	1.38442
H	1.62159	4.64100	-0.20061
H	-4.09938	2.53521	1.43012
H	-3.08401	3.98971	-0.04926
H	-1.19642	4.96327	-2.36366
H	5.30499	0.93183	2.90379

H	3.89097	0.35007	3.34747
H	-5.03667	-1.44515	2.19839
H	-6.30347	-1.85720	1.34228
H	-5.00922	-3.79757	2.23749
H	-4.39425	-4.68420	3.35508
H	4.81352	-2.84655	-1.33850
H	5.75105	-3.30019	-0.22762
H	-3.26052	4.95270	-3.00871
H	-2.81044	3.49874	-2.67964
H	3.98645	-4.06663	0.63790
H	-4.87221	2.95052	-0.36636
H	3.46081	5.50967	1.50532
H	2.75473	4.34562	2.27423
H	-4.95218	-2.25211	-3.33713
H	-5.15078	-3.78016	-3.12077
H	2.94235	-1.40016	3.80282
H	-3.98739	0.57009	2.75081
H	2.89084	5.94152	-2.33184
H	4.76340	1.39040	-0.60094
H	-0.82595	6.15527	-1.41398
H	0.16589	4.35166	-0.61491
H	2.33706	3.66460	-2.01948
H	1.35437	5.58817	-2.19156
H	-5.76215	4.05978	0.35947
H	-3.88222	-0.38046	4.00352
H	2.13935	-0.28483	4.47632
H	4.49443	-5.03092	1.76628
H	4.86034	0.61499	-1.92974
H	-1.81568	3.86120	0.85611
H	-2.78172	2.48131	2.27913
H	1.38487	2.25341	3.04647
H	3.62678	3.24104	0.86107
H	-0.19303	1.98376	-2.26928
H	-0.58135	1.20070	1.90533
H	2.34704	0.16011	-1.98360
H	1.27191	0.13468	2.17387
H	-0.08768	-1.61442	2.02449
H	0.38937	-1.91238	-2.10694
H	-1.48503	-0.50201	-2.33039
H	-2.69988	-0.62446	1.75135
H	-1.43488	-3.54057	2.19649
H	-1.87539	-4.98565	-0.32748
H	-2.83733	-3.17572	-2.67353
H	1.81585	-3.07335	2.54752

H	4.24732	-0.52748	1.41045
H	-4.17838	-2.84827	-1.19871
O	0.92409	-5.16775	-1.51887
H	0.78121	-4.77088	-2.39386
H	1.61381	-4.57524	-1.09516

109
Hf4_4_2_term_perox_conf1_ion12_diconf9.log Energy: -3143086.2613503

Hf	1.63097	-1.79816	0.63603
O	1.77767	0.20034	1.40418
O	1.65394	-0.19592	-0.88044
O	3.23852	-2.47689	-0.85732
O	1.99056	-2.14323	2.68183
O	1.25859	-4.13095	0.79034
O	3.22570	-2.22940	1.85450
Hf	-1.76600	-2.06999	-0.35344
O	0.25382	-2.47293	-0.94910
O	-0.42470	-1.68745	1.22362
O	-2.83190	-2.78014	1.73433
O	-1.81478	-3.07534	-2.44966
O	-3.86618	-2.62268	-0.78613
O	-1.41361	-4.27158	0.17119
Hf	1.48929	1.70399	-0.03778
O	-0.09552	2.03206	-1.40848
O	-0.45170	1.60913	0.86200
O	1.65093	2.91476	2.12303
O	2.53485	1.89763	-2.14420
O	3.69196	1.87097	0.39293
O	1.85564	3.87299	-0.36536
Hf	-2.05999	1.49852	-0.59071
O	-2.75690	-0.34879	0.40194
O	-1.57992	-0.38767	-1.58907
O	-2.75191	2.15595	-2.38744
O	-3.28352	1.97305	1.49379
O	-1.98608	3.76943	-0.19200
O	-3.84403	2.00886	-1.36305
Cl	-1.71058	0.01714	3.55596
Cl	0.33936	-1.31056	-3.91324
Cl	-0.49491	5.21087	2.15465
Cl	4.40510	-0.49368	-3.03637
O	0.13943	5.56006	-1.28991
O	4.71117	0.06289	2.10335
O	-5.98471	-1.37207	0.19996
O	-5.41408	-3.14963	2.16432

O	5.67019	-2.98223	-0.01188
O	-1.69776	4.59738	-3.05055
O	2.00962	-4.73463	3.24934
O	-3.59844	4.60858	1.84195
O	4.20311	4.02726	1.87439
O	-4.35539	-3.60227	-3.25327
O	1.59692	0.19220	4.08969
O	-5.92458	1.09739	1.15659
O	3.98398	4.23980	-2.02071
O	6.74932	-0.68518	-0.93829
H	3.44289	-1.82745	-1.58226
H	1.70230	-4.62204	0.03495
H	-3.82354	-2.92272	1.87809
H	-1.20165	-2.64009	-3.09242
H	-4.61248	-2.04726	-0.43705
H	-0.43790	-4.33981	0.37271
H	0.93690	3.60880	2.17360
H	3.09756	1.10719	-2.35273
H	4.02978	1.13543	0.99640
H	2.68060	4.13917	-0.84069
H	-3.42816	2.93346	1.73175
H	-2.84237	4.16982	0.05880
H	-0.54418	5.15953	-1.89922
H	4.46963	0.42398	2.97230
H	4.17647	-0.77478	2.02841
H	-5.94595	-0.42323	0.53529
H	-6.76732	-1.43436	-0.37186
H	-5.82467	-2.51830	1.52257
H	-5.61727	-2.78750	3.04246
H	6.15591	-2.16015	-0.30508
H	6.00845	-3.68854	-0.58661
H	-2.13421	3.76686	-2.71907
H	-1.28966	4.34363	-3.89372
H	2.02834	-3.73597	3.26528
H	-4.33828	4.96526	2.35978
H	4.19503	4.87434	1.39954
H	3.27834	3.89906	2.17776
H	-4.85748	-3.04907	-3.87491
H	-4.63564	-4.51897	-3.41376
H	1.84156	-0.73808	3.84702
H	-4.98620	1.37847	1.26608
H	4.90926	4.23429	-1.72402
H	7.57729	-0.84696	-1.41943
H	-0.34448	5.80298	-0.48031

H	1.11801	4.47803	-0.74777
H	3.13071	2.67512	-2.25399
H	3.92229	4.93415	-2.69788
H	-2.77121	4.96677	2.23692
H	-6.27631	1.04860	2.06072
H	0.62270	0.15607	4.18801
H	1.21434	-4.97702	3.75180
H	6.07680	-0.53568	-1.64569
H	-1.37421	4.04602	0.53423
H	-2.86628	1.55248	2.28142
H	1.55665	2.36700	2.92566
H	3.99094	2.71856	0.83822
H	0.08916	2.29844	-2.32079
H	-0.55543	1.18956	1.73541
H	1.37071	-0.35215	-1.80133
H	1.75699	0.31638	2.38465
H	-0.69998	-1.19941	2.02978
H	0.48865	-2.31402	-1.88478
H	-1.01999	-0.40740	-2.39526
H	-2.98595	-0.34822	1.34444
H	-2.50047	-2.32490	2.53097
H	-1.87409	-4.35173	1.03131
H	-2.65793	-3.25344	-2.93061
H	1.55906	-4.52882	1.66560
H	4.15055	-2.69481	-0.45331
H	-4.18083	-3.03057	-1.63126
O	2.48245	-5.11173	-1.36716
H	1.80231	-5.20710	-2.05460
H	2.84270	-4.20693	-1.49737

109
Hf4_4_2_term_perox_conf1_ion13_diconf5.log Energy: -3143090.4453763

Hf	2.42465	-0.22012	-0.22466
O	2.02037	1.59179	0.75209
O	1.19722	1.07418	-1.34823
O	3.08377	-0.37940	-2.48050
O	3.37636	-0.48850	1.98443
O	3.90224	-1.91240	-0.19187
O	4.34032	0.87088	-0.38948
Hf	-0.48721	-2.23551	0.17214
O	1.24547	-1.83476	-1.06631
O	0.93708	-0.97674	1.08006
O	-0.22129	-2.96846	2.35499
O	-1.00881	-3.12067	-2.02949

O	-2.20466	-3.57931	0.49217
O	0.51677	-4.22675	0.11618
Hf	0.44017	2.79092	-0.18909
O	-1.43964	2.11710	-1.04313
O	-0.79673	1.82575	1.25873
O	1.10145	3.98324	1.35568
O	0.71079	3.53595	-2.39528
O	1.78682	4.34460	0.08621
O	-0.96441	4.66797	-0.44714
Hf	-2.45158	0.77489	0.29556
O	-1.84153	-1.05343	1.30439
O	-1.34679	-0.66479	-0.90629
O	-3.79615	0.61226	-1.25788
O	-3.16948	0.81507	2.54585
O	-3.62993	2.70541	0.77089
O	-4.35543	0.06441	0.00988
Cl	1.10487	0.82251	3.74138
Cl	0.11922	-0.71268	-3.84990
Cl	2.75712	-3.21255	3.28968
Cl	-3.96305	-3.88006	-2.68835
O	-3.56346	4.42376	-1.28370
O	4.35077	3.48301	-0.11308
O	-4.63040	-2.52887	0.18047
O	-0.44078	-5.70889	2.18733
O	4.84314	-2.34583	-2.69116
O	-4.94667	2.61145	-2.60998
O	6.42783	-1.53984	0.62207
O	-5.73489	1.34644	2.18206
O	-1.00075	5.52269	2.32174
O	-2.61851	-5.90445	-0.72262
O	6.01527	0.31642	2.44936
O	-6.60858	-1.22295	1.78968
O	0.95050	6.10916	-1.67072
O	6.39170	-0.35895	-1.77000
H	2.33352	-0.36338	-3.11352
H	3.27250	-1.43732	2.29943
H	4.07845	-2.37903	-1.04410
H	5.04832	0.59526	-1.02493
H	-0.53300	-3.89298	2.49189
H	-0.78676	-2.46116	-2.73138
H	-3.11734	-3.14498	0.49146
H	0.72875	-4.65846	-0.76822
H	1.45730	3.08938	-2.83079
H	-0.52435	5.43945	-0.87460

H	-4.16186	0.98066	2.55578
H	-4.54682	2.44778	1.01067
H	-4.08528	3.82955	-1.91060
H	3.40004	3.76111	0.01977
H	4.78699	3.68785	0.73031
H	-4.44216	-1.55461	-0.00333
H	-4.75762	-2.93314	-0.70701
H	-1.22109	-6.27740	2.07930
H	0.18348	-6.21513	2.73384
H	5.63011	-1.75414	-2.58010
H	5.01935	-2.95816	-3.42272
H	-5.87335	2.73563	-2.34720
H	-4.62625	1.83263	-2.06760
H	6.42528	-0.86338	1.36684
H	-6.07950	0.44390	1.92980
H	-1.45693	5.46859	1.46570
H	-0.16300	5.06613	2.08300
H	-3.12867	-5.48820	-1.45992
H	-3.28129	-6.40720	-0.21978
H	5.04895	0.13524	2.38416
H	-6.50403	-1.61065	2.67356
H	1.46738	5.78589	-0.88792
H	6.70319	-0.77098	-0.92284
H	-4.08051	5.23819	-1.17135
H	-1.82928	4.51788	-0.90410
H	0.89599	4.51198	-2.41907
H	1.30970	6.96702	-1.94617
H	-6.24589	1.62092	2.96113
H	-6.02385	-1.76767	1.21534
H	6.13210	1.14761	1.96027
H	6.94129	-2.30663	0.92446
H	7.15067	0.10547	-2.15874
H	-3.67061	3.38696	0.04248
H	-2.77539	1.59275	2.97759
H	-1.66550	2.21429	-1.97899
H	-0.36869	1.57827	2.10528
H	0.71963	0.74722	-2.13713
H	2.08523	1.77715	1.70575
H	0.76885	-0.53597	1.94145
H	1.15161	-1.83632	-2.03567
H	-1.13831	-0.47227	-1.83885
H	-1.95149	-1.14971	2.26183
H	0.73428	-2.97280	2.64663
H	0.22896	-4.92662	0.75340

H	-1.97509	-3.33185	-2.18166
H	2.79787	-0.00164	2.62896
H	4.80543	-1.80501	0.23276
H	4.33812	1.88289	-0.28675
H	3.67781	-1.13052	-2.75808
H	-2.31225	-4.48649	0.06917
O	0.78817	-5.25138	-2.29715
H	0.09112	-4.61635	-2.56744
H	1.59422	-4.94459	-2.74510

109
Hf4_4_2_term_perox_conf1_ion13_diconf9.log Energy: -3143088.2973738

Hf	-1.24306	2.23107	0.07993
O	-2.33869	0.59684	0.95575
O	-1.64421	0.48045	-1.28972
O	-2.02862	3.03306	-1.87896
O	-1.79984	3.05853	1.91335
O	-0.29708	4.31391	-0.12722
O	-2.75489	3.41301	0.82772
Hf	2.15640	1.01727	0.04876
O	0.64942	2.07692	-1.08053
O	0.45722	1.54609	1.20358
O	2.82641	1.46622	2.24036
O	2.99418	1.35857	-2.23427
O	4.32346	0.43551	0.01845
O	3.08396	3.03654	0.05062
Hf	-2.30244	-1.15679	-0.17297
O	-0.79049	-2.25753	-1.17003
O	-0.68549	-1.52275	1.06324
O	-3.18259	-1.92389	2.03508
O	-3.18107	-1.46478	-2.44250
O	-4.50981	-0.60630	-0.19274
O	-3.34060	-3.18982	-0.25133
Hf	1.01804	-2.39536	0.06765
O	2.15012	-0.82193	1.11404
O	1.46926	-0.61392	-1.07751
O	1.83031	-3.44895	-1.45799
O	1.36713	-3.03810	2.35440
O	-0.08823	-4.37725	0.49534
O	2.69620	-3.51011	-0.22755
Cl	-0.82597	-1.25755	4.12608
Cl	0.38345	0.53219	-3.85798
Cl	2.76231	4.53530	2.73523
Cl	5.15209	-0.47152	-3.52791

O	-1.87003	-5.08036	-1.46579
O	-5.01438	2.04017	0.31933
O	4.84635	-1.97879	-0.70574
O	5.35794	0.70726	2.59358
O	-3.58988	5.11484	-2.04674
O	-1.50507	-3.41688	-3.56473
O	-0.35026	5.32836	2.27754
O	1.55734	-5.73125	2.20453
O	-5.90635	-1.41662	1.91375
O	6.16922	1.66352	-1.46011
O	-2.98619	1.19549	3.48814
O	3.92249	-4.49281	2.63404
O	-5.45898	-2.82142	-1.91543
O	-5.88985	3.75767	-1.66873
H	-2.47579	2.34259	-2.39541
H	0.60425	4.14870	-0.45418
H	3.76764	1.21489	2.47659
H	2.25508	1.18504	-2.87021
H	4.49554	-0.55551	-0.22789
H	3.22172	3.57075	-0.79255
H	-3.19528	-2.88791	1.88242
H	-3.24150	-0.58782	-2.86098
H	-4.62263	0.38226	-0.08389
H	-4.22505	-3.19955	-0.69952
H	1.23802	-4.01455	2.48248
H	0.47241	-5.08975	0.87821
H	-1.73444	-4.69653	-2.36825
H	-5.62444	2.04492	1.07658
H	-4.17844	2.49699	0.63843
H	4.04258	-2.56099	-0.56138
H	4.90214	-1.81201	-1.67185
H	5.28273	0.46643	1.64493
H	5.38338	-0.14207	3.06502
H	-4.48359	4.68551	-1.91721
H	-3.58683	5.42155	-2.96835
H	-1.11128	-3.43456	-4.45139
H	-2.22478	-2.75251	-3.57612
H	-0.92507	4.52914	2.40257
H	2.52259	-5.53022	2.33380
H	-6.38653	-2.25315	1.79558
H	-5.07101	-1.66331	2.36225
H	6.09229	1.05246	-2.23180
H	7.03022	1.45335	-1.06116
H	-2.56113	2.02170	3.14244

H	3.39468	-3.67137	2.63933
H	-6.22551	-2.30424	-1.61596
H	-5.98732	3.20219	-2.45900
H	-2.25810	-5.96362	-1.57968
H	-2.80953	-3.93039	-0.67040
H	-4.10731	-1.82294	-2.40404
H	-5.80778	-3.51688	-2.49836
H	1.28457	-6.28887	2.95074
H	4.21130	-4.60044	3.55567
H	-2.26352	0.69030	3.91169
H	0.54156	5.06199	2.59429
H	-5.64411	3.12343	-0.95054
H	-0.58314	-4.73812	-0.27910
H	0.75842	-2.58874	2.98605
H	-2.54592	-1.77414	2.78067
H	-5.08867	-0.97908	0.54340
H	-0.83767	-2.58688	-2.09218
H	-0.65333	-1.15161	1.97037
H	-1.06627	0.34748	-2.07244
H	-2.68448	0.68940	1.88497
H	0.42953	1.34206	2.15078
H	0.53097	1.90358	-2.03445
H	1.10444	-0.51077	-1.98023
H	2.32614	-0.83813	2.06556
H	2.71737	2.40677	2.53608
H	3.05062	3.64042	0.84014
H	3.71077	0.74042	-2.55393
H	-0.24071	4.83968	0.73657
H	-2.60137	3.87442	-1.92461
H	4.98646	0.97924	-0.51215
O	3.53370	4.08968	-2.31442
H	3.44563	3.16319	-2.62933
H	2.76716	4.55381	-2.69033

109
Hf4_4_2_term_perox_conf1_ion14_diconf5.log Energy: -3143092.7765740

Hf	-2.39830	-0.90864	0.17855
O	-0.95710	-2.29571	0.70662
O	-0.98226	-1.23276	-1.33572
O	-3.60030	-0.99482	-1.82442
O	-2.70473	-1.42731	2.60618
O	-4.42623	-0.26004	0.88127
O	-3.51949	-2.82749	0.18288
Hf	-0.92258	2.32997	0.39590

O	-2.41417	1.10913	-0.58915
O	-1.34286	0.51207	1.38413
O	-1.05643	2.99425	2.70121
O	-1.52778	3.40160	-1.66587
O	-0.10506	4.34880	0.50788
O	-2.81764	3.38663	0.90443
Hf	0.78290	-2.35780	-0.67272
O	1.72901	-0.62143	-1.63754
O	1.44714	-1.00690	0.78624
O	1.05688	-3.89602	0.72043
O	0.67778	-2.99739	-2.85591
O	0.50218	-4.41494	-0.55753
O	3.01427	-2.90887	-0.95769
Hf	2.26839	0.79106	-0.06017
O	1.01452	1.95293	1.24566
O	0.40916	1.54989	-0.97278
O	3.20915	1.94173	-1.50259
O	3.17423	0.58604	2.19175
O	4.08580	-0.47967	-0.29344
O	3.63503	2.34438	-0.12920
Cl	0.20193	-0.73376	3.76209
Cl	-1.65182	0.88938	-3.65961
Cl	4.58930	-2.11498	2.98435
Cl	0.00128	5.73114	-2.92837
O	4.41304	-2.65070	-3.18827
O	-2.14868	-5.00115	-0.37715
O	2.52983	4.60598	0.73703
O	1.53135	3.83911	3.15262
O	-6.03963	-0.12667	-1.26842
O	3.90973	0.05688	-3.30733
O	-6.06183	-2.01762	2.04907
O	6.35477	-0.34770	1.00723
O	3.64834	-4.55492	0.97007
O	-1.22189	6.60025	-0.22366
O	-4.33363	-3.65826	3.21063
O	5.56343	2.14280	1.80316
O	1.68300	-5.41363	-2.74892
O	-6.18581	-2.70056	-0.52851
H	-3.12477	-0.59215	-2.58473
H	-3.20945	-0.70105	3.01787
H	-5.02176	0.13578	0.19672
H	-4.40918	-2.88926	-0.24976
H	-0.22232	3.44413	2.98765
H	-1.53296	2.75433	-2.41396

H	0.88768	4.48975	0.48514
H	-3.43454	3.77233	0.19922
H	0.95403	-2.39139	-3.56215
H	3.38497	-3.61729	-0.33702
H	3.61375	-0.29679	2.34950
H	4.97958	-0.42343	0.18359
H	4.35051	-1.67184	-3.30115
H	-1.17442	-4.78270	-0.40416
H	-2.24593	-5.61964	0.36536
H	2.98413	3.80260	0.32940
H	2.96817	5.39794	0.38606
H	2.04788	4.32765	2.46632
H	2.10197	3.73781	3.93089
H	-6.41355	-1.03468	-1.13779
H	-6.66855	0.39258	-1.79403
H	3.65841	0.52260	-4.12079
H	3.94173	0.74791	-2.59338
H	-5.52381	-2.68914	2.56980
H	6.25071	0.57076	1.37160
H	3.97885	-3.89253	1.61862
H	2.65892	-4.50455	1.05873
H	-0.87901	6.55833	-1.15310
H	-0.74359	7.33923	0.18859
H	-3.60966	-3.00613	3.08838
H	4.80772	1.78452	2.30889
H	1.40226	-5.31896	-1.80229
H	-6.41474	-2.62312	0.43247
H	3.99665	-3.02269	-3.98242
H	3.49707	-2.92944	-1.84122
H	1.07861	-3.90882	-3.02746
H	1.09086	-6.08755	-3.12261
H	6.07086	-0.94019	1.73941
H	5.13420	2.31429	0.93400
H	-4.17188	-4.31599	2.51388
H	-6.75430	-1.67725	2.63895
H	-6.69227	-3.44837	-0.88525
H	3.82659	-1.42688	-0.40075
H	2.42256	0.58142	2.81797
H	2.38109	-0.61771	-2.36881
H	1.12822	-1.08563	1.70874
H	-0.94750	-0.68476	-2.14618
H	-0.85320	-2.90367	1.45400
H	-0.73685	0.20335	2.09990
H	-2.54653	1.19885	-1.55056

H	0.17277	1.17096	-1.83711
H	1.32809	2.45366	2.03071
H	-1.17499	2.23848	3.30377
H	-2.77728	3.96974	1.68124
H	-0.94093	4.15016	-1.99242
H	-1.81636	-1.37287	3.04832
H	-5.01539	-0.88911	1.40311
H	-2.98273	-3.66204	-0.04149
H	-4.52077	-0.60964	-1.82488
H	-0.56577	5.22170	0.27509
O	-4.12366	4.32411	-1.14367
H	-3.31728	4.11710	-1.66440
H	-4.79364	3.69251	-1.45531

109
Hf4_4_2_term_perox_conf1_ion14_diconf7.log Energy: -3143079.4976077

Hf	0.62649	2.42401	0.16693
O	-1.31636	1.81891	1.01325
O	-0.80337	1.65288	-1.29315
O	1.79479	3.67925	-1.07196
O	0.57670	3.11900	2.46608
O	2.16620	3.72497	0.38047
O	-0.67391	4.24540	0.08924
Hf	2.40087	-0.69880	0.03757
O	1.83079	1.04878	-0.98212
O	1.34157	0.69411	1.26833
O	3.24526	-0.88923	2.21790
O	3.43046	-0.80131	-2.09141
O	3.74688	-2.47632	-0.01390
O	4.24373	0.55106	0.17896
Hf	-2.34071	0.56416	-0.33959
O	-1.69968	-1.10643	-1.46292
O	-1.53110	-0.95537	0.89197
O	-3.58486	0.42360	1.97244
O	-3.04746	1.05258	-2.51638
O	-3.87057	2.20255	-0.26540
O	-4.30148	-0.54505	-0.48463
Hf	-0.61069	-2.54380	-0.25101
O	1.14721	-2.12996	0.95403
O	0.99503	-1.52944	-1.30646
O	-0.71434	-3.74881	-1.90088
O	-0.95952	-3.70010	1.90895
O	-2.81484	-3.30305	-0.04393
O	-0.11557	-4.47010	-0.73204

Cl	-0.77903	0.56602	3.79487
Cl	-0.39645	0.07795	-4.04252
Cl	-3.81329	-2.62576	2.83295
Cl	6.44361	-1.01078	-2.77066
O	-4.89036	-2.49322	-2.23191
O	-3.44748	4.47286	1.17071
O	3.69503	-4.25441	2.00912
O	5.47097	-2.32131	2.74108
O	1.86890	6.35092	-1.76686
O	-3.08825	-4.26353	-3.12363
O	2.08012	6.41373	0.97771
O	-1.94557	-5.81206	0.55850
O	-5.43201	2.41931	1.84519
O	6.12052	-1.34172	0.22405
O	-1.54411	4.99833	3.04603
O	1.40002	-3.60490	3.27750
O	-5.52363	0.05378	-2.79509
O	-0.76396	6.00643	-1.82829
H	1.43559	3.48358	2.74680
H	-0.69058	4.90947	-0.68381
H	4.10617	-1.35772	2.43316
H	3.07655	-1.58294	-2.55034
H	3.62343	-3.19333	0.67068
H	4.32926	1.33192	-0.45691
H	-3.82391	-0.53167	2.09465
H	-2.40709	0.79012	-3.21657
H	-3.48279	3.06935	0.02801
H	-4.99549	-0.07484	-1.00579
H	-1.27311	-4.61122	1.65353
H	-2.84104	-4.28711	0.00158
H	-4.19487	-3.13649	-2.56560
H	-4.20225	4.04298	1.62077
H	-2.80465	4.67581	1.90241
H	2.86199	-4.17539	2.54186
H	3.81893	-5.19675	1.81061
H	5.02356	-3.19705	2.65122
H	5.74075	-2.25320	3.67176
H	1.94511	5.37030	-1.67114
H	1.98964	6.63381	-0.82695
H	-3.41702	-5.13971	-2.86511
H	-2.24414	-4.14781	-2.61034
H	2.10794	5.43202	0.84877
H	-1.20681	-5.61623	-0.08363
H	-6.38805	2.25567	1.88885

H	-4.98886	1.62906	2.22823
H	6.65274	-1.38546	-0.60577
H	6.58402	-1.72751	0.98986
H	-0.79640	4.40540	2.82441
H	0.48595	-3.85015	3.00258
H	-6.28035	0.37176	-3.31170
H	-0.95065	5.54708	-2.66355
H	-5.59030	-3.04479	-1.84662
H	-4.26076	-1.42365	-0.96735
H	-3.94922	0.73563	-2.79185
H	-5.45672	-0.92501	-2.91711
H	-2.02404	-6.77409	0.65358
H	1.34634	-3.26914	4.18628
H	-1.83190	4.71030	3.92760
H	2.97506	6.64296	1.27621
H	0.20809	6.25964	-1.88452
H	-3.23984	-3.00435	0.80278
H	-1.73408	-3.30562	2.38821
H	-2.97093	0.59012	2.72018
H	-4.62241	2.11787	0.39100
H	-1.48005	-1.00664	-2.41262
H	-1.31681	-0.77154	1.82618
H	-0.50681	1.34980	-2.18020
H	-1.32657	1.58221	1.96336
H	0.86510	0.38182	2.06283
H	2.22201	1.28161	-1.83581
H	0.73952	-1.01429	-2.09779
H	1.28892	-2.43825	1.87637
H	3.32265	0.01179	2.57547
H	5.10591	0.06538	0.24968
H	4.42006	-0.82790	-2.24988
H	0.34562	2.40333	3.10981
H	-1.59571	4.11004	0.37784
H	4.71679	-2.22302	-0.00551
O	4.34073	2.68312	-1.40824
H	4.51536	2.49547	-2.34451
H	3.42809	3.07732	-1.37344

109
Hf4_4_2_term_perox_conf1_ion14_diconf9.log Energy: -3143092.3253320

Hf	2.43545	-0.82421	-0.20339
O	0.86994	-2.14584	-0.97578
O	0.85776	-1.31822	1.18321
O	3.47547	-1.38131	1.72669

O	3.29377	-1.56209	-2.00714
O	4.25123	0.63370	-0.53716
O	3.79910	-2.25638	-0.79160
Hf	0.85979	2.36078	-0.13414
O	2.16844	1.03571	0.96646
O	1.39288	0.66897	-1.30398
O	1.06026	3.09369	-2.40473
O	1.57899	3.46046	1.72286
O	0.10480	4.44213	-0.16768
O	2.97873	3.03788	-0.66798
Hf	-0.74144	-2.33224	0.38923
O	-2.04094	-0.90161	1.33047
O	-1.46019	-0.81695	-0.92799
O	-1.57273	-3.49367	-1.55402
O	-0.60621	-2.80432	2.73150
O	0.14195	-4.36639	0.54455
O	-2.53488	-3.64143	0.91220
Hf	-2.38294	0.84718	0.08382
O	-1.07459	2.19183	-0.97095
O	-0.55376	1.48023	1.15884
O	-3.39229	1.58961	1.69907
O	-3.09160	1.21551	-2.21351
O	-4.32639	-0.35439	-0.21705
O	-3.75614	2.32712	0.44727
Cl	-0.42761	0.37320	-3.83751
Cl	1.13401	-0.06624	3.89423
Cl	-4.54119	-2.91799	-2.05305
Cl	0.05258	5.17915	3.68506
O	-4.57920	-2.64534	2.33038
O	2.52209	-4.75441	-0.59616
O	-2.59274	4.66407	0.02346
O	-0.35366	5.06063	-3.44918
O	6.10109	-1.62617	1.92187
O	-5.34903	-0.08656	2.60458
O	5.42330	-0.16321	-2.77609
O	-5.45262	0.03802	-2.64308
O	-1.27203	-6.17892	-0.79395
O	1.14681	6.52781	1.07877
O	1.90451	-3.59188	-3.04491
O	-2.72863	4.00744	-2.63711
O	-2.71950	-4.21654	3.53828
O	6.44863	-2.75799	-0.43484
H	3.08703	-1.08312	2.57316
H	4.88542	0.78043	0.23631

H	0.56212	3.90914	-2.73661
H	2.32668	3.05452	2.19079
H	-0.88457	4.55312	-0.08093
H	3.54183	2.21136	-0.62432
H	-2.54222	-3.28308	-1.71167
H	-0.20223	-2.14378	3.32801
H	1.07530	-4.46516	0.16247
H	-2.41358	-4.26736	1.66247
H	-3.93579	0.79323	-2.53333
H	-4.98414	0.05763	-0.81968
H	-4.81000	-1.67300	2.45070
H	2.26882	-4.74852	-1.54347
H	3.03369	-3.91187	-0.53429
H	-3.03728	3.82340	0.35541
H	-2.99426	5.41107	0.49596
H	-1.26103	4.70005	-3.28413
H	-0.22587	4.99824	-4.41005
H	6.35531	-2.11559	1.07744
H	6.46743	-2.12337	2.67109
H	-6.01095	-0.08276	1.89366
H	-4.64646	0.52807	2.25305
H	4.66774	-0.80887	-2.70636
H	-6.14824	0.33087	-3.25346
H	-2.05051	-6.50937	-0.31587
H	-1.60045	-5.41466	-1.31207
H	0.84117	6.30129	1.99199
H	0.62970	7.31238	0.83097
H	2.55434	-2.85098	-2.89542
H	-3.10270	3.10195	-2.63409
H	-2.84608	-4.81164	4.29350
H	6.50302	-3.72490	-0.35934
H	-5.41777	-3.08848	2.12062
H	-3.33595	-3.12229	1.21797
H	-1.32201	-3.28058	3.23001
H	-3.52967	-3.65957	3.44858
H	-5.32594	-0.92962	-2.77978
H	-2.85907	4.35955	-1.72441
H	1.63643	-3.55031	-3.97645
H	5.15777	0.45334	-3.47865
H	5.51203	-2.57945	-0.70994
H	-4.23393	-1.26657	-0.58858
H	-2.36731	0.91742	-2.81905
H	-1.12192	-3.23730	-2.37824
H	-0.38534	-5.12645	0.15305

H	-2.25710	-0.93602	2.27273
H	-1.03383	-0.69193	-1.79941
H	0.85382	-0.91505	2.08411
H	1.04930	-2.67976	-1.78222
H	0.91584	0.45363	-2.13920
H	1.96338	0.90334	1.91186
H	-0.30199	1.04169	1.99070
H	-1.37581	2.73310	-1.72240
H	0.80095	2.37042	-3.01428
H	2.90330	3.26608	-1.61624
H	1.02153	3.95917	2.39605
H	4.80809	0.42717	-1.35005
H	4.46432	-1.51396	1.85287
H	0.54622	5.22847	0.28683
O	5.98747	1.04760	1.42423
H	5.52098	1.44826	2.17611
H	6.20449	0.13060	1.72139

109
Hf4_4_2_term_perox_conf1_ion15_diconf5.log Energy: -3143087.1163319

Hf	-1.53690	-1.76474	-0.34285
O	-2.12997	-0.03029	-1.33962
O	-1.62528	-0.11760	0.93108
O	-2.29714	-2.56778	1.64360
O	-1.79526	-2.42735	-2.70099
O	-1.33416	-3.96249	-0.60554
O	-3.74783	-2.09901	-0.65121
Hf	1.98109	-1.35076	-0.05423
O	0.21909	-2.24405	0.83287
O	0.32567	-1.43392	-1.36037
O	2.84725	-1.94309	-2.16518
O	2.55370	-2.02663	2.20634
O	4.17042	-1.14111	0.18351
O	2.44176	-3.56187	-0.09699
Hf	-1.99434	1.78719	-0.11310
O	-0.31535	2.38742	1.14615
O	-0.17600	2.02163	-1.23527
O	-2.91410	2.45099	-1.83190
O	-3.14842	1.87740	1.88999
O	-3.92884	2.12343	-0.79520
O	-2.25753	4.05897	0.38393
Hf	1.54498	2.18268	0.08026
O	2.33776	0.49031	-1.05060
O	1.48261	0.28342	1.10280

O	2.41918	2.83420	1.82273
O	2.45121	3.12935	-1.98285
O	1.06243	4.45278	-0.16153
O	3.40623	2.79928	0.69994
Cl	-0.48107	0.08292	-4.04638
Cl	0.14723	-0.55805	3.73803
Cl	-4.36059	-0.73054	3.20812
Cl	5.42450	-2.82099	3.07533
O	-0.42024	5.40202	1.87870
O	-5.15802	-0.11835	-1.59842
O	5.67136	0.06940	-1.69165
O	5.49495	-2.54093	-2.37149
O	-3.58636	-4.85361	2.04731
O	1.61214	4.80259	3.44581
O	-2.94462	-5.70758	-1.57561
O	3.67140	5.03504	-0.61213
O	-2.19158	5.08302	-2.32615
O	5.12742	-3.63507	0.10851
O	-4.28966	-3.80377	-2.90335
O	3.83897	1.17850	-3.29525
O	-4.85121	3.81860	0.99353
O	-5.40173	-2.95108	1.31659
H	-2.85467	-1.93953	2.17002
H	-1.14342	-3.14467	-2.80678
H	-0.72042	-4.36550	0.03008
H	-4.32771	-2.43872	0.08790
H	3.80243	-2.22082	-2.28120
H	2.08242	-1.49693	2.89101
H	4.67800	-0.55435	-0.44596
H	2.09173	-4.07084	0.69467
H	-3.50401	1.02079	2.24258
H	-3.18387	4.29832	0.63256
H	3.01846	3.90822	-1.70458
H	1.86920	5.01147	-0.21229
H	0.26245	5.20074	2.59222
H	-4.69077	0.72111	-1.31105
H	-5.06076	-0.13067	-2.56489
H	5.12887	0.58964	-2.34266
H	6.43285	0.61776	-1.44298
H	5.82770	-1.61444	-2.27694
H	5.77218	-2.84240	-3.25218
H	-4.44372	-4.40377	1.86302
H	-3.59652	-5.03748	3.00125
H	2.04280	4.15297	2.82236

H	1.37449	4.27311	4.22431
H	-3.52779	-5.12571	-2.14432
H	3.83055	4.31533	0.06595
H	-1.98123	5.21430	-1.38673
H	-2.55456	4.16995	-2.27951
H	5.58800	-3.64007	0.98064
H	5.75140	-3.53275	-0.63779
H	-3.50462	-3.37531	-3.29678
H	3.45453	2.05384	-3.06490
H	-4.84715	3.31855	0.13737
H	-6.33915	-2.96632	1.06098
H	-0.52293	6.36743	1.85404
H	-1.65081	4.42911	1.07211
H	-3.90642	2.50858	1.84966
H	-5.68933	4.30147	1.06396
H	4.48839	5.54450	-0.72886
H	3.77276	1.07504	-4.25762
H	-4.38992	-3.26482	-2.09191
H	-2.45025	-6.26631	-2.19855
H	-5.30133	-2.22896	1.98924
H	0.49732	4.82894	0.56949
H	1.70001	3.51188	-2.47165
H	-0.36950	2.40218	2.11281
H	-0.15333	1.61530	-2.12346
H	-1.24663	-0.14878	1.83423
H	-2.03126	0.14778	-2.29414
H	0.31934	-0.89484	-2.18378
H	0.06746	-2.18116	1.79466
H	1.03945	0.20388	1.97942
H	2.70548	0.52898	-1.95752
H	2.30639	-2.65392	-2.54982
H	3.40963	-3.77737	-0.13615
H	3.50994	-2.11656	2.49135
H	-1.46994	-1.70324	-3.30031
H	-1.97859	-4.68673	-0.96348
H	-4.24020	-1.28739	-1.03967
H	-2.68168	-3.48752	1.78556
H	4.66743	-2.00519	0.25259
O	1.86337	-4.75150	2.21061
H	2.01836	-3.86678	2.60226
H	0.94552	-4.97321	2.43672

109
Hf4_4_2_term_perox_conf1_ion15_diconf9.log Energy: -3143094.0111361

Hf	1.34930	-2.07316	0.49049
O	2.16263	-0.22661	1.26166
O	1.55762	-0.43320	-0.98053
O	2.32519	-2.99318	-1.29841
O	1.92968	-2.61014	2.45099
O	0.55901	-4.23554	0.62125
O	2.93642	-2.98300	1.41540
Hf	-2.13209	-1.29436	0.04357
O	-0.45553	-2.30274	-0.81096
O	-0.52089	-1.48710	1.41718
O	-3.07113	-1.67158	2.16159
O	-2.72352	-1.97718	-2.21632
O	-4.32259	-0.88001	-0.17554
O	-2.74428	-3.43154	0.16519
Hf	2.10285	1.36398	-0.09279
O	0.51177	2.25453	-1.22803
O	0.38504	1.75563	1.05644
O	2.82786	2.48402	2.00656
O	2.93204	1.41687	-2.26305
O	4.31654	1.00695	0.09470
O	2.85112	3.50880	-0.40234
Hf	-1.35683	2.20330	-0.08626
O	-2.39986	0.60627	0.95523
O	-1.50897	0.30390	-1.14007
O	-2.19988	2.96732	-1.79851
O	-2.01037	2.87598	2.09881
O	-0.70172	4.36827	0.32309
O	-3.09282	3.17522	-0.62092
Cl	0.67080	1.66654	4.14414
Cl	-0.22578	-0.80359	-3.75095
Cl	4.17935	-1.29740	-3.23904
Cl	-5.79457	-2.39342	-2.38352
O	1.07891	5.24937	-1.46783
O	4.97021	-1.10221	1.62347
O	-5.17611	1.67421	-0.29584
O	-5.76378	-2.01326	2.26172
O	4.07945	-4.96394	-1.11049
O	-0.86932	4.84685	-3.18674
O	1.10889	-5.04559	3.06793
O	-3.08309	5.23830	1.54254
O	5.62760	2.63798	1.74266
O	-5.28430	-4.03327	0.39450
O	3.12203	-0.59228	3.78598
O	-5.51857	4.02579	1.30758

O	4.85889	3.39583	-2.20185
O	6.05095	-3.13117	-1.41841
H	2.81748	-2.37357	-1.89450
H	-0.38975	-4.22425	0.40945
H	-4.06263	-1.75241	2.21752
H	-2.21168	-1.50251	-2.91418
H	-4.59923	0.08781	-0.15939
H	-2.47708	-3.97996	-0.63250
H	2.66101	3.41429	1.76503
H	3.28867	0.52788	-2.53356
H	4.51622	0.15015	0.59710
H	3.69204	3.62282	-0.91581
H	-2.38602	3.80348	2.07540
H	-1.48425	4.94237	0.47268
H	0.45319	5.10348	-2.24595
H	4.69436	-0.75354	2.49464
H	4.30376	-1.82377	1.47382
H	-4.35428	2.19714	-0.57995
H	-5.79787	1.72855	-1.04175
H	-6.20171	-1.25791	1.83390
H	-6.18136	-2.10298	3.13531
H	4.88548	-4.38515	-1.20545
H	4.03526	-5.46543	-1.94102
H	-0.66983	4.34581	-3.99389
H	-1.44941	4.24084	-2.64326
H	1.48798	-4.11965	3.05856
H	-3.98703	4.86195	1.34693
H	5.83806	3.53059	1.42202
H	4.78459	2.73672	2.22971
H	-5.59878	-3.66852	-0.46271
H	-5.64560	-3.42311	1.07519
H	2.66285	-1.43966	3.53971
H	-5.69257	3.74638	2.22088
H	5.78116	3.17970	-1.98420
H	6.78635	-3.45199	-1.96545
H	1.32805	6.18816	-1.47223
H	2.18074	4.10318	-0.84854
H	3.67847	2.04863	-2.39808
H	4.89941	4.08743	-2.88378
H	-3.20856	5.88249	2.25827
H	-5.48517	3.18488	0.79669
H	2.43884	-0.02875	4.20353
H	0.31527	-4.98278	3.62463
H	5.56344	-2.50384	-2.00217

H	-0.07295	4.80950	-0.30995
H	-1.26118	2.87967	2.72654
H	2.23412	2.29539	2.78200
H	4.86932	1.68839	0.58116
H	0.58040	2.29985	-2.19327
H	0.39164	1.50308	2.00636
H	1.12910	-0.47019	-1.86130
H	2.55948	-0.21164	2.16508
H	-0.52619	-1.03453	2.27458
H	-0.30139	-2.21378	-1.76995
H	-1.07481	0.17672	-2.01196
H	-2.65998	0.73996	1.87853
H	-2.70470	-2.46726	2.58400
H	-3.71476	-3.68215	0.34564
H	-3.68198	-1.99309	-2.47694
H	0.67549	-4.67895	1.51869
H	2.92544	-3.79657	-1.17574
H	-4.88383	-1.32651	-0.86687
O	-2.19674	-4.73571	-2.09595
H	-2.27513	-3.85944	-2.52658
H	-1.26440	-4.98551	-2.20547

109
Hf4_4_2_term_perox_conf1_ion1_diconf5.log Energy: -3143091.4225341

Hf	-1.63564	-1.74151	0.23635
O	0.27657	-2.15743	1.02136
O	-0.10561	-1.59871	-1.19667
O	-2.55322	-2.47835	-1.70844
O	-2.01512	-2.11117	2.56636
O	-3.79536	-1.77630	0.67333
O	-1.69354	-3.98910	0.45425
Hf	-1.64612	1.84553	0.05546
O	-2.42804	0.00121	-0.75876
O	-1.19274	0.10999	1.20021
O	-2.04070	2.43753	2.26532
O	-2.43515	2.33929	-2.10244
O	-1.72854	4.03998	0.03100
O	-3.82256	2.06189	0.31842
Hf	1.92723	-1.74632	-0.39166
O	2.07733	0.05291	-1.68594
O	2.10334	0.01658	0.76792
O	2.82498	-2.65465	1.23421
O	1.95778	-2.84822	-2.43887
O	2.52909	-3.66817	0.19173

O	4.07978	-1.68165	-1.18708
Hf	1.96473	1.84343	-0.40044
O	0.26093	2.40868	0.83346
O	-0.05482	1.56552	-1.28140
O	2.28688	2.92762	-2.10252
O	2.75639	2.70821	1.62346
O	4.23538	1.60959	-0.51886
O	2.39945	3.80492	-0.89445
Cl	-3.31089	0.21163	4.05874
Cl	2.73787	0.47640	3.84059
Cl	-0.68197	-4.15237	-3.60161
Cl	-4.84053	4.15300	-2.91435
O	5.61454	-0.42953	0.51858
O	0.53059	-5.21947	1.05992
O	0.37194	5.49041	-0.47714
O	-4.28123	4.08711	1.98278
O	-4.70862	-4.01297	-1.89531
O	8.29933	-0.29253	0.04702
O	-5.34842	-3.44672	1.84802
O	5.13329	3.76798	0.83850
O	4.88594	-1.69291	2.73001
O	-3.95497	5.52318	-0.28857
O	-3.19310	-4.70351	2.81737
O	4.45178	5.55298	-0.98070
O	4.16228	-4.30696	-1.75900
O	-2.51463	-5.60520	-1.54902
H	-1.94355	-2.93987	-2.34140
H	-2.51417	-1.33553	2.97749
H	-4.31488	-1.15414	0.13884
H	-2.03522	-4.56053	-0.29206
H	-2.68319	3.17774	2.36030
H	-1.68100	2.66704	-2.62250
H	-0.88337	4.58458	-0.13613
H	-4.54287	1.79940	-0.33918
H	1.11415	-3.27828	-2.73319
H	4.40675	-2.58277	-1.42736
H	3.63089	3.16442	1.52787
H	4.69339	2.41859	-0.16978
H	6.59488	-0.39122	0.36567
H	1.30713	-4.66139	0.75744
H	0.65372	-5.34696	2.01461
H	0.65373	5.89382	0.36066
H	1.11145	4.85163	-0.70640
H	-4.32702	4.80053	1.30042

H	-5.07593	4.16046	2.53520
H	-4.14160	-4.81723	-1.84707
H	-5.03813	-3.98864	-2.80897
H	8.63235	0.51541	0.47157
H	8.41046	-0.12341	-0.90329
H	-4.66406	-4.03765	2.27665
H	5.02206	4.56114	0.23455
H	4.30430	-1.04285	3.18424
H	4.24636	-2.24457	2.21673
H	-4.38556	5.19222	-1.12019
H	-3.81371	6.47657	-0.41148
H	-2.82197	-3.86165	3.14842
H	4.09956	6.36213	-0.57521
H	3.75136	-4.37987	-0.85918
H	-2.38646	-6.55017	-1.36149
H	5.44116	-0.84789	1.41604
H	4.74444	-1.28160	-0.54196
H	2.66275	-3.53695	-2.48058
H	4.77369	-5.04950	-1.88184
H	6.01055	3.82019	1.24854
H	3.65761	4.96261	-1.09099
H	-2.73501	-4.76443	1.95432
H	-5.79408	-2.99638	2.58516
H	-1.88967	-5.37337	-2.28259
H	4.68012	0.85075	-0.04721
H	2.84163	2.06159	2.37016
H	2.86358	0.01029	-2.25222
H	2.20334	-0.00713	1.74615
H	-0.23678	-1.28717	-2.10389
H	0.63386	-2.61113	1.79923
H	-0.37231	0.14566	1.71764
H	-2.75240	-0.05979	-1.67024
H	-0.03569	0.95634	-2.03328
H	0.36186	2.85963	1.68430
H	-2.40581	1.68930	2.81587
H	-4.18559	2.74889	0.94180
H	-3.19489	2.95188	-2.30271
H	-1.17352	-2.12401	3.05479
H	-4.43097	-2.43535	1.14874
H	-0.80588	-4.41501	0.72893
H	-3.43659	-2.96113	-1.75609
H	-2.51531	4.60606	-0.19532
O	-5.78318	1.58930	-1.37031
H	-5.66559	2.37514	-1.95719

H	-5.63877	0.82350	-1.95041

109
Hf4_4_2_term_perox_conf1_ion1_diconf7.log Energy: -3143079.3450852

Hf	0.62253	2.48916	-0.04344
O	1.95093	1.14343	-1.22131
O	1.54152	0.91695	1.11280
O	0.62027	3.74491	1.57425
O	0.31860	3.21142	-2.24338
O	0.03244	4.38246	0.35083
O	2.65635	3.54333	-0.21128
Hf	-2.46328	0.57472	0.00643
O	-1.21868	1.93326	1.03876
O	-0.74955	1.08186	-1.15217
O	-3.32457	1.32389	-1.98582
O	-3.24600	0.17305	2.21761
O	-4.45719	-0.41657	-0.25429
O	-3.83217	2.28058	0.47886
Hf	2.44737	-0.57624	-0.10470
O	1.22547	-1.89743	0.97679
O	0.78868	-1.32386	-1.30365
O	3.37880	-0.94024	-2.29955
O	3.49203	-0.81687	1.90737
O	4.45732	0.51082	-0.21119
O	3.64766	-2.44387	-0.31136
Hf	-0.58423	-2.47486	-0.07320
O	-2.15008	-1.28753	-0.95866
O	-1.10892	-0.72546	1.07506
O	-0.98803	-3.58922	1.59237
O	-1.13132	-3.52916	-2.18950
O	0.96458	-4.19008	-0.53867
O	-1.88464	-3.99843	0.47053
Cl	-2.47136	4.21593	-2.86087
Cl	1.69717	-3.25431	-3.61999
Cl	2.53234	1.16521	4.05622
Cl	-5.80973	-1.45488	2.80054
O	3.74060	-4.30542	1.61168
O	4.47084	2.47309	-2.05625
O	-4.47404	-3.04548	0.26210
O	-5.91614	2.16288	-1.16164
O	2.40913	5.82145	2.25061
O	1.37922	-3.93884	2.83418
O	1.42376	6.66365	-0.28234
O	-0.98754	-5.96557	-1.02476

O	6.17699	-1.56713	-0.14800
O	-7.01566	0.19262	0.43635
O	2.44554	2.02714	-3.80161
O	-3.84678	-2.69476	-2.56465
O	5.58634	-2.46532	2.32253
O	4.28972	2.68755	1.75091
H	-0.37430	3.91746	-2.36525
H	3.18101	3.41033	0.63059
H	-4.30021	1.44870	-1.94613
H	-2.52835	-0.41293	2.53024
H	-4.42477	-1.41138	-0.11192
H	-3.96295	2.56002	1.43315
H	3.03801	-1.75987	-2.74146
H	3.27013	-0.24382	2.68752
H	4.54987	1.13417	-0.98624
H	4.61383	-2.30850	-0.49702
H	-1.17130	-4.50622	-2.01548
H	0.50487	-5.05387	-0.68626
H	2.87993	-4.31447	2.11299
H	5.27195	2.96719	-2.29576
H	3.92585	2.37767	-2.87530
H	-3.56592	-3.36790	0.50073
H	-4.95826	-2.92318	1.10713
H	-6.56028	1.62804	-0.64662
H	-6.38123	2.95986	-1.46376
H	1.83020	5.03725	2.13855
H	2.24890	6.28884	1.40480
H	1.22142	-4.05217	3.78501
H	0.52944	-4.15438	2.37545
H	0.95297	5.80904	-0.10621
H	-1.48718	-5.54140	-0.27835
H	6.30601	-1.91562	0.76815
H	6.99630	-1.71825	-0.64594
H	-6.86036	-0.18884	1.33727
H	-7.55551	-0.47125	-0.02557
H	1.79933	2.73995	-3.61952
H	-3.05864	-3.25295	-2.71206
H	6.03075	-2.45989	3.18592
H	4.48910	1.88449	1.22885
H	3.89211	-5.21109	1.29521
H	3.57032	-3.17836	0.36662
H	4.29470	-1.36251	2.12874
H	5.08116	-3.31406	2.25317
H	-1.27177	-6.88920	-1.10779

H	-4.28700	-3.08316	-1.78324
H	2.40882	1.86087	-4.75803
H	0.76875	7.34107	-0.04915
H	3.77950	2.34935	2.51887
H	1.44689	-4.00204	-1.37629
H	-0.41511	-3.41905	-2.86195
H	3.31770	-0.23811	-2.97031
H	5.25102	-0.09074	-0.19168
H	1.45457	-2.30430	1.83656
H	0.95159	-1.57740	-2.23484
H	1.65316	0.98952	2.09175
H	1.93714	1.15699	-2.19546
H	-0.29495	0.27967	-1.48593
H	-1.44006	2.58401	1.72195
H	-0.35127	-0.29231	1.50503
H	-2.77561	-1.65667	-1.63412
H	-2.96186	2.20112	-2.29823
H	-4.67869	2.39967	-0.03132
H	-4.09629	-0.34289	2.34725
H	-0.20591	2.41470	-2.48745
H	3.25465	3.19927	-0.91713
H	-5.36887	-0.12579	0.01184
O	-4.04116	2.70471	3.08502
H	-3.65507	1.82007	3.24615
H	-3.43990	3.33966	3.50758

109
Hf4_4_2_term_perox_conf1_ion1_diconf9.log Energy: -3143090.1302850

Hf	-0.07130	-2.41391	0.51309
O	1.58935	-1.28149	1.35344
O	1.18068	-1.35407	-0.93280
O	-0.03153	-3.90830	-1.21174
O	0.07638	-3.27536	2.44482
O	-2.14761	-3.67509	0.63876
O	0.64175	-4.12872	1.35988
Hf	-2.52099	0.06302	-0.06350
O	-1.49791	-1.59006	-0.89122
O	-1.28498	-0.88341	1.36670
O	-3.68149	0.38037	1.92230
O	-3.35237	-0.24269	-2.34021
O	-4.16402	1.50866	-0.56472
O	-3.97812	-1.65843	0.03793
Hf	2.48891	0.01516	-0.10100
O	1.59841	1.52601	-1.28654

O	1.06553	1.23558	1.00731
O	3.55656	0.62335	1.97258
O	3.22744	-0.35082	-2.34364
O	4.06497	-1.56948	0.09759
O	4.43788	1.06682	-0.44396
Hf	-0.01444	2.58250	-0.25580
O	-1.76274	1.86111	0.76591
O	-1.12418	1.04930	-1.32681
O	-0.19143	3.70963	-1.97022
O	-0.22918	3.84489	1.83174
O	1.82270	3.95476	-0.00213
O	-0.93083	4.35328	-0.84328
Cl	-1.73496	-0.04514	4.30100
Cl	4.10581	3.64825	2.02782
Cl	1.13916	-2.28143	-3.93063
Cl	-6.34462	-0.75929	-2.93529
O	4.59850	3.51954	-1.28871
O	3.42762	-3.82891	1.37025
O	-3.57245	4.12741	-0.36777
O	-5.99413	-0.98646	1.63727
O	1.84953	-5.73394	-1.18888
O	2.36621	3.59005	-2.93457
O	-1.98659	-4.84546	2.96952
O	0.38573	6.13863	0.57484
O	5.94235	-0.83371	1.83886
O	-6.72727	0.71417	-0.29717
O	2.36056	-2.58362	3.61637
O	-3.02774	3.72132	2.34104
O	5.92483	-0.55617	-2.07499
O	3.45784	-4.22096	-2.76091
H	0.09934	-3.53125	-2.10729
H	-2.05330	-4.30883	-0.09585
H	-4.54368	-0.08539	2.05549
H	-3.25020	0.64091	-2.73694
H	-3.98515	2.48439	-0.43535
H	-3.43661	-2.46502	0.24543
H	3.78129	1.60275	1.95511
H	2.70311	-0.96299	-2.90544
H	3.74015	-2.44293	0.49402
H	5.10562	0.56146	-0.96992
H	0.00826	4.79321	1.65466
H	1.57742	4.90189	0.13523
H	3.79960	3.70100	-1.84023
H	3.42277	-3.48369	2.28811

H	2.46926	-4.03902	1.24302
H	-2.64288	4.23219	-0.71931
H	-4.13786	4.72674	-0.88168
H	-6.52555	-0.40824	1.03104
H	-6.60491	-1.50713	2.18190
H	2.51273	-5.26665	-1.76714
H	1.55499	-6.49992	-1.70840
H	2.34276	3.71242	-3.89676
H	1.50713	3.93301	-2.58367
H	-1.15215	-4.29384	2.99214
H	-0.22225	5.80917	-0.13803
H	6.64316	-0.28863	1.44436
H	5.28523	-0.18991	2.17777
H	-6.78149	0.23178	-1.17106
H	-7.44542	1.36883	-0.29358
H	1.45034	-2.94111	3.41301
H	-2.11845	4.06141	2.43895
H	6.29583	-1.35579	-1.66698
H	3.89685	-4.71640	-3.47165
H	4.44159	3.96116	-0.43157
H	4.46379	2.02537	-0.79764
H	4.17249	-0.61996	-2.42403
H	6.58868	-0.23964	-2.70991
H	0.31910	7.10498	0.62374
H	-3.33784	4.10217	1.49007
H	2.32834	-2.21468	4.51299
H	-2.59500	-4.40605	3.58655
H	2.78827	-3.66646	-3.21888
H	2.48524	3.74649	0.71004
H	0.36428	3.53357	2.53780
H	2.93780	0.52952	2.71835
H	4.85308	-1.32138	0.66994
H	2.02257	1.95762	-2.05895
H	0.59330	0.72872	1.68823
H	0.99820	-1.45161	-1.89047
H	1.96445	-1.56780	2.21820
H	-1.29988	-0.65928	2.33166
H	-1.71561	-1.96876	-1.77978
H	-0.60842	0.49950	-1.93688
H	-2.25970	2.37619	1.45246
H	-3.15039	0.26821	2.75586
H	-4.77107	-1.63591	0.63923
H	-4.33015	-0.44365	-2.43342
H	-2.21869	-4.21680	1.49330

H	0.65087	-4.65813	-1.13611
H	-5.13786	1.33227	-0.44064
O	-2.06415	-2.47646	-3.42150
H	-2.56998	-1.64071	-3.46502
H	-1.21000	-2.28777	-3.85952

109
Hf4_4_2_term_perox_conf1_ion2_diconf5.log Energy: -3143082.2489481

Hf	-2.06347	-1.07991	0.22009
O	-0.37233	-1.95432	1.07498
O	-0.52184	-1.44779	-1.16055
O	-2.97604	-1.95681	-1.69204
O	-2.41894	-0.82225	2.61333
O	-4.18680	-0.74624	0.50045
O	-2.77964	-3.14386	0.86039
Hf	-1.26463	2.33435	-0.45420
O	-2.40355	0.62256	-1.10400
O	-1.22972	0.75654	0.91392
O	-1.56694	3.39054	1.63902
O	-2.00538	2.81293	-2.61551
O	-0.90296	4.48375	-0.81615
O	-3.50715	2.94641	-0.18966
Hf	1.38438	-2.05788	-0.31557
O	1.99761	-0.46740	-1.72759
O	1.82003	-0.28644	0.73301
O	2.05063	-2.98353	1.40045
O	1.00389	-3.37830	-2.22054
O	1.49583	-3.99912	0.46796
O	3.44245	-2.62289	-1.16979
Hf	2.19298	1.40497	-0.56754
O	0.65306	2.59689	0.40461
O	0.26803	1.54897	-1.62403
O	3.09166	2.16403	-2.21101
O	2.89531	2.07818	1.73382
O	4.27303	0.53682	-0.30801
O	3.16145	3.13374	-1.06193
Cl	0.51562	0.42702	3.54939
Cl	-4.09007	1.85472	2.84468
Cl	5.34152	0.38057	2.68012
Cl	-1.90212	-4.68400	-2.67872
O	5.73641	-2.62680	0.02437
O	-0.89789	-4.93861	1.30584
O	1.54453	5.28339	-0.79073
O	-3.31115	5.42140	0.95093

O	-5.60550	-2.39509	-2.24676
O	7.48969	-0.51636	0.37577
O	-5.69458	-1.07746	2.55941
O	6.58014	1.52817	-1.38774
O	4.58072	-2.84844	2.47430
O	-2.35637	5.45840	-2.91991
O	-3.98416	-2.96293	3.50772
O	1.89832	4.64297	1.88794
O	2.81520	-5.24050	-1.43043
O	-4.47971	-4.46517	-0.83961
H	-2.52935	-2.76877	-2.05053
H	-2.95454	0.01240	2.71742
H	-4.69645	-0.26388	-0.20806
H	-3.44756	-3.59635	0.27697
H	-2.00746	4.26691	1.52718
H	-2.63854	2.19087	-3.00735
H	0.08773	4.79401	-0.80393
H	-3.87754	2.45973	0.58854
H	0.06765	-3.67878	-2.32388
H	3.47564	-3.58907	-1.37124
H	3.73952	1.66658	2.05506
H	5.00924	1.01592	-0.76424
H	6.35316	-1.85218	0.05891
H	-0.01243	-4.56705	1.02306
H	-0.82236	-5.06206	2.26629
H	1.72669	5.32581	0.17500
H	2.10128	4.50038	-1.07074
H	-3.02770	6.21097	0.46105
H	-3.99582	5.72359	1.57111
H	-5.51650	-3.21459	-1.70185
H	-5.67224	-2.70243	-3.16638
H	7.04970	-0.17188	1.18015
H	7.34441	0.18886	-0.28865
H	-5.20525	-1.80201	3.03859
H	6.64659	1.43218	-2.35275
H	4.64047	-1.89168	2.67363
H	3.67490	-2.97195	2.09362
H	-1.94239	5.92883	-3.66299
H	-3.21264	5.89210	-2.76669
H	-3.31513	-2.26087	3.63318
H	2.54153	3.90749	1.98970
H	2.45966	-5.09078	-0.51535
H	-4.88678	-5.26833	-0.47294
H	5.43777	-2.76666	0.96183

H	4.32429	-2.44942	-0.68339
H	1.54359	-4.20458	-2.19746
H	3.21791	-6.12158	-1.46900
H	6.80220	2.45662	-1.20515
H	1.75312	5.00929	2.77434
H	-3.72976	-3.27686	2.61564
H	-5.47307	-0.24819	3.02720
H	-3.78367	-4.77286	-1.47172
H	4.59698	0.30569	0.59369
H	2.21101	1.72150	2.34481
H	2.82112	-0.73263	-2.16663
H	1.51832	-0.23003	1.66325
H	-0.60229	-1.14601	-2.07630
H	-0.16498	-2.20556	1.98687
H	-0.57271	0.77622	1.64614
H	-3.27239	0.66325	-1.54698
H	0.14106	0.96343	-2.38369
H	0.81461	3.28701	1.07943
H	-2.19019	2.86867	2.20160
H	-3.60932	3.90107	0.06073
H	-2.27232	3.72637	-2.89164
H	-1.55362	-0.58738	3.02627
H	-4.79812	-0.90576	1.30815
H	-2.02581	-3.81002	1.02051
H	-3.94168	-2.05417	-1.90003
H	-1.36387	4.99762	-1.52175
O	-5.22990	0.31093	-1.69123
H	-5.94690	0.96246	-1.62588
H	-5.62937	-0.52322	-2.02350

109
Hf4_4_2_term_perox_conf1_ion2_diconf7.log Energy: -3143078.3381898

Hf	-2.41090	-0.15621	-0.09549
O	-1.25680	-1.58960	1.12979
O	-1.09580	-1.46014	-1.22878
O	-3.83220	0.26218	-1.61710
O	-3.21503	0.23254	2.12537
O	-4.09413	0.94419	-0.31008
O	-3.74323	-1.93302	-0.01205
Hf	-0.09056	2.57342	-0.38652
O	-1.39698	1.25796	-1.44995
O	-1.02290	1.21021	0.88636
O	-0.37238	3.68155	1.63956
O	-0.29864	3.36135	-2.55117

O	1.17017	4.48796	-0.59320
O	-2.00435	3.81392	-0.50481
Hf	0.37017	-2.32781	-0.01047
O	1.80622	-1.32863	-1.20568
O	1.38278	-0.80902	1.07514
O	0.69907	-3.02754	2.47903
O	0.30992	-3.62791	-1.89188
O	-0.54119	-4.33500	0.39841
O	2.11647	-3.72524	0.29027
Hf	2.68649	0.37092	-0.13437
O	1.65179	2.05660	0.72421
O	1.20822	1.26983	-1.41865
O	3.95279	0.57773	-1.74189
O	3.72490	0.69129	2.04468
O	4.15910	-1.39576	0.31360
O	4.38382	1.45579	-0.61320
Cl	-0.42544	-0.20684	3.78501
Cl	-3.41164	3.38153	2.31397
Cl	3.65325	-2.20122	3.33513
Cl	-1.27024	-2.28175	-4.21759
O	4.07363	-4.14266	-1.43887
O	-3.95600	-3.57223	2.04155
O	3.72553	4.13313	-0.13223
O	0.29077	6.29464	1.23760
O	-6.46287	-0.65031	-2.12735
O	4.01556	-1.86452	-2.81013
O	-6.64296	0.34370	0.52042
O	6.16383	0.31391	0.92487
O	-1.45702	-4.71724	2.82573
O	1.24224	5.38933	-3.26772
O	-5.02780	-1.50271	3.47941
O	3.23177	3.36559	2.53632
O	2.04797	-5.46825	-2.68843
O	-3.71993	-3.32858	-2.33465
H	-3.41669	1.21048	2.16189
H	-3.75633	-2.45166	-0.86690
H	-0.21678	4.65728	1.67076
H	-0.26095	2.64949	-3.21043
H	2.16696	4.31794	-0.41336
H	-2.57167	3.55087	-1.28151
H	1.67913	-3.01226	2.63161
H	-0.11814	-3.26373	-2.70865
H	-0.94271	-4.75845	-0.37874
H	1.84095	-4.62650	0.53279

H	4.70483	0.65751	1.87945
H	5.07383	-1.04845	0.45222
H	4.23324	-3.30272	-1.95157
H	-3.10960	-3.85517	2.44159
H	-4.35089	-2.91475	2.66890
H	3.72777	4.00430	0.84290
H	3.96957	3.24123	-0.48398
H	0.92402	6.76360	1.80683
H	-0.38738	6.94625	0.99158
H	-5.51491	-0.40343	-2.07701
H	-6.76811	-0.38767	-1.23424
H	4.19600	-1.79417	-3.76108
H	4.32214	-1.01917	-2.39317
H	-5.70771	0.55434	0.27064
H	5.81819	0.87991	0.18376
H	-1.42503	-5.62437	3.17288
H	-0.62066	-4.27960	3.09899
H	1.50497	5.43293	-2.32689
H	2.03544	5.07142	-3.73132
H	-4.51619	-0.81119	3.00768
H	3.54692	2.45379	2.71575
H	2.11759	-5.40140	-3.65496
H	-3.50292	-4.25976	-2.16624
H	4.92665	-4.42397	-1.06982
H	2.91505	-3.80612	-0.31960
H	0.99096	-4.31283	-2.18246
H	2.91847	-5.15507	-2.34592
H	7.10928	0.49593	1.04184
H	3.08990	3.79245	3.39592
H	-4.69461	-1.46896	4.39081
H	-7.10235	1.19582	0.44989
H	-2.99232	-3.00545	-2.91370
H	3.93158	-1.84349	1.16894
H	3.55590	-0.09541	2.62783
H	0.39155	-2.29263	3.05630
H	-1.03086	-4.57672	1.24040
H	2.32086	-1.70447	-1.94972
H	1.02311	-0.47364	1.91883
H	-1.07235	-1.46135	-2.21328
H	-1.09356	-1.33130	2.05819
H	-0.67930	1.05940	1.78839
H	-2.04923	1.67111	-2.04517
H	0.77899	0.64368	-2.02438
H	1.95845	2.57675	1.49867

H	-1.27433	3.53335	2.02752
H	-2.58007	3.72061	0.29886
H	0.27974	4.10991	-2.89592
H	-2.49654	0.11745	2.79241
H	-3.70015	-2.59210	0.75243
H	0.91276	5.25767	-0.02269
O	-3.58636	2.78434	-2.50689
H	-3.44996	2.85255	-3.46524
H	-3.85755	1.84276	-2.31793

109
Hf4_4_2_term_perox_conf1_ion2_diconf9.log Energy: -3143083.6229428

Hf	-0.14640	-2.40971	0.34518
O	1.35983	-1.21456	1.30038
O	1.12603	-1.25412	-0.99701
O	0.49515	-3.89921	-1.27347
O	-0.33568	-3.11266	2.30977
O	-2.09192	-3.76909	0.18446
O	0.51996	-3.99107	1.46013
Hf	-2.63170	-0.04358	-0.61069
O	-1.44691	-1.70190	-1.31851
O	-1.48312	-0.84690	0.96312
O	-3.87125	0.34838	1.30736
O	-3.40311	-0.59741	-2.76277
O	-4.26028	1.31204	-1.24627
O	-3.98363	-1.86778	-0.28778
Hf	2.36851	0.10731	-0.02082
O	1.60355	1.47839	-1.46034
O	0.89729	1.38184	0.77971
O	3.08050	0.88758	2.24434
O	3.45759	-0.50770	-1.99610
O	3.97774	-1.35852	0.62035
O	4.25207	1.29477	-0.13516
Hf	-0.14004	2.56281	-0.67659
O	-2.00784	1.82158	0.20447
O	-1.19229	0.98371	-1.77096
O	-0.08170	3.58118	-2.44763
O	-0.62648	3.68878	1.45516
O	1.60518	4.02700	-0.25201
O	-0.87700	4.29862	-1.39017
Cl	-0.31398	1.08625	3.58644
Cl	-4.85631	-2.26854	2.69255
Cl	3.57401	4.01317	2.15021
Cl	2.53374	-3.10246	-3.51200

O	4.48401	3.66021	-1.17461
O	3.14502	-3.40237	2.20102
O	-4.90850	3.61187	-0.11652
O	-6.18465	1.67735	1.31500
O	1.87111	-6.04047	-0.62342
O	2.52236	3.52006	-3.07684
O	-2.56158	-4.62533	2.57582
O	0.97852	5.80181	1.76144
O	5.57048	-0.34075	2.49959
O	-5.99130	0.16291	-2.96355
O	1.36122	-1.82857	3.95065
O	-3.15135	4.91411	1.38750
O	6.12367	-0.24186	-1.38925
O	4.15011	-4.75732	-1.32607
H	1.11661	-3.52425	-1.95477
H	-2.15743	-4.31647	-0.63434
H	-4.75336	0.83381	1.27226
H	-3.18497	-1.48568	-3.08794
H	-4.40280	2.22350	-0.84924
H	-3.35592	-2.63564	-0.18110
H	3.27219	1.86156	2.16801
H	3.12929	-1.34440	-2.41449
H	3.60342	-2.14681	1.12428
H	5.04678	0.81599	-0.47980
H	-0.05910	4.48867	1.66263
H	1.26449	4.92592	-0.07644
H	3.76990	3.76080	-1.85451
H	2.93477	-2.90396	3.01366
H	2.24710	-3.69088	1.89192
H	-4.22673	4.10674	0.43279
H	-5.31557	4.26259	-0.71125
H	-5.91308	2.51789	0.87359
H	-6.35083	1.91846	2.24107
H	2.77302	-5.67485	-0.84047
H	1.70376	-6.71247	-1.30460
H	2.61241	3.65849	-4.03255
H	1.59799	3.80181	-2.82817
H	-1.72699	-4.10924	2.73325
H	0.68019	6.55276	2.30015
H	6.24249	0.27955	2.17211
H	4.79876	0.22225	2.72426
H	-6.32487	0.61682	-3.75574
H	-6.70429	-0.42728	-2.66677
H	0.65006	-2.39450	3.54205

H	-2.28025	4.45537	1.41759
H	6.61465	-0.92682	-0.90586
H	4.82129	-5.32597	-1.73762
H	4.22357	4.22543	-0.42500
H	4.29006	2.22744	-0.55334
H	4.43552	-0.59758	-1.92091
H	6.76075	0.16782	-1.99804
H	1.80846	5.46959	2.17287
H	-3.47594	4.89803	2.30267
H	0.89182	-1.01657	4.22744
H	-3.28127	-3.98130	2.76270
H	3.76395	-4.24250	-2.07333
H	2.19155	3.83225	0.52185
H	-0.51645	3.07280	2.21556
H	2.33896	0.84306	2.88107
H	4.68665	-0.99943	1.23357
H	2.11133	1.87818	-2.19618
H	0.50586	1.15813	1.65392
H	0.79080	-1.08981	-1.89051
H	1.51038	-1.33315	2.26850
H	-1.30611	-0.35261	1.78822
H	-1.76596	-2.41604	-1.90404
H	-0.78713	0.56383	-2.54314
H	-2.30680	1.99572	1.10921
H	-4.01736	-0.42190	1.91126
H	-4.49885	-1.89750	0.55856
H	-4.35951	-0.45059	-2.97886
H	-2.32948	-4.29715	1.02041
H	0.94589	-4.75463	-0.95506
H	-5.05424	1.05627	-1.77466
O	-1.96487	-4.22766	-2.43493
H	-2.30954	-4.77401	-3.15882
H	-0.99694	-4.37851	-2.38705

109
Hf4_4_2_term_perox_conf1_ion3_diconf5.log Energy: -3143080.8519677

Hf	1.58380	1.80718	-0.01895
O	-0.29517	2.39448	0.69767
O	0.08717	1.40903	-1.43548
O	2.57628	2.18962	-2.14109
O	1.81129	2.21879	2.32688
O	3.68637	2.46852	0.48222
O	1.47718	3.98426	-0.41800
Hf	1.73187	-1.75456	0.02071

O	2.63987	0.04849	-0.72451
O	1.12597	0.01090	0.99673
O	2.16821	-2.12739	2.21566
O	2.31342	-2.39612	-2.16491
O	1.75562	-3.96061	0.10166
O	3.91101	-2.22958	0.12998
Hf	-1.97099	1.85433	-0.60833
O	-2.27144	-0.04961	-1.59527
O	-2.07773	0.23483	0.75428
O	-2.80587	2.97790	0.91201
O	-1.95929	2.66294	-2.78077
O	-2.47277	3.85894	-0.24016
O	-4.15279	1.85266	-1.25822
Hf	-1.88755	-1.66649	-0.24684
O	-0.16821	-2.31995	0.87042
O	0.10985	-1.34360	-1.29510
O	-2.05731	-2.83649	-1.91865
O	-2.50017	-2.16158	2.07898
O	-4.18186	-1.70978	-0.14580
O	-2.35498	-3.63422	-0.69358
Cl	-0.69354	0.26708	3.57165
Cl	3.74960	0.22570	3.59637
Cl	-5.34839	-1.11454	2.65058
Cl	4.87294	-3.76149	-3.22179
O	-5.33440	-0.28014	-2.31984
O	-0.47860	5.34871	0.69760
O	-0.53172	-5.30888	0.10577
O	3.60632	-4.36404	2.66774
O	4.90977	3.35225	-1.75219
O	-3.29882	-1.39147	-3.79825
O	3.84460	4.90142	1.64949
O	-5.03123	-4.02803	0.76837
O	-5.29406	2.26753	1.97788
O	4.22021	-4.84419	-0.40019
O	1.46902	5.04089	2.82831
O	-2.74749	-5.00690	1.99943
O	-4.00342	4.34342	-2.32362
O	3.65109	5.54341	-0.91597
H	1.93403	2.59427	-2.74719
H	2.57398	1.68059	2.71003
H	4.33330	2.59781	-0.25839
H	2.20894	4.58865	-0.71435
H	2.71157	-2.94833	2.39519
H	2.08761	-1.78969	-2.88991

H	0.90257	-4.50197	0.10929
H	4.57556	-1.74204	-0.44890
H	-1.07789	2.95695	-3.06633
H	-4.47269	2.68102	-1.67854
H	-3.42184	-1.87057	2.33461
H	-4.47858	-2.66428	0.05299
H	-4.76545	-0.63045	-3.04283
H	-0.57996	6.25332	0.35797
H	-1.28493	4.83205	0.37282
H	-1.17317	-4.67128	-0.35057
H	-0.51201	-6.11106	-0.44279
H	2.97815	-5.10464	2.63342
H	3.94757	-4.37541	3.57779
H	4.70596	4.31128	-1.60917
H	5.75477	3.27980	-2.22363
H	-3.08512	-1.63834	-4.71149
H	-3.02838	-2.15087	-3.22186
H	2.97121	5.09563	2.11063
H	-4.21922	-4.48711	1.11155
H	-5.20985	1.30578	2.10724
H	-4.47447	2.52487	1.50241
H	4.58049	-4.77093	-1.31870
H	4.75247	-5.49197	0.08869
H	1.48546	4.06392	2.88203
H	-2.52198	-4.08316	2.23033
H	-3.61674	4.49950	-1.42361
H	3.86187	5.59029	0.05392
H	-5.08970	-0.86067	-1.56689
H	-4.55905	1.06604	-1.73922
H	-2.59437	3.41849	-2.89185
H	-4.43799	5.16036	-2.61412
H	-5.44372	-3.63601	1.56029
H	-2.01159	-5.28179	1.41299
H	0.74531	5.23784	2.19479
H	4.55236	5.09636	2.28539
H	3.57479	6.45335	-1.24623
H	-4.57229	-1.20181	0.61052
H	-1.91995	-1.62093	2.66343
H	-2.48409	-0.23131	-2.53219
H	-1.79800	0.39627	1.68136
H	0.08650	0.46837	-1.73104
H	-0.61501	2.83033	1.50214
H	0.49663	-0.03424	1.75145
H	3.03524	0.14002	-1.60517

H	-0.00287	-1.91000	-2.07779
H	-0.14951	-2.65013	1.78129
H	2.64878	-1.36856	2.64925
H	4.18496	-3.18542	0.13021
H	3.15083	-2.85870	-2.45466
H	1.03045	1.79637	2.75688
H	3.76746	3.29712	1.04115
H	0.72504	4.53796	-0.03952
H	3.44540	2.67020	-2.23244
H	2.53103	-4.51611	-0.16546
O	5.79551	-1.29344	-1.46739
H	5.67561	-1.97699	-2.16854
H	5.66882	-0.44185	-1.91573

109
Hf4_4_2_term_perox_conf1_ion3_diconf7.log Energy: -3143074.3412055

Hf	-2.53211	0.13162	-0.08012
O	-1.67250	-1.73520	0.84328
O	-1.14015	-0.85825	-1.42722
O	-3.74479	0.88806	-1.58539
O	-3.35419	0.16478	2.10402
O	-4.13150	1.35093	-0.21137
O	-3.84389	-1.68908	-0.58662
Hf	0.19987	2.49821	0.08975
O	-1.37990	1.75419	-1.11753
O	-0.96984	1.04572	1.09214
O	-0.09640	3.23745	2.25875
O	0.45076	3.41638	-2.12640
O	1.69785	4.08183	0.27168
O	-1.13420	4.28841	0.03442
Hf	-0.04045	-2.41011	-0.50778
O	1.75071	-1.62537	-1.16620
O	1.00581	-1.36095	1.04207
O	-0.07633	-3.89786	1.35396
O	-0.00937	-2.62392	-2.95628
O	-1.86074	-3.58403	-1.16682
O	0.76518	-4.39497	-1.06141
Hf	2.62410	-0.18315	0.25228
O	1.75263	1.54611	1.22556
O	1.35878	1.08631	-0.98989
O	4.00295	0.10923	-1.23819
O	3.30317	-0.13047	2.51201
O	3.85020	-2.08696	0.60817
O	4.48762	0.67987	0.05538

Cl	-0.69237	-1.02780	3.68470
Cl	-3.04814	2.95662	3.29314
Cl	2.81402	-4.77741	1.85163
Cl	3.21182	4.17781	-3.19607
O	3.31789	-4.69712	-1.34589
O	-3.89710	-3.28768	1.58335
O	4.17240	3.40264	-0.20318
O	-0.37610	5.94925	2.06097
O	-6.22901	0.76961	-2.74332
O	4.00241	-2.27407	-2.52505
O	-6.87302	1.48806	-0.16677
O	5.70723	-1.27232	2.37503
O	-2.33186	-5.42371	0.69959
O	1.77222	6.24251	-1.27808
O	-5.85040	-1.34862	2.33053
O	7.08284	0.22852	0.70810
O	-0.41475	-5.30499	-3.32637
O	-5.90302	-1.80217	-2.17573
H	-3.39296	1.11983	2.42612
H	-4.64414	-1.64573	-1.22095
H	0.06130	4.20263	2.38371
H	0.04419	2.79096	-2.75244
H	2.66732	3.76391	0.20500
H	-1.36490	4.73730	-0.83783
H	0.84254	-4.29601	1.46163
H	-0.75103	-2.06210	-3.23992
H	-2.63314	-2.96210	-1.13939
H	0.32792	-4.88021	-1.80615
H	4.23097	-0.47721	2.64119
H	4.64482	-1.94467	1.18899
H	3.70108	-3.85717	-1.69549
H	-3.66782	-4.21941	1.38140
H	-3.02372	-2.83846	1.61294
H	4.30221	2.42319	-0.10606
H	4.10033	3.55773	-1.17107
H	0.28998	6.63588	1.89060
H	-1.04276	6.35954	2.63703
H	-5.28154	0.89623	-2.48963
H	-6.68639	1.07252	-1.92008
H	4.32671	-2.14592	-3.43046
H	4.30357	-1.48944	-1.99977
H	-5.88856	1.43599	-0.07666
H	6.37943	-0.72706	1.86283
H	-2.35111	-6.37771	0.51712

H	-1.47909	-5.23396	1.14764
H	2.30435	5.82396	-1.99542
H	2.36779	6.89592	-0.87453
H	-5.12554	-0.69864	2.36400
H	6.20234	0.46325	0.31511
H	-1.32198	-5.64972	-3.27946
H	-5.58743	-2.23000	-2.98865
H	3.53956	-4.73060	-0.39203
H	1.77934	-4.49770	-1.19381
H	-0.22618	-3.53119	-3.27934
H	0.06210	-5.87282	-3.95449
H	6.17908	-1.80552	3.03382
H	7.39384	1.04904	1.12466
H	-5.36349	-2.18630	2.22115
H	-7.06651	2.43800	-0.11512
H	-6.12494	-0.85952	-2.44949
H	3.37428	-2.85784	1.00934
H	2.74423	-0.61906	3.14096
H	-0.23835	-3.43210	2.19821
H	-2.10024	-4.35999	-0.57972
H	2.26743	-1.90635	-1.95312
H	0.60812	-1.19314	1.92248
H	-0.67876	-0.16952	-1.93510
H	-1.34755	-1.54435	1.75051
H	-0.69704	0.69051	1.95901
H	-2.06102	2.21097	-1.63974
H	1.45289	0.99312	-1.94817
H	1.84183	1.70525	2.17715
H	-1.02487	3.08152	2.59295
H	-0.96220	5.00608	0.69498
H	1.37475	3.60241	-2.47621
H	-2.74555	-0.25793	2.75346
H	-4.09094	-2.28972	0.16978
H	1.65187	4.93133	-0.26723
O	-1.49124	5.48897	-2.28689
H	-0.71037	5.01415	-2.63369
H	-2.24133	5.14842	-2.80291

109
Hf4_4_2_term_perox_conf1_ion3_diconf9.log Energy: -3143095.2661488

Hf	1.29059	2.19312	-0.06141
O	-0.66395	2.16888	0.87705
O	-0.43040	1.86055	-1.40897
O	1.78036	3.36457	-1.95074

O	1.66043	3.15504	1.78372
O	3.65386	2.25937	-0.06580
O	1.51864	4.12334	0.66245
Hf	2.03780	-1.29839	-0.28150
O	1.92415	0.54312	-1.33087
O	1.61973	0.37281	1.01436
O	3.02346	-2.06037	1.55962
O	3.01485	-1.65643	-2.37144
O	2.41927	-3.49199	-0.67300
O	4.15785	-0.42202	-0.19046
Hf	-2.18678	1.43069	-0.35838
O	-2.13618	-0.37911	-1.48422
O	-1.87090	-0.25987	0.85860
O	-3.37811	1.89999	1.70489
O	-2.78375	1.97734	-2.59106
O	-2.69643	3.60227	-0.42133
O	-4.40537	1.02246	-0.53199
Hf	-1.47750	-2.06229	-0.28542
O	0.39539	-2.09849	0.80945
O	0.34607	-1.78080	-1.48235
O	-2.01428	-3.20833	-1.90574
O	-1.83056	-3.00061	1.89493
O	-3.77631	-2.08655	0.08802
O	-1.80767	-4.03525	-0.67843
Cl	-0.23692	-0.82268	3.63281
Cl	5.20825	-0.26700	2.77859
Cl	-4.96347	-0.60569	2.69658
Cl	5.93009	-2.57269	-2.72787
O	-5.57252	-0.70597	-2.16474
O	-1.05588	5.21290	0.90705
O	0.48837	-5.34718	-0.41426
O	1.82411	-3.49438	3.37749
O	4.15815	4.46756	-1.51816
O	-4.50816	-3.02852	-2.91652
O	4.30315	2.81378	2.39639
O	-4.40100	-3.66847	2.22349
O	-4.94805	4.10848	0.88438
O	4.89642	-4.41235	-0.39610
O	-0.58574	3.60942	3.15644
O	-0.01597	-5.17888	2.32507
O	-5.44236	1.90056	-2.86253
O	3.46701	6.02297	0.49413
H	1.83606	2.82522	-2.77893
H	4.02691	2.95388	-0.67003

H	2.54812	-2.68359	2.20969
H	2.70920	-2.55842	-2.58310
H	1.70456	-4.17626	-0.54087
H	4.04672	0.55250	-0.35163
H	-3.85970	1.08006	2.01623
H	-2.44173	2.87444	-2.74894
H	-2.03025	4.20119	0.06160
H	-4.94656	1.70916	-0.97807
H	-2.75884	-3.30941	2.10434
H	-4.12143	-2.94882	0.39709
H	-5.13294	-1.56518	-2.45750
H	-1.16504	4.91985	1.83606
H	-0.13179	4.91605	0.71509
H	-0.38357	-4.92112	-0.67160
H	0.59637	-6.13650	-0.96931
H	1.19138	-4.16734	2.99400
H	1.24822	-2.81504	3.77976
H	4.03631	5.18342	-0.82257
H	4.81240	4.77132	-2.16653
H	-5.06745	-3.69570	-2.48653
H	-3.61574	-3.13052	-2.47896
H	3.33237	2.98235	2.47663
H	-4.66105	-4.41491	2.78766
H	-5.83331	3.98008	0.50692
H	-4.76750	3.31310	1.42474
H	5.31449	-3.87235	-1.11503
H	4.94367	-5.32662	-0.72130
H	0.36754	3.53323	2.86772
H	-0.71056	-4.49896	2.19338
H	-5.96049	2.38738	-3.52260
H	3.01111	6.81736	0.17054
H	-6.40559	-0.97425	-1.74311
H	-4.68614	0.18904	-1.02518
H	-3.75543	2.00629	-2.82685
H	-5.66497	0.94281	-2.95067
H	-4.76677	-2.85237	2.63818
H	0.25242	-5.39938	1.40443
H	-0.61789	3.35078	4.09135
H	4.45902	1.90286	2.73315
H	2.73745	5.37829	0.68914
H	-4.05119	-1.45740	0.80104
H	-1.56211	-2.39031	2.62167
H	-2.84312	2.20214	2.46126
H	-3.59772	3.86990	-0.07078

H	-2.33413	-0.39763	-2.43205
H	-1.45482	-0.15317	1.73837
H	-0.27542	1.35666	-2.22190
H	-0.74798	2.50798	1.79672
H	1.21786	0.22929	1.89254
H	2.10899	0.59734	-2.28925
H	0.26021	-1.52681	-2.41307
H	0.35814	-1.89958	1.76694
H	3.62975	-1.48484	2.09456
H	4.64130	-0.46542	0.67368
H	4.01224	-1.74857	-2.39481
H	4.01693	2.48238	0.85874
H	2.61478	3.91045	-1.91736
H	3.31958	-3.89902	-0.48068
O	2.13807	1.52900	-3.95145
H	3.00695	1.59458	-4.38227
H	1.50372	1.36905	-4.67015

109
Hf4_4_2_term_perox_conf1_ion4_diconf5.log Energy: -3143084.6718876

Hf	2.22849	-1.22118	0.20582
O	2.18977	0.72048	1.03151
O	1.44764	0.16039	-1.12787
O	2.99031	-1.87160	-1.84315
O	2.82687	-1.55864	2.54091
O	3.10186	-3.25373	0.60308
O	4.36406	-0.67005	0.27920
Hf	-1.19808	-2.22718	0.23829
O	0.76724	-2.60059	-0.65048
O	0.40768	-1.38170	1.27924
O	-1.55861	-2.64871	2.51609
O	-1.69313	-3.40761	-1.68923
O	-3.37298	-2.87702	0.35389
O	-0.90929	-4.37365	0.76103
Hf	1.28232	2.20896	-0.31659
O	-0.43359	1.89480	-1.69395
O	-0.52387	1.94409	0.75441
O	1.82267	3.33891	1.32941
O	2.45865	2.48453	-2.26629
O	2.91167	3.34805	0.32260
O	0.67309	4.24789	-1.21819
Hf	-2.12907	1.20929	-0.52407
O	-2.22622	-0.49458	0.85632
O	-1.21165	-0.71253	-1.24174

O	-3.05246	0.96533	-2.32786
O	-3.33975	1.80453	1.36400
O	-2.74574	3.39526	-0.86119
O	-4.04043	0.96170	-1.20361
Cl	0.40019	-0.89379	4.33853
Cl	-1.58304	2.90344	3.68712
Cl	4.25231	0.34637	-3.69525
Cl	-4.35577	-3.32392	-3.21075
O	-1.27455	5.39744	0.11839
O	5.02770	1.79678	0.93184
O	-5.14363	-1.32125	-0.78476
O	-4.13474	-2.85868	3.08836
O	4.96231	-3.59857	-2.25701
O	-1.97953	7.94163	-0.58950
O	5.56103	-3.62232	1.24637
O	-5.35920	3.12149	0.21695
O	0.14252	5.24434	2.34628
O	-4.17179	-5.21464	-0.77031
O	5.62170	-1.68862	3.13292
O	-6.92424	0.86894	-0.04603
O	3.21499	5.04690	-1.63703
O	6.10990	-1.18098	-1.72233
H	3.22362	-1.12555	-2.45264
H	2.79653	-2.53294	2.59789
H	2.69908	-3.99121	0.11581
H	5.02935	-0.91428	-0.42209
H	-2.49907	-2.67654	2.86574
H	-1.00335	-3.58352	-2.34988
H	-4.04772	-2.21546	-0.04260
H	-1.18330	-5.18571	0.20829
H	3.01637	1.75771	-2.64559
H	1.44613	4.83587	-1.38846
H	-4.14208	2.34381	1.12202
H	-3.70510	3.46930	-0.65174
H	-1.52642	6.32639	-0.12515
H	4.23941	2.38978	0.76098
H	5.23792	1.90830	1.87322
H	-4.63205	-0.47093	-1.01825
H	-5.21114	-1.81794	-1.63018
H	-4.24982	-2.89088	2.11668
H	-4.55883	-2.02942	3.36555
H	5.63999	-2.89540	-2.12154
H	4.99209	-3.79593	-3.20800
H	-2.68430	8.23161	0.01306

H	-2.41614	7.88813	-1.45581
H	5.68302	-2.93553	1.96228
H	-5.91469	2.32243	0.00042
H	-0.36698	4.59016	2.87688
H	0.86515	4.69656	1.94668
H	-4.40187	-4.81794	-1.64944
H	-4.99160	-5.60018	-0.41776
H	4.68389	-1.42139	3.03014
H	-7.17031	0.68728	0.87537
H	3.31996	4.68979	-0.71709
H	7.02199	-0.87341	-1.58913
H	-0.83346	5.41513	1.02361
H	-0.03734	4.77739	-0.73983
H	2.97155	3.32434	-2.30933
H	3.79641	5.81700	-1.73281
H	-5.92677	3.71882	0.73016
H	-6.42850	0.06846	-0.32537
H	6.12654	-0.95071	2.75446
H	5.66496	-4.47945	1.69218
H	5.71659	-0.60714	-2.42944
H	-2.26795	4.13532	-0.38857
H	-2.85881	2.26776	2.09810
H	-0.59639	2.66397	-2.26019
H	-0.60030	2.08081	1.72111
H	0.62949	-0.08452	-1.60670
H	2.57586	1.06349	1.85045
H	0.28090	-0.86056	2.10089
H	0.95945	-2.73503	-1.59179
H	-1.50496	-0.86747	-2.15371
H	-2.58087	-0.32122	1.74064
H	-0.99726	-2.16833	3.17332
H	-1.14263	-4.51949	1.69512
H	-2.55112	-3.30784	-2.20046
H	2.13616	-1.25547	3.19822
H	4.09452	-3.45661	0.80100
H	4.58351	0.27631	0.57280
H	3.68242	-2.59004	-1.98692
H	-3.63758	-3.77725	0.01028
O	-1.73240	-6.44415	-0.58691
H	-2.66718	-6.16091	-0.73991
H	-1.32340	-6.43849	-1.46799

109
Hf4_4_2_term_perox_conf1_ion4_diconf7.log Energy: -3143089.1332227

Hf	-0.70447	2.52614	0.06502
O	-1.82648	1.01497	1.21768
O	-1.62292	1.04891	-1.15587
O	-0.83389	3.85896	-1.50177
O	-0.77840	3.56816	2.20566
O	-0.02351	4.41174	-0.36728
O	-2.76660	3.43588	0.34372
Hf	2.48474	0.82518	-0.00182
O	1.11479	2.04312	-1.13630
O	0.91310	1.55010	1.22991
O	3.43830	1.22417	2.09943
O	3.38164	1.23439	-2.12129
O	4.50609	-0.04759	-0.11384
O	3.51819	2.82696	0.05815
Hf	-2.28641	-0.63411	-0.04193
O	-0.97264	-1.73094	-1.26891
O	-0.66694	-1.44167	1.06347
O	-3.10736	-1.27510	2.16333
O	-3.39640	-0.78570	-2.04414
O	-4.33451	0.33769	0.23653
O	-3.42099	-2.56438	0.01034
Hf	0.80863	-2.33768	-0.18361
O	2.19757	-1.05773	0.93533
O	1.43347	-0.54659	-1.20164
O	1.27566	-3.36021	-1.89783
O	1.18590	-3.52074	1.91376
O	-0.66532	-4.17777	-0.00291
O	2.19924	-3.72621	-0.77531
Cl	-0.46744	0.05089	3.89544
Cl	-1.72928	-4.07375	2.98915
Cl	-2.65666	1.39549	-4.09483
Cl	5.12294	-0.62325	-3.83602
O	-3.46830	-4.31541	-2.01433
O	-4.37738	2.17083	2.19197
O	5.43901	-1.86898	1.64033
O	5.86671	0.53486	2.83711
O	-2.60092	6.03135	-1.41690
O	-1.07823	-3.79242	-3.11499
O	-1.22283	6.02096	1.32921
O	1.41895	-5.82711	0.55205
O	-5.98881	-1.80147	0.00891
O	6.49903	0.93740	-1.59150
O	-2.60860	2.50418	4.15866
O	3.27175	-2.30485	3.15566

O	-5.42595	-2.51443	-2.53215
O	-4.41638	2.61887	-1.60911
H	-0.97857	4.54896	2.04467
H	-3.31954	3.31040	-0.48266
H	4.36299	0.93699	2.40101
H	2.62149	1.50412	-2.66591
H	4.79836	-0.81094	0.45587
H	4.25591	3.09057	-0.59574
H	-2.78600	-2.20115	2.31450
H	-3.23560	-0.14588	-2.78501
H	-4.39967	0.88084	1.07469
H	-4.38967	-2.47683	0.21493
H	1.39348	-4.46163	1.65957
H	-0.15286	-5.01484	0.09792
H	-2.59460	-4.26140	-2.48911
H	-5.20388	2.62247	2.42868
H	-3.78943	2.19182	3.00562
H	4.72401	-2.22653	2.22722
H	6.01351	-2.61004	1.38955
H	5.94861	-0.39102	2.50434
H	5.91319	0.46498	3.80495
H	-2.03620	5.23262	-1.52642
H	-2.53728	6.19835	-0.46225
H	-0.87127	-3.79134	-4.06302
H	-0.22684	-3.96735	-2.63665
H	-0.77028	5.61653	0.53152
H	1.89806	-5.26961	-0.12544
H	-6.12632	-2.08580	-0.92767
H	-6.76354	-2.07865	0.52374
H	6.27039	0.43548	-2.42184
H	7.41501	0.70418	-1.36515
H	-1.97724	3.00120	3.59610
H	2.54141	-2.93207	2.94317
H	-5.89317	-2.46278	-3.38177
H	-4.52311	1.77605	-1.12205
H	-3.57352	-5.23669	-1.72546
H	-3.33371	-3.24844	-0.71633
H	-4.16954	-1.36085	-2.28457
H	-4.87863	-3.33845	-2.54544
H	1.84416	-6.69746	0.59797
H	3.20272	-2.08289	4.09761
H	-2.10880	1.68858	4.36591
H	-0.62293	6.71557	1.64857
H	-3.91041	2.36362	-2.41166

H	-1.20885	-4.11427	0.82204
H	0.32606	-3.58498	2.41228
H	-2.68551	-0.77211	2.88768
H	-5.10402	-0.28955	0.20078
H	-1.22100	-2.20895	-2.08694
H	-0.47984	-1.12166	1.97053
H	-1.69619	1.15255	-2.13251
H	-1.50649	0.83443	2.12452
H	0.67147	1.07414	2.05161
H	1.41347	2.93782	-1.37240
H	0.82709	-0.20458	-1.87747
H	2.56062	-1.29079	1.81655
H	2.86850	1.27349	2.88326
H	3.84699	2.97357	0.96313
H	3.87096	0.53684	-2.64748
H	0.10798	3.53368	2.60945
H	-3.30898	3.01747	1.06236
H	5.30204	0.32493	-0.59173
O	5.44984	3.47936	-1.57729
H	5.95761	2.63259	-1.63266
H	5.01739	3.55045	-2.44478

109
Hf4_4_2_term_perox_conf1_ion4_diconf9.log Energy: -3143087.2745710

Hf	0.63597	-2.32646	0.60408
O	1.72473	-0.64160	1.41364
O	1.38287	-0.91581	-0.88181
O	1.41527	-3.70051	-1.01416
O	0.91085	-2.93701	2.61638
O	-0.83565	-4.24225	0.76265
O	1.87685	-3.55578	1.66265
Hf	-2.49672	-0.89586	-0.26981
O	-0.96219	-2.22547	-0.88966
O	-1.11552	-1.29583	1.29313
O	-3.72773	-1.02885	1.84037
O	-3.05768	-1.75874	-2.34429
O	-4.58109	-0.35479	-0.67898
O	-3.29012	-3.03141	0.28813
Hf	2.20542	0.81842	-0.06079
O	0.97144	1.87085	-1.40493
O	0.42959	1.59619	0.87213
O	2.90789	1.91200	2.01628
O	3.23119	0.38355	-2.14276
O	4.21910	-0.07771	0.40769

O	3.64902	2.48523	-0.45571
Hf	-1.00408	2.33629	-0.56930
O	-2.48677	1.07620	0.48750
O	-1.52330	0.45676	-1.53007
O	-1.34935	3.19503	-2.39232
O	-1.78594	3.41014	1.47342
O	0.20479	4.29704	-0.30737
O	-2.29906	3.67808	-1.33208
Cl	-1.58326	0.91161	3.55275
Cl	2.29206	4.97166	1.90684
Cl	3.64148	-2.64200	-2.99617
Cl	-0.35369	-1.26028	-3.88845
O	3.02938	4.80318	-1.45542
O	4.31852	-2.25867	1.95600
O	-5.85036	1.76232	0.26854
O	-6.18966	-0.11851	2.19698
O	2.84034	-5.86130	-0.46947
O	1.07971	3.96168	-3.18390
O	-0.31446	-5.22566	3.11272
O	-0.75479	5.86241	1.73012
O	5.67969	1.51199	1.97934
O	-5.69062	-1.83686	-2.55333
O	2.58263	-1.32357	3.91285
O	-4.53855	3.87974	1.17507
O	5.70810	1.60115	-1.98954
O	5.14610	-4.52280	-0.93297
H	2.00707	-3.27086	-1.68520
H	-0.64648	-4.83405	0.01303
H	-4.66832	-0.67358	1.94614
H	-2.38402	-1.62762	-3.05374
H	-4.99488	0.50448	-0.36357
H	-2.46598	-3.57848	0.41653
H	2.71306	2.89003	1.96037
H	3.29402	-0.58721	-2.33349
H	4.19963	-0.94108	0.93427
H	4.50075	2.26110	-0.90565
H	-1.42658	4.31843	1.68900
H	-0.36212	5.06037	-0.07938
H	2.27194	4.65396	-2.07552
H	4.09145	-1.86826	2.82523
H	3.50998	-2.80163	1.77225
H	-5.33045	2.56271	0.59015
H	-6.56023	2.10034	-0.30146
H	-6.24486	0.64901	1.57582

H	-6.23435	0.26880	3.08653
H	3.74597	-5.46366	-0.59871
H	2.72017	-6.45216	-1.23094
H	1.07414	4.01491	-4.15229
H	0.12592	3.93938	-2.88803
H	0.19696	-4.36694	3.16001
H	-1.21006	6.54322	2.25162
H	6.12250	2.23570	1.50639
H	4.81284	1.88256	2.24885
H	-6.43292	-1.69888	-3.16183
H	-5.77532	-2.74486	-2.13726
H	1.91105	-2.02184	3.66999
H	-3.57678	3.67853	1.25189
H	6.45946	1.11745	-1.60821
H	5.78773	-5.05854	-1.42723
H	2.66009	5.26504	-0.68089
H	3.35749	3.38236	-0.84626
H	4.15198	0.72044	-2.23333
H	6.07943	2.18030	-2.67580
H	0.15984	5.79406	2.08577
H	-4.83624	4.01835	2.08914
H	2.26565	-0.89753	4.72490
H	-1.08758	-5.09150	3.68579
H	4.78177	-3.89419	-1.60085
H	0.90086	4.30006	0.39533
H	-1.64729	2.85069	2.27259
H	2.41829	1.60593	2.80009
H	4.86351	0.50694	0.90599
H	1.26226	2.36431	-2.20106
H	0.14112	1.21146	1.71917
H	1.01594	-0.90202	-1.78734
H	2.06758	-0.70324	2.33506
H	-1.09874	-0.76322	2.11650
H	-0.73432	-2.29237	-1.83644
H	-1.07327	0.15743	-2.35082
H	-2.57192	1.16091	1.45501
H	-3.22324	-0.69680	2.61086
H	-3.63482	-2.83510	1.18696
H	-3.96581	-1.70794	-2.73392
H	-0.70861	-4.77431	1.62012
H	1.90985	-4.53892	-0.73600
H	-5.16967	-0.78758	-1.35783
O	-5.47415	-4.13646	-1.23268
H	-4.70055	-3.87339	-0.68821

H	-5.12772	-4.81209	-1.83864

109
Hf4_4_2_term_perox_conf1_ion5_diconf5.log Energy: -3143081.0220478

Hf	1.03632	2.09367	0.15689
O	-0.88988	2.16168	0.92296
O	-0.32280	1.23033	-1.19280
O	1.63708	3.06761	-1.78302
O	1.23664	2.40170	2.55936
O	3.11204	2.78650	0.50107
O	0.65836	4.36487	0.53939
Hf	2.17868	-1.29272	-0.13041
O	2.38761	0.68739	-0.91735
O	1.29767	0.21241	1.07513
O	2.93255	-1.63690	2.02891
O	2.86112	-1.60065	-2.42203
O	2.89589	-3.34382	-0.23191
O	4.40231	-1.00303	-0.10852
Hf	-2.37104	1.14468	-0.37106
O	-2.25827	-0.76889	-1.40365
O	-1.77773	-0.43385	0.92084
O	-3.55579	1.74328	1.20729
O	-2.53205	2.28993	-2.36433
O	-3.48276	2.84873	0.21706
O	-4.42601	0.67478	-1.39651
Hf	-1.33667	-2.27754	-0.11400
O	0.62831	-2.38910	0.83367
O	0.39762	-1.39364	-1.29851
O	-1.39195	-3.50903	-1.71429
O	-1.54795	-2.97803	2.16556
O	-3.53773	-2.76669	0.13815
O	-1.26793	-4.29961	-0.43961
Cl	-0.42479	-0.30809	3.75022
Cl	3.75114	0.96101	3.68533
Cl	-0.51968	4.34548	-3.62130
Cl	2.40491	-4.30779	-3.73793
O	-5.58712	-1.06612	0.21835
O	-1.91500	4.62978	1.41500
O	1.21341	-5.20279	-0.81612
O	5.41159	-2.74451	1.73368
O	3.32428	5.10975	-2.03553
O	-7.89144	-2.30007	-0.55699
O	4.23184	3.93268	2.49698
O	-3.74760	-4.50703	2.24384

O	-5.82899	0.70757	2.18733
O	4.87058	-4.24083	-1.77818
O	1.85620	5.10526	3.09861
O	-1.44627	-5.87628	2.52273
O	-5.05737	3.24723	-1.82526
O	0.85997	6.13365	-1.48786
H	0.91774	3.32786	-2.41610
H	2.05739	1.93797	2.89591
H	3.71989	2.11197	0.14959
H	0.77592	5.00963	-0.21635
H	3.74710	-2.19199	2.09715
H	2.38883	-0.99761	-3.02330
H	2.18399	-4.08020	-0.35677
H	4.89790	-0.79967	-0.96024
H	-1.79702	2.87018	-2.68437
H	-4.96640	1.48052	-1.57094
H	-2.45275	-3.30765	2.40500
H	-3.75605	-3.49932	0.75933
H	-6.43710	-1.50654	-0.04769
H	-2.62172	4.07470	0.96357
H	-2.26195	4.89987	2.27946
H	0.27796	-4.88111	-0.63765
H	1.33890	-5.10431	-1.78373
H	5.56046	-3.68332	1.53242
H	6.12360	-2.48428	2.34186
H	2.59703	5.76116	-1.90358
H	3.56357	5.18492	-2.97417
H	-7.85593	-3.22173	-0.25166
H	-7.86605	-2.37008	-1.52570
H	3.47043	4.47649	2.83953
H	-3.08128	-5.23315	2.37688
H	-5.53400	0.36032	3.04476
H	-5.04209	1.20971	1.83689
H	4.27375	-4.43159	-2.54007
H	5.13527	-5.11497	-1.44585
H	1.47333	4.22161	3.27358
H	-1.04496	-4.98686	2.46769
H	-4.73306	3.32986	-0.89037
H	0.49840	7.01489	-1.29543
H	-5.76345	-0.51060	1.03302
H	-4.97322	0.04145	-0.84228
H	-3.36441	2.81380	-2.43526
H	-5.77439	3.88581	-1.95995
H	-4.39471	-4.56834	2.96402

H	-1.28917	-6.15752	3.43941
H	1.57989	5.23240	2.16984
H	4.28081	3.15070	3.08978
H	0.30404	5.74789	-2.21335
H	-4.25997	-2.07933	0.22746
H	-1.31623	-2.25227	2.79138
H	-2.91586	-0.98168	-2.08083
H	-1.47646	-0.20757	1.82479
H	-0.05564	0.35070	-1.54576
H	-1.24418	2.87491	1.49030
H	0.77645	-0.05011	1.86727
H	2.59121	0.98542	-1.81678
H	0.35957	-1.82901	-2.16480
H	0.76924	-2.67557	1.74873
H	3.13514	-0.79700	2.52002
H	4.95001	-1.62439	0.43017
H	2.71525	-2.51555	-2.82225
H	0.50482	1.88763	2.96761
H	3.57334	3.27435	1.28713
H	-0.26301	4.53286	0.88133
H	2.35320	3.77488	-1.84319
H	3.69790	-3.63464	-0.76463
O	5.56061	-0.66397	-2.45883
H	4.75958	-1.03696	-2.87693
H	5.57925	0.26564	-2.74232

109
Hf4_4_2_term_perox_conf1_ion5_diconf7.log Energy: -3143083.2416680

Hf	-0.88760	2.08708	-0.12074
O	-1.91265	0.61466	1.15768
O	-1.82166	0.44982	-1.21419
O	-1.05314	3.30099	-1.78088
O	-0.73131	3.05888	2.04576
O	-0.39121	4.01436	-0.64255
O	-2.93666	2.96998	0.12978
Hf	2.36120	0.50125	-0.34559
O	0.81400	1.51844	-1.36176
O	0.80394	1.14582	0.90508
O	3.32634	1.16332	1.67226
O	2.99860	0.50485	-2.63200
O	4.46430	-0.24829	-0.48821
O	3.31249	2.44934	-0.72429
Hf	-2.28614	-1.14259	0.07029
O	-0.99609	-2.41015	-1.01566

O	-0.63901	-1.80494	1.24660
O	-3.10639	-1.45077	2.44772
O	-3.45835	-1.68242	-2.00468
O	-4.40403	-0.37378	0.14799
O	-3.47793	-3.04182	0.41210
Hf	0.90654	-2.75303	0.01003
O	2.26916	-1.26452	0.83818
O	1.38485	-1.12620	-1.32743
O	1.33703	-4.01278	-1.51818
O	1.57244	-3.57485	2.22788
O	-0.30457	-4.64171	0.70813
O	2.43179	-4.01562	-0.48720
Cl	-0.52843	0.15231	3.84985
Cl	2.10623	3.92788	2.73379
Cl	-3.15710	0.58600	-4.05457
Cl	5.78252	1.39871	-3.74805
O	-2.45917	-5.18037	-0.83920
O	-4.46921	3.05796	2.25468
O	5.66938	-1.42840	1.62288
O	6.08472	1.25007	1.87775
O	-3.08440	5.15481	-2.38171
O	-2.10721	-3.81882	-3.10706
O	-1.88363	6.26135	-0.05046
O	2.01307	-5.96007	1.18294
O	-5.15175	0.36072	2.62260
O	5.91624	1.96023	-0.75070
O	-2.61831	4.49820	3.65336
O	3.56758	-1.96784	3.21935
O	-5.78159	-2.62857	-0.93479
O	-4.70080	1.69914	-1.56974
H	0.19494	3.44029	2.17895
H	-3.55450	2.70477	-0.59178
H	4.31297	1.26735	1.75028
H	2.93926	-0.41888	-2.93218
H	4.83537	-0.80373	0.25166
H	2.85315	3.22121	-1.19585
H	-3.27162	-2.41102	2.49743
H	-3.46368	-0.97579	-2.70921
H	-4.56442	0.37287	-0.49977
H	-4.41836	-2.97866	0.09499
H	1.84188	-4.53024	2.08263
H	0.29735	-5.41406	0.80424
H	-2.37877	-4.90333	-1.78962
H	-4.64889	2.15820	2.59743

H	-3.89834	3.52271	2.91580
H	5.00844	-1.74250	2.29134
H	6.29366	-2.15656	1.47291
H	6.19000	0.27050	1.94284
H	6.38801	1.61033	2.72691
H	-2.43775	4.42566	-2.26263
H	-2.86995	5.71108	-1.60466
H	-1.95723	-4.01718	-4.04516
H	-2.80051	-3.12598	-3.05474
H	-1.36288	5.43505	-0.21022
H	2.37000	-5.43527	0.40425
H	-6.04541	0.09761	2.89896
H	-4.53895	-0.32304	2.96827
H	6.36635	1.91247	-1.62429
H	6.53251	1.91774	0.00631
H	-1.89911	4.16858	3.07447
H	2.93020	-2.70998	3.12133
H	-6.31245	-1.91691	-0.53937
H	-5.60046	2.01725	-1.75487
H	-2.93664	-6.02578	-0.81263
H	-3.11174	-3.87435	-0.00912
H	-4.40055	-1.92942	-1.82578
H	-6.40528	-3.30011	-1.25795
H	2.61257	-6.69916	1.36913
H	3.38087	-1.53973	4.06983
H	-2.39297	4.15799	4.53441
H	-1.30991	6.96732	-0.38915
H	-4.30488	1.45513	-2.44567
H	-1.01485	-4.91437	0.07377
H	0.77434	-3.61273	2.78558
H	-2.40296	-1.24729	3.10357
H	-4.72832	-0.04712	1.03639
H	-1.19563	-2.81999	-1.88424
H	-0.39417	-1.30307	2.04991
H	-1.95490	0.48235	-2.18817
H	-1.60191	0.51354	2.08240
H	0.74163	0.80192	1.81502
H	0.86955	1.86006	-2.26538
H	0.67376	-0.87535	-1.93795
H	2.69071	-1.31245	1.72217
H	2.93472	2.02566	1.97119
H	4.29679	2.54881	-0.72239
H	3.89443	0.83097	-2.93161
H	-0.75953	2.33872	2.71564

H	-3.47944	2.91437	0.98360
H	5.13026	0.47778	-0.66943
O	2.00896	4.45838	-1.75472
H	1.83680	4.35307	-2.70430
H	1.11701	4.32937	-1.31825

109
Hf4_4_2_term_perox_conf1_ion5_diconf9.log Energy: -3143082.5038550

Hf	-0.81614	-2.30604	-0.07499
O	-1.90683	-0.83127	-1.20419
O	-1.57134	-0.54987	1.08284
O	-1.68079	-3.24923	1.83952
O	-1.08742	-3.33248	-1.87793
O	0.65397	-4.17426	0.13732
O	-2.05547	-3.74934	-0.82441
Hf	2.35215	-0.71211	0.23860
O	0.81793	-1.86371	1.33185
O	0.83602	-1.36321	-1.07800
O	3.34754	-1.02608	-1.85901
O	2.99760	-0.95873	2.44089
O	4.46835	-0.12081	0.37111
O	3.05676	-2.88314	0.17828
Hf	-2.32040	0.94546	-0.16009
O	-1.12183	2.28632	0.98771
O	-0.62500	1.55908	-1.19058
O	-2.95248	1.42944	-2.55449
O	-3.53273	1.24099	1.91649
O	-4.37727	0.06705	-0.44297
O	-3.59286	2.80746	-0.38795
Hf	0.84655	2.56119	0.05030
O	2.33510	1.14800	-0.74115
O	1.11912	0.72681	1.18191
O	1.37520	3.60366	1.69572
O	1.52582	3.22031	-2.16310
O	-0.31267	4.43226	-0.56370
O	2.39372	3.77016	0.59810
Cl	-0.18904	0.53133	-4.04137
Cl	3.55224	-4.07972	-2.70272
Cl	-2.79515	-1.09092	3.91481
Cl	4.93394	0.87639	3.96460
O	-2.56573	4.93835	0.88582
O	-4.41718	-2.41396	-1.47410
O	4.68457	2.37009	1.11326
O	5.88037	-1.86849	-2.24080

O	-3.92692	-4.56175	1.61606
O	-2.39194	3.47889	3.13383
O	0.57174	-5.46119	-2.11922
O	1.32489	5.90623	-2.14592
O	-5.70307	0.90010	-2.59182
O	6.24738	-1.23799	2.00854
O	-2.50751	-1.88235	-3.63903
O	3.88653	5.07135	-2.12477
O	-5.86931	2.29710	1.00880
O	-5.34588	-2.40690	2.43536
H	-1.95422	-2.60465	2.53896
H	0.64318	-4.60705	1.03005
H	4.34162	-1.12185	-1.88212
H	2.19095	-0.95426	2.98462
H	4.56571	0.87775	0.58547
H	2.22565	-3.43382	0.22876
H	-2.98687	2.40386	-2.54291
H	-3.46890	0.47695	2.54458
H	-4.32641	-0.90618	-0.71669
H	-4.52360	2.73355	-0.05121
H	1.28093	4.16101	-2.37264
H	0.18520	5.20317	-0.91796
H	-2.54781	4.61844	1.82534
H	-4.14832	-2.17963	-2.38381
H	-3.63737	-2.93850	-1.15561
H	3.82730	2.85913	0.95648
H	4.72200	2.18824	2.07723
H	6.21896	-1.48993	-3.06914
H	5.47520	-2.72105	-2.50895
H	-4.54627	-3.83765	1.90965
H	-3.97172	-5.23329	2.31644
H	-2.31095	3.63991	4.08720
H	-3.01839	2.73357	3.01196
H	-0.08858	-4.73875	-2.28537
H	2.31830	5.86369	-2.11678
H	-6.19206	1.73837	-2.54673
H	-4.84003	1.12942	-2.99306
H	6.05199	-0.63505	2.76460
H	7.13893	-0.98659	1.71500
H	-1.94621	-2.56751	-3.18447
H	3.51581	4.17025	-2.17404
H	-6.62321	1.79619	0.65497
H	-6.06185	-2.61907	3.05656
H	-3.06496	5.77163	0.86991

H	-3.21331	3.63112	0.04255
H	-4.49261	1.39545	1.73134
H	-6.25260	3.02266	1.53045
H	1.08583	6.41413	-2.93766
H	4.31100	5.20582	-2.98854
H	-1.87662	-1.32990	-4.14143
H	1.42191	-5.10598	-2.45798
H	-4.65475	-1.97625	2.98640
H	-1.03636	4.74019	0.03537
H	1.13040	2.66026	-2.86065
H	-2.21617	1.19653	-3.17274
H	-4.96777	0.46041	-1.15417
H	-1.33700	2.62035	1.88114
H	-0.41093	1.12545	-2.04798
H	-1.67196	-0.57401	2.05709
H	-2.17312	-1.04794	-2.13051
H	0.68310	-0.93828	-1.94215
H	1.04900	-2.57689	1.95594
H	0.32361	0.35287	1.59670
H	2.86600	1.27449	-1.54116
H	3.03381	-1.82647	-2.33468
H	3.47118	-3.20269	-0.66223
H	3.62463	-0.31898	2.88835
H	0.62382	-4.85400	-0.61238
H	-2.50726	-3.83280	1.69656
H	5.14435	-0.61006	0.93320
O	0.65194	-4.39450	2.75845
H	0.85381	-5.08237	3.41222
H	-0.30829	-4.21061	2.81568

109
Hf4_4_2_term_perox_conf1_ion6_diconf1.log Energy: -3143076.2556490

Hf	-2.24650	-0.54339	-0.23043
O	-1.88917	1.29092	-1.27703
O	-1.39744	0.91883	1.00887
O	-3.20991	-0.86999	1.83432
O	-2.77209	-0.89249	-2.58885
O	-3.29384	-2.46146	-0.48149
O	-4.29165	0.24807	-0.46099
Hf	1.01228	-2.00217	0.06731
O	-0.94151	-1.80958	0.95799
O	-0.44502	-1.12336	-1.20586
O	1.33477	-2.81538	-2.05753
O	1.10023	-2.82154	2.35388

O	2.93761	-3.06342	0.29203
O	0.23670	-4.12726	0.04117
Hf	-0.74095	2.69307	-0.01908
O	0.99284	2.44185	1.21331
O	0.96975	1.98052	-1.17082
O	-1.18740	3.74306	-2.25429
O	-1.58353	3.69076	1.57882
O	-2.39081	3.83524	0.32595
O	0.14057	4.83433	-0.37470
Hf	2.54501	1.25994	0.21936
O	2.34188	-0.64404	-0.89515
O	1.45831	-0.32676	1.21066
O	3.54324	1.38973	2.00894
O	3.75721	1.40406	-1.86118
O	3.49982	3.31179	-0.02914
O	4.34950	0.72309	0.92883
Cl	-0.10978	-0.31180	3.87459
Cl	-1.23815	-3.21154	-3.90293
Cl	-5.31306	0.93701	3.19692
Cl	2.96134	-4.97323	3.53770
O	2.57094	5.42999	-1.48558
O	-4.78993	2.79278	-0.34593
O	5.07209	-2.81296	-1.30996
O	3.38680	-4.25277	-2.92850
O	-4.77523	-3.04375	1.67431
O	4.63846	3.76535	2.30844
O	-4.12980	-3.75007	-2.55759
O	6.34849	2.05466	-1.75107
O	-3.66058	2.76324	-2.86790
O	2.43763	-5.65049	0.61086
O	-5.42766	-1.51906	-3.40115
O	5.63032	-0.52079	-2.63990
O	-0.65167	6.15911	1.74672
O	-6.29341	-0.94419	0.97565
H	-3.76882	-0.14921	2.23738
H	-2.27349	-1.64220	-3.03308
H	-3.74287	-2.90049	0.28211
H	-5.04721	-0.23498	-0.03170
H	2.08474	-3.41850	-2.35454
H	0.93938	-2.10870	3.01869
H	3.72750	-2.81462	-0.26583
H	-0.36590	-4.34293	0.81618
H	-0.89525	4.62301	-1.92850
H	-0.05451	5.46668	0.38774

H	4.63858	1.86467	-1.71055
H	3.94099	3.66693	0.79914
H	2.95669	6.29910	-1.28236
H	-3.98558	3.17747	0.09524
H	-4.63011	2.97777	-1.29795
H	5.33366	-1.96718	-1.76621
H	5.88223	-3.17834	-0.91794
H	4.13776	-3.84094	-2.43624
H	3.36138	-5.17481	-2.62604
H	-5.57323	-2.48812	1.48386
H	-5.02462	-3.73654	2.30579
H	5.59972	3.69930	2.18628
H	4.32072	2.81386	2.37080
H	-4.71654	-3.08022	-2.99690
H	6.49704	1.13793	-2.06896
H	-3.96259	2.59236	-3.77437
H	-2.91726	3.39975	-2.92970
H	2.59776	-5.67450	1.59511
H	2.97679	-6.35432	0.21466
H	-4.59659	-1.07313	-3.13302
H	4.79004	-0.01276	-2.58574
H	-1.10313	5.27346	1.87713
H	-7.21032	-0.88005	0.66040
H	2.58780	5.34887	-2.45420
H	1.04965	5.01902	-0.71016
H	0.05869	6.17312	2.40930
H	6.58962	2.61810	-2.50502
H	5.75547	-0.72163	-3.58314
H	-5.46698	-1.40495	-4.36489
H	-3.32800	-3.80263	-3.12257
H	-6.21079	-0.32031	1.74822
H	3.16462	4.06582	-0.56489
H	3.28138	1.94848	-2.51302
H	-0.53485	3.48753	-2.93044
H	1.02398	2.65212	2.15763
H	0.76447	1.46769	-1.96699
H	-1.07448	0.69802	1.90685
H	-2.55908	1.69435	-1.87314
H	-0.22572	-0.90050	-2.12208
H	-1.01481	-1.62860	1.91343
H	1.05776	-0.15337	2.09226
H	2.52190	-0.75096	-1.83976
H	0.52154	-3.07617	-2.55534
H	0.92112	-4.83999	0.04370

H	1.83771	-3.39525	2.70908
H	-2.47950	-0.08620	-3.05052
H	-3.61827	-2.93963	-1.32903
H	-4.48887	1.25030	-0.37626
H	-3.70866	-1.71146	1.99917
H	2.93164	-4.05916	0.38252
O	-1.00949	-4.70699	2.31551
H	-0.38319	-4.05809	2.70008
H	-1.88139	-4.28659	2.39314

109
Hf4_4_2_term_perox_conf1_ion6_diconf2.log Energy: -3143092.3452052

Hf	-2.17065	-0.88431	-0.23977
O	-2.03524	1.02733	-1.19084
O	-1.41552	0.62824	1.04456
O	-3.05676	-1.23956	1.85569
O	-2.83989	-1.22001	-2.41872
O	-3.18300	-2.88373	-0.40770
O	-4.30106	-0.22660	-0.36245
Hf	1.16432	-2.16549	-0.14417
O	-0.74825	-2.04618	0.88040
O	-0.41918	-1.37091	-1.35452
O	1.52472	-3.06437	-2.29579
O	1.52252	-2.80181	2.14993
O	3.09158	-3.20056	-0.08999
O	0.45149	-4.27940	-0.12194
Hf	-0.88718	2.46380	0.10087
O	1.11965	2.38746	0.80008
O	0.58766	1.52006	-1.39214
O	-0.54897	3.83541	-1.69684
O	-1.20796	3.25651	1.98147
O	-3.07626	3.11053	-0.09412
O	-0.94090	4.34999	1.00611
Hf	2.47880	1.18983	-0.34917
O	2.37947	-0.81916	-1.21511
O	1.54755	-0.37496	0.86825
O	3.81049	1.40226	1.17467
O	3.16954	1.20755	-2.63165
O	3.06580	3.32864	-0.88474
O	4.51129	0.89041	-0.05008
Cl	0.05280	-0.53305	3.70694
Cl	-0.61117	-2.11324	-4.38481
Cl	-4.92714	0.70216	3.38958
Cl	4.39648	-2.84170	3.35230

O	1.43097	5.50778	-0.97931
O	-5.07731	1.96218	-1.98567
O	5.15176	-1.70541	0.41693
O	1.88037	-5.75569	-1.90398
O	-4.67924	-3.36289	1.82504
O	1.08797	5.90748	1.63525
O	-5.30696	-3.13867	-1.99390
O	5.03761	3.11605	-2.69135
O	-3.30915	5.59416	0.79734
O	3.70604	-5.26715	1.48321
O	-5.34154	-0.62452	-3.24900
O	6.65457	2.32810	-0.77757
O	1.21446	3.57587	3.24823
O	-6.17910	-1.15052	1.30624
H	-3.53177	-0.49625	2.31860
H	-2.26237	-1.55892	-3.14696
H	-3.57705	-3.30037	0.39465
H	-5.06549	-0.53430	0.20541
H	1.80240	-4.01000	-2.31907
H	1.09800	-2.13282	2.75264
H	3.90837	-2.58833	0.00872
H	0.16379	-4.67148	0.75995
H	0.05830	4.59652	-1.47426
H	-3.66204	2.75616	-0.78871
H	3.91189	1.83804	-2.83870
H	3.76580	3.48523	-1.56725
H	1.38688	5.83408	-0.03484
H	-5.89255	2.45492	-1.78358
H	-4.71027	2.38513	-2.78237
H	4.91079	-0.74841	0.26269
H	5.09873	-1.84288	1.38786
H	2.72913	-6.17010	-1.67576
H	1.42311	-6.38448	-2.48713
H	-5.46727	-2.77800	1.70651
H	-4.85651	-3.95656	2.57186
H	0.80312	6.78038	1.95297
H	0.24783	5.37444	1.49414
H	-5.50384	-2.27881	-2.42596
H	5.79386	2.87513	-2.07067
H	-2.36741	5.33677	0.98965
H	-3.24578	6.21040	0.04902
H	4.05497	-4.69968	2.21217
H	4.49081	-5.70295	1.11085
H	-5.48244	-0.54161	-4.20690

H	5.90088	1.79398	-0.39369
H	0.25198	3.46519	3.04524
H	-7.11657	-1.04157	1.07359
H	1.75566	6.24105	-1.52706
H	1.39850	4.48642	2.93687
H	5.38109	3.69582	-3.38843
H	7.29155	1.66406	-1.08811
H	-5.52125	0.26045	-2.86609
H	-5.14248	-3.75254	-2.72834
H	-5.99857	-0.53475	2.07026
H	2.45382	4.10755	-0.88151
H	2.39952	1.52303	-3.13671
H	-0.00608	3.21969	-2.23418
H	-3.35387	4.03792	0.15766
H	1.33980	2.78428	1.68120
H	0.23205	0.68677	-1.74324
H	-1.11966	0.40031	1.95209
H	-2.06309	1.03412	-2.15894
H	-0.40524	-1.43505	-2.33713
H	-0.81531	-1.86817	1.83761
H	1.14286	-0.15677	1.73169
H	2.68254	-1.01002	-2.11454
H	0.84374	-2.94025	-3.00235
H	0.92912	-4.97223	-0.63996
H	2.47384	-2.82101	2.45537
H	-3.72721	-0.97110	-2.78910
H	-3.90688	-2.94514	-1.10672
H	-4.52281	0.61639	-0.80728
H	-3.58765	-2.05903	2.03817
H	3.27379	-4.01946	0.46288
O	-0.00255	-5.13441	2.32683
H	0.56341	-4.38073	2.60380
H	-0.89133	-4.91313	2.65134

109
Hf4_4_2_term_perox_conf1_ion6_diconf4.log Energy: -3143088.4284229

Hf	-1.90839	-1.29607	-0.20908
O	-2.14534	0.47489	-1.37004
O	-1.50192	0.36752	0.99170
O	-2.79637	-1.74294	1.83895
O	-2.50341	-1.97392	-2.51611
O	-2.14286	-3.48018	-0.28357
O	-4.13673	-1.28852	-0.48015
Hf	1.64557	-1.69788	-0.03650

O	-0.25319	-2.06131	0.97113
O	-0.07313	-1.44049	-1.27400
O	2.32219	-2.53974	-2.13507
O	2.08822	-2.29225	2.24536
O	3.80857	-1.96916	0.09104
O	1.51804	-3.91953	0.01657
Hf	-1.55959	2.22362	-0.11294
O	0.33935	2.68860	0.81218
O	0.13094	1.82989	-1.39560
O	-2.42962	3.33426	-1.63336
O	-1.95436	2.94138	2.10696
O	-3.79296	1.90510	0.36283
O	-1.93875	4.19597	-0.51133
Hf	1.99803	1.87905	-0.27292
O	2.36801	-0.06537	-1.18716
O	1.57661	0.13253	0.96272
O	3.15821	2.45447	1.32641
O	2.76771	2.16662	-2.52544
O	2.05614	4.10800	-0.82811
O	3.98770	2.19616	0.10971
Cl	0.19313	-0.28625	3.74611
Cl	-0.03889	-2.80699	-4.14875
Cl	-4.25347	0.80037	3.25493
Cl	4.71165	-3.32067	3.49577
O	1.39561	5.79033	1.10875
O	-4.71118	0.50698	-2.42596
O	5.47609	0.00082	-0.17960
O	3.56948	-4.89412	-1.36763
O	-4.63736	-3.54205	2.48304
O	3.51030	4.85581	2.44765
O	-4.09407	-5.01537	-0.94799
O	4.53709	4.13262	-2.29396
O	-5.02994	3.05878	-1.65218
O	5.27722	-4.17148	0.62075
O	-4.79561	-3.57693	-3.09401
O	5.58972	1.52344	-2.58372
O	-3.35134	5.14127	1.54857
O	-5.89568	-1.28802	1.57484
H	-3.11929	-0.95108	2.33168
H	-1.76254	-2.44554	-2.99365
H	-1.53278	-3.93129	0.32325
H	-4.77589	-1.28216	0.28583
H	2.91298	-3.32645	-2.06848
H	1.67845	-1.66129	2.88946

H	4.44129	-1.18398	-0.09399
H	1.28456	-4.36857	0.88487
H	-2.49903	2.29782	2.60979
H	-4.10710	1.60457	1.24741
H	3.29285	3.01248	-2.60484
H	2.96813	4.37039	-1.07067
H	2.15471	5.54479	1.71365
H	-5.01648	1.43610	-2.24399
H	-4.98016	0.29219	-3.33338
H	5.67388	0.26405	-1.10387
H	4.93346	0.78327	0.12202
H	4.29798	-4.85620	-0.70181
H	3.60419	-5.76491	-1.79454
H	-5.35078	-2.89703	2.27084
H	-4.65348	-3.62947	3.45052
H	3.45532	3.95610	2.01141
H	3.31343	4.68419	3.38270
H	-4.45295	-4.56703	-1.76672
H	5.19376	3.39835	-2.26667
H	-5.62087	3.79306	-1.88040
H	-4.07505	3.36472	-1.76740
H	5.15858	-4.11299	1.60945
H	6.21836	-3.99378	0.45557
H	-4.04692	-2.95176	-2.98032
H	4.67570	1.35648	-2.88396
H	-2.89578	5.94882	1.83860
H	-6.81328	-1.08752	1.32503
H	1.59462	6.69118	0.80533
H	-2.49890	3.78496	2.06780
H	-2.99848	4.96007	0.63606
H	4.75615	4.65511	-3.08331
H	6.14693	1.36116	-3.36340
H	-5.58555	-3.05337	-2.88194
H	-3.73437	-5.86353	-1.25681
H	-5.60187	-0.56046	2.17626
H	1.74509	4.74230	-0.10649
H	1.99335	2.26627	-3.10681
H	-4.49624	2.40896	-0.11326
H	0.34055	3.06122	1.70533
H	-0.09110	1.11149	-2.00855
H	-1.03242	0.26651	1.84712
H	-2.98894	0.62806	-1.84899
H	-0.02100	-1.46397	-2.25009
H	-0.34219	-1.88894	1.92691

H	1.20731	0.23741	1.86533
H	2.67448	-0.22062	-2.09151
H	1.61183	-2.76851	-2.78952
H	2.19932	-4.46834	-0.45829
H	3.01965	-2.46895	2.56289
H	-2.59222	-1.14169	-3.01602
H	-2.92314	-4.10279	-0.53589
H	-4.50537	-0.67777	-1.17159
H	-3.40893	-2.50807	2.07009
H	4.36110	-2.76449	0.32048
O	1.08550	-4.89034	2.44226
H	1.38045	-4.00440	2.74396
H	0.14856	-4.94271	2.69328

109
Hf4_4_2_term_perox_conf1_ion6_diconf5.log Energy: -3143091.2167047

Hf	2.35217	0.59571	-0.18286
O	1.97404	-1.14636	-1.31153
O	1.32588	-0.85367	0.92545
O	3.18069	0.73413	1.92152
O	3.20781	1.10626	-2.37330
O	3.33672	2.56110	-0.15654
O	4.41367	-0.33815	-0.29682
Hf	-0.83637	2.22415	-0.21226
O	1.00464	1.91805	0.90406
O	0.70482	1.30490	-1.33072
O	-0.92444	3.17618	-2.35030
O	-1.23132	2.98293	2.03512
O	-2.72874	3.32064	-0.33964
O	0.07667	4.25281	-0.12994
Hf	0.71532	-2.61358	-0.21761
O	-1.15795	-2.22210	0.82638
O	-0.77385	-1.75163	-1.49010
O	1.36973	-3.59978	-1.91717
O	1.34610	-3.38774	1.86420
O	2.23205	-3.93974	-0.75359
O	-0.37112	-4.65850	0.04634
Hf	-2.47648	-0.98774	-0.35831
O	-2.05359	0.90015	-1.37330
O	-1.48317	0.53714	0.81793
O	-3.69527	-1.06571	1.30437
O	-3.51089	-1.00096	-2.47754
O	-3.25772	-3.08181	-0.78321
O	-4.42350	-0.47287	0.14724

Cl	-0.16567	0.45683	3.62576
Cl	1.82420	3.42820	-3.80553
Cl	3.66142	-1.98365	3.47834
Cl	-3.96601	4.11864	2.90297
O	-2.82650	-4.81829	1.22443
O	4.57948	-2.76942	-1.25680
O	-4.89116	2.16823	0.43868
O	-1.41993	5.88045	-1.61508
O	5.44627	1.89832	2.66870
O	-4.27583	-3.24374	2.76191
O	5.66922	3.40999	-0.81037
O	-5.54696	-2.68505	-2.12687
O	-0.65561	-5.30930	-2.76099
O	-3.38948	5.85646	0.35833
O	6.05859	1.13095	-2.16664
O	-6.89429	-1.53511	-0.18350
O	1.80883	-5.92091	0.93978
O	5.97053	-0.66507	1.88443
H	3.22033	-0.11263	2.43499
H	2.77540	1.92748	-2.76587
H	2.88579	3.17161	0.45081
H	4.97102	-0.42009	0.53006
H	-1.31513	4.07751	-2.33725
H	-1.02873	2.26684	2.68945
H	-3.58910	2.80376	-0.11425
H	0.36053	4.61760	0.76302
H	2.07349	-2.88849	2.32002
H	0.22547	-5.38105	0.36234
H	-4.35146	-1.54155	-2.49683
H	-4.15301	-3.17101	-1.19517
H	-3.33113	-4.30365	1.92828
H	3.72399	-3.26100	-1.07841
H	4.74550	-2.85341	-2.20954
H	-4.72737	1.18481	0.44097
H	-4.81520	2.48064	1.36463
H	-2.09906	6.16173	-0.96306
H	-1.07100	6.68619	-2.02930
H	5.92599	1.05263	2.50895
H	5.44006	2.00767	3.63407
H	-4.20567	-2.43091	2.18824
H	-3.85443	-2.98998	3.59912
H	5.97966	2.62039	-1.34051
H	-6.21733	-2.30996	-1.47768
H	-1.01449	-5.36214	-1.85968

H	0.14804	-4.77257	-2.57960
H	-3.53275	5.57032	1.29619
H	-4.28475	5.99018	0.00269
H	5.21218	1.23308	-2.64436
H	-6.03487	-1.10035	0.06429
H	2.20748	-5.48839	0.14350
H	6.78409	-1.16535	1.70486
H	-3.26765	-5.67857	1.13359
H	-1.17983	-4.65648	0.61819
H	1.62636	-4.33393	1.83367
H	2.21468	-6.79494	1.04941
H	-6.01973	-3.20761	-2.79320
H	-7.45086	-0.81047	-0.51291
H	5.77323	0.53504	-1.44421
H	5.57922	4.13098	-1.45596
H	5.40832	-1.23516	2.46983
H	-3.15521	-3.76547	-0.06648
H	-2.94965	-1.37138	-3.18015
H	-1.24381	-2.31341	1.78636
H	-0.46744	-1.44236	-2.35431
H	0.88528	-0.61881	1.76868
H	2.43736	-1.60677	-2.02742
H	0.51215	0.93814	-2.20580
H	0.98672	1.72484	1.86056
H	-1.19642	0.33272	1.73487
H	-2.38555	1.13895	-2.25076
H	-0.03574	3.26804	-2.79585
H	-0.34407	4.98899	-0.65226
H	-2.15220	3.30355	2.26170
H	3.00507	0.40264	-3.01452
H	4.26363	2.93000	-0.41454
H	4.44051	-1.26310	-0.72360
H	3.98050	1.28234	2.19253
H	-2.91060	4.26494	-0.08574
O	0.54500	5.10844	2.32806
H	-0.07968	4.39913	2.59314
H	1.40578	4.83338	2.68518

109
Hf4_4_2_term_perox_conf1_ion6_diconf6.log Energy: -3143081.7171903

Hf	0.75808	2.22628	-0.04338
O	2.13191	1.04165	-1.25965
O	1.63341	0.48677	0.97999
O	1.42242	3.26129	1.58939

O	0.86211	3.22170	-2.22047
O	-0.85402	3.85002	-0.12613
O	2.22722	3.61386	0.37629
Hf	-2.24351	0.30614	0.20625
O	-0.80936	1.55307	1.25416
O	-0.77397	1.08453	-1.12749
O	-3.42458	0.93268	-1.74138
O	-2.83945	0.47261	2.47757
O	-4.27359	-0.45268	0.43589
O	-3.13176	2.41516	0.38221
Hf	2.59257	-0.82526	-0.29015
O	1.47429	-2.38016	0.61538
O	0.81581	-1.31618	-1.43702
O	3.24384	-1.11323	-2.54176
O	3.68321	-1.12849	1.68418
O	4.63483	0.20066	-0.51608
O	4.03187	-2.59882	-0.57555
Hf	-0.46586	-2.72240	-0.34751
O	-2.09030	-1.41574	-1.00366
O	-1.07990	-1.22206	1.06636
O	-0.73048	-4.08965	1.14175
O	-1.10275	-3.38603	-2.61597
O	0.96749	-4.27757	-1.28896
O	-1.72261	-4.29740	0.03977
Cl	-0.04949	-0.13591	3.81821
Cl	-1.69219	2.59664	-3.81754
Cl	4.14708	0.52693	4.15062
Cl	-5.19909	-0.67732	4.07914
O	3.07486	-4.97254	0.22057
O	4.69289	2.51480	0.71089
O	-5.39666	-2.04088	-1.43028
O	-5.94848	0.44363	-2.40458
O	-0.68590	4.91630	2.22987
O	1.31273	-5.59735	2.06024
O	-1.41090	5.46322	-2.09389
O	-1.05907	-5.93681	-1.90154
O	4.32013	1.59206	-2.85564
O	-6.23461	0.81751	1.59801
O	1.16369	6.11101	-2.56322
O	-3.46238	-2.17547	-3.29913
O	6.18702	-1.74728	0.71455
O	2.02868	6.32411	0.01999
H	0.02727	3.11321	-2.75988
H	-0.83797	4.38676	0.74513

H	-4.38413	0.74469	-1.98461
H	-2.08435	0.21668	3.06508
H	-4.63569	-1.12193	-0.21003
H	-2.34849	3.02273	0.25435
H	3.74396	-1.95246	-2.55966
H	3.68697	-0.48674	2.46485
H	4.66762	1.06121	0.03812
H	4.95556	-2.45282	-0.23505
H	-1.18033	-4.38390	-2.60935
H	0.51731	-5.11299	-1.55183
H	2.52696	-5.22908	1.02810
H	5.28268	3.07890	0.18381
H	3.79078	2.93276	0.62357
H	-4.75391	-2.29963	-2.13827
H	-5.91472	-2.82948	-1.20234
H	-6.03925	-0.49265	-2.10995
H	-6.52975	0.95216	-1.81565
H	0.18166	4.44835	2.27007
H	-1.32722	4.32474	2.70314
H	0.49503	-5.17075	1.68445
H	1.40732	-5.22814	2.95317
H	-0.51465	5.82739	-2.34761
H	-1.45180	-5.63174	-1.03679
H	4.80855	2.41410	-3.02810
H	4.30186	1.10053	-3.69372
H	-6.10191	0.41030	2.49406
H	-7.08713	0.46932	1.28673
H	1.34846	5.15700	-2.64704
H	-2.68872	-2.77753	-3.35090
H	6.30680	-0.90483	0.23752
H	2.93975	6.65892	0.03845
H	3.54518	-5.76926	-0.07559
H	3.71984	-3.47069	-0.20289
H	4.62176	-1.41642	1.59594
H	7.06720	-2.10767	0.90935
H	-1.49832	-6.75596	-2.17880
H	-3.54424	-1.73385	-4.15912
H	1.48583	6.30743	-1.64338
H	-1.65265	4.83920	-2.80701
H	2.11760	5.35019	0.18460
H	1.77064	-4.54049	-0.76044
H	-0.35695	-3.17679	-3.20738
H	2.39323	-1.29081	-2.98788
H	4.74220	0.53970	-1.44094

H	1.76192	-2.76011	1.45946
H	0.34062	-0.50068	-1.69498
H	1.29752	0.23194	1.86432
H	2.82062	1.37498	-1.87294
H	-1.00129	1.29899	-2.05594
H	-0.55246	1.32508	2.16971
H	-0.61757	-1.10137	1.92456
H	-2.51275	-1.44866	-1.88791
H	-3.01146	1.42814	-2.48695
H	-3.68842	2.52846	-0.41103
H	-3.64014	0.02937	2.88540
H	1.53171	2.73360	-2.73182
H	-1.03743	4.49609	-0.89595
H	-5.05639	0.05137	0.84871
O	-2.60167	3.28805	3.39668
H	-2.71024	2.44288	2.91564
H	-2.33117	3.02103	4.29000

109
Hf4_4_2_term_perox_conf1_ion6_diconf9.log Energy: -3143095.3047908

Hf	-1.22290	-2.15448	-0.18656
O	-2.09307	-0.48751	-1.25029
O	-1.54885	-0.28537	0.99684
O	-2.00249	-2.81454	1.81627
O	-1.99899	-3.04054	-1.95170
O	-0.19419	-4.21156	-0.11719
O	-2.84198	-3.27233	-0.74611
Hf	2.16886	-1.10222	-0.13848
O	0.60660	-1.97780	1.02785
O	0.52553	-1.65615	-1.34945
O	3.12986	-1.75119	-2.17483
O	2.95172	-1.33572	2.18874
O	4.32190	-0.66262	-0.11399
O	2.75319	-3.28087	0.05978
Hf	-2.13927	1.30722	-0.18336
O	-0.61126	2.40056	0.77821
O	-0.47515	1.62663	-1.49595
O	-2.99110	1.84952	-2.52848
O	-3.07613	1.70756	2.00096
O	-4.32334	0.84415	-0.27527
O	-3.02873	3.37992	-0.25949
Hf	1.25015	2.38544	-0.34667
O	2.22574	0.67058	-1.31663
O	1.51823	0.62610	0.86280

O	2.02456	3.40976	1.22945
O	1.91795	3.02577	-2.50362
O	0.26456	4.39090	-0.87229
O	3.02851	3.32271	0.11806
Cl	0.38410	-0.17842	3.68982
Cl	1.16099	-2.98981	-4.18064
Cl	-3.96332	-0.90639	3.46473
Cl	5.71412	-0.31050	3.14731
O	-1.54673	5.23758	1.01454
O	-4.98933	-1.55686	-1.16264
O	5.12074	1.68049	0.60239
O	5.06571	-3.54610	-1.24970
O	-3.57461	-4.92679	2.08836
O	-1.35528	3.55843	3.14282
O	-0.56844	-5.21349	-2.53332
O	2.16792	5.66837	-2.24642
O	-5.63906	2.46126	-1.94922
O	6.46020	-2.12169	0.69981
O	-3.40456	-1.35328	-3.45924
O	3.99030	5.79650	-0.36023
O	-5.20635	3.33247	1.37610
O	-5.70523	-3.25151	2.17230
H	-2.53496	-2.13480	2.30102
H	0.75366	-4.02729	0.03754
H	3.97295	-2.24589	-2.06679
H	2.29927	-0.93221	2.81258
H	4.60729	0.30159	0.09273
H	2.82802	-3.64913	0.99825
H	-2.22416	2.31516	-2.91100
H	-3.31455	0.84090	2.43639
H	-4.55107	-0.10500	-0.56678
H	-3.94139	3.47895	0.10723
H	2.12382	4.00085	-2.57802
H	0.83579	5.07963	-1.29912
H	-1.46403	4.86682	1.92688
H	-4.81059	-1.44538	-2.12003
H	-4.27801	-2.19660	-0.89517
H	4.34369	2.30254	0.54261
H	5.23983	1.44426	1.54554
H	5.71691	-3.27944	-0.56319
H	5.40236	-4.35465	-1.66815
H	-4.42752	-4.41236	2.12347
H	-3.44647	-5.25475	2.99353
H	-0.91231	3.45883	4.00035

H	-2.07657	2.89232	3.10364
H	-1.28205	-4.52182	-2.48610
H	2.92481	5.86787	-1.61234
H	-5.97187	3.32670	-1.66160
H	-4.80282	2.64209	-2.42318
H	6.36583	-1.76074	1.61818
H	7.23678	-1.66477	0.33393
H	-2.91636	-2.14549	-3.08348
H	3.69726	4.88610	-0.07798
H	-6.08405	2.92995	1.26427
H	-6.37126	-3.52159	2.82527
H	-1.90909	6.13507	1.09724
H	-2.48440	4.09771	0.17856
H	-3.93272	2.19757	1.91310
H	-5.34581	4.12231	1.92602
H	2.14364	6.35942	-2.92638
H	4.87885	5.66470	-0.72972
H	-3.25306	-1.36084	-4.41819
H	0.11006	-4.75308	-3.07436
H	-5.26024	-2.47283	2.58094
H	-0.24333	4.80196	-0.13278
H	1.19861	2.85828	-3.13749
H	-3.11620	1.05822	-3.08778
H	-4.90801	1.44757	-0.82090
H	-0.67839	2.75760	1.69193
H	-0.28879	0.82278	-2.01077
H	-1.10132	-0.15151	1.85845
H	-2.45060	-0.64780	-2.14740
H	0.57809	-1.91088	-2.29802
H	0.47260	-1.71237	1.95790
H	1.09925	0.58883	1.74891
H	2.63877	0.68112	-2.19212
H	2.58071	-2.25104	-2.83749
H	3.56255	-3.58311	-0.43620
H	3.83381	-0.93357	2.42712
H	-0.25044	-4.70668	-0.99673
H	-2.53791	-3.66932	1.86879
H	5.07467	-1.24131	0.17907
O	3.01789	-4.05980	2.56308
H	3.02458	-3.10053	2.78047
H	2.17381	-4.39096	2.91306

109
Hf4_4_2_term_perox_conf1_ion7_diconf5.log Energy: -3143090.6474846

Hf	-2.02336	-1.28148	0.54378
O	-0.22017	-2.07351	1.23146
O	-0.61160	-1.55753	-0.97822
O	-3.21428	-1.93746	-1.26898
O	-2.26043	-1.51284	2.87396
O	-4.12540	-0.74576	1.04956
O	-2.59805	-3.45143	0.96215
Hf	-1.20996	2.17685	0.15140
O	-2.44528	0.53597	-0.54849
O	-1.27123	0.50910	1.49120
O	-1.17376	3.05842	2.33481
O	-2.23585	2.81600	-1.93068
O	-0.73448	4.33560	-0.09812
O	-3.24778	2.87974	0.66744
Hf	1.37826	-2.17717	-0.27335
O	1.87910	-0.56395	-1.69647
O	2.06358	-0.46149	0.74282
O	2.17668	-3.18464	1.34054
O	1.00003	-3.37659	-2.22316
O	1.54716	-4.15468	0.40980
O	3.44308	-2.66762	-1.19518
Hf	2.21517	1.26737	-0.55104
O	0.81086	2.27965	0.79629
O	0.13546	1.47112	-1.24406
O	2.64280	2.14166	-2.34086
O	3.35138	1.98829	1.42657
O	4.40357	0.60612	-0.78796
O	3.09108	3.00398	-1.20058
Cl	-1.46174	0.37470	-3.70550
Cl	2.83457	0.00995	3.79169
Cl	-1.93775	-4.16636	-3.13013
Cl	-2.50547	5.90230	-2.03692
O	5.34595	-1.62183	0.30759
O	-0.67429	-5.10306	1.53563
O	1.74723	5.09915	-0.60262
O	-1.39544	5.76319	2.51523
O	-5.67556	-2.93501	-1.24531
O	7.95391	-2.20015	-0.26223
O	-6.01272	-1.87819	2.43182
O	5.67517	2.86958	0.38915
O	4.47836	-2.55804	2.63587
O	-3.69545	5.44545	0.96796
O	-4.01886	-3.48443	3.34717
O	3.93813	4.84419	1.19689

O	2.85888	-5.26964	-1.55976
O	-3.88990	-4.96355	-0.86512
H	-2.75642	-2.54124	-1.90782
H	-2.50997	-0.65750	3.26361
H	-4.49525	-0.10896	0.41644
H	-3.09946	-3.96879	0.26807
H	-1.22959	4.04847	2.42855
H	-1.91943	2.27950	-2.70124
H	0.23528	4.58860	-0.25198
H	-3.95750	2.60357	0.01935
H	0.05794	-3.60008	-2.43496
H	3.55051	-3.63505	-1.35997
H	4.31286	2.12891	1.22704
H	4.98498	1.38005	-0.62085
H	6.29541	-1.84411	0.12113
H	0.17604	-4.74444	1.13740
H	-0.51675	-5.13027	2.49360
H	2.21605	4.27243	-0.98242
H	1.74374	5.76495	-1.31064
H	-0.68884	6.15196	1.97199
H	-1.31673	6.17867	3.39095
H	-5.30678	-3.84396	-1.15168
H	-6.03829	-2.89981	-2.14598
H	8.48023	-1.41146	-0.05044
H	8.02091	-2.27670	-1.22848
H	-5.49404	-2.56893	2.90909
H	5.18254	3.72813	0.48116
H	4.05611	-1.79361	3.08719
H	3.71637	-3.00582	2.19309
H	-3.45095	5.76010	0.06932
H	-2.97220	5.76165	1.55374
H	-3.66218	-3.84828	2.50674
H	3.50839	4.08231	1.62885
H	2.48814	-5.17083	-0.64297
H	-3.96034	-5.89748	-0.60602
H	5.12544	-1.92048	1.24134
H	4.21969	-2.36190	-0.63352
H	1.51364	-4.21818	-2.24749
H	3.23700	-6.15830	-1.64580
H	6.45586	2.94366	0.96158
H	3.25166	5.13788	0.55791
H	-3.91831	-4.17427	4.02393
H	-6.29889	-1.25490	3.12049
H	-3.28245	-4.93035	-1.64944

H	4.77126	-0.16672	-0.27007
H	3.28996	1.38622	2.21372
H	2.60024	-0.81898	-2.29188
H	2.15621	-0.44123	1.72011
H	-0.70183	-1.12555	-1.85049
H	-0.02169	-2.32192	2.14568
H	-0.50165	0.40021	2.07307
H	-2.54118	0.39432	-1.51106
H	-0.11734	1.06421	-2.10053
H	1.04912	2.57918	1.68535
H	-1.89420	2.68601	2.87145
H	-3.42270	3.86456	0.85579
H	-2.24311	3.77625	-2.18619
H	-2.89107	-2.19532	3.23166
H	-4.88328	-1.18170	1.57622
H	-1.79823	-4.04735	1.20769
H	-4.18373	-2.20792	-1.24808
H	-1.27324	4.92183	-0.69739
O	-4.97631	2.48353	-1.33259
H	-4.18022	2.49664	-1.90243
H	-5.42407	1.64620	-1.53373

109
Hf4_4_2_term_perox_conf1_ion7_diconf9.log Energy: -3143075.3316665

Hf	-1.00045	-2.22278	-0.52855
O	-2.03075	-0.48089	-1.32906
O	-1.50999	-0.69089	0.92794
O	-1.54349	-3.28100	1.38573
O	-1.68117	-2.90561	-2.41126
O	0.18002	-4.29871	-0.72541
O	-2.52123	-3.37283	-1.27030
Hf	2.29956	-0.93300	-0.20831
O	0.79175	-2.08937	0.70561
O	0.71327	-1.43645	-1.57783
O	3.30122	-1.33352	-2.33301
O	3.10426	-1.68697	1.89093
O	4.41148	-0.41313	-0.04722
O	2.86402	-3.15305	-0.53057
Hf	-2.27382	1.04951	0.09942
O	-0.80794	1.94807	1.34180
O	-0.59955	1.74015	-1.02662
O	-3.11597	2.14123	-1.94370
O	-3.25332	0.71502	2.23434
O	-4.40862	0.44772	-0.19158

O	-3.26558	3.01706	0.63960
Hf	1.02014	2.36955	0.22618
O	2.17629	0.98355	-1.06323
O	1.57879	0.52189	1.13670
O	1.66450	3.30602	1.93272
O	1.52465	3.59101	-1.85051
O	-0.21596	4.38598	0.10687
O	2.61558	3.52210	0.79474
Cl	0.54046	-1.00367	3.67817
Cl	-1.33605	4.51845	-2.85398
Cl	-4.27175	-2.46103	2.53909
Cl	5.71019	-1.03336	3.41065
O	-1.93665	3.94658	2.77958
O	-4.85125	-1.83487	-1.46758
O	5.50933	1.41477	-1.70296
O	5.82672	-0.95026	-2.98607
O	-1.55855	-5.88851	0.89204
O	0.29811	5.34969	3.07073
O	-0.36176	-5.06273	-3.19300
O	2.05219	5.78401	-0.38315
O	-5.84878	2.30379	-1.46082
O	6.31165	-2.08456	0.58043
O	-3.27423	-1.17038	-3.64482
O	3.41776	2.18846	-3.20551
O	-5.45831	2.39576	2.11879
O	-4.22126	-5.43816	1.04590
H	-2.40867	-2.98371	1.78366
H	-0.26600	-4.97276	-0.16097
H	4.26630	-1.17834	-2.59700
H	2.43204	-1.51309	2.59586
H	4.77597	0.33783	-0.59392
H	2.03381	-3.67590	-0.40878
H	-2.52637	2.90388	-2.21194
H	-3.49325	-0.24028	2.30901
H	-4.55994	-0.44937	-0.64538
H	-4.19744	2.94352	0.96422
H	1.84089	4.48934	-1.56143
H	0.40444	5.15107	0.04146
H	-1.15803	4.57468	2.88332
H	-4.66817	-1.56472	-2.39229
H	-4.08671	-2.43786	-1.28074
H	4.83474	1.86609	-2.27416
H	6.11944	2.09542	-1.37628
H	5.97395	-0.03944	-2.63568

H	5.90582	-0.87060	-3.95106
H	-2.55803	-5.86913	0.87028
H	-1.31507	-6.45794	1.64030
H	0.29934	6.12026	2.48066
H	0.88475	4.68029	2.62099
H	-0.96777	-4.27301	-3.10653
H	2.49777	5.13180	0.22839
H	-6.22696	3.03654	-0.94814
H	-4.99979	2.64004	-1.81499
H	6.33141	-1.85542	1.54628
H	7.16184	-1.77344	0.22664
H	-2.68858	-1.94861	-3.41988
H	2.79809	2.90699	-2.93909
H	-6.31060	1.99864	1.87335
H	-4.65037	-6.05288	1.66338
H	-2.33200	3.83054	3.65786
H	-2.78236	3.50403	1.36897
H	-4.10284	1.20643	2.34033
H	-5.65333	3.00742	2.84892
H	2.56568	6.60681	-0.39031
H	3.35996	2.09391	-4.16945
H	-3.07310	-0.91752	-4.55991
H	0.33045	-4.77970	-3.81308
H	-4.29447	-4.56128	1.48470
H	-0.75001	4.43187	-0.72533
H	0.68095	3.77105	-2.34306
H	-3.13314	1.55120	-2.71909
H	-5.04723	1.09816	-0.60669
H	-1.09436	2.54947	2.06856
H	-0.45521	1.32236	-1.88817
H	-1.07501	-0.66948	1.80346
H	-2.44887	-0.54813	-2.21702
H	0.57580	-1.01684	-2.43925
H	0.62590	-2.07458	1.66881
H	1.16221	0.26425	1.98960
H	2.52790	1.20813	-1.95137
H	2.77158	-1.32708	-3.14552
H	3.11524	-3.22250	-1.47071
H	3.96968	-1.37887	2.28869
H	0.09381	-4.66554	-1.66239
H	-1.55413	-4.27702	1.34554
H	5.16870	-1.06333	0.15480
O	2.82856	-4.59525	2.14595
H	2.98991	-3.64945	1.96577

H	2.53391	-4.60284	3.06983

109
Hf4_4_2_term_perox_conf1_ion8_diconf5.log Energy: -3143084.8543548

Hf	-2.13701	-0.90667	0.39477
O	-0.50745	-1.93882	1.21544
O	-0.67441	-1.29459	-1.05711
O	-3.32657	-1.66627	-1.32627
O	-2.31924	-0.78500	2.80405
O	-4.20563	-0.22472	0.84742
O	-3.08702	-2.90844	1.15929
Hf	-1.02222	2.39759	-0.28882
O	-2.45474	0.90004	-0.75949
O	-0.96576	0.73809	1.06435
O	-1.36153	3.37302	1.75783
O	-1.73166	2.79970	-2.51046
O	-0.40895	4.52645	-0.69504
O	-3.04368	3.56011	-0.32873
Hf	1.17927	-2.11923	-0.23689
O	2.07542	-0.61857	-1.52776
O	1.67766	-0.31108	0.87967
O	1.94849	-3.07773	1.40968
O	0.56199	-3.40222	-2.08128
O	1.19336	-4.05909	0.58772
O	3.06728	-3.02600	-1.28778
Hf	2.39255	1.29080	-0.47263
O	0.93537	2.54292	0.54852
O	0.42406	1.48514	-1.44266
O	3.09377	2.07847	-2.20299
O	3.34619	2.04474	1.61041
O	4.44909	0.30087	-0.32717
O	3.51713	2.89935	-1.01710
Cl	-0.91956	0.17324	-4.05289
Cl	-3.25393	1.95638	3.84342
Cl	3.62126	-0.19444	3.69846
Cl	-2.39435	-4.22740	-2.84347
O	5.16645	-2.22063	0.04717
O	-1.01273	-4.50300	2.01422
O	2.10374	5.16171	-0.51529
O	-2.45114	5.77493	1.07262
O	-5.91805	-2.27087	-1.35606
O	7.72132	-2.69498	-0.77826
O	-5.53887	-0.23189	3.03824
O	5.90617	1.28347	1.79150

O	4.45347	-3.07166	2.44645
O	-1.03667	5.31277	-3.24408
O	-4.30071	-2.53101	3.79079
O	2.18435	4.47171	2.17544
O	2.13470	-5.54301	-1.35505
O	-4.48775	-4.45965	-0.55478
H	-2.95219	-2.39356	-1.88750
H	-2.57133	0.13460	3.11122
H	-4.33987	0.64553	0.43353
H	-3.62911	-3.44721	0.51514
H	-1.72219	4.29299	1.73792
H	-1.47985	2.04872	-3.10596
H	0.59659	4.72982	-0.60507
H	-3.38329	3.60488	-1.23966
H	-0.40486	-3.54246	-2.23784
H	3.02170	-4.00857	-1.36299
H	4.33471	2.09075	1.57855
H	5.13505	0.74265	0.21767
H	6.09886	-2.41057	-0.23733
H	-0.15519	-4.50710	1.49082
H	-0.79602	-4.77439	2.92024
H	2.22544	5.14518	0.46114
H	2.61040	4.35362	-0.81663
H	-1.74394	6.27624	0.63237
H	-2.99663	6.41844	1.55418
H	-5.69378	-3.19454	-1.09720
H	-6.21571	-2.33220	-2.27875
H	8.24088	-1.89740	-0.58385
H	7.70750	-2.73805	-1.74879
H	-5.23303	-1.08885	3.44345
H	6.70249	1.74516	2.10003
H	4.30555	-2.23154	2.93383
H	3.54896	-3.28127	2.10123
H	-0.27168	5.51195	-3.80957
H	-1.74566	5.91469	-3.52609
H	-3.46935	-2.01725	3.83460
H	2.80410	3.70900	2.19057
H	1.88715	-5.31702	-0.42175
H	-4.71919	-5.33626	-0.20504
H	5.03498	-2.54723	0.98996
H	3.92358	-2.80352	-0.81087
H	0.97207	-4.29813	-2.07106
H	2.42126	-6.46879	-1.38387
H	5.60447	0.70946	2.52810

H	2.19231	4.85838	3.06488
H	-4.22589	-2.89440	2.88662
H	-5.04104	0.47052	3.51076
H	-3.85331	-4.60931	-1.30208
H	4.62312	-0.67647	-0.19525
H	3.20767	1.39022	2.34681
H	2.66618	-0.92979	-2.22887
H	1.99434	-0.44377	1.79382
H	-0.72122	-0.88738	-1.94714
H	-0.59552	-2.72051	1.79736
H	-0.04236	0.47813	1.28321
H	-3.03899	0.88718	-1.56421
H	0.25204	0.98506	-2.26513
H	1.11647	3.13012	1.30672
H	-1.92166	2.85710	2.39686
H	-3.02435	4.48050	0.03878
H	-1.44954	3.63296	-2.96369
H	-1.38106	-0.88046	3.05098
H	-4.76297	-0.25601	1.71585
H	-2.40041	-3.53793	1.50803
H	-4.32825	-1.75903	-1.33499
H	-0.68826	4.97148	-1.53034
O	-3.95223	0.74550	-3.05104
H	-4.06285	1.63156	-3.43370
H	-3.18358	0.37433	-3.53586

109
Hf4_4_2_term_perox_conf1_ion8_diconf9.log Energy: -3143079.1401218

Hf	1.23327	-2.09725	0.69943
O	1.76602	-0.11014	1.35821
O	1.52187	-0.62053	-0.89274
O	2.37954	-3.20935	-0.89512
O	1.76974	-2.40756	2.74218
O	0.52955	-4.23524	1.11604
O	2.85972	-2.73668	1.77689
Hf	-2.18797	-1.63602	-0.17256
O	-0.37427	-2.58108	-0.74885
O	-0.73517	-1.55069	1.37132
O	-3.31187	-2.02595	1.86060
O	-2.47813	-2.66080	-2.38247
O	-4.32412	-1.42707	-0.73396
O	-2.84384	-3.77699	0.08331
Hf	1.85987	1.32069	-0.19376
O	0.33672	1.93426	-1.54966

O	0.00557	1.79300	0.76778
O	2.43987	2.58197	1.86628
O	2.79139	1.06774	-2.33782
O	4.03254	0.93002	0.17822
O	2.82989	3.26893	-0.69219
Hf	-1.66841	1.88411	-0.64474
O	-2.64946	0.30998	0.53941
O	-1.62149	-0.11539	-1.50558
O	-2.28929	2.58234	-2.42403
O	-2.69417	2.78823	1.42457
O	-0.99642	4.14522	-0.35720
O	-3.36450	2.66460	-1.36433
Cl	0.04987	-1.50954	-3.79893
Cl	-1.79013	0.53957	3.56473
Cl	0.58578	5.07225	2.36667
Cl	4.31193	-1.65292	-2.88389
O	2.21650	5.73757	-0.28944
O	4.75233	-0.80189	2.05505
O	-6.13516	0.19680	0.31464
O	-5.94678	-1.86345	2.08433
O	4.26870	-4.96121	-0.27891
O	0.40407	5.58080	-2.31363
O	1.62949	-4.98855	3.37706
O	-2.41642	5.45690	1.51711
O	5.15339	3.13977	1.23218
O	-5.07770	-2.43133	-3.13465
O	2.73103	-0.20164	3.89681
O	-5.47185	2.55181	1.31392
O	4.18968	3.28972	-3.06216
O	6.12579	-3.02935	-0.66482
H	2.87461	-2.64225	-1.53971
H	0.45716	-4.81990	0.34643
H	-4.32041	-1.97096	1.91453
H	-1.79410	-2.30802	-3.00918
H	-4.90839	-0.69481	-0.38116
H	-2.47190	-4.50864	-0.49751
H	1.79565	3.31401	2.06841
H	3.27685	0.20616	-2.42101
H	4.27103	0.22973	0.87133
H	3.31376	3.36343	-1.54816
H	-2.64402	3.76796	1.59525
H	-1.70478	4.75975	-0.05586
H	1.56472	5.85809	-1.03029
H	4.38944	-0.40671	2.87366

H	4.13369	-1.56898	1.91009
H	-5.88982	1.10025	0.68564
H	-6.90888	0.33004	-0.25677
H	-6.18463	-1.09174	1.51257
H	-6.14472	-1.57925	2.99162
H	5.03531	-4.33097	-0.37575
H	4.34484	-5.56036	-1.03959
H	-0.11615	6.38517	-2.47285
H	-0.18059	5.00818	-1.76899
H	1.73142	-3.99574	3.38064
H	-3.09039	6.08245	1.82877
H	5.15711	3.80489	0.52429
H	4.26174	3.23315	1.62919
H	-5.38982	-1.80155	-3.80594
H	-5.59397	-3.24469	-3.26312
H	2.37695	-1.11762	3.69355
H	-4.48592	2.58860	1.31940
H	5.15786	3.36084	-3.02135
H	6.92923	-3.36067	-1.09806
H	1.69151	5.78130	0.53961
H	2.54440	4.22398	-0.44579
H	3.37541	1.75108	-2.74186
H	3.90599	3.84236	-3.80928
H	-1.59099	5.63125	2.02354
H	-5.72480	2.55780	2.25161
H	2.32422	0.07394	4.73399
H	0.89812	-5.16614	3.99134
H	5.64770	-2.53606	-1.37305
H	-0.34684	4.18063	0.38437
H	-2.39269	2.33634	2.24683
H	2.46929	2.02900	2.66934
H	4.55066	1.74462	0.43956
H	0.51940	1.96385	-2.50025
H	-0.12910	1.42169	1.65722
H	1.20192	-0.77168	-1.80488
H	2.01505	0.01540	2.29800
H	-0.85589	-0.96343	2.14740
H	-0.10792	-2.59782	-1.68693
H	-1.09084	-0.30323	-2.30855
H	-2.70059	0.42281	1.50711
H	-2.96972	-1.49005	2.60393
H	-2.89038	-4.06337	1.01050
H	-3.35406	-2.56917	-2.83447
H	0.95742	-4.72417	1.88399

H	3.04098	-3.91387	-0.60010
H	-4.76067	-1.81346	-1.53006
O	-2.11116	-5.38748	-1.85323
H	-2.14238	-4.54729	-2.36043
H	-1.18472	-5.67424	-1.90244

109
Hf4_4_2_term_perox_conf1_ion9_diconf5.log Energy: -3143091.6163655

Hf	1.25823	2.12270	0.03108
O	-0.71818	2.36003	0.76366
O	-0.18690	1.51155	-1.34509
O	2.03162	2.72235	-2.07418
O	1.48642	2.61272	2.34293
O	3.31897	2.95972	0.46569
O	0.92931	4.29734	-0.05267
Hf	1.88800	-1.41325	0.18960
O	2.50791	0.50584	-0.56347
O	0.92908	0.27986	1.11091
O	2.25234	-1.74188	2.44714
O	2.95984	-1.72590	-1.84933
O	2.24985	-3.58598	0.21594
O	4.10009	-1.46053	0.55687
Hf	-2.23310	1.48877	-0.59532
O	-2.10515	-0.37656	-1.76924
O	-2.05343	-0.16202	0.71516
O	-3.33169	2.40909	0.90130
O	-2.45675	2.41496	-2.71849
O	-3.21236	3.30378	-0.27771
O	-4.37123	0.89549	-1.33049
Hf	-1.62496	-2.02068	-0.38041
O	0.07601	-2.28464	0.93695
O	0.33448	-1.45590	-1.19586
O	-1.70575	-3.22909	-2.01266
O	-2.38125	-2.81916	1.73345
O	-3.91377	-2.26419	-0.54697
O	-1.80833	-4.02745	-0.74826
Cl	1.31727	0.13679	-3.87009
Cl	3.36931	0.80607	3.86502
Cl	-2.75427	-0.47947	3.78238
Cl	5.00026	-3.98517	-2.64078
O	-5.66817	-0.53237	0.45258
O	-1.47704	5.34032	0.03976
O	0.25677	-5.36500	0.02575
O	4.59040	-3.27702	2.46007

O	4.39074	3.90226	-1.81544
O	-8.29799	-1.08228	-0.02053
O	3.64463	5.35244	1.64953
O	-4.18829	-4.66226	0.96384
O	-5.20943	1.15702	2.44046
O	4.57731	-4.92518	0.27692
O	1.57290	5.29834	3.29249
O	-1.84622	-5.74635	1.89284
O	-4.92286	3.37057	-2.25984
O	2.95167	5.95224	-0.85485
H	1.89798	2.01303	-2.74857
H	2.20111	2.05359	2.79520
H	3.93401	3.10585	-0.29672
H	1.56024	4.94133	-0.46864
H	2.94901	-2.41059	2.64528
H	2.53233	-1.32412	-2.64170
H	1.48161	-4.23433	0.19542
H	4.80396	-1.37462	-0.15866
H	-2.31681	1.79755	-3.45638
H	-4.88553	1.66983	-1.65342
H	-3.20314	-3.36208	1.61092
H	-4.11967	-3.18761	-0.27962
H	-6.63119	-0.71959	0.29773
H	-2.14548	4.59975	-0.03421
H	-1.64262	5.75369	0.90276
H	-0.49323	-4.83451	-0.41608
H	0.49852	-6.06700	-0.60130
H	4.75730	-4.02055	1.83371
H	5.35154	-3.22784	3.06034
H	4.08071	4.82919	-1.65452
H	5.21049	3.93489	-2.33313
H	-8.46232	-1.99024	0.28369
H	-8.40975	-1.13187	-0.98438
H	2.91291	5.47342	2.32702
H	-3.40756	-5.25592	1.12995
H	-4.52044	0.70023	2.97281
H	-4.68499	1.76307	1.86158
H	4.91536	-4.70074	-0.62993
H	4.44250	-5.88766	0.28233
H	1.43455	4.34898	3.08287
H	-1.71996	-4.85140	2.25721
H	-4.53722	3.64249	-1.38681
H	3.29452	6.02332	0.07389
H	-5.57823	0.02698	1.28331

H	-4.94989	0.40279	-0.66939
H	-3.34432	2.84208	-2.84871
H	-5.53411	4.06240	-2.55710
H	-4.87673	-4.94041	1.58955
H	-1.10014	-5.82139	1.25614
H	0.84000	5.75205	2.84431
H	4.48756	5.51730	2.10261
H	2.79718	6.85530	-1.17680
H	-4.54792	-1.67139	-0.05246
H	-2.56980	-2.14044	2.43207
H	-2.95468	-0.55009	-2.20660
H	-2.25185	-0.10051	1.67777
H	0.04709	1.00229	-2.14860
H	-1.11757	2.96957	1.40169
H	-0.00607	0.12347	1.33872
H	3.19971	0.55381	-1.23894
H	0.40065	-1.11343	-2.10768
H	-0.00802	-2.52608	1.87043
H	2.53985	-0.90533	2.91123
H	4.46293	-2.03720	1.27837
H	3.45424	-2.53792	-2.12896
H	0.66190	2.23355	2.69970
H	3.42250	3.78062	1.03044
H	-0.00023	4.70208	-0.01906
H	2.93938	3.10601	-2.20708
H	3.10182	-4.10014	0.17063
O	6.06639	-1.37591	-1.21862
H	5.87485	-2.18976	-1.74381
H	5.95303	-0.64870	-1.85250

109
Hf4_4_2_term_perox_conf1_ion9_diconf7.log Energy: -3143082.1344213

Hf	-1.74073	-1.81764	-0.10907
O	-2.26052	0.09440	-1.10985
O	-1.57848	-0.15627	1.22797
O	-2.26694	-3.09340	1.42802
O	-2.19812	-2.40905	-2.31339
O	-2.28514	-3.75446	0.08186
O	-4.06196	-1.38213	0.12809
Hf	1.85821	-1.55027	-0.16760
O	0.17469	-2.40918	0.74533
O	0.05378	-1.19943	-1.22159
O	2.24760	-2.35881	-2.24474
O	2.44821	-2.05403	2.26520

O	4.04713	-1.47942	-0.18027
O	2.46726	-3.75489	0.06582
Hf	-1.84923	1.70195	0.29138
O	-0.00137	2.27418	1.18672
O	-0.24990	1.83175	-1.11858
O	-2.84995	2.77240	-1.55185
O	-2.32195	1.98324	2.57122
O	-4.05867	1.32959	0.56044
O	-2.20726	3.86780	0.63971
Hf	1.67536	2.01205	-0.19921
O	2.30927	0.26884	-1.25067
O	1.63046	0.19436	0.96844
O	2.82646	2.80710	1.30667
O	2.27454	2.74668	-2.45638
O	1.04458	4.26138	-0.53074
O	3.59160	2.78025	0.02534
Cl	0.21455	0.14523	3.79609
Cl	-0.05477	-4.32377	-3.25264
Cl	-0.56652	3.90652	-3.41116
Cl	5.31417	-2.50801	3.36176
O	-0.67767	5.45926	2.05278
O	-4.54774	1.00250	-2.82997
O	5.31148	0.82889	-0.63568
O	4.50604	-3.83933	-2.45908
O	-4.24079	-4.59966	2.58926
O	1.95126	5.16750	2.37692
O	-4.46166	-5.38179	-0.04811
O	3.47442	4.96102	-1.44449
O	-6.12702	2.22911	-1.00875
O	5.12999	-3.74654	0.58561
O	-5.00921	-1.79174	-2.32553
O	4.16153	0.71936	-3.21746
O	-2.33018	4.30150	3.88547
O	-5.60106	-2.37679	2.02915
H	-1.58318	-3.16121	-2.59752
H	-4.57972	-1.84587	0.86547
H	3.07031	-2.91820	-2.33514
H	1.99542	-1.42454	2.86351
H	4.56149	-0.63042	-0.31856
H	2.01428	-4.19613	0.83454
H	-2.20664	3.21599	-2.16603
H	-1.78452	1.41771	3.16203
H	-4.19103	0.34305	0.47189
H	-2.66201	4.35387	-0.06836

H	2.79379	3.58609	-2.35272
H	1.81080	4.82615	-0.79525
H	0.31656	5.29901	2.11469
H	-5.32894	1.41258	-2.37998
H	-4.62735	1.21010	-3.77720
H	4.75347	1.55545	-0.23489
H	6.21076	0.93724	-0.28536
H	5.14607	-3.34817	-3.00069
H	4.32823	-4.64823	-2.96741
H	-3.43044	-4.09478	2.32820
H	-4.44785	-5.07672	1.74853
H	2.37059	5.89687	1.89223
H	2.29028	4.34456	1.93355
H	-3.67913	-4.77321	-0.10063
H	3.84347	4.34600	-0.75906
H	-6.98545	1.87200	-0.72235
H	-6.26691	3.18482	-1.12485
H	5.38150	-3.54197	1.52644
H	5.89384	-4.13306	0.12863
H	-4.18113	-2.21636	-2.62656
H	3.67457	1.56422	-3.27548
H	-1.89042	4.12046	4.73224
H	-5.48259	-1.77927	2.78553
H	-0.79023	6.39791	1.82943
H	-1.53187	4.47285	1.09272
H	-2.36315	2.88449	3.01831
H	-1.68702	4.84964	3.37310
H	4.13502	5.64444	-1.63785
H	4.77784	0.84741	-2.46313
H	-4.96514	-0.87958	-2.68497
H	-4.08829	-6.26363	-0.20770
H	-5.18289	-3.24144	2.32061
H	0.41032	4.31764	-1.28097
H	1.48337	3.00371	-2.98883
H	-3.41727	2.19746	-2.12576
H	-4.79229	1.77056	0.06224
H	0.13153	2.12164	2.13763
H	-0.43666	2.00167	-2.06120
H	-1.06126	-0.24727	2.06068
H	-3.04141	0.19420	-1.67868
H	-0.00345	-0.34290	-1.67647
H	0.13046	-3.10821	1.42383
H	1.19477	0.21127	1.84712
H	2.86970	0.27706	-2.06512

H	1.48945	-2.91696	-2.56497
H	3.43380	-3.94994	0.16448
H	3.39868	-2.08622	2.57143
H	-1.87364	-1.65340	-2.83766
H	-4.55093	-1.55536	-0.73328
H	4.64693	-2.23952	0.06200
O	1.20257	-4.47295	2.32918
H	1.72464	-3.75735	2.75232
H	1.32673	-5.27617	2.85961

109
Hf4_4_2_term_perox_conf1_ion9_diconf9.log Energy: -3143095.8699572

Hf	-2.59464	0.11693	0.04660
O	-1.65780	-1.67259	0.90389
O	-1.24826	-0.95632	-1.25919
O	-3.58716	0.12546	-1.98743
O	-3.84543	-0.33738	1.71133
O	-3.74801	2.12559	0.43031
O	-4.40912	-0.80010	0.41240
Hf	0.08278	2.43071	0.31258
O	-1.56879	1.79761	-0.92672
O	-1.12640	1.00675	1.31366
O	0.09426	2.94348	2.65160
O	-0.11225	3.91920	-1.41023
O	1.52301	4.09285	0.59636
O	-1.64263	3.80569	0.92257
Hf	-0.13713	-2.43758	-0.29524
O	1.40332	-1.50015	-1.48700
O	1.13100	-1.23854	0.87291
O	0.24275	-3.43559	2.00195
O	-0.55039	-3.26118	-2.44546
O	-1.46345	-4.23538	-0.17972
O	1.28218	-4.19342	-0.42241
Hf	2.51744	-0.10322	-0.26965
O	1.80946	1.45756	1.05636
O	1.09915	1.27855	-1.14429
O	3.64620	0.24158	-1.95529
O	3.80706	-0.27742	1.80061
O	3.78586	-2.09020	-0.24046
O	4.30064	0.84729	-0.75781
Cl	-0.93020	0.76584	-3.83528
Cl	0.04684	-0.48857	3.78030
Cl	3.34586	-3.30919	2.62151
Cl	2.11483	5.06007	-3.12187

O	3.14124	-4.50735	-2.31727
O	-4.02082	-3.63373	0.32748
O	4.11324	3.33807	0.24919
O	2.09143	4.08046	3.94881
O	-6.06012	1.01721	-2.34235
O	3.39244	-2.03578	-3.35789
O	-5.39861	1.69327	2.46115
O	6.05488	-0.76015	0.35393
O	-1.01565	-5.86201	1.87385
O	1.38389	6.51914	-0.44533
O	-3.31446	-2.68566	2.82620
O	3.86603	2.35340	2.82217
O	0.68091	-5.63254	-2.62003
O	-6.98510	-0.15274	-0.16697
H	-3.01658	0.34343	-2.75632
H	-4.17066	2.58950	-0.36211
H	0.85294	3.44535	3.09389
H	-0.89856	3.79197	-1.96591
H	2.48008	3.84129	0.46660
H	-2.47682	3.27740	0.76567
H	1.23096	-3.48230	2.11482
H	-0.28760	-2.67112	-3.17157
H	-2.44173	-3.98649	-0.09446
H	0.86051	-4.98323	-0.83323
H	4.74908	-0.42700	1.52189
H	4.75017	-1.88252	-0.17914
H	3.38657	-3.65381	-2.75733
H	-3.92867	-3.65468	1.30455
H	-4.17734	-2.67201	0.17560
H	4.18308	2.51948	-0.31655
H	4.73868	3.98717	-0.11218
H	2.81179	3.45441	3.69329
H	1.93142	3.91375	4.89225
H	-6.54468	0.58191	-1.57219
H	-6.52260	0.76549	-3.15810
H	3.35782	-1.78140	-4.29372
H	3.80823	-1.28075	-2.86971
H	-4.94189	0.81284	2.37188
H	5.72501	-0.03410	-0.23801
H	-0.39209	-6.57527	1.65821
H	-0.46130	-5.14054	2.24599
H	1.65472	6.26696	-1.36281
H	2.13587	7.02559	-0.09533
H	-3.66358	-1.77430	2.61814

H	4.02187	1.38922	2.75899
H	0.41283	-6.42202	-3.11615
H	-7.40946	-0.99981	-0.38120
H	3.97220	-4.93435	-2.05410
H	2.11457	-4.10271	-0.97167
H	-0.18518	-4.16596	-2.65687
H	1.62454	-5.44696	-2.83485
H	7.02303	-0.71587	0.39139
H	4.17959	2.73414	1.96837
H	-3.14145	-2.71292	3.78034
H	-5.00068	2.09831	3.24978
H	-6.07920	-0.39962	0.15866
H	3.59714	-2.61864	0.57943
H	3.56197	-1.10497	2.28967
H	-0.02709	-2.76054	2.66314
H	-1.30504	-4.91552	0.54601
H	1.88472	-1.83617	-2.27295
H	0.85993	-0.95255	1.77594
H	-0.96536	-0.56362	-2.11466
H	-2.05837	-2.10470	1.69279
H	-0.83792	0.49882	2.11055
H	-1.38428	1.65782	-1.87951
H	0.70667	1.06321	-2.01264
H	2.30095	1.74506	1.85237
H	-0.03191	2.13268	3.18234
H	-1.53251	3.86363	1.89284
H	0.64278	4.20727	-2.00816
H	-4.43361	2.09567	1.16603
H	-4.52190	0.43738	-2.17873
H	1.40623	5.02519	0.22554
O	-4.93569	3.37399	-1.58326
H	-4.26835	3.58405	-2.25710
H	-5.47296	2.64467	-1.97871

109
Hf4_4_2_term_perox_conf3_ion6_diconf1.log Energy: -3143080.3654596

Hf	2.06414	-1.09472	0.14143
O	2.32469	0.77683	1.22928
O	1.62143	0.57051	-1.05566
O	2.87109	-1.63732	-1.91322
O	2.59704	-1.47600	2.48701
O	2.51419	-3.22910	0.35450
O	4.27155	-0.93766	0.35986
Hf	-1.46219	-1.64350	-0.03643

O	0.40503	-1.86697	-1.03021
O	0.21963	-1.20913	1.20917
O	-2.05153	-2.32167	2.12749
O	-1.87403	-2.59381	-2.23471
O	-3.60397	-2.15290	-0.18985
O	-1.20772	-3.86317	0.13819
Hf	1.46102	2.44462	0.02011
O	-0.27425	2.60532	-1.18529
O	-0.35409	1.97376	1.11211
O	2.01425	3.24677	2.28493
O	2.56342	3.25865	-1.52761
O	3.33883	3.16989	-0.24714
O	0.93183	4.65777	0.44111
Hf	-2.09769	1.86888	-0.24173
O	-2.31954	0.01463	0.97669
O	-1.68417	0.03782	-1.28491
O	-2.72507	2.64397	-2.07522
O	-2.86096	2.73500	1.76270
O	-2.97747	3.57316	-0.93505
O	-4.32712	1.34892	-0.16653
Cl	-0.17486	-0.48381	-3.91402
Cl	0.40475	-3.01354	3.99951
Cl	5.22281	-0.19162	-3.27303
Cl	-4.32134	-4.41026	-2.85610
O	-1.38435	5.64477	-0.36579
O	5.10529	1.49752	0.87211
O	-5.40557	-0.88948	1.43822
O	-4.53343	-3.35740	2.49313
O	3.93088	-4.08832	-1.76036
O	-5.27270	2.10785	-2.49810
O	2.87079	-4.59460	2.51472
O	-5.22784	3.87367	2.00876
O	4.76031	3.02751	3.07980
O	-3.78726	-4.75834	0.15284
O	4.91562	-2.92294	3.19674
O	-4.94080	1.24231	3.04301
O	2.54111	5.89930	-1.27098
O	5.92310	-2.36504	-1.23527
H	3.55413	-1.04205	-2.33652
H	1.94588	-1.98279	3.04924
H	2.95904	-3.74016	-0.36772
H	4.90854	-1.48706	-0.17574
H	-2.92849	-2.76171	2.31627
H	-1.63569	-1.98309	-2.97128

H	-4.23057	-1.65650	0.39170
H	-0.74934	-4.30353	-0.64491
H	1.61627	4.13495	2.14755
H	1.54182	5.24634	-0.10422
H	-3.66904	3.34041	1.75185
H	-4.85357	1.58212	-0.99247
H	-1.95271	4.89275	-0.69756
H	4.64649	2.09944	0.23139
H	5.13342	2.01120	1.72468
H	-5.27891	-0.15848	2.10674
H	-6.34227	-0.86790	1.17704
H	-5.06224	-2.54671	2.31723
H	-4.72433	-3.60400	3.41319
H	4.84578	-3.72945	-1.64118
H	3.96890	-4.83248	-2.38169
H	-5.75373	2.94417	-2.38632
H	-4.30727	2.37707	-2.54626
H	3.67259	-4.14226	2.88949
H	-5.52025	3.04682	2.44896
H	5.22325	3.87224	2.95657
H	3.81797	3.23221	2.89834
H	-4.19166	-4.98245	-0.72220
H	-4.45236	-4.80209	0.86541
H	4.30480	-2.20583	2.92466
H	-4.03394	1.54690	2.82736
H	2.64608	4.95374	-1.57792
H	6.84468	-2.47993	-0.94890
H	-1.87466	6.00695	0.39021
H	0.00152	4.95810	0.18638
H	1.96426	6.31311	-1.93402
H	-5.24811	4.54924	2.70703
H	-4.94640	1.08507	4.00262
H	5.54866	-2.98766	2.46304
H	2.12973	-4.34861	3.10855
H	5.93231	-1.70838	-1.98516
H	-4.61617	0.48019	0.16890
H	-2.14707	3.17608	2.25596
H	1.47206	2.80444	2.96174
H	-0.39810	2.97882	-2.07035
H	-0.31844	1.27237	1.78041
H	1.19012	0.46433	-1.92589
H	3.26418	1.02455	1.36584
H	0.16435	-1.29346	2.17746
H	0.46586	-1.69384	-1.99237

H	-1.28868	0.05678	-2.18917
H	-2.38526	-0.08097	1.93818
H	-1.36278	-2.76718	2.67720
H	-2.04002	-4.37175	0.29999
H	-2.75196	-3.02094	-2.45408
H	2.53184	-0.54297	2.77488
H	2.64021	-3.75332	1.22836
H	4.70490	-0.05557	0.56850
H	3.17114	-2.56751	-2.08751
H	-3.81710	-3.13231	-0.11855
O	-0.23973	-4.86629	-2.10508
H	-0.71278	-4.11259	-2.51862
H	0.70148	-4.64387	-2.19449

109
Hf4_4_2_term_perox_conf3_ion6_diconf2.log Energy: -3143067.1582427

Hf	2.27955	0.24183	-0.06193
O	1.81415	-1.34628	-1.39510
O	1.69212	-1.53691	0.96586
O	3.27279	0.31599	1.94830
O	3.11892	0.97576	-2.14799
O	3.06498	2.35426	0.21480
O	4.38470	-0.51696	-0.31636
Hf	-0.80768	1.98324	0.18754
O	0.82417	1.11189	1.22814
O	0.71173	1.25115	-1.08695
O	-0.87430	3.30312	-1.82279
O	-0.85249	2.88418	2.30744
O	-2.55963	3.30698	0.31914
O	0.60067	3.80509	0.24594
Hf	0.57545	-2.86094	-0.35036
O	-1.05278	-2.20674	0.85615
O	-1.05341	-1.85736	-1.51172
O	0.53839	-3.63840	-2.59211
O	0.71905	-4.30173	1.10558
O	2.65516	-3.82372	-0.73978
O	0.02145	-4.81226	-0.12174
Hf	-2.55899	-1.06851	-0.09537
O	-2.05734	0.85046	-1.09542
O	-1.91031	0.51499	1.24108
O	-3.72430	-1.71554	1.48264
O	-3.55791	-1.28538	-2.21983
O	-3.90255	-2.55242	0.24652
O	-4.59935	0.12217	-0.13266

Cl	-0.34811	0.36530	4.05136
Cl	0.78400	1.81761	-4.09821
Cl	5.14562	-1.55207	3.50856
Cl	-2.35914	5.54844	3.15100
O	-3.58629	-4.92265	1.65104
O	5.37871	-0.53855	-2.97095
O	-4.74858	2.76371	-1.28631
O	-3.09731	4.77491	-2.35426
O	5.32676	1.66889	2.94335
O	-4.97060	-3.25102	3.37137
O	5.26692	3.08801	-1.17019
O	-6.18629	-1.57597	-2.50330
O	2.13627	-6.41351	-0.53367
O	-2.06056	5.82567	0.01731
O	5.74250	2.30713	-3.70239
O	-5.02624	0.90997	-3.21862
O	-1.30853	-3.94938	2.86839
O	6.31516	1.17489	0.39775
H	3.71066	-0.49707	2.32096
H	2.51104	1.29969	-2.85935
H	2.29908	2.97715	0.21459
H	5.14654	0.04431	0.02867
H	-1.68168	3.82452	-2.09366
H	-0.77994	2.23069	3.04886
H	-3.33166	3.07042	-0.24743
H	0.58847	4.48790	1.00966
H	0.60716	-4.60685	-2.65812
H	3.07172	-3.54716	-1.57184
H	-4.51893	-1.58720	-2.20683
H	-4.90387	-0.13478	0.75959
H	-3.61867	-4.18833	0.99152
H	6.32037	-0.65497	-2.75131
H	5.18398	-1.22195	-3.63633
H	-4.88058	2.13556	-2.05393
H	-5.62890	3.10233	-1.04848
H	-3.84436	4.16836	-2.14837
H	-3.21693	5.04559	-3.27929
H	5.86796	1.61687	2.12307
H	5.49853	0.80386	3.37726
H	-5.90211	-3.22837	3.09958
H	-4.52923	-2.60496	2.76360
H	5.39707	2.85088	-2.13335
H	-6.18023	-0.64569	-2.81457
H	1.22412	-6.04504	-0.38400

H	2.09263	-6.87351	-1.38769
H	-2.43266	6.18623	0.84965
H	-2.67297	6.02238	-0.71805
H	5.06408	2.59052	-4.33702
H	-4.26922	0.29842	-3.08870
H	-0.53397	-4.28295	2.34961
H	6.09948	1.94053	-0.20343
H	-4.17432	-4.56021	2.35627
H	-2.09473	-4.39914	2.46207
H	-6.37779	-2.09987	-3.29912
H	-4.96611	1.22019	-4.13801
H	5.69682	1.33087	-3.70457
H	5.58694	3.99873	-1.06157
H	7.22372	0.89992	0.19118
H	-4.60160	1.09818	-0.20709
H	-3.05369	-1.93278	-2.74353
H	-0.35644	-3.41017	-2.90686
H	2.64173	-4.82846	-0.70836
H	-1.24714	-2.70468	1.70180
H	-0.74506	-1.21330	-2.16880
H	1.33986	-1.43268	1.86445
H	1.83427	-1.22331	-2.35563
H	0.65105	1.29166	-2.06953
H	0.76731	0.87364	2.17977
H	-1.60477	0.27165	2.14281
H	-2.00707	0.98439	-2.05275
H	-0.42419	2.98496	-2.64239
H	0.42882	4.28118	-0.59010
H	-1.51461	3.57510	2.56422
H	3.88018	0.54101	-2.57850
H	3.75077	2.69440	-0.42377
H	4.65831	-0.81190	-1.21322
H	3.89634	1.04963	2.23078
H	-2.39771	4.31208	0.23724
O	0.62781	5.60808	2.12495
H	-0.29541	5.67816	2.47662
H	1.13794	5.24133	2.86659

109
Hf4_4_2_term_perox_conf3_ion6_diconf4.log Energy: -3143076.8117981

Hf	-1.69647	-1.49868	-0.19406
O	-2.08799	0.12579	-1.49309
O	-1.56879	0.28016	0.90231
O	-2.61531	-1.92760	1.83401

O	-2.04176	-2.42213	-2.46389
O	-1.62970	-3.69502	-0.11873
O	-3.87427	-1.83178	-0.57715
Hf	1.85405	-1.35686	0.14399
O	0.01095	-1.92788	1.10196
O	0.20201	-1.45322	-1.17743
O	2.70128	-2.15921	-1.86483
O	2.35116	-1.87462	2.45748
O	4.04598	-1.34686	0.41793
O	2.10936	-3.58883	0.30651
Hf	-1.84405	2.03101	-0.33871
O	-0.14638	2.85529	0.66168
O	0.01078	1.75239	-1.40018
O	-2.71276	2.88501	-2.01465
O	-2.59902	2.81557	1.75418
O	-4.05384	1.36528	-0.03035
O	-2.47476	3.89033	-0.92956
Hf	1.72551	2.22862	-0.10923
O	2.39800	0.32050	-1.05283
O	1.60388	0.47510	1.14309
O	2.50010	3.12116	1.59523
O	2.32575	2.97594	-2.20180
O	2.35521	4.09785	0.46748
O	4.13440	2.25105	-0.19607
Cl	0.12340	-0.07909	3.80428
Cl	0.55896	-3.40650	-3.73586
Cl	-4.54416	0.43843	2.95155
Cl	5.12908	-2.93897	3.37919
O	0.21722	5.32292	1.72974
O	-4.55034	-0.29874	-2.70506
O	5.63145	0.00833	-1.35966
O	5.35772	-2.70974	-2.04487
O	-4.20186	-3.91923	2.55834
O	1.45124	4.14570	3.88425
O	-3.37165	-5.46674	-0.76465
O	4.38022	4.54783	-2.68508
O	-5.24593	2.24627	-2.20515
O	4.82465	-3.87086	0.44695
O	-4.10713	-4.30001	-3.05921
O	4.71864	1.76040	-3.21884
O	-4.26922	4.71294	0.87225
O	-5.73459	-1.98956	1.37163
H	-3.07704	-1.16047	2.25008
H	-1.24313	-2.90667	-2.82621

H	-1.04802	-4.03506	0.58028
H	-4.55909	-1.87942	0.14770
H	3.65059	-2.44313	-1.98042
H	1.92508	-1.25912	3.10020
H	4.57998	-0.81685	-0.22349
H	1.75657	-4.00486	1.15076
H	-3.07246	2.12402	2.26622
H	-4.39828	1.12176	0.85876
H	2.97783	3.74019	-2.31170
H	4.21864	2.57175	0.72575
H	1.02085	5.13068	1.18684
H	-4.98693	0.59200	-2.63969
H	-4.71719	-0.63242	-3.60104
H	5.35505	0.60084	-2.11422
H	6.54060	0.26117	-1.12443
H	5.68504	-1.78337	-1.98815
H	5.64370	-3.04108	-2.91206
H	-4.99142	-3.42119	2.24375
H	-4.26744	-3.91382	3.52772
H	2.13040	4.73837	4.24442
H	1.88833	3.71863	3.09975
H	-3.73361	-5.12749	-1.63321
H	4.87054	3.74106	-2.95203
H	-5.90362	2.88120	-2.52854
H	-4.33095	2.66547	-2.27578
H	5.24343	-3.86665	1.34201
H	5.50090	-3.83244	-0.25670
H	-3.45046	-3.57801	-2.95238
H	3.77115	1.90377	-3.01045
H	-3.98266	5.59831	1.15080
H	-6.65602	-1.95777	1.06408
H	0.52456	5.07996	2.63660
H	-3.27077	3.54261	1.59444
H	-3.77270	4.53676	0.02810
H	4.26882	5.05448	-3.50700
H	4.74311	1.47295	-4.14754
H	-4.96872	-3.86683	-2.94470
H	-2.91104	-6.29380	-0.98390
H	-5.59262	-1.18149	1.92394
H	4.60580	1.39989	-0.27425
H	1.54765	3.13839	-2.76374
H	-4.76947	1.75847	-0.58580
H	-0.19302	3.68848	1.19825
H	0.00375	0.95220	-1.94852

H	-1.12685	0.30958	1.77573
H	-2.90895	0.11683	-2.03249
H	0.30642	-1.62612	-2.13253
H	-0.12554	-1.69765	2.04275
H	1.20989	0.52818	2.04402
H	2.49789	0.12283	-1.99552
H	2.12748	-2.74435	-2.42158
H	3.04021	-3.90910	0.21483
H	3.29570	-2.02906	2.74880
H	-2.13058	-1.65169	-3.05474
H	-2.32926	-4.41106	-0.37003
H	-4.27631	-1.32621	-1.33241
H	-3.12227	-2.75677	2.10210
H	4.46842	-2.25340	0.50219
O	1.45271	-4.51732	2.70710
H	1.66517	-3.61182	3.01585
H	0.51910	-4.65294	2.93708

109
Hf4_4_2_term_perox_conf3_ion6_diconf5.log Energy: -3143090.4085102

Hf	2.21155	-1.15424	0.33922
O	2.23268	0.71496	1.30163
O	1.78701	0.43318	-0.94944
O	3.23488	-1.62451	-1.62905
O	2.57480	-1.68234	2.61227
O	2.71790	-3.32919	0.42498
O	4.44312	-0.78766	0.73821
Hf	-1.25698	-1.94577	0.12614
O	0.68132	-2.16445	-0.83496
O	0.34418	-1.30198	1.30453
O	-1.72135	-2.60674	2.38104
O	-1.66291	-3.11584	-1.90334
O	-3.37208	-2.54263	0.15172
O	-0.72574	-4.08841	0.56730
Hf	1.42424	2.34259	0.09729
O	-0.20754	2.18589	-1.31688
O	-0.41242	1.83345	0.99923
O	1.88736	3.27362	1.87126
O	2.55097	2.95802	-1.82554
O	3.03103	3.38572	0.91674
O	0.64446	4.52873	-0.29119
Hf	-2.04838	1.48614	-0.45689
O	-2.22727	-0.24026	0.98219
O	-1.49329	-0.42239	-1.28417

O	-2.61858	1.93454	-2.37178
O	-2.88161	2.75990	1.31445
O	-2.92152	3.08107	-1.45947
O	-4.20352	0.77345	-0.47935
Cl	0.04132	-1.37332	-3.86211
Cl	-0.42369	-0.02611	3.92586
Cl	4.63797	0.89755	-3.05939
Cl	-4.36408	-3.44644	-3.33067
O	-1.07029	4.81673	-2.28681
O	5.05382	1.66764	1.48492
O	-5.21108	-0.86943	1.61771
O	-4.23363	-2.97781	3.19120
O	5.22377	-3.35289	-2.06318
O	-5.62150	2.81024	-1.36945
O	4.04344	-4.58371	2.30681
O	-5.47756	3.61662	1.30577
O	-1.05435	4.64078	1.96280
O	-4.55436	-4.74789	-0.54344
O	5.15449	-2.17676	3.04672
O	-4.76722	1.45446	2.92630
O	3.14903	5.41018	-0.72190
O	6.28831	-0.98429	-1.22709
H	3.55650	-0.83531	-2.13109
H	1.96182	-1.31306	3.27391
H	1.93294	-3.82839	0.13365
H	5.10516	-0.92279	0.00082
H	-2.67400	-2.74382	2.67282
H	-1.12386	-2.70522	-2.63213
H	-3.98746	-1.94290	0.62602
H	-0.79713	-4.84241	-0.10305
H	3.21777	2.30571	-2.16546
H	1.39863	5.15796	-0.40896
H	-3.72195	3.25698	1.13781
H	-4.89345	1.41650	-0.82920
H	-1.82415	4.22767	-1.98283
H	4.29305	2.29353	1.30821
H	5.19647	1.70691	2.44478
H	-5.06543	-0.07735	2.20836
H	-6.17269	-0.93340	1.48287
H	-4.72970	-2.25080	2.75207
H	-4.28423	-2.78194	4.14122
H	5.87485	-2.64524	-1.84881
H	5.30370	-3.48721	-3.02196
H	-5.81589	3.20505	-0.49228

H	-4.69346	3.11452	-1.54732
H	4.60448	-3.86376	2.67857
H	-5.59445	2.91787	1.98791
H	-0.50662	4.72082	1.14739
H	-0.43684	4.19223	2.56586
H	-4.64010	-4.50260	-1.50183
H	-5.46496	-4.75691	-0.20311
H	5.79111	-1.83277	3.69413
H	-3.88772	1.78398	2.63212
H	3.30685	4.85895	0.09425
H	7.17652	-0.70505	-0.94891
H	-1.42487	5.72043	-2.27537
H	0.02859	4.63982	-1.08609
H	3.00201	3.82798	-1.71376
H	3.71871	6.19344	-0.67309
H	-5.68517	4.45832	1.74341
H	-4.75174	1.46857	3.89803
H	5.29581	-1.68578	2.20806
H	3.45313	-4.83785	3.03547
H	5.96165	-0.29829	-1.86573
H	-4.57954	0.21460	0.23271
H	-2.19139	3.44163	1.59475
H	-0.25604	2.52424	-2.22243
H	-0.42712	1.47932	1.90679
H	1.28087	0.29426	-1.76757
H	2.41316	0.93644	2.22629
H	0.17978	-0.79489	2.13787
H	0.78592	-2.08573	-1.80575
H	-1.12410	-0.50505	-2.19177
H	-2.06519	-0.08796	1.92920
H	-1.30804	-2.02783	3.05767
H	-1.06126	-4.36289	1.43868
H	-2.59660	-3.12590	-2.27310
H	3.48108	-1.74226	3.01194
H	3.16781	-3.82464	1.18812
H	4.60529	0.16853	1.05827
H	3.89539	-2.36822	-1.77194
H	-3.84384	-3.41878	-0.06706
O	-0.97563	-5.77191	-1.41304
H	-1.23881	-4.98010	-1.93127
H	-0.10131	-6.01992	-1.75794

109
Hf4_4_2_term_perox_conf3_ion6_diconf6.log Energy: -3143084.6170433

Hf	-2.26354	-1.00029	-0.06472
O	-2.29316	0.80458	-1.26918
O	-1.71955	0.86492	0.99138
O	-3.42400	-1.30687	1.60008
O	-3.15753	-1.50893	-2.11127
O	-2.25168	-3.31805	-0.14877
O	-4.26621	-0.88504	0.43541
Hf	1.20408	-1.80624	0.11269
O	-0.62645	-1.60652	1.19569
O	-0.39437	-1.30477	-1.17848
O	1.58954	-3.00653	-1.91563
O	1.51279	-2.60176	2.32799
O	3.22807	-2.64086	0.22339
O	0.36114	-3.91843	0.16582
Hf	-1.36240	2.44197	-0.30694
O	0.45578	2.62645	0.74840
O	0.33592	1.59682	-1.34562
O	-1.50166	3.06176	-2.66491
O	-1.99345	3.53866	1.53431
O	-3.44287	3.22340	-0.68999
O	-0.83651	4.65761	-0.73564
Hf	2.18211	1.61429	-0.08192
O	2.25462	-0.39553	-1.08788
O	1.68213	-0.03760	1.17623
O	2.88965	2.55126	1.63450
O	2.90760	2.22725	-2.17972
O	3.11026	3.37779	0.41069
O	4.34975	0.95740	-0.13713
Cl	0.18066	-0.21923	3.90162
Cl	-0.83746	-2.64887	-3.98567
Cl	-3.01942	2.66124	4.21724
Cl	3.88643	-4.01944	3.68901
O	1.42628	5.42831	0.36749
O	-5.07786	1.73529	0.79944
O	5.17992	-1.48440	-1.42981
O	4.00594	-3.62333	-2.82992
O	-3.21818	-3.98958	2.14925
O	5.43222	1.94766	2.03670
O	-2.86672	-4.70727	-2.30758
O	5.31848	3.20338	-2.55799
O	-4.02821	2.07904	-3.08899
O	3.81151	-5.09253	0.81443
O	-5.18399	-3.21628	-2.36445
O	4.93628	0.49284	-3.26630

O	-0.96995	6.02181	1.64079
O	-6.16127	-2.78685	0.05395
H	-2.52453	-1.79031	-2.81390
H	-2.68296	-3.71670	0.68930
H	2.49988	-3.23401	-2.28022
H	1.27296	-1.91201	2.99597
H	3.90428	-2.22915	-0.36270
H	-0.63318	-3.79602	0.10622
H	-1.26182	4.00924	-2.65330
H	-2.32971	3.14786	2.40160
H	-4.06951	2.75269	-0.04795
H	-1.39835	5.31746	-0.28171
H	3.74922	2.78490	-2.25358
H	4.92367	1.25859	0.63471
H	2.08053	4.65992	0.43894
H	-5.94988	1.75145	0.37224
H	-4.76617	0.79554	0.70164
H	5.14669	-0.80623	-2.16220
H	6.11953	-1.60641	-1.20922
H	4.58697	-2.93424	-2.43690
H	4.04168	-3.46661	-3.78801
H	-3.46394	-3.03351	2.19485
H	-2.34916	-4.05915	2.62397
H	5.95230	2.73436	1.80399
H	4.48720	2.27565	2.08978
H	-3.77433	-4.38045	-2.50451
H	5.58101	2.31313	-2.87796
H	-4.84896	2.14420	-3.60343
H	-3.32934	2.51080	-3.61287
H	3.92083	-4.94544	1.79171
H	4.69824	-5.32613	0.49160
H	-5.82739	-3.00120	-3.05883
H	4.03782	0.85191	-3.11152
H	-1.13196	6.62505	2.38313
H	-7.02392	-2.34250	0.01564
H	1.89730	6.14794	-0.08396
H	0.10065	4.90534	-0.43768
H	-1.64396	4.45176	1.72475
H	0.00398	5.97239	1.51655
H	5.37465	3.77654	-3.34111
H	4.95403	0.21925	-4.19946
H	-5.66278	-3.13144	-1.48218
H	-2.28699	-4.27692	-2.97086
H	-5.50968	-2.06561	0.26945

H	4.55966	0.02799	-0.36057
H	2.22327	2.61952	-2.74880
H	-0.72357	2.59974	-3.02980
H	-3.76823	2.93296	-1.58424
H	0.58719	3.03435	1.61760
H	0.11337	0.71073	-1.68981
H	-1.29058	0.81911	1.86535
H	-2.90342	0.88253	-2.02684
H	-0.42623	-1.56794	-2.12529
H	-0.60792	-1.29931	2.12644
H	1.32707	0.11250	2.08324
H	2.20322	-0.51616	-2.04728
H	0.95766	-2.96596	-2.67151
H	0.64268	-4.31096	-0.68390
H	2.35448	-3.02257	2.66960
H	-3.96785	-2.09246	-2.20584
H	-2.53514	-3.85259	-0.96096
H	3.48700	-3.61276	0.41167
O	-0.71048	-4.25869	3.28680
H	-0.01905	-3.75690	2.80673
H	-0.70070	-3.87956	4.18043

109

Hf4_4_2_term_perox_conf3_ion6_diconf9.log Energy: -3143089.6787920

Hf	-1.78886	-1.74075	-0.50739
O	-1.59732	0.23290	-1.38320
O	-2.44959	-0.08544	0.72861
O	-2.95014	-2.73311	1.28786
O	-2.57715	-2.04848	-2.44079
O	-1.24644	-3.99986	-0.68602
O	-3.59196	-2.17514	-1.35146
Hf	1.70307	-1.63366	-0.03488
O	-0.17052	-2.00880	0.90482
O	0.15073	-1.74205	-1.48366
O	2.64513	-2.22936	-2.26049
O	2.21484	-2.84689	1.84770
O	3.90701	-1.73703	0.09665
O	1.53407	-3.88068	-0.57932
Hf	-1.89077	1.79404	-0.05626
O	-0.33579	1.83637	1.34438
O	0.04509	2.34414	-0.90526
O	-2.32071	2.60601	-2.41644
O	-2.90260	2.29378	1.99556
O	-4.05735	1.92689	-0.45788

O	-2.06419	4.03146	0.04082
Hf	1.68975	1.85493	0.54491
O	2.12467	0.24520	-0.90068
O	1.76123	-0.10317	1.43031
O	2.01443	2.60019	2.41439
O	2.50293	3.11471	-1.31524
O	2.03041	3.70135	1.39906
O	3.93576	1.66921	0.67928
Cl	0.46814	-1.44765	3.99366
Cl	0.66630	0.49787	-3.68323
Cl	-3.72611	-0.40731	3.53863
Cl	4.98333	-3.78440	2.97550
O	-0.07584	5.27568	1.26483
O	-5.21734	-0.01145	-1.77323
O	5.45133	0.26700	-1.25967
O	5.29677	-2.18405	-2.62846
O	-5.48698	-3.24895	0.92072
O	4.75258	4.03827	1.49200
O	-2.36918	-4.64416	-2.97666
O	4.75489	4.58301	-1.26066
O	-4.61116	4.09705	-1.92145
O	5.14672	-3.99505	-0.08869
O	-3.28507	0.34379	-3.69658
O	4.73223	2.30787	-2.86240
O	-2.41434	4.85475	2.58491
O	-6.32882	-0.81106	1.73227
H	-3.01578	-2.18801	2.10436
H	-1.50196	-4.58122	0.09380
H	3.63494	-2.21446	-2.42845
H	1.73723	-2.53647	2.65935
H	4.39105	-1.03013	-0.38272
H	0.55221	-4.04468	-0.61240
H	-1.55215	2.98551	-2.87599
H	-3.22475	1.59895	2.61351
H	-4.51994	1.13398	-0.90500
H	-2.58872	4.37790	0.80497
H	3.22253	3.78779	-1.15106
H	4.41579	2.48726	1.01842
H	0.72845	4.68436	1.40983
H	-4.81009	0.19814	-2.64418
H	-4.73471	-0.84276	-1.52334
H	5.24528	0.95842	-1.95045
H	6.37197	0.42303	-0.98503
H	5.54174	-1.28953	-2.30418

H	5.52941	-2.19168	-3.57142
H	-5.89617	-2.37948	1.19045
H	-5.73873	-3.87081	1.62343
H	4.95496	4.41325	0.60891
H	3.77509	4.16596	1.57877
H	-2.53405	-3.65860	-2.98740
H	5.10364	3.93461	-1.91373
H	-4.42682	4.89277	-1.39564
H	-3.74909	3.87046	-2.33204
H	5.33163	-4.09611	0.88077
H	5.99899	-3.81992	-0.52220
H	-2.94371	-0.51211	-3.31543
H	3.76586	2.37804	-2.71250
H	-2.89197	5.54391	3.07199
H	-7.12623	-0.85395	2.28511
H	0.26202	6.13945	0.97813
H	-1.18080	4.47817	0.20752
H	-2.71749	3.12701	2.49371
H	-1.49789	5.18138	2.41687
H	4.71011	5.43587	-1.72389
H	4.85566	2.24352	-3.82457
H	-3.31000	0.22815	-4.66017
H	-1.68891	-4.79249	-3.65410
H	-5.59725	-0.61823	2.36271
H	4.47599	1.21703	-0.00514
H	1.73153	3.61058	-1.64470
H	-2.62171	1.82523	-2.96156
H	-4.38225	2.75218	-0.92407
H	-0.46447	1.74613	2.30005
H	0.22219	1.98549	-1.79739
H	-2.82605	-0.19229	1.63010
H	-1.05729	0.33263	-2.19281
H	0.23662	-1.22931	-2.31255
H	-0.23903	-1.87771	1.87581
H	1.43592	-0.29008	2.33868
H	1.92548	0.38089	-1.85171
H	2.23035	-1.77252	-3.01411
H	1.81691	-3.84272	-1.51659
H	3.14687	-3.04786	2.13650
H	-1.62614	-4.40932	-1.52846
H	-3.92300	-2.95977	1.06725
H	4.42212	-2.61535	-0.01269
O	-1.93735	-5.29651	1.52783
H	-1.14291	-5.38805	2.07999

H	-2.33853	-4.44218	1.79931

109
Hf4_4_2_term_perox_conf4_ion11_diconf9.log Energy: -3143102.0634192

Hf	-1.10869	-2.21467	-0.18357
O	-1.79197	-0.48976	-1.30002
O	-1.56344	-0.44235	1.01529
O	-2.24085	-3.05066	1.60683
O	-1.49185	-3.07762	-2.05833
O	-0.22358	-4.39229	0.18603
O	-2.60486	-3.28824	-1.08939
Hf	2.30147	-1.34848	0.38412
O	0.52447	-2.10412	1.29556
O	0.81608	-1.86593	-1.05654
O	3.64440	-2.03819	-1.30032
O	2.92753	-1.88616	2.55362
O	4.36796	-0.43785	0.83637
O	2.47922	-3.66328	0.46814
Hf	-1.98372	1.23152	-0.11292
O	-0.50427	2.16745	1.08755
O	-0.18523	1.70741	-1.16353
O	-2.55739	2.09238	-2.40616
O	-2.96350	1.55001	1.98367
O	-4.12869	0.69236	-0.41576
O	-2.90095	3.30689	-0.13098
Hf	1.46585	2.14735	0.10097
O	2.34732	0.38704	-0.82973
O	1.67228	0.39742	1.36849
O	2.06946	2.99585	2.16951
O	2.32426	2.88125	-1.62913
O	0.69946	4.41297	0.14383
O	3.22146	3.14574	-0.47065
Cl	-0.31964	1.00940	-4.33844
Cl	2.17253	0.65536	4.44670
Cl	2.93101	-4.84144	-2.40628
Cl	-3.67056	-1.01799	3.75626
O	-1.24503	4.59884	-1.89984
O	-4.60106	-1.51397	-1.84626
O	5.22646	1.46284	-0.87152
O	4.21775	0.01727	-2.88072
O	-4.53365	-4.32309	1.27853
O	-0.09313	4.44820	2.77025
O	-0.28451	-5.48256	-2.15708
O	2.88018	5.78657	-0.45247

O	-5.32113	2.43784	-2.04683
O	5.59602	-2.42831	2.25460
O	-2.56602	-1.31923	-3.80449
O	0.73523	4.01557	-3.48959
O	-4.24990	3.95211	2.08963
O	-5.90644	-2.02314	1.71479
H	-2.53903	-2.37782	2.26293
H	-0.71908	-4.81646	0.90739
H	3.94798	-1.34343	-1.95638
H	2.85702	-1.11936	3.17442
H	4.75688	0.22648	0.20150
H	1.54486	-3.93490	0.64377
H	-2.22104	3.01985	-2.40653
H	-3.26935	0.72696	2.43870
H	-4.28278	-0.17330	-0.92003
H	-3.32319	3.72325	0.66589
H	2.24640	2.31419	2.86058
H	1.44341	5.05303	-0.09171
H	-1.57443	5.47722	-2.15684
H	-4.19654	-1.28474	-2.70818
H	-3.97016	-2.20268	-1.50818
H	4.51698	2.16547	-0.72401
H	6.08769	1.88813	-0.73088
H	4.79264	0.60702	-2.32809
H	4.63865	-0.07239	-3.75015
H	-5.13780	-3.54157	1.40719
H	-4.66601	-4.87013	2.07010
H	-0.02109	4.74985	1.83609
H	-0.03790	5.24592	3.32132
H	-0.76268	-4.63350	-2.36151
H	3.25453	4.86468	-0.49047
H	-5.34578	3.30415	-1.60715
H	-4.44840	2.42670	-2.49539
H	6.21776	-2.25999	2.98233
H	5.86312	-3.28062	1.87157
H	-2.11079	-2.09520	-3.38010
H	1.43642	3.79069	-2.82596
H	-5.19259	4.14547	1.95312
H	-6.74433	-2.15469	2.18790
H	-0.49432	4.37857	-2.56041
H	-2.33398	3.97084	-0.58585
H	-3.61301	2.26461	2.17232
H	-3.93614	4.58790	2.75452
H	3.23182	6.16314	0.37125

H	0.50162	3.15022	-3.89126
H	-1.86956	-0.79780	-4.25392
H	0.65399	-5.30800	-2.39344
H	-5.29510	-1.64831	2.38980
H	1.36133	3.58755	2.55297
H	-0.01972	4.55386	-0.51983
H	-2.01882	1.65516	-3.11555
H	-4.68018	1.37582	-0.90015
H	-0.72288	2.53416	1.95899
H	-0.04720	1.33105	-2.05840
H	-1.14282	-0.34773	1.90197
H	-2.10645	-0.62577	-2.22393
H	0.88434	-1.56886	-1.97555
H	0.29903	-1.83997	2.20991
H	1.41542	0.42758	2.30916
H	2.65823	0.46440	-1.74998
H	3.39899	-2.85301	-1.81285
H	2.71216	-4.13010	-0.37573
H	3.86214	-2.20855	2.61570
H	-0.27517	-4.98647	-0.64039
H	-3.06992	-3.60021	1.41408
H	5.07282	-1.04259	1.15871
O	-0.50671	-0.79999	3.53477
H	-1.37526	-0.84956	3.98618
H	0.10427	-0.26329	4.08362

109
Hf4_4_2_term_perox_conf4_ion12_diconf10.log Energy: -3143093.4614379

Hf	-2.56763	-0.88591	-0.47752
O	-1.71438	0.93424	-1.35142
O	-1.69322	0.54187	0.98624
O	-3.71898	-1.49564	1.37941
O	-3.39530	-1.07607	-2.32565
O	-3.83627	-2.18002	-1.41515
O	-4.34022	0.52637	-0.27708
Hf	0.53586	-2.70742	-0.35367
O	-1.35440	-2.43666	0.53782
O	-0.77754	-1.61363	-1.55718
O	0.84042	-3.57980	-2.53837
O	0.55254	-3.93786	1.69149
O	2.41397	-3.92953	-0.36374
O	-0.43432	-4.76276	-0.69460
Hf	-0.65568	2.10064	0.03768
O	0.93877	1.45319	1.34181

O	1.06736	1.39067	-1.03982
O	-0.60235	3.31637	-2.04235
O	-1.18670	3.05797	2.07949
O	-2.56550	3.25090	-0.11578
O	0.39496	4.13000	0.29891
Hf	2.42568	0.29543	0.18660
O	1.88657	-1.31588	-1.19388
O	1.24952	-1.32232	1.03135
O	3.15795	0.04326	2.44866
O	3.87914	0.43807	-1.28359
O	3.45580	2.22873	0.67345
O	4.35986	-0.40536	-0.15064
Cl	-0.21271	0.82937	-4.07105
Cl	0.85936	-1.75355	4.05432
Cl	1.92311	5.13349	-2.10674
Cl	-2.66528	1.19185	4.03216
O	3.17681	2.65359	3.36644
O	-4.21052	2.50632	-2.14703
O	4.59366	-2.75635	-1.27710
O	3.06805	-2.43420	-3.45453
O	-6.28789	-0.90978	1.88615
O	5.74443	-0.26402	2.12430
O	-6.55614	-2.01691	-0.82405
O	5.84208	3.08953	-0.12695
O	-1.90583	5.81000	0.27251
O	2.56540	-5.77419	1.62091
O	-3.61134	0.87643	-4.17376
O	6.12657	1.51962	-2.29072
O	1.07185	4.26095	2.87459
O	-5.12040	1.51578	2.15354
H	-3.27586	-1.83865	2.18880
H	-4.49850	0.98768	0.58435
H	1.68949	-3.28366	-2.97761
H	0.64623	-3.37171	2.49475
H	3.28026	-3.51544	-0.66474
H	-0.69581	-5.25979	0.10018
H	0.18582	3.90824	-2.17307
H	-1.72676	2.52361	2.71946
H	-3.05094	3.09941	-0.96756
H	0.83538	4.24397	1.18873
H	2.69699	-0.64249	2.98143
H	4.36839	2.47852	0.32988
H	3.09463	1.67236	3.35856
H	-5.03069	2.98084	-2.35771

H	-3.95105	1.99084	-2.96962
H	4.56903	-1.84629	-0.82996
H	5.46329	-3.14948	-1.09911
H	3.83875	-2.62573	-2.86291
H	3.39003	-2.42073	-4.36928
H	-6.09695	0.03709	2.09898
H	-6.61449	-1.31428	2.70622
H	6.17519	0.55951	2.40763
H	5.55297	-0.14429	1.16090
H	-5.59844	-2.02805	-1.05354
H	6.05608	2.57785	-0.95696
H	-0.98084	5.48559	0.31308
H	-1.96016	6.28878	-0.57146
H	3.27412	-5.74023	2.28525
H	2.39368	-6.71622	1.45433
H	-3.74378	0.06230	-3.63066
H	5.28675	1.06930	-2.00410
H	1.13400	5.11069	3.33937
H	-5.50358	2.40464	2.23055
H	3.94221	2.87153	3.92276
H	1.03461	4.44819	-0.40680
H	-0.43142	3.44420	2.59124
H	1.82476	3.69411	3.18191
H	6.51650	2.81352	0.51398
H	6.82417	0.87481	-2.09018
H	-2.64580	0.89241	-4.33206
H	-6.57097	-1.59990	0.05589
H	-4.39011	1.46457	2.82391
H	4.15282	-0.14674	2.47382
H	3.38258	2.56437	1.59809
H	-0.57420	2.70510	-2.81346
H	-2.46911	4.23737	0.02966
H	0.64937	1.11093	2.20048
H	0.99058	1.20636	-1.99624
H	-1.89573	0.51089	1.94358
H	-1.41888	0.87858	-2.28349
H	-0.42323	-1.03509	-2.25574
H	-1.55422	-2.74260	1.44766
H	0.91677	-1.30879	1.95544
H	2.27973	-1.33294	-2.08681
H	0.11738	-3.24314	-3.09624
H	0.05245	-5.35997	-1.28991
H	1.21827	-4.66033	1.80559
H	-4.35049	1.22569	-0.98322

H	-4.68621	-1.34405	1.56661
H	2.61831	-4.65354	0.27542
O	-2.10166	-2.69426	3.21335
H	-2.29960	-3.52363	3.67715
H	-1.32431	-2.30180	3.66978

109
Hf4_4_2_term_perox_conf4_ion12_diconf9.log Energy: -3143100.5461829

Hf	-2.57032	-0.90579	-0.26402
O	-1.87737	0.88634	-1.23254
O	-1.56931	0.51012	1.03795
O	-3.76066	-1.07945	1.66864
O	-3.67800	-1.01853	-2.05306
O	-3.30752	-3.18811	-0.22509
O	-4.47333	-0.49369	-0.90481
Hf	0.50061	-2.66262	-0.16393
O	-1.20358	-2.13809	0.94244
O	-0.99948	-1.78324	-1.45292
O	0.60260	-3.67687	-2.34038
O	0.63570	-3.83984	1.90244
O	2.27460	-3.98707	-0.29688
O	-0.84178	-4.50551	-0.32233
Hf	-0.71213	2.11491	0.02726
O	0.97723	1.51836	1.26452
O	0.94133	1.35875	-1.09495
O	-0.68899	3.21707	-2.17023
O	-1.22007	2.91618	2.14741
O	-2.64178	3.24582	-0.09871
O	0.17181	4.14717	0.23486
Hf	2.40515	0.34706	0.08406
O	1.68714	-1.30291	-1.20599
O	1.55201	-1.35019	1.11121
O	3.39890	0.39146	2.27109
O	3.77664	0.39085	-1.47302
O	3.39030	2.37073	0.34140
O	4.27597	-0.45705	-0.34772
Cl	0.00029	0.62751	-4.04068
Cl	2.02341	-1.86857	4.12486
Cl	1.70254	5.14982	-2.18379
Cl	-3.21737	1.18312	4.03468
O	3.17003	3.05003	2.99616
O	-4.64129	2.19955	-1.52686
O	4.38722	-2.86052	-1.37159
O	2.73870	-2.57517	-3.47492

O	-6.33295	-0.49741	1.69193
O	5.95400	0.35049	1.62311
O	-4.98300	-3.31156	-2.20415
O	6.05065	2.65018	0.09339
O	-2.36984	5.44033	-1.60901
O	2.16883	-6.05886	1.44568
O	-3.18455	1.07472	-3.67779
O	6.08507	1.51662	-2.29116
O	0.86220	4.43200	2.81006
O	-5.65845	2.08259	2.17426
H	-3.47006	-0.47400	2.39030
H	-3.69628	-3.34503	0.65427
H	1.43519	-3.44296	-2.84568
H	1.11820	-3.38342	2.63024
H	3.14681	-3.62501	-0.64969
H	-1.77983	-4.17856	-0.26655
H	0.13841	3.76421	-2.29383
H	-1.81803	2.39020	2.72981
H	-3.38561	2.80623	-0.62291
H	0.53612	4.37563	1.13608
H	3.15496	-0.32895	2.90059
H	4.36413	2.49263	0.15249
H	3.19818	2.06869	3.07956
H	-4.23900	2.12373	-2.41630
H	-4.68598	1.25176	-1.23490
H	4.39745	-1.92987	-0.96655
H	5.27702	-3.23562	-1.27083
H	3.52868	-2.73760	-2.89990
H	3.01706	-2.70031	-4.39568
H	-6.21831	0.47910	1.85263
H	-6.68990	-0.84456	2.52599
H	6.17524	1.26662	1.33951
H	5.62777	-0.03730	0.77586
H	-4.58478	-2.40746	-2.36537
H	6.37871	3.56329	0.11661
H	-1.72720	6.07512	-1.25101
H	-1.82952	4.83755	-2.15990
H	2.85954	-6.26197	2.09862
H	1.86034	-6.91524	1.10510
H	-3.45202	0.20357	-3.28014
H	5.20747	1.09179	-2.08314
H	0.87830	5.28560	3.27151
H	-6.30600	2.58192	2.69814
H	3.97204	3.39014	3.42587

H	0.79111	4.51549	-0.46075
H	-0.55429	3.40635	2.68796
H	1.71250	3.96419	3.01363
H	6.22567	2.29624	-0.83101
H	6.71580	0.77846	-2.29940
H	-2.32473	0.90670	-4.11837
H	-4.61519	-3.87904	-2.90189
H	-4.91746	1.90167	2.79735
H	4.40973	0.37221	2.15739
H	3.24073	2.78396	1.22635
H	-0.62601	2.52610	-2.87380
H	-2.56415	4.16421	-0.48405
H	0.80904	1.31782	2.19637
H	0.77280	1.07155	-2.02187
H	-1.17156	0.16294	1.86953
H	-2.24748	1.10743	-2.11713
H	-0.68454	-1.15977	-2.13671
H	-1.13991	-1.96961	1.90481
H	1.54939	-1.41949	2.09017
H	1.93230	-1.32704	-2.15015
H	-0.12529	-3.25505	-2.83201
H	-0.73046	-4.93322	-1.19113
H	1.02226	-4.74681	1.86111
H	-4.02014	-3.38883	-0.92424
H	-4.76179	-0.93117	1.60258
H	2.43424	-4.77069	0.28295
O	-0.86135	-0.78845	3.35260
H	-1.48098	-0.31748	3.94849
H	-0.03082	-0.97006	3.84350

109
Hf4_4_2_term_perox_conf4_ion13_diconf9.log Energy: -3143115.2856399

Hf	-2.60379	0.21696	0.39263
O	-1.53079	1.65902	-0.82910
O	-1.25263	1.55118	1.48902
O	-3.26672	0.30403	2.62228
O	-4.03681	0.64335	-1.08167
O	-4.06163	-1.61669	0.68273
O	-4.34659	1.30748	0.21693
Hf	-0.32042	-2.45417	-0.10623
O	-1.41086	-1.32553	1.29955
O	-1.74429	-1.11323	-1.04543
O	-0.69213	-3.46849	-2.10974
O	-0.22681	-3.73968	1.79402

O	1.19750	-4.10604	-0.38179
O	-2.29890	-3.64487	0.04292
Hf	0.09241	2.51677	0.14921
O	1.52455	1.29300	1.09186
O	1.21721	1.40400	-1.30233
O	0.04152	3.76650	-1.96966
O	0.45599	3.56093	2.17584
O	-1.26992	4.27326	0.41109
O	1.99684	3.78355	-0.21758
Hf	2.38924	-0.12929	-0.34017
O	0.97216	-1.38157	-1.38299
O	1.33221	-1.52310	0.93807
O	3.87440	-0.35462	1.45232
O	3.35578	-0.33076	-2.14941
O	3.84140	1.74770	-0.31084
O	3.84810	-1.36435	-1.18878
Cl	-0.91947	1.50344	-3.86955
Cl	0.75149	0.16087	3.91053
Cl	-3.66100	-3.93108	-2.78715
Cl	4.11872	-2.68354	3.45234
O	4.50300	2.19883	2.29839
O	-3.72472	3.94110	-0.36984
O	2.99684	-3.58663	-2.30218
O	1.09834	-2.57298	-3.86339
O	-5.61974	-0.85800	2.73525
O	6.13651	-0.71473	0.10766
O	-5.50431	-1.61216	-1.48493
O	6.19707	1.54126	-1.52462
O	-0.69103	6.36083	-1.14784
O	2.27228	-4.63467	2.01288
O	-3.90227	2.77149	-2.84311
O	5.44974	0.29749	-3.73070
O	2.94877	4.43305	2.23290
O	-6.86112	0.86296	1.17888
H	-3.21091	1.21462	2.95818
H	-4.64927	-1.57335	1.48175
H	-0.09364	-3.23099	-2.87354
H	-0.62872	-3.35697	2.61119
H	1.83995	-3.97916	-1.13965
H	-2.93284	-3.01147	0.46966
H	0.99015	3.90894	-2.14510
H	-0.20510	4.27500	2.22775
H	-2.24132	4.09810	0.11587
H	2.38427	4.23794	0.57564

H	3.78415	-1.12973	2.07722
H	4.66418	1.72476	-0.88729
H	4.19765	1.27174	2.42523
H	-3.69611	3.73780	-1.34123
H	-4.00269	3.06300	-0.00977
H	3.40789	-2.75957	-1.88953
H	3.71223	-4.22704	-2.44583
H	1.92804	-3.02906	-3.56860
H	1.05844	-2.60976	-4.83174
H	-6.25092	-0.23951	2.25242
H	-6.08204	-1.25322	3.49085
H	6.40469	0.13146	-0.31567
H	5.51257	-1.09419	-0.55854
H	-5.10023	-0.71452	-1.58817
H	6.05663	1.13477	-2.43326
H	0.12910	6.82885	-0.91864
H	-0.42302	5.69898	-1.81611
H	2.90703	-4.02048	2.48078
H	2.47944	-5.53689	2.30563
H	-4.00063	1.95347	-2.29378
H	4.63252	0.01265	-3.23915
H	3.30516	5.23707	2.64332
H	-7.08546	1.67199	1.66741
H	5.44545	2.20990	2.53539
H	2.68330	3.10801	-0.46961
H	1.35051	3.94170	2.39516
H	3.56548	3.68660	2.43752
H	6.71748	2.35141	-1.64597
H	5.97081	-0.51571	-3.83206
H	-3.06924	2.61617	-3.32674
H	-4.96903	-2.21622	-2.04852
H	-6.00103	1.07231	0.72770
H	4.80234	-0.45644	1.05565
H	4.16822	1.97574	0.60003
H	-0.29028	3.20779	-2.72263
H	-1.01597	5.11964	-0.06358
H	1.39697	1.04417	2.03620
H	0.79621	1.20427	-2.16103
H	-0.86561	1.22598	2.32795
H	-1.55312	1.57166	-1.80792
H	-1.56905	-0.80317	-1.94766
H	-1.45205	-1.51170	2.26584
H	1.16400	-1.22995	1.85555
H	1.01800	-1.44892	-2.35820

H	-1.62022	-3.50790	-2.46222
H	-2.74483	-3.86894	-0.81443
H	0.66628	-4.09420	2.05424
H	-4.69033	-1.69931	-0.11502
H	-4.18023	-0.03974	2.84505
H	1.75458	-4.32034	0.41253
O	-1.17294	-2.24904	3.86150
H	-1.93275	-2.23621	4.46506
H	-0.56551	-1.51662	4.13309

109
Hf4_4_2_term_perox_conf4_ion14_diconf9.log Energy: -3143105.8520767

Hf	-2.73841	-0.11781	0.13011
O	-1.64376	1.54276	-0.71543
O	-1.57485	1.04972	1.54737
O	-3.64781	-0.48888	2.23273
O	-4.07998	0.51794	-1.37152
O	-4.03465	-2.13129	-0.21626
O	-4.54302	0.87593	-0.00191
Hf	-0.24784	-2.47693	-0.55125
O	-1.59509	-1.76202	0.87250
O	-1.68147	-1.12190	-1.46469
O	-0.63778	-3.15595	-2.80345
O	0.01216	-3.97179	1.31294
O	1.19849	-4.05601	-1.11596
O	-1.98923	-3.94848	-0.63998
Hf	-0.17558	2.34456	0.54775
O	1.30474	1.11103	1.41411
O	1.14760	1.53149	-0.94029
O	-0.18451	3.84729	-1.39095
O	-0.16106	2.89350	2.82954
O	-1.69878	3.91967	0.98945
O	1.27809	4.02172	0.82893
Hf	2.33966	-0.05875	-0.15645
O	1.07871	-1.21886	-1.55012
O	1.12696	-1.59147	0.77552
O	3.54015	-0.84896	1.74206
O	3.45651	0.02055	-1.89827
O	3.81617	1.55247	0.39578
O	3.88331	-1.13387	-1.05247
Cl	-0.85308	1.75519	-3.67312
Cl	0.29795	-0.62997	3.83533
Cl	2.64943	4.99822	-1.70029
Cl	2.89929	-3.94165	2.57226

O	3.96975	1.50910	3.13654
O	-4.06547	3.60364	-0.05536
O	3.30717	-3.23748	-2.48541
O	1.47964	-2.20499	-4.11302
O	-5.80629	-1.93483	1.79216
O	5.96821	-1.10920	0.69268
O	-5.43735	-1.54821	-2.37285
O	6.38325	1.42313	-0.33763
O	-1.13914	6.21833	-0.24648
O	1.63145	-6.04140	0.60064
O	-3.92803	2.91926	-2.71739
O	5.83020	0.86822	-2.85769
O	2.34366	3.67891	3.27054
O	-7.08031	0.03119	0.58610
H	-3.81997	0.35471	2.68459
H	-4.69628	-2.30104	0.50629
H	0.12804	-2.96123	-3.41668
H	0.90642	-3.81200	1.72839
H	2.02300	-3.80275	-1.63447
H	-2.81342	-3.41615	-0.44987
H	0.73851	4.15541	-1.62354
H	-0.81727	3.60961	2.90688
H	-2.63012	3.74186	0.59740
H	1.83782	3.98409	1.65080
H	3.25332	-1.75802	2.01221
H	4.75506	1.55126	0.04740
H	3.70828	0.56810	3.01464
H	-3.92955	3.59268	-1.03759
H	-4.31396	2.66153	0.11048
H	3.60418	-2.43433	-1.94099
H	4.07179	-3.82721	-2.58566
H	2.30527	-2.64721	-3.79006
H	1.57461	-2.05084	-5.06599
H	-6.45464	-1.26658	1.40868
H	-6.28606	-2.52703	2.39242
H	6.35456	-0.21491	0.55885
H	5.45201	-1.22559	-0.13996
H	-5.07003	-0.64777	-2.15556
H	6.33627	1.26451	-1.32957
H	-0.34111	6.64599	0.10650
H	-0.80586	5.62774	-0.95431
H	2.28073	-5.64940	1.23145
H	1.99322	-6.89454	0.31070
H	-4.02695	2.01599	-2.32404

H	4.91813	0.56969	-2.58844
H	2.68197	4.37776	3.85279
H	-7.41573	0.66783	1.23865
H	4.86436	1.50026	3.51517
H	1.85556	4.33067	0.07164
H	0.69700	3.21598	3.21249
H	2.94236	2.89539	3.36036
H	6.90362	2.23067	-0.19956
H	6.28470	0.05215	-3.12286
H	-3.06007	2.87200	-3.15892
H	-4.96581	-1.82128	-3.17746
H	-6.21317	0.41131	0.28759
H	4.51291	-0.94154	1.47341
H	3.88873	1.71097	1.36984
H	-0.49635	3.38150	-2.20570
H	-1.46375	4.83807	0.66212
H	1.09274	0.69246	2.27962
H	0.84674	1.49587	-1.86824
H	-1.25931	0.62320	2.37048
H	-1.60598	1.63109	-1.69377
H	-1.32488	-0.52251	-2.14490
H	-1.73936	-2.15597	1.77904
H	0.83997	-1.42593	1.70106
H	1.26225	-1.20668	-2.51193
H	-1.36911	-2.59793	-3.12385
H	-2.10375	-4.36986	-1.51063
H	0.02804	-4.92993	1.10970
H	-4.57975	-2.04935	-1.06312
H	-4.50226	-1.01083	2.25714
H	1.42435	-4.84494	-0.54462
O	-1.77877	-2.98380	3.27013
H	-1.16990	-3.64429	2.88658
H	-1.17724	-2.33149	3.69338

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Hf4_4_2_term_perox_conf4_ion15_diconf9.log Energy: -3143093.5634144

Hf	-2.09789	-1.48483	-0.51294
O	-2.00035	0.56856	-1.19043
O	-1.52064	-0.02975	1.00680
O	-3.32828	-2.10483	1.24657
O	-2.97805	-1.65440	-2.42546
O	-2.15300	-3.88118	-0.81159
O	-3.97589	-1.59523	-1.31936
Hf	1.34052	-2.28911	-0.26686

O	-0.52243	-2.43598	0.67883
O	-0.22933	-1.66266	-1.58834
O	1.92333	-3.09621	-2.44920
O	1.66994	-3.35908	1.81806
O	3.44710	-2.99366	-0.27411
O	0.62231	-4.44229	-0.65243
Hf	-1.21243	1.88802	0.24524
O	0.59128	1.79256	1.38994
O	0.51692	1.64315	-0.95835
O	-1.31016	3.37232	-1.71565
O	-1.94665	2.09107	2.46254
O	-3.36533	2.56806	0.12977
O	-1.03566	4.07626	0.83535
Hf	2.30003	1.14939	0.04642
O	2.25833	-0.63491	-1.20412
O	1.77543	-0.71113	1.05316
O	3.48984	1.33119	1.99849
O	3.22618	1.73940	-1.71022
O	2.52470	3.43977	0.39883
O	4.23463	1.35623	-0.69050
Cl	-0.20334	1.49497	-4.04539
Cl	0.36730	-1.01705	3.79754
Cl	-3.86372	-0.11237	3.65174
Cl	5.66587	-0.98621	2.38603
O	1.08910	4.58674	2.46726
O	-4.98082	1.01886	-1.34924
O	5.28022	-1.13948	-0.83226
O	4.02347	-1.63508	-3.24776
O	-5.90458	-2.66116	1.08673
O	5.27332	3.13209	1.08157
O	-3.46128	-4.17367	-3.03775
O	1.09232	4.71663	-1.53384
O	-3.66310	4.74855	-1.36645
O	4.30857	-3.73401	2.12492
O	-3.30667	0.74322	-3.61726
O	3.06126	4.00272	-3.15299
O	-3.11788	4.59507	2.48260
O	-6.49773	-0.15030	1.89848
H	-3.32341	-1.49616	2.02874
H	-2.58700	-4.29585	-0.04472
H	2.77116	-2.70546	-2.80543
H	1.33002	-2.76013	2.52106
H	4.09234	-2.25564	-0.52710
H	-0.36703	-4.39648	-0.71850

H	-0.48782	3.93375	-1.63091
H	-2.53172	1.34216	2.75073
H	-3.96128	1.90892	-0.35554
H	-1.82245	4.45627	1.30461
H	4.01272	0.51115	2.19579
H	2.04022	3.93913	-0.31875
H	1.03417	4.14238	3.33015
H	-4.60946	1.22284	-2.23290
H	-4.71884	0.06904	-1.24152
H	4.87487	-0.22496	-0.85323
H	5.72495	-1.17235	0.04460
H	4.77074	-1.61986	-2.61343
H	4.41134	-1.71833	-4.13359
H	-6.24622	-1.76492	1.35996
H	-6.10000	-3.23995	1.84193
H	4.61809	3.84740	0.99302
H	5.09644	2.61121	0.25736
H	-3.35616	-3.17759	-3.02712
H	1.75605	4.53499	-2.27052
H	-3.52959	5.59753	-0.91394
H	-2.78433	4.51175	-1.73880
H	4.81627	-2.90776	2.35285
H	4.85866	-4.49726	2.36453
H	-3.23240	-0.22564	-3.40584
H	3.27806	3.18847	-2.61972
H	-4.03176	4.65153	2.15718
H	-7.26802	-0.10914	2.48848
H	1.28923	5.51895	2.65965
H	-0.26609	4.25059	1.44096
H	-2.46095	2.91325	2.63875
H	-3.04150	5.25738	3.18982
H	1.06873	5.68129	-1.41886
H	3.79200	4.61795	-2.97702
H	-2.45710	0.97893	-4.04885
H	-2.85235	-4.48543	-3.72781
H	-5.71949	-0.04890	2.49733
H	4.19401	2.03231	1.84469
H	2.07692	3.72837	1.23069
H	-1.15242	2.85780	-2.54754
H	-3.54022	3.43983	-0.33922
H	0.52088	1.52988	2.32210
H	0.42609	1.53167	-1.93270
H	-1.03339	-0.36474	1.78500
H	-2.42798	0.79748	-2.04799

H	-0.04895	-0.92516	-2.19695
H	-0.72793	-2.98452	1.47941
H	1.36411	-0.68846	1.94842
H	2.64352	-0.56418	-2.09529
H	1.21929	-2.81027	-3.05786
H	0.95797	-4.75260	-1.51370
H	2.59559	-3.58481	2.09440
H	-2.67787	-4.15745	-1.63935
H	-4.29845	-2.36212	1.11173
H	3.84770	-3.42198	0.53149
O	-1.08937	-3.78495	3.00231
H	-0.37930	-4.43526	3.13257
H	-0.80873	-3.00997	3.53494

109
Hf4_4_2_term_perox_conf4_ion1_diconf9.log Energy: -3143097.3381286

Hf	2.60167	-0.42639	0.15424
O	1.48415	0.94608	1.38375
O	1.33760	0.98372	-0.94081
O	3.82403	0.15720	-1.72066
O	3.67826	-0.57121	1.96098
O	3.80652	-2.41530	-0.18407
O	4.32373	0.33829	0.97235
Hf	-0.04480	-2.73109	-0.21845
O	1.53906	-1.72668	-1.30808
O	1.28136	-1.79340	1.09956
O	-0.07159	-4.03252	1.76703
O	0.14874	-3.64048	-2.37862
O	-1.57508	-4.32991	-0.43093
O	1.71808	-4.23906	-0.19284
Hf	0.17262	2.18354	0.33414
O	-1.36619	1.53150	-1.01252
O	-1.32923	0.97129	1.28973
O	0.07774	2.98353	2.56647
O	0.48559	3.50438	-1.52406
O	1.94725	3.51865	0.59515
O	-1.13508	4.05110	0.48690
Hf	-2.52741	-0.13530	-0.12477
O	-1.56030	-1.83389	0.91602
O	-1.17975	-1.35899	-1.31605
O	-3.32669	-0.15207	-2.29608
O	-3.90676	-0.62618	1.35535
O	-3.89074	1.67676	-0.06953
O	-4.26951	-1.20605	0.02089

Cl	0.74706	-2.06388	4.16353
Cl	-2.71986	4.12612	3.08197
Cl	3.01549	2.81858	-3.31172
Cl	-0.33114	0.25145	-3.79973
O	-4.33472	3.44973	-2.14118
O	3.88723	2.73437	2.25982
O	-4.00584	-3.76974	0.37187
O	-2.59543	-3.81609	2.65513
O	6.25399	1.10964	-1.42315
O	-5.65681	1.16270	-2.71795
O	5.55227	-2.44118	1.79144
O	-6.56877	1.27478	-0.17880
O	0.93522	5.99351	0.84118
O	-1.13572	-6.02350	-2.50106
O	2.36798	0.75165	3.90844
O	-6.52614	-0.38880	1.85852
O	-1.90731	4.59068	-2.02184
O	5.28797	3.62780	-1.25938
H	3.43072	0.90637	-2.24056
H	4.16725	-2.49401	-1.11836
H	-1.00724	-4.22063	2.04820
H	1.09787	-3.67250	-2.58698
H	-2.53846	-4.13455	-0.19626
H	2.54164	-3.67649	-0.14515
H	-0.81891	3.24813	2.91523
H	1.25510	3.30267	-2.11560
H	2.62903	3.26053	1.28747
H	-1.58166	4.29648	-0.37599
H	-2.69325	0.07245	-3.00810
H	-4.86737	1.51665	0.03327
H	-4.84886	2.74538	-2.60969
H	3.48682	2.41218	3.08697
H	4.12448	1.90139	1.76979
H	-4.15966	-2.77527	0.21083
H	-4.76165	-4.25172	-0.00024
H	-3.31454	-3.94947	1.99087
H	-2.93205	-4.11552	3.51377
H	6.01716	2.07396	-1.32502
H	6.66734	1.04554	-2.30007
H	-6.17564	1.09850	-1.87325
H	-6.24915	0.90471	-3.44273
H	4.93401	-1.71062	2.07618
H	-6.69360	0.59359	0.55515
H	0.06467	5.54691	0.77473

H	0.99571	6.27203	1.77012
H	-1.80695	-6.19799	-3.18219
H	-0.66305	-6.86159	-2.36329
H	3.02260	0.23236	3.36486
H	-5.53074	-0.44777	1.79938
H	-1.98721	5.52879	-2.25967
H	5.86674	4.29120	-1.66942
H	-4.99198	4.08692	-1.81571
H	-1.80344	4.10524	1.23341
H	-0.28927	3.81437	-2.04794
H	-2.76701	4.16071	-2.26065
H	-7.09141	2.05294	0.07433
H	-6.82461	-1.26997	1.58025
H	1.80183	0.04555	4.29018
H	5.34962	-3.18530	2.38210
H	4.55759	3.49630	-1.91067
H	-4.19687	0.28492	-2.50288
H	-3.81702	2.36267	-0.77561
H	0.52147	2.47340	3.26608
H	1.73078	4.48870	0.69221
H	-1.11478	1.44331	-1.95277
H	-1.14637	0.59067	2.16155
H	1.06208	0.87418	-1.87131
H	1.66747	0.92606	2.35568
H	1.11711	-1.72199	2.06983
H	1.27711	-1.32622	-2.15384
H	-0.88470	-1.01738	-2.19108
H	-1.94110	-2.17310	1.74842
H	0.29874	-3.54099	2.54192
H	1.65140	-4.71469	0.65619
H	-0.21889	-4.53564	-2.58689
H	4.56027	-2.54757	0.47253
H	4.77902	0.46261	-1.53539
H	-1.54978	-5.05128	-1.10491
O	4.61440	-2.30953	-2.72477
H	3.97899	-2.78911	-3.28126
H	4.29037	-1.38224	-2.71412

109
Hf4_4_2_term_perox_conf4_ion6_diconf1.log Energy: -3143090.5410904

Hf	2.44610	-0.50422	0.11589
O	1.96025	1.32730	1.11244
O	1.36213	0.86632	-1.06373
O	3.21765	-0.71458	-2.04105

O	3.26670	-0.67541	2.26062
O	3.78836	-2.28587	0.18647
O	4.42667	0.61395	0.09399
Hf	-0.60513	-2.35316	0.20428
O	1.16158	-1.91035	-0.94685
O	0.92003	-1.37502	1.29936
O	-0.61944	-3.41884	2.32205
O	-1.04301	-3.17053	-2.06227
O	-2.45793	-3.55809	0.27870
O	0.34676	-4.37244	0.16312
Hf	0.48108	2.50621	0.03201
O	-1.27398	1.90448	-1.02838
O	-0.96683	1.59381	1.36698
O	0.94827	3.67535	2.16183
O	0.87278	3.62501	-1.65139
O	1.74880	4.00521	-0.49793
O	-1.00890	4.25483	0.54868
Hf	-2.55342	0.65363	0.27338
O	-1.87193	-1.11875	1.35562
O	-1.44329	-0.79839	-0.88989
O	-3.68190	0.43000	-1.70502
O	-3.58565	0.78046	2.05615
O	-3.47331	2.77026	0.08531
O	-4.45582	0.19937	0.99428
Cl	-0.02995	-0.60102	-3.68524
Cl	1.27584	-1.85316	4.34763
Cl	4.55693	1.45453	-3.78662
Cl	-3.98591	-2.51275	-2.94275
O	-3.35528	4.08597	-2.35441
O	4.31091	3.17523	-0.08227
O	-4.60321	-2.41533	1.44699
O	-2.89031	-2.58605	3.49764
O	5.14965	-2.55876	-2.13724
O	-6.20894	1.48854	-1.96988
O	5.74926	-2.66207	1.92708
O	-6.01873	2.38856	0.69215
O	3.78434	4.00614	2.48130
O	-3.42178	-5.26578	-1.49595
O	5.82572	0.04576	2.43655
O	-3.80055	3.16264	3.43894
O	-0.99513	5.56089	-1.70615
O	6.26501	-0.12933	-1.79627
H	3.50635	0.08001	-2.56909
H	2.79100	-1.11275	3.01069

H	4.22861	-2.62211	-0.63192
H	5.09420	0.33578	-0.59281
H	-1.49380	-3.31011	2.78523
H	-0.60929	-2.55403	-2.70360
H	-3.28015	-3.11504	0.63702
H	0.38595	-4.94403	-0.67313
H	0.31544	4.40133	1.96992
H	-1.07642	4.88257	-0.24945
H	-3.69990	-0.49529	-2.06092
H	-4.44239	2.80447	0.36985
H	-3.32991	3.51263	-3.13943
H	3.42499	3.43017	-0.45020
H	4.23838	3.48601	0.85817
H	-4.62017	-1.42000	1.28262
H	-5.49444	-2.75602	1.26906
H	-3.71466	-2.64901	2.95464
H	-3.14376	-2.64627	4.43145
H	5.83374	-1.84455	-2.10310
H	5.37899	-3.16771	-2.85681
H	-6.21816	2.12099	-2.70849
H	-6.88530	0.82641	-2.19302
H	6.01965	-1.75673	2.19962
H	-5.66839	1.49600	0.94251
H	4.04048	4.93574	2.59437
H	2.80615	4.02230	2.42369
H	-3.80935	-4.56409	-2.06953
H	-4.18556	-5.72307	-1.10592
H	5.62155	0.47917	1.57849
H	-3.84605	2.34806	2.88739
H	-0.24479	4.92843	-1.88571
H	7.17761	0.15529	-1.62134
H	-4.14415	4.64221	-2.47568
H	-1.89550	3.84130	0.64972
H	-1.78100	5.13015	-2.10735
H	-6.32839	2.23461	-0.22597
H	-3.44550	2.84238	4.28222
H	6.21532	0.71994	3.01651
H	5.43261	-3.08227	2.74369
H	5.93021	0.43075	-2.54934
H	-4.60867	0.77619	-1.78163
H	-3.42102	3.16191	-0.82370
H	0.60211	3.25567	2.97004
H	-1.29093	1.82335	-1.99281
H	-0.74316	1.16504	2.20551

H	1.02316	0.59527	-1.94173
H	2.21643	1.38906	2.04359
H	0.85291	-1.24397	2.27051
H	1.13461	-1.70395	-1.90102
H	-1.10142	-0.57014	-1.78258
H	-2.17753	-1.27704	2.26980
H	0.04479	-3.06981	2.96814
H	0.03556	-4.90581	0.91602
H	-2.00902	-3.02659	-2.26798
H	4.16875	-0.38021	2.54779
H	4.46321	-2.40411	0.92743
H	4.33463	1.64796	0.01639
H	3.84248	-1.44735	-2.28024
H	-2.75933	-4.27474	-0.36189
O	0.23708	-5.62831	-2.12278
H	-0.32064	-4.88470	-2.44115
H	1.07151	-5.54469	-2.61440

109
Hf4_4_2_term_perox_conf4_ion6_diconf2.log Energy: -3143076.6991727

Hf	-2.38674	-0.32938	-0.14482
O	-1.85423	1.37169	-1.33088
O	-1.34694	1.08151	1.00675
O	-3.28915	-0.45002	1.93343
O	-3.36980	-0.70776	-2.38831
O	-3.55076	-2.22613	-0.21521
O	-4.34714	0.67115	-0.21119
Hf	0.57867	-2.33657	-0.05127
O	-1.17857	-1.70972	1.01845
O	-0.87039	-1.31495	-1.27198
O	0.52772	-3.62331	-2.02096
O	0.97220	-2.94848	2.27088
O	2.38576	-3.60845	0.00746
O	-0.49075	-4.29174	0.19564
Hf	-0.32939	2.62543	-0.11657
O	1.49420	1.99516	0.77171
O	0.84310	1.27044	-1.40620
O	0.09432	3.67391	-2.10815
O	-0.46064	3.73711	1.62043
O	-2.36675	3.69588	-0.37295
O	0.14536	4.52510	0.50351
Hf	2.61279	0.59328	-0.43913
O	1.90583	-1.30915	-1.30315
O	1.46423	-0.71060	0.89036

O	3.91788	0.31945	1.41348
O	3.38502	0.58810	-2.35823
O	3.75466	2.56160	-0.49666
O	4.39145	0.03168	-1.40686
Cl	-0.09614	-0.36139	3.71101
Cl	-1.59248	-2.55444	-4.07220
Cl	-4.56490	1.88597	3.54348
Cl	3.94019	-2.37749	3.13456
O	3.76682	4.63432	1.35956
O	-5.88895	1.66257	-2.22496
O	4.48912	-2.64067	-1.41893
O	2.72607	-2.99302	-3.40499
O	-5.24547	-2.16634	2.46566
O	6.57895	1.02412	1.37749
O	-6.12113	-2.32645	-0.51721
O	6.23407	1.97524	-1.26223
O	-1.86296	6.23346	0.15038
O	3.31774	-5.20257	1.89751
O	-6.22411	-1.07241	-2.88637
O	2.39515	3.05119	-3.36540
O	1.81878	3.45906	3.04548
O	-6.27566	0.24424	1.59452
H	-3.55510	0.37069	2.42926
H	-2.89133	-1.40495	-2.92353
H	-3.27149	-2.85620	0.47083
H	-5.08353	0.48481	0.44455
H	1.37183	-3.55007	-2.55121
H	0.55849	-2.25581	2.85055
H	3.19865	-3.23164	-0.43313
H	-0.55760	-4.76564	1.08887
H	0.13993	4.64326	-2.05687
H	-2.82148	3.42650	-1.18650
H	3.83357	-0.53242	1.91136
H	4.71349	2.50518	-0.79045
H	4.65181	4.75330	1.74405
H	-6.59516	2.18214	-1.80366
H	-5.54394	2.23123	-2.93447
H	4.49442	-1.63168	-1.43962
H	5.40554	-2.93321	-1.29003
H	3.54673	-3.03579	-2.85271
H	2.94875	-3.32466	-4.28857
H	-5.89565	-1.51843	2.10881
H	-5.39849	-2.16778	3.42538
H	6.77499	1.62473	2.11660

H	7.17305	0.26486	1.50382
H	-6.29496	-1.86438	-1.38734
H	5.73369	1.14482	-1.48005
H	-0.99594	5.77323	0.34397
H	-1.69546	6.75293	-0.65293
H	3.70640	-4.46666	2.42708
H	4.08149	-5.68890	1.54423
H	-5.24970	-1.12618	-2.93623
H	2.84291	2.30796	-2.89473
H	0.92777	3.69286	2.67214
H	-7.15528	0.56401	1.33362
H	3.58328	5.46322	0.88625
H	2.44154	4.06581	2.59578
H	6.59756	1.76911	-0.37526
H	2.16521	2.67834	-4.23252
H	-6.36698	-0.11492	-2.72899
H	-6.39644	-3.24787	-0.65458
H	-5.94893	0.85321	2.31087
H	4.88250	0.54523	1.38531
H	3.68599	3.24483	0.21138
H	0.93911	3.36633	-2.56923
H	-2.36803	4.69515	-0.28243
H	1.76218	2.40637	1.63172
H	0.40669	0.53141	-1.85629
H	-1.06343	0.85386	1.91737
H	-1.59893	1.28545	-2.26060
H	-0.91827	-1.48233	-2.23797
H	-1.14828	-1.44768	1.96143
H	1.10817	-0.33233	1.71974
H	2.12273	-1.49165	-2.23463
H	-0.19561	-3.41588	-2.66551
H	-0.18529	-4.91864	-0.48415
H	1.94246	-2.82438	2.46801
H	-3.31303	0.09342	-2.93825
H	-4.56978	-2.28787	-0.32843
H	-4.76504	1.09178	-1.00521
H	-3.96196	-1.15768	2.17047
H	2.68520	-4.27592	0.70019
O	-0.42143	-5.31454	2.59830
H	0.17450	-4.56881	2.83191
H	-1.24153	-5.14542	3.09186

109
Hf4_4_2_term_perox_conf4_ion6_diconf4.log Energy: -3143087.6839644

Hf	2.36141	-0.58897	0.05643
O	1.88400	1.10326	1.26921
O	1.39380	0.86906	-1.07022
O	3.33126	-0.59760	-2.01256
O	3.23796	-1.03648	2.35597
O	3.34942	-2.56407	-0.01265
O	4.38650	0.25422	0.31802
Hf	-0.73237	-2.32681	-0.05819
O	1.07160	-1.87578	-1.15839
O	0.79290	-1.49322	1.13471
O	-0.77360	-3.56694	1.95004
O	-1.22173	-2.90041	-2.35500
O	-2.61410	-3.47932	-0.09065
O	0.18769	-4.36186	-0.28430
Hf	0.60098	2.52773	0.13309
O	-1.27375	2.11540	-0.86243
O	-0.84682	1.56423	1.44118
O	0.86982	3.70484	1.80909
O	0.69442	3.33620	-2.06614
O	2.73734	3.32420	-0.31035
O	0.23624	4.44266	0.66278
Hf	-2.49715	0.78361	0.38582
O	-1.96206	-1.18203	1.20820
O	-1.48766	-0.60588	-0.97181
O	-3.82907	0.75466	-1.52156
O	-3.42467	0.73122	2.24608
O	-3.40947	2.85658	0.44799
O	-4.35485	0.25145	1.19396
Cl	0.03051	-0.39267	-3.80481
Cl	0.76403	-1.76510	4.17234
Cl	3.83032	2.39064	-3.13100
Cl	-4.11883	-2.01675	-3.14234
O	-3.08760	4.69182	-1.66009
O	4.50795	1.34535	2.73454
O	-4.61837	-2.38563	1.30603
O	-3.14780	-3.75092	3.14979
O	5.72758	-1.54983	-2.68313
O	-6.24646	1.29384	-0.30695
O	5.70943	-3.44257	0.57616
O	-5.92630	3.64015	1.01777
O	3.44988	3.77052	2.22021
O	-3.68444	-4.93585	-2.02551
O	5.35502	-2.75122	3.12644
O	-2.10991	2.55543	3.70917

O	-0.55223	5.66980	-2.37152
O	6.12905	0.94118	-1.61080
H	3.38046	0.29531	-2.43308
H	2.53214	-1.31590	2.99578
H	2.88604	-3.16115	-0.62466
H	5.05108	0.50888	-0.38159
H	-1.68474	-3.68251	2.36385
H	-0.73600	-2.27851	-2.95596
H	-3.40214	-3.04478	0.35040
H	0.13549	-4.88000	-1.15275
H	1.59210	3.33289	-2.45367
H	3.26446	2.90296	-1.02599
H	-3.84065	-0.11178	-2.00083
H	-4.32244	3.12547	0.75180
H	-3.40926	4.24032	-2.45988
H	4.08619	2.24653	2.67201
H	5.35535	1.45601	3.19497
H	-4.52496	-1.37915	1.30124
H	-5.54339	-2.58960	1.09353
H	-3.80452	-3.24363	2.61129
H	-3.10210	-3.29482	4.00552
H	6.16220	-0.71049	-2.40628
H	5.77880	-1.55266	-3.65323
H	-7.02955	0.73137	-0.42490
H	-5.73388	0.91073	0.45877
H	5.71388	-3.25542	1.55845
H	-6.32483	2.91323	0.48298
H	3.83928	4.61309	2.50314
H	2.44469	3.89672	2.16305
H	-4.03759	-4.15893	-2.51884
H	-4.46923	-5.38718	-1.67189
H	4.60054	-2.15871	2.90536
H	-2.86647	2.12008	3.25298
H	-0.62684	5.86648	-3.31970
H	6.91250	1.44104	-1.32642
H	-3.73762	5.39715	-1.49592
H	0.30395	4.25334	-2.19589
H	-1.46076	5.39757	-2.10177
H	-6.04511	4.43987	0.47936
H	-1.95258	1.99769	4.48815
H	6.05120	-2.15405	3.44541
H	5.71090	-4.41109	0.49881
H	5.58590	1.55475	-2.16707
H	-4.77272	0.95616	-1.29244

H	-3.16111	3.44326	-0.30375
H	3.29016	3.43285	0.50354
H	-1.24792	2.10924	-1.83091
H	-1.03442	1.95744	2.32682
H	1.08497	0.69030	-1.98179
H	1.48367	0.95026	2.13834
H	0.64324	-1.36117	2.09980
H	1.04214	-1.58733	-2.09247
H	-1.14722	-0.31736	-1.84381
H	-2.09458	-1.26189	2.16343
H	-0.21112	-3.19659	2.66988
H	-0.09857	-4.92613	0.45622
H	-2.17521	-2.66379	-2.53981
H	3.60573	-0.18497	2.70921
H	4.28894	-2.91524	0.19133
H	4.56822	0.76904	1.15555
H	4.18571	-1.07319	-2.24500
H	-2.96257	-4.09796	-0.80424
O	-0.15234	-5.45053	-2.63807
H	-0.67336	-4.65075	-2.86986
H	0.65575	-5.38598	-3.17447

109
Hf4_4_2_term_perox_conf4_ion6_diconf5.log Energy: -3143095.3995950

Hf	-2.29707	-0.98480	-0.11986
O	-2.00298	0.72966	-1.30444
O	-1.55093	0.65922	0.95336
O	-3.23189	-1.10350	1.94376
O	-3.09637	-1.67754	-2.21769
O	-3.09042	-3.04899	0.11883
O	-4.45282	-0.29145	-0.39929
Hf	1.05456	-2.14134	0.01271
O	-0.81198	-2.00301	1.10503
O	-0.63215	-1.73714	-1.19235
O	1.37893	-3.36557	-2.02605
O	1.53886	-2.71874	2.34395
O	3.08997	-2.93765	0.06436
O	0.56499	-4.35557	0.20130
Hf	-1.04106	2.40741	-0.27069
O	0.79045	2.23696	0.92422
O	0.66827	1.87570	-1.42843
O	-1.67907	3.24373	-2.04638
O	-1.91641	3.20984	1.71721
O	-2.67240	3.49806	-0.96856

O	-0.20952	4.57517	-0.01005
Hf	2.33465	1.19922	-0.26286
O	1.98378	-0.73593	-1.22763
O	1.54297	-0.39797	1.01911
O	3.50488	1.20330	1.70451
O	3.35452	1.45876	-2.05305
O	3.01828	3.35942	-0.11298
O	4.29396	0.98362	-1.00239
Cl	-0.03698	-0.28026	3.72598
Cl	-0.86688	-2.50597	-4.18349
Cl	-4.05889	1.61467	3.38251
Cl	4.27379	-1.60332	3.22407
O	1.86097	4.94782	1.80216
O	-4.81696	2.00533	-1.56835
O	4.97229	-1.56084	-1.20992
O	3.74673	-2.81721	-3.26273
O	-5.45013	-2.42437	2.61919
O	5.85351	2.46911	1.97810
O	-4.51577	-4.30727	-1.63905
O	5.65077	3.19056	-0.61996
O	0.11110	5.24079	-2.79386
O	4.21622	-4.53817	1.80548
O	-6.27671	-2.24414	-1.53426
O	2.51776	-0.38895	-3.85926
O	-2.59905	5.61314	0.59337
O	-6.12093	0.06109	1.69223
H	-3.38533	-0.25153	2.42385
H	-2.46068	-1.95565	-2.93436
H	-2.44447	-3.61128	0.58060
H	-5.03264	-0.18108	0.40967
H	2.27896	-3.26364	-2.44414
H	0.96622	-2.17591	2.93817
H	3.82256	-2.38371	-0.33672
H	0.88336	-4.89016	0.98344
H	-2.59401	2.64676	2.17452
H	-0.92476	5.22742	0.19884
H	3.63936	0.31674	2.11738
H	3.96460	3.55620	-0.33180
H	1.75710	4.57318	2.69279
H	-4.01788	2.57477	-1.36021
H	-4.82378	1.91997	-2.53574
H	4.73324	-0.57882	-1.18616
H	5.89533	-1.64059	-0.91963
H	4.36494	-2.43149	-2.58995

H	4.24384	-3.49969	-3.74162
H	-5.98020	-1.62481	2.39599
H	-5.48577	-2.48833	3.58785
H	6.52666	1.77809	2.09034
H	6.00988	2.83111	1.07241
H	-5.23323	-3.61800	-1.68799
H	5.32161	2.28718	-0.90789
H	0.41956	5.32856	-1.87654
H	-0.60979	4.58605	-2.65671
H	3.46652	-5.05388	2.17705
H	4.41736	-3.84256	2.46834
H	-6.62694	-1.91819	-2.37901
H	3.04859	0.29882	-3.38541
H	-2.87356	5.07087	-0.19088
H	-6.95444	0.49463	1.44351
H	2.16782	5.86109	1.93320
H	0.47335	4.64971	0.70022
H	-2.31299	4.10674	1.61416
H	-3.08967	6.44961	0.57583
H	6.17155	3.56471	-1.34791
H	3.09272	-1.18038	-3.92714
H	-5.71428	-1.51943	-1.18943
H	-4.04224	-4.21889	-2.48270
H	-5.63873	0.69116	2.28874
H	4.38112	1.68745	1.78876
H	2.72585	3.90292	0.65603
H	0.72668	2.06100	1.87543
H	0.64364	1.80869	-2.39397
H	-1.16558	0.52593	1.84451
H	-2.17315	0.85501	-2.24881
H	-0.56377	-1.65640	-2.16814
H	-0.84543	-1.71208	2.03721
H	1.17782	-0.21025	1.91087
H	2.03485	-0.74338	-2.21926
H	0.72156	-3.21581	-2.74813
H	0.92402	-4.75535	-0.61463
H	2.45687	-2.37910	2.56580
H	-3.84302	-1.23164	-2.64790
H	-3.58219	-3.58976	-0.59642
H	-4.54774	0.59875	-0.90248
H	-3.99079	-1.71937	2.17829
H	3.51037	-3.59475	0.71218
O	1.63415	-5.40392	2.42604
H	1.48380	-4.51378	2.81763

H	1.20562	-6.05140	3.01010

109
Hf4_4_2_term_perox_conf4_ion6_diconf6.log Energy: -3143084.0621304

Hf	-2.44578	0.45543	0.03523
O	-1.37973	2.13652	-1.10895
O	-0.92962	1.56584	1.16115
O	-3.62978	0.85425	1.65786
O	-3.27257	0.76025	-2.19428
O	-3.97289	-1.23582	-0.29375
O	-3.99143	1.73005	0.50029
Hf	-0.34834	-2.42561	0.01498
O	-1.58116	-1.11037	1.21424
O	-1.27388	-0.90580	-1.13353
O	-0.92922	-3.54170	-1.95230
O	-0.25569	-3.42757	2.07020
O	0.89502	-4.27042	-0.11041
O	-2.44375	-3.39917	0.20648
Hf	0.50116	2.51898	-0.01929
O	1.87997	1.20213	0.95779
O	1.14365	0.94415	-1.24446
O	0.74374	3.34564	-2.30115
O	0.88250	3.31668	2.08567
O	-0.34776	4.56888	0.01710
O	2.47183	3.60350	-0.35535
Hf	2.55949	-0.42079	-0.38120
O	1.25362	-1.88694	-1.27437
O	1.15695	-1.36085	0.98660
O	3.85308	-1.05654	1.36202
O	3.31380	-0.48812	-2.29380
O	4.14756	1.32728	-0.32583
O	4.06612	-1.41004	-1.39448
Cl	-1.78421	-1.87931	4.26847
Cl	-2.47440	-1.65179	-3.99477
Cl	-1.30995	4.55318	3.74315
Cl	2.74873	-3.38203	3.23423
O	4.97346	2.39941	2.11707
O	-2.99948	4.16794	-0.04474
O	3.20046	-4.00519	-1.60010
O	1.29925	-3.61367	-3.44251
O	-5.48337	-1.18977	1.80458
O	6.25810	-1.27068	0.06686
O	-5.38126	-1.62166	-2.44527
O	6.61979	1.08814	-1.27646

O	0.41948	6.05903	-1.99773
O	1.63340	-5.95328	1.79260
O	-6.08385	0.96686	-2.73463
O	2.99372	2.21100	-3.31545
O	3.29300	4.56526	1.97605
O	-6.66336	1.62283	-0.14200
H	-3.11428	-0.00289	-2.81438
H	-4.65998	-1.25244	0.46729
H	-0.13808	-3.77830	-2.51231
H	-0.80666	-3.03695	2.80222
H	1.74956	-4.16429	-0.61021
H	-3.07952	-2.64889	-0.01810
H	1.56107	2.92421	-2.71069
H	0.11311	3.75204	2.57666
H	-1.33368	4.61605	0.13236
H	2.83419	4.11561	0.42434
H	3.50830	-1.79899	1.92872
H	5.02835	1.24717	-0.81159
H	4.90532	1.84588	2.91460
H	-3.67139	4.66932	-0.53312
H	-3.45970	3.39803	0.38512
H	3.56866	-3.07732	-1.55642
H	3.95020	-4.61659	-1.52044
H	2.10568	-3.97199	-2.99674
H	1.35973	-3.83053	-4.38576
H	-4.94797	-0.39829	2.05098
H	-5.05767	-1.96309	2.26334
H	6.83305	-2.05379	0.08562
H	5.63657	-1.39477	-0.69961
H	-5.75744	-0.71393	-2.63550
H	6.81705	0.28293	-0.74334
H	1.23446	6.53783	-1.77150
H	0.71994	5.22992	-2.43056
H	2.12358	-5.29732	2.34391
H	2.32330	-6.51742	1.40497
H	-5.13567	1.19675	-2.68613
H	3.22866	1.34148	-2.92159
H	3.62088	5.45739	2.17351
H	-6.95313	2.54861	-0.10479
H	5.92378	2.58632	2.01922
H	3.14992	2.90507	-0.54054
H	1.67196	3.89641	2.22222
H	4.00637	3.91972	2.20378
H	7.12838	1.80240	-0.85814

H	2.90827	2.03709	-4.26718
H	-6.40905	1.20698	-1.82722
H	-4.70759	-1.77734	-3.13810
H	-5.71901	1.64727	0.15503
H	4.79794	-1.24664	1.12270
H	4.39354	1.58776	0.59797
H	-0.03035	2.97639	-2.76517
H	-0.08612	5.22250	-0.71220
H	2.11762	1.38924	1.87723
H	0.68143	0.69098	-2.05636
H	-0.71000	1.27147	2.05936
H	-1.95106	2.93341	-1.00010
H	-1.31170	-0.97993	-2.10694
H	-1.71860	-1.20393	2.18402
H	0.94031	-0.86923	1.79192
H	1.32640	-2.10620	-2.22314
H	-1.52464	-3.04829	-2.57134
H	-2.58063	-4.09991	-0.45803
H	0.67509	-3.39049	2.41814
H	-2.60925	1.43610	-2.45143
H	-4.50458	-1.36180	-1.16019
H	1.07169	-4.93821	0.62450
O	-4.15189	-3.38881	2.75574
H	-3.63633	-3.63214	1.96428
H	-3.47667	-2.99223	3.35130

109
Hf4_4_2_term_perox_conf4_ion7_diconf9.log Energy: -3143092.3214226

Hf	-2.44097	-1.11971	-0.60819
O	-1.65066	0.79309	-1.26850
O	-1.62991	0.17169	0.95472
O	-3.71917	-1.44065	1.19705
O	-3.36807	-0.78312	-2.51330
O	-3.30837	-3.19236	-1.02882
O	-4.28502	-0.62369	-1.34943
Hf	0.79211	-2.56695	-0.38399
O	-1.16449	-2.61230	0.39812
O	-0.65887	-1.72285	-1.72859
O	1.23446	-3.45672	-2.51957
O	0.93319	-3.58092	1.75746
O	2.83451	-3.43207	-0.32427
O	0.43574	-4.84663	-0.50980
Hf	-0.89396	2.02223	0.24050
O	0.82616	1.58156	1.40440

O	0.90741	1.89295	-0.91446
O	-1.30003	3.44754	-1.82506
O	-1.47439	2.29632	2.47701
O	-2.93889	2.89306	0.28752
O	-0.36316	4.16936	0.64431
Hf	2.36360	0.67263	0.07647
O	1.90518	-0.97062	-1.30987
O	1.24662	-1.02359	0.89119
O	3.24473	0.26659	2.12720
O	3.57416	1.06649	-1.56522
O	3.23520	2.76986	0.69767
O	4.34773	0.42269	-0.46390
Cl	-0.17843	-1.20731	3.68058
Cl	1.26239	3.76994	-3.49145
Cl	-4.19673	0.89399	3.34305
Cl	5.54010	-1.92622	2.23437
O	1.90979	4.78694	-0.62184
O	-4.85298	2.01707	-1.28339
O	4.98950	-2.06900	-0.99888
O	3.50931	-2.27749	-3.29519
O	-6.28681	-2.08033	1.06554
O	3.35642	2.58806	3.42299
O	-4.36681	-3.05667	-3.41943
O	5.79834	2.66644	0.06863
O	-2.75905	5.44886	-0.51519
O	3.52334	-4.26812	2.10353
O	-3.07363	1.72009	-3.43198
O	5.16012	3.05600	-2.54448
O	-0.54845	4.73124	3.27948
O	-6.89751	0.47913	1.70400
H	-3.75173	-0.69652	1.84870
H	-2.61967	-3.86645	-0.91243
H	2.12348	-3.17501	-2.88151
H	0.63569	-2.94458	2.44918
H	3.61812	-2.85138	-0.59100
H	-0.26373	-5.26711	0.01750
H	-0.51516	3.62797	-2.41253
H	-2.39222	1.98229	2.67990
H	-3.67505	2.50113	-0.29527
H	-0.28137	4.45322	1.59216
H	4.01801	-0.35326	2.17022
H	4.21746	2.84578	0.45793
H	2.24565	5.69852	-0.58444
H	-4.49362	2.22846	-2.16956

H	-4.74695	1.02678	-1.24891
H	4.75981	-1.09892	-0.84954
H	5.53288	-2.29033	-0.21408
H	4.28341	-2.38274	-2.69912
H	3.84595	-2.30352	-4.20495
H	-6.62584	-1.16939	1.28806
H	-6.47928	-2.61525	1.85290
H	3.25633	2.95149	2.51189
H	4.23650	2.87901	3.71364
H	-4.04715	-2.11664	-3.29061
H	5.77063	2.98592	-0.87005
H	-2.11174	5.79052	0.12480
H	-2.18554	5.02316	-1.18953
H	4.20100	-3.56055	2.28465
H	3.92192	-5.11979	2.34536
H	-3.28673	0.75295	-3.25714
H	4.53097	2.33115	-2.28682
H	-1.08081	5.51279	3.50414
H	-7.63697	0.53715	2.33077
H	1.80416	4.55964	-1.58447
H	0.46551	4.47351	0.16944
H	-1.32340	3.15018	2.94452
H	0.21647	4.74324	3.87914
H	5.57516	1.71195	-0.04820
H	5.80571	2.62209	-3.12527
H	-2.95867	1.81037	-4.39215
H	-3.76375	-3.43688	-4.07948
H	-6.09965	0.69394	2.24298
H	3.41595	1.05513	2.72073
H	2.76810	3.50774	0.22823
H	-1.95989	3.01681	-2.41307
H	-2.96063	3.88035	0.11557
H	0.65691	1.24727	2.30048
H	1.01038	2.14919	-1.85388
H	-1.36685	-0.18941	1.82546
H	-1.82561	1.08377	-2.18078
H	-0.28738	-1.00169	-2.26267
H	-1.45162	-3.04316	1.24601
H	0.89090	-0.96832	1.80509
H	2.41962	-1.02087	-2.13711
H	0.56299	-3.09384	-3.12430
H	0.39703	-5.19051	-1.41993
H	1.83139	-3.88402	2.04850
H	-3.73255	-3.31447	-1.93854

H	-4.67070	-1.75611	1.08137
H	3.13489	-3.92596	0.48607
O	-1.94870	-3.74473	2.77222
H	-1.33089	-4.47201	2.95506
H	-1.60326	-2.99749	3.30623

109
Hf4_4_2_term_perox_conf4_ion8_diconf9.log Energy: -3143110.4329774

Hf	2.42504	0.84843	-0.26055
O	0.98839	-0.47868	-1.20610
O	2.18168	-1.07254	0.69055
O	3.67316	1.13604	1.59728
O	3.36437	0.76307	-2.12501
O	3.20866	3.10956	-0.20111
O	4.27079	0.34789	-1.00760
Hf	-0.58503	2.64097	0.15292
O	1.01239	1.70683	1.11697
O	0.95479	2.10613	-1.22242
O	-0.96888	3.88701	-1.78251
O	-0.45161	3.56639	2.35259
O	-2.38672	3.95537	0.37158
O	0.78196	4.50369	0.19757
Hf	0.57544	-2.22002	-0.14660
O	-0.72865	-1.32557	1.23140
O	-1.40025	-1.69003	-0.97476
O	0.65430	-2.91780	-2.42991
O	1.01137	-3.13876	1.92632
O	2.36884	-3.49810	-0.45737
O	-0.44135	-4.24763	-0.16591
Hf	-2.49133	-0.39525	0.33170
O	-1.69455	1.21737	-0.94289
O	-1.73673	1.32499	1.38891
O	-3.14209	-0.67998	2.57991
O	-3.95406	-0.28123	-1.12833
O	-3.57309	-2.46455	0.63559
O	-4.42983	0.31578	0.16059
Cl	-1.18663	1.11367	4.45189
Cl	1.07295	3.45407	-4.08964
Cl	-2.07396	-2.65558	-3.92205
Cl	3.87127	-2.66580	2.98461
O	-2.86316	-4.22276	-1.35023
O	4.45427	-2.34895	-1.56974
O	-4.61850	2.83960	-0.48867
O	-3.18278	2.76027	-2.76692

O	6.22260	0.62572	1.82404
O	-2.92308	-3.43081	3.04658
O	3.99293	3.32475	-2.66956
O	-6.10188	-1.79890	0.64418
O	1.51124	-5.54747	-1.97657
O	-2.12609	5.71935	2.41836
O	2.70619	-1.50372	-3.51099
O	-6.03111	-1.78209	-2.06809
O	-0.82308	-5.00644	2.37672
O	6.50943	-2.01690	1.39742
H	3.22817	1.07750	2.46959
H	3.93539	3.16468	0.44434
H	-1.86375	3.68080	-2.17307
H	-0.78545	2.99014	3.07580
H	-3.28959	3.56954	0.15305
H	1.70003	4.12854	0.11666
H	-0.16895	-2.81241	-2.97661
H	1.95188	-3.21062	2.22719
H	3.20734	-3.04603	-0.81675
H	-0.61563	-4.67187	0.72146
H	-2.69168	-0.11242	3.24631
H	-4.58476	-2.31704	0.64599
H	-3.33125	-5.06547	-1.47552
H	4.04532	-2.24148	-2.45765
H	4.48442	-1.41099	-1.24488
H	-4.62370	1.86998	-0.19644
H	-5.48945	3.21541	-0.28225
H	-3.91302	2.82975	-2.10173
H	-3.56357	2.96372	-3.63570
H	6.39047	-0.34380	1.65220
H	6.47023	0.76047	2.75333
H	-3.25253	-3.33455	2.11544
H	-3.65303	-3.82954	3.55057
H	3.91898	2.33232	-2.65783
H	-6.31075	-1.92963	-0.31790
H	0.78597	-5.71913	-1.34827
H	1.14640	-4.80537	-2.50389
H	-2.74144	5.77884	3.16843
H	-1.90562	6.63481	2.17750
H	2.84820	-0.62252	-3.06078
H	-5.24272	-1.22216	-1.84228
H	-0.80501	-5.90280	2.74768
H	7.24932	-2.36516	1.92136
H	-2.75063	-3.81806	-2.25028

H	-1.31588	-4.26759	-0.65158
H	0.48994	-3.89827	2.28791
H	-1.61325	-4.53120	2.75127
H	-5.75586	-0.87422	0.64229
H	-6.67898	-1.15514	-2.42828
H	2.78965	-1.34796	-4.46549
H	3.17705	3.58648	-3.15290
H	5.70126	-2.32353	1.87471
H	-3.04322	-1.60598	2.91351
H	-3.37233	-3.06451	-0.13025
H	1.35987	-2.36959	-2.88547
H	2.20746	-4.32479	-0.99495
H	-0.38953	-1.17787	2.12724
H	-1.65469	-1.77453	-1.91774
H	2.78659	-1.41699	1.38227
H	0.25108	-0.02652	-1.64864
H	0.99046	2.32576	-2.17744
H	1.17754	1.70676	2.08919
H	-1.46985	1.21611	2.32614
H	-2.11546	1.39026	-1.80910
H	-0.33567	3.77711	-2.54116
H	0.63022	5.02567	-0.61111
H	-0.87946	4.44465	2.49322
H	3.57792	3.34900	-1.12415
H	4.65273	0.88321	1.69007
H	-2.47862	4.60957	1.10637
O	1.87421	1.49128	3.70999
H	2.01156	2.36695	4.10862
H	1.04907	1.15130	4.12666

109
Hf4_4_2_term_perox_conf5_ion6_diconf10.log Energy: -3143087.7128613

Hf	-2.20038	-1.47963	-0.02938
O	-2.36446	0.19935	-1.46563
O	-1.33663	0.36177	0.73473
O	-2.55676	-1.67188	2.26029
O	-3.18789	-2.49147	-1.49774
O	-3.14544	-3.27980	-0.22236
O	-4.19372	-0.53573	0.47095
Hf	1.31627	-2.11267	-0.16472
O	-0.46897	-2.46580	0.93329
O	-0.38622	-1.68735	-1.26204
O	1.79507	-2.77721	-2.38488
O	1.98661	-2.93868	1.96628

O	3.50378	-2.78262	-0.08809
O	1.13233	-4.32868	-0.37664
Hf	-1.41098	1.89864	-0.71176
O	0.31077	2.53624	0.51734
O	0.43372	1.29582	-1.42981
O	-1.32833	2.17486	-3.21671
O	-2.51932	2.68703	1.04603
O	-3.37415	2.85440	-1.47316
O	-1.06092	4.06726	-1.24927
Hf	2.10720	1.41959	-0.01785
O	2.37739	-0.48937	-1.08004
O	1.33532	-0.33918	1.06657
O	2.35343	2.21477	2.13487
O	3.03544	2.32116	-1.62048
O	3.27120	3.06761	-0.35050
O	4.09650	0.55793	0.66022
Cl	0.97994	-1.12671	4.10698
Cl	0.35862	-0.42979	-4.11160
Cl	-2.85436	1.16478	3.82446
Cl	4.54920	1.76947	4.26283
O	-0.06443	5.77025	0.50612
O	-5.49669	1.18779	-1.14023
O	5.34345	-1.22802	-1.38103
O	4.37753	-3.21821	-3.07278
O	-4.74221	-2.86136	3.30648
O	2.33724	4.86293	1.29433
O	-5.65122	-3.94162	0.79186
O	6.08834	2.05262	1.58472
O	-3.80182	3.01770	-4.10983
O	3.64177	-5.13533	-1.29848
O	-4.61020	-0.67331	-2.83323
O	5.19931	1.08512	-2.58487
O	-2.41144	5.20359	1.83445
O	-5.40119	-0.28461	2.91204
H	-2.54839	-0.79861	2.72414
H	-4.62347	-0.49385	1.36286
H	2.73096	-2.88221	-2.71028
H	1.71418	-2.38647	2.76693
H	4.15526	-2.17775	-0.52494
H	0.95463	-4.85816	0.46314
H	-0.66430	2.87584	-3.35292
H	-2.51020	2.12197	1.86152
H	-4.18625	2.39306	-1.14541
H	-1.89327	4.52083	-1.47374

H	3.07178	1.93531	2.76926
H	4.84755	1.16834	0.94267
H	0.82315	5.49439	0.87175
H	-6.43849	1.31976	-0.94462
H	-5.43307	0.57592	-1.91855
H	5.29359	-0.35108	-1.89870
H	6.27035	-1.33386	-1.10562
H	4.91353	-2.51817	-2.62581
H	4.61201	-3.19825	-4.01500
H	-5.20228	-1.98985	3.37947
H	-4.66611	-3.21090	4.20925
H	3.01016	5.51462	1.55343
H	2.66189	4.44205	0.44966
H	-4.79635	-3.72522	0.35626
H	6.87382	1.48104	1.61120
H	-3.80822	3.94493	-4.40067
H	-2.88222	2.71516	-4.25300
H	4.18142	-5.88955	-1.01063
H	4.06610	-4.75650	-2.10365
H	-4.36141	-1.49363	-2.32708
H	4.42852	1.59894	-2.19534
H	-2.29586	5.19466	2.79887
H	-6.24473	0.19699	2.90290
H	0.05715	6.65970	0.13380
H	-0.56343	4.67150	-0.61398
H	-2.52779	3.65639	1.33699
H	-1.54817	5.52166	1.47453
H	5.74698	2.04810	2.51592
H	4.98373	0.98324	-3.52629
H	-4.77088	-0.94185	-3.75140
H	-5.47508	-3.70142	1.72073
H	-4.73462	0.30722	3.35046
H	2.40985	3.20185	2.08485
H	4.47296	-0.09527	0.03625
H	-0.93109	1.36409	-3.62118
H	-3.53991	2.94379	-2.46045
H	0.18256	2.75668	1.45227
H	0.54205	0.76216	-2.24346
H	-0.43552	0.23033	1.09733
H	-3.01544	0.12220	-2.19504
H	-0.39980	-1.29228	-2.15823
H	-0.53594	-2.41871	1.90185
H	1.30065	-0.41118	2.05013
H	2.48338	-0.48731	-2.04345

H	1.32168	-2.24626	-3.06382
H	1.84830	-4.78592	-0.87498
H	2.96224	-2.94851	1.94435
H	-4.66197	0.12854	-0.09743
H	-3.29998	-2.20763	2.65661
H	3.70586	-3.71589	-0.38450
O	0.87011	-5.51560	1.96153
H	1.28259	-4.71204	2.34233
H	-0.05244	-5.48993	2.26639

109
Hf4_4_2_term_perox_conf5_ion6_diconf1.log Energy: -3143094.4659174

Hf	2.48076	0.17075	-0.04920
O	1.88304	-1.47542	-1.20081
O	1.09927	-1.08132	0.94385
O	3.21462	0.06384	2.09184
O	3.30316	0.58320	-2.22458
O	3.96143	1.81942	0.03847
O	4.35141	-1.11489	-0.11898
Hf	-0.28386	2.41510	-0.00668
O	1.43503	1.73118	1.08561
O	0.97379	1.20325	-1.17165
O	-0.20639	3.31101	-2.20601
O	-0.44094	3.43724	2.09708
O	-1.76599	4.10194	0.00182
O	1.18733	4.16124	-0.03257
Hf	0.14908	-2.53125	-0.39959
O	-1.57716	-1.96652	0.76482
O	-1.13595	-1.12142	-1.37647
O	0.46249	-3.05519	-2.75900
O	0.51006	-3.95155	1.05986
O	1.35776	-4.16566	-0.15815
O	-1.31566	-4.11437	-1.19938
Hf	-2.65255	-0.25280	-0.10819
O	-1.87746	1.56245	-1.07721
O	-1.28817	0.97590	1.12372
O	-3.60022	-0.84992	1.93298
O	-3.75484	-0.32262	-1.84600
O	-4.32729	-1.20855	-0.79219
O	-4.07020	1.40258	0.56995
Cl	0.15775	1.14172	4.03915
Cl	0.52039	-0.09851	-4.02801
Cl	4.13203	-2.38865	3.70287
Cl	-6.49168	0.43554	2.27126

O	-3.91785	-3.85709	-0.88459
O	3.98989	-3.67205	-0.37550
O	-4.16879	3.58829	-1.02796
O	-0.64333	5.92801	-2.95144
O	4.40837	2.36305	2.65659
O	-4.50758	-3.39254	1.82335
O	6.19182	2.05747	-1.36240
O	-7.07682	-2.64786	1.75506
O	3.20348	-3.16693	-2.99899
O	-0.35102	6.33682	-0.31592
O	5.77153	-0.44773	-2.37962
O	-4.90074	1.86536	-2.86489
O	-0.79869	-6.17413	0.43800
O	6.15652	-0.95043	1.81855
H	3.42065	-0.78003	2.58152
H	2.62977	0.34790	-2.90022
H	4.15136	2.20881	0.93011
H	5.02320	-0.99848	0.62748
H	-0.42176	4.24259	-2.46996
H	-0.33090	2.81784	2.86762
H	-2.62650	3.98089	-0.49376
H	1.73144	4.09041	0.77192
H	-0.32621	-3.61551	-2.90075
H	-1.15322	-4.98029	-0.72097
H	-4.43655	-0.37828	2.16551
H	-4.96724	1.17881	0.91776
H	-4.06377	-3.92460	0.08622
H	3.04879	-3.86541	-0.10343
H	3.93007	-3.70193	-1.35559
H	-4.41824	3.03829	-1.83840
H	-4.89718	4.21046	-0.86796
H	-1.51125	6.11126	-3.35089
H	0.01249	6.21469	-3.61035
H	5.30454	2.42624	3.02393
H	3.78263	2.76375	3.33067
H	-4.32901	-3.94100	2.60448
H	-5.49338	-3.20629	1.83037
H	6.28450	1.18817	-1.81685
H	-6.98238	-1.67673	1.90733
H	3.59755	-2.96407	-3.86223
H	2.28790	-3.47041	-3.17419
H	-0.36129	7.18441	0.15724
H	-0.42673	6.51907	-1.28389
H	5.50497	-0.93466	-1.56624

H	-4.58522	1.01120	-2.44475
H	-0.27981	-5.43614	0.86947
H	6.89881	-1.51928	1.55442
H	-4.09138	-2.88859	-1.03551
H	-2.30838	-3.94000	-1.07825
H	-1.59749	-6.26385	0.98313
H	-7.55764	-2.96929	2.53537
H	-4.44568	1.90598	-3.72137
H	6.15461	-1.09356	-2.99491
H	6.04230	2.69686	-2.07839
H	5.68323	-1.46023	2.52393
H	-3.86628	-1.81516	1.92389
H	-4.13990	2.23144	0.02672
H	0.36638	-2.23426	-3.30385
H	-1.67473	-2.20477	1.69738
H	-0.94994	-0.72728	-2.24812
H	0.67343	-0.78745	1.76403
H	2.42034	-1.86035	-1.92451
H	0.69528	0.81260	-2.03370
H	1.35076	1.53359	2.03979
H	-1.06046	0.80630	2.05884
H	-1.94679	1.73386	-2.02818
H	0.66407	3.11350	-2.59253
H	0.80668	5.08190	-0.06766
H	-1.33408	3.81973	2.16547
H	4.16035	0.16481	-2.50053
H	4.79297	1.90754	-0.52764
H	4.16867	-2.12745	-0.17990
H	3.79298	0.79369	2.44504
H	-1.46100	5.04659	-0.05304
O	2.65834	3.20640	4.48182
H	2.25212	4.05843	4.25331
H	1.91618	2.56307	4.44704

109
Hf4_4_2_term_perox_conf5_ion6_diconf2.log Energy: -3143083.9330893

Hf	-2.40907	-0.44763	-0.10239
O	-2.01819	1.09528	-1.49646
O	-1.37848	1.16845	0.73889
O	-3.35020	-0.11255	1.92361
O	-3.31539	-1.28198	-2.24465
O	-3.61844	-2.27432	0.19410
O	-4.44378	0.37292	-0.59977
Hf	0.67675	-2.21236	0.35878

O	-1.11665	-1.54246	1.29566
O	-0.79785	-1.49809	-1.03997
O	0.79273	-3.61690	-1.47396
O	1.11940	-2.52703	2.74652
O	2.59360	-3.37580	0.65314
O	-0.17014	-4.21287	0.86083
Hf	-0.53246	2.61883	-0.69704
O	1.29147	2.42642	0.40738
O	0.67521	0.96608	-1.42580
O	0.95410	3.36032	-2.35403
O	-1.12491	3.92408	0.75448
O	-2.05058	3.58952	-2.15488
O	-0.28945	4.63312	-0.25910
Hf	2.47448	0.82870	-0.22373
O	2.07701	-1.25688	-0.96257
O	1.42090	-0.44556	1.14844
O	3.31589	1.36235	1.84634
O	3.18885	1.61153	-2.01965
O	3.98954	2.12945	-0.87318
O	4.38203	-0.42361	0.08241
Cl	-0.21053	0.14735	3.80774
Cl	-1.31254	-3.09034	-3.70667
Cl	-4.98025	2.55773	2.22807
Cl	3.84587	-1.23902	3.71475
O	2.81454	5.93652	1.67997
O	-4.50661	3.04884	-0.85824
O	4.57822	-2.81102	-1.46937
O	2.99492	-4.97082	-2.15953
O	-5.13643	-2.01592	2.42264
O	4.48833	3.76368	1.15713
O	-3.28734	-4.40475	-1.29372
O	6.35203	0.84867	-1.19267
O	-1.79660	6.20306	-1.73801
O	1.98741	-5.91011	0.21223
O	-5.47760	-3.31737	-2.47622
O	4.67997	-0.53086	-3.02488
O	0.98799	4.04231	2.51731
O	-6.46582	-0.00026	1.18562
H	-3.76069	0.78281	2.06366
H	-2.74321	-1.70078	-2.93816
H	-4.05932	-2.49681	1.04564
H	-5.22939	0.15914	-0.02678
H	1.60618	-4.07893	-1.81984
H	0.65496	-1.81108	3.25177

H	3.27452	-3.14977	-0.01750
H	-0.34177	-4.46253	1.82578
H	1.28468	4.24714	-2.12890
H	-2.94895	3.37380	-1.80486
H	3.68490	0.59828	2.35729
H	5.22221	0.01081	-0.25485
H	3.48649	5.23943	1.49253
H	-4.59670	3.16174	0.12193
H	-5.33095	3.39834	-1.23770
H	4.56418	-2.09078	-2.15867
H	5.51492	-3.05292	-1.36031
H	3.71679	-4.30113	-2.07746
H	3.03063	-5.31787	-3.06607
H	-5.88527	-1.45387	2.10632
H	-5.36641	-2.35369	3.30301
H	5.44478	3.93571	1.15700
H	4.27040	3.48258	0.23379
H	-4.14543	-4.26996	-1.77275
H	6.14045	0.36439	-2.01834
H	-1.18884	5.79760	-1.05096
H	-1.19998	6.61700	-2.38306
H	2.32117	-6.66906	0.71811
H	2.41361	-5.93986	-0.67497
H	-4.94211	-2.50422	-2.38992
H	4.09314	0.23446	-2.78004
H	0.12955	4.15304	2.04246
H	-7.38140	0.06721	0.86632
H	3.15562	6.39972	2.46179
H	1.54220	4.81663	2.25141
H	5.65257	1.55027	-1.17254
H	4.66917	-0.57852	-3.99476
H	-6.16104	-3.22843	-1.79174
H	-2.61150	-4.18950	-1.96959
H	-6.26711	0.85186	1.64950
H	3.94544	2.12264	1.84616
H	4.36015	-1.31376	-0.32460
H	1.74748	2.75704	-2.35158
H	-2.00240	4.59268	-2.15335
H	1.38346	2.98373	1.23222
H	0.18327	0.13631	-1.53212
H	-1.07355	1.12617	1.66597
H	-2.15477	1.04216	-2.45341
H	-0.84394	-1.81204	-1.97118
H	-1.07659	-1.11816	2.18094

H	1.10055	-0.09077	2.00617
H	2.02013	-1.46212	-1.90745
H	0.13557	-3.58532	-2.21123
H	0.33359	-4.95781	0.46033
H	2.07878	-2.30639	2.91944
H	-3.82087	-0.55877	-2.65335
H	-3.43836	-3.12349	-0.33975
H	-4.47135	1.35501	-0.78587
H	-3.97494	-0.79093	2.30294
H	2.50796	-4.37386	0.66769
O	-0.30860	-4.79503	3.41764
H	0.31283	-4.04927	3.56412
H	-1.13669	-4.52194	3.84684

109
Hf4_4_2_term_perox_conf1_ion5_diconf6.log Energy: -3143083.1618237

Hf	2.24094	-0.63634	0.07327
O	1.05145	-1.80652	-1.32345
O	0.59104	-1.75916	0.97722
O	3.26290	-1.53310	1.61966
O	3.29451	-0.30152	-2.08955
O	3.99255	0.91081	0.32291
O	3.63054	-2.13439	0.29662
Hf	0.39070	2.36976	0.40452
O	1.55655	0.86052	1.42126
O	1.18372	0.98300	-0.92902
O	0.85772	3.52362	-1.59501
O	0.57033	3.00240	2.65525
O	-0.42131	4.39828	0.73247
O	2.53623	3.21789	0.52630
Hf	-0.81528	-2.36835	-0.39684
O	-2.29312	-1.27754	0.67740
O	-1.45552	-0.64309	-1.43054
O	-0.95751	-2.96693	-2.80981
O	-1.32785	-3.69916	1.51962
O	0.18348	-4.38373	-0.64137
O	-2.61004	-3.67198	-0.92312
Hf	-2.70680	0.66645	-0.19252
O	-1.34219	2.24195	-0.81546
O	-1.16465	1.24890	1.24312
O	-3.99890	0.96137	1.35141
O	-3.33507	1.45082	-2.34235
O	-4.37751	-0.64253	-1.05377
O	-4.11557	2.06996	0.34721

Cl	0.48820	-0.32446	-3.98823
Cl	3.65796	2.76484	-2.78310
Cl	0.46796	-3.19202	3.85790
Cl	-0.63549	0.92773	4.52646
O	-4.89025	-2.93263	0.30487
O	2.49843	-4.57075	0.56590
O	-3.02820	4.47097	0.99618
O	0.68957	6.21584	-2.18024
O	4.86326	0.29148	2.75387
O	-3.63500	-2.66959	2.64853
O	6.07199	1.27694	-1.23744
O	-5.98554	1.11314	-2.28042
O	0.88692	-5.00677	-3.13996
O	0.74851	6.73599	0.50793
O	5.96449	-1.12091	-2.54870
O	-6.71189	2.54387	-0.19822
O	-1.83854	-6.00419	0.18162
O	6.32594	-2.31147	0.98894
H	3.43513	0.67467	-2.25304
H	4.37211	0.78596	1.25328
H	0.72664	4.48889	-1.76944
H	0.09028	2.39936	3.29628
H	-1.43477	4.46921	0.77172
H	3.13538	2.41604	0.51821
H	-1.90483	-3.15869	-2.94122
H	-0.67854	-3.64621	2.28914
H	1.05416	-4.43926	-0.10917
H	-2.48414	-4.62973	-0.68947
H	-4.32763	1.48030	-2.44935
H	-5.15370	-0.17752	-1.45743
H	-4.65599	-2.91143	1.26915
H	3.02195	-5.16981	0.00820
H	2.93596	-3.67783	0.46430
H	-3.39416	3.56288	0.79687
H	-3.19382	4.60398	1.94401
H	-0.11949	6.48692	-2.64697
H	1.42255	6.45982	-2.77125
H	4.50335	-0.58464	2.46348
H	4.16173	0.62404	3.35354
H	-3.85211	-2.61839	3.59288
H	-2.87130	-3.27860	2.55147
H	6.19766	0.43511	-1.74797
H	-6.41439	1.69686	-1.58161
H	0.56124	-5.89795	-3.35039

H	0.20055	-4.39783	-3.47854
H	0.15065	7.45064	0.78285
H	0.78821	6.79083	-0.47517
H	4.98978	-1.03795	-2.47607
H	-5.77969	2.41506	0.12963
H	-0.94815	-6.04509	-0.21723
H	6.21367	-2.54386	1.92294
H	-5.68177	-3.48615	0.20339
H	-3.47875	-3.40344	-0.50287
H	-1.44978	-4.65306	1.28989
H	-2.16567	-6.91257	0.28309
H	-6.60066	1.02199	-3.02475
H	-6.76344	3.48630	-0.42735
H	6.14884	-1.01511	-3.49640
H	5.63173	1.88767	-1.86440
H	5.40332	-2.27464	0.65490
H	-4.70099	-1.38566	-0.48784
H	-3.02211	0.85994	-3.04918
H	-0.72913	-2.21245	-3.40254
H	0.46776	-4.60848	-1.58086
H	-2.69801	-1.56682	1.52097
H	-0.94350	-0.33050	-2.20285
H	0.60550	-1.94329	1.94443
H	0.98096	-1.48198	-2.24477
H	0.90079	0.94198	-1.86000
H	1.89600	0.96767	2.34026
H	-1.03767	0.77891	2.09018
H	-1.34949	2.62323	-1.70561
H	1.67889	3.25152	-2.07872
H	2.79100	3.71351	-0.27423
H	0.11657	3.86431	2.68732
H	2.70063	-0.55959	-2.82722
H	4.80032	1.00327	-0.28910
H	0.00324	5.31426	0.66509
O	2.49737	1.25097	4.00572
H	2.41047	2.21992	3.98360
H	1.66075	0.94878	4.42952

109
Hf4_4_2_term_perox_conf4_ion10_diconf1.log Energy: -3143091.7873869

Hf	-2.24219	-0.60237	-0.44475
O	-1.14421	-2.02672	0.66743
O	-0.56270	-1.22936	-1.46835
O	-2.80842	-0.72983	-2.70529

O	-3.41005	-0.74765	1.75696
O	-4.29373	0.35825	-0.49328
O	-3.41010	-2.44615	-0.71886
Hf	-0.45993	2.42422	0.02443
O	-1.79098	1.33662	-1.26875
O	-1.30112	0.71102	0.92762
O	-1.16128	2.99099	2.18452
O	-0.28397	3.62886	-2.06011
O	0.33474	4.44495	0.53488
O	-2.27358	3.77193	-0.26230
Hf	0.82382	-2.43760	-0.26508
O	2.16207	-1.04905	-1.21397
O	1.59788	-0.91179	1.15439
O	0.69553	-3.56769	1.91544
O	1.05874	-3.47881	-2.01581
O	0.08342	-4.13793	-1.09217
O	2.69979	-3.56870	0.18372
Hf	2.61820	0.61318	0.09970
O	1.16120	1.86726	1.18719
O	1.08454	1.56897	-1.12978
O	3.69563	1.05866	-2.00001
O	3.73861	1.26108	1.78711
O	4.44684	-0.69534	0.11877
O	3.90131	2.17412	0.62072
Cl	-0.79762	-1.20692	3.62635
Cl	1.04775	0.26756	-3.99082
Cl	-4.03165	2.03087	3.06029
Cl	3.54326	-3.86135	3.12690
O	4.95280	-1.44267	-2.44704
O	-3.19325	-4.53989	0.85012
O	2.80380	4.48072	1.42309
O	-3.24798	4.84771	1.92090
O	-5.27821	0.12288	-3.00601
O	5.62335	2.73146	-1.35265
O	-6.55670	-0.79882	0.38113
O	6.21877	0.27864	1.84972
O	-0.75862	-5.77508	0.84323
O	-0.52531	6.22148	-1.34447
O	-5.84591	-1.94758	2.64344
O	2.25511	2.72946	3.53581
O	3.74098	-4.00152	-2.17684
O	-5.91659	-2.19095	-1.78971
H	-2.71646	-1.64893	-3.00907
H	-3.65626	0.17591	2.04743

H	-4.63975	0.62705	-1.37822
H	-4.31906	-2.47108	-1.12072
H	-1.32277	3.94505	2.31096
H	0.64419	3.56063	-2.34890
H	1.29439	4.51598	0.84950
H	-2.94010	3.23289	-0.72523
H	1.58747	-3.75245	2.32348
H	3.29915	-3.73669	-0.60583
H	3.08990	1.32492	-2.71935
H	5.24882	-0.41084	0.64199
H	4.50883	-0.58209	-2.61281
H	-2.31282	-5.00757	0.77689
H	-3.18547	-4.18225	1.75267
H	3.24556	3.65341	1.06316
H	3.37532	5.22986	1.18875
H	-3.84916	5.60765	1.85231
H	-3.76549	4.11347	2.33034
H	-5.74573	-0.72463	-2.79403
H	-5.72495	0.54086	-3.75912
H	6.47169	2.26088	-1.40941
H	5.30163	2.57711	-0.43107
H	-6.44047	-1.26155	1.26595
H	5.37444	0.77224	2.03498
H	-0.35949	-5.50629	-0.01520
H	-0.29250	-5.16351	1.45199
H	0.02477	6.90784	-1.75842
H	-1.40422	6.61682	-1.21755
H	-4.91829	-1.67834	2.46577
H	2.93914	2.15937	3.10368
H	2.76395	-3.94835	-2.33209
H	-6.39190	-1.82881	-0.99548
H	5.85788	-1.34877	-2.78727
H	3.21091	-3.53341	1.02901
H	4.08717	-3.11614	-2.42251
H	6.81298	0.93947	1.45939
H	2.44683	3.60248	3.13652
H	-5.85352	-2.91341	2.54072
H	-7.32425	-0.20911	0.46120
H	-6.42102	-2.95866	-2.10520
H	4.43260	1.74489	-1.92372
H	4.72192	-1.10768	-0.73756
H	0.22605	-3.03748	2.59787
H	2.01622	-0.89503	-2.16559
H	1.21583	-0.77185	2.03778

H	-0.28870	-0.86694	-2.33337
H	-1.12636	-1.92282	1.64016
H	-0.93415	0.38539	1.77280
H	-1.83499	1.50076	-2.25293
H	0.91222	1.18761	-2.02149
H	1.33641	2.16686	2.11633
H	-1.99685	2.54514	2.48489
H	-2.72642	4.23053	0.51553
H	-0.47791	4.59977	-1.97624
H	-2.74908	-1.01093	2.44234
H	-5.08822	-0.04233	-0.03193
H	-3.28183	-3.24553	-0.10176
H	-3.69585	-0.40224	-3.02720
H	0.11010	5.23090	-0.01985
O	-1.71245	1.99566	-3.89211
H	-1.27350	2.82264	-3.61443
H	-0.96128	1.41776	-4.14613

Appendix 6. Supporting Information for Chapter 7

Optimized Geometries of Al Clusters with Cl^- Counterions

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Al10c_Cl.log Energy: -5647406.6243001

Al	5.32415	0.37048	-0.19442
O	4.91966	1.96252	-1.12028
O	3.96471	1.10471	0.85416
Al	3.28673	2.47287	-0.28394
O	6.82468	1.22492	0.73867
O	6.90121	-0.15556	-1.46530
O	4.15557	3.85198	0.87867
O	3.14042	4.05766	-1.49918
O	5.62155	-1.19895	0.79631
O	4.40324	-0.89777	-1.20816
O	1.71490	2.62963	0.70768
O	2.07770	1.52685	-1.34101
Al	4.52797	-2.40772	-0.13240
Al	0.51809	1.47015	-0.27537
O	6.21696	-3.00807	-1.06616
O	4.96232	-3.85850	1.22707
O	-0.49003	2.83075	-1.22739
O	-0.87477	1.93768	0.94125
O	2.89751	-2.23679	0.77616
O	3.49027	-3.63548	-1.13075
O	0.93831	-0.20325	0.70457
O	-0.35040	0.15843	-1.30865
Al	1.83003	-3.45289	-0.20847
Al	-0.28914	-1.40316	-0.29741
O	-1.72008	-1.17949	0.90438
O	-1.74504	-2.23207	-1.21058
O	0.25170	-3.05258	0.75723
O	1.05050	-2.21885	-1.34830
H	3.31754	0.57439	1.33682
H	2.43687	-1.36922	0.76611
H	0.70278	-0.11967	1.64392
H	1.48879	-1.74694	-2.08712
H	3.86823	-0.79425	-2.02816
H	2.24504	0.90414	-2.07751
H	3.81771	-4.46113	-1.51342
H	-1.08982	0.40155	-1.87811
H	5.09615	2.15009	-2.05153

H	5.71605	-1.29772	1.76957
H	1.30176	3.41329	1.09893
H	0.44486	-2.89457	1.69516
H	6.73179	-0.10745	-2.42330
H	-0.05755	3.52117	-1.76078
H	7.73082	0.32585	-1.29282
H	3.61111	4.82028	-1.11822
H	6.13059	-3.34787	-1.97468
H	2.24491	4.41329	-1.73745
H	-1.59638	-3.05631	-1.70148
H	6.78131	-2.20686	-1.12955
H	6.92041	2.23053	0.78011
H	-1.10616	1.51483	1.79265
H	7.04105	0.88166	1.62178
H	3.89873	3.72028	1.80754
H	5.22568	-3.45347	2.12811
H	5.15817	3.95668	0.88053
H	5.70484	-4.43015	0.95804
H	-1.72369	-0.74088	1.77774
Al	-3.11253	-2.12613	0.08741
O	-4.46678	-1.87226	1.37180
O	-4.03790	-0.59910	-0.57958
H	-3.47831	0.18205	-0.73986
H	-4.66996	-2.41389	2.14419
Al	-5.26502	-0.26700	0.81914
Al	-1.76057	3.26598	0.04113
O	-6.45202	-0.34150	2.44938
O	-5.88370	1.42731	0.16539
O	-6.81103	-1.07465	-0.02083
O	-4.23179	1.01043	1.79125
H	-7.11044	-0.63215	-0.86538
H	-6.88814	-2.06817	-0.12864
H	-7.40348	-0.24246	2.27195
H	-6.20792	0.30119	3.13758
Al	-4.50403	2.51751	0.74052
H	-6.35543	1.42765	-0.70244
H	-3.43936	0.81526	2.33602
O	-3.10149	3.61347	1.34661
O	-3.22484	2.20796	-0.62637
O	-5.76194	3.41800	2.03063
O	-0.49796	4.69798	0.77387
H	-3.45737	2.28704	-1.56333
H	-2.86744	3.65419	2.28551
H	-0.10490	5.20658	0.01109

H	-0.89169	5.36075	1.36888
H	-5.52709	3.43468	2.97577
H	-6.65591	3.03350	1.97168
O	-2.44326	4.82532	-1.01045
H	-3.38882	4.85114	-1.25172
H	-1.88576	5.20852	-1.71940
O	-5.15280	4.11473	-0.44839
H	-5.54805	4.82932	0.08605
H	-5.80502	3.90823	-1.14385
O	2.36731	-4.82502	1.14390
H	2.25923	-5.74751	0.85375
H	3.32027	-4.69534	1.36888
O	1.05278	-5.00710	-1.16367
H	1.29041	-5.01553	-2.10796
H	0.06044	-5.14723	-1.15315
O	-2.40296	-3.77769	1.01388
H	-1.42662	-3.60900	1.07976
H	-2.44736	-4.56935	0.42739
O	-4.18804	-3.35352	-1.00745
H	-3.70919	-4.13813	-1.36023
H	-5.10722	-3.64395	-0.73420
Cl	0.50102	5.71572	-1.99388
Cl	7.15165	4.19599	0.95919
Cl	-7.05183	-4.09890	-0.31735
Cl	5.74518	-2.39014	3.69257
Cl	2.60423	-0.61005	-3.71777
Cl	-7.50578	0.77109	-2.38177
Cl	-1.64499	0.45336	3.60247
Cl	-1.96043	-5.57103	-1.53195

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Al13c_Cl.log Energy: -6869631.7945587

Al	4.24405	-4.02837	-0.24557
O	3.04049	-5.00854	0.83427
O	2.75493	-4.18330	-1.36028
Al	1.43400	-4.60975	-0.09858
O	5.03589	-5.65456	-1.12885
O	5.76244	-4.29778	1.07956
O	1.38430	-6.57159	-0.60162
O	0.32920	-5.35158	1.48795
O	5.32390	-2.89878	-1.31515
O	3.98158	-2.39330	0.60597
O	-0.07225	-4.32380	-1.15158

O	0.91544	-2.97418	0.59840
Al	5.03572	-1.22120	-0.43967
Al	-0.71659	-2.64246	-0.40988
O	6.61084	-1.54360	0.70966
O	6.40676	-0.29042	-1.58313
O	-1.87612	-3.57364	0.88280
O	-2.37384	-2.73736	-1.35002
O	3.77746	-0.52518	-1.61070
O	4.58673	0.35725	0.46108
O	0.06638	-1.45691	-1.64356
O	-1.01695	-0.96171	0.44000
Al	2.93913	0.83804	-0.58563
Al	0.09013	0.18665	-0.68467
O	3.94561	2.29590	-1.43021
O	2.69141	2.29975	0.61466
O	-1.34726	1.00783	-1.62154
O	-0.33293	1.71612	0.42626
O	1.45646	0.99083	-1.71867
O	1.69476	-0.25732	0.35757
H	2.58597	-3.62357	-2.15553
H	3.28276	-1.03659	-2.28552
H	0.73896	-1.69166	-2.30930
H	1.60428	0.00449	1.29922
H	3.84026	-2.35107	1.56712
H	1.50142	-2.18617	0.55501
H	4.60624	0.29891	1.43860
H	-0.82153	-0.95821	1.38822
H	3.13897	-4.85676	1.79847
H	5.22507	-2.92775	-2.27911
H	-0.73116	-4.98616	-1.40073
H	1.26463	1.76763	-2.27978
H	2.35938	2.15919	1.52293
H	5.37416	-4.22695	2.01455
H	-1.54425	-4.45710	1.10643
H	6.26765	-5.13013	1.04926
H	0.45806	-4.81716	2.29224
H	6.59109	-0.98866	1.54937
H	0.41632	-6.28696	1.74263
H	-0.26236	1.56259	1.38746
H	6.64551	-2.48646	0.97670
H	4.43805	-5.97126	-1.83048
H	3.67869	2.49690	-2.34016
H	-2.60015	-2.07709	-2.03792
H	5.90539	-5.53354	-1.55182

H	1.32103	-6.76601	-1.55368
H	6.00702	-0.00431	-2.42345
H	2.16960	-7.04455	-0.27126
H	7.23177	-0.76387	-1.78527
H	-1.91561	0.51324	-2.24215
Al	-1.99103	2.25726	-0.36920
O	-3.75219	2.49267	-1.16630
O	-2.22680	3.65919	0.96052
O	-3.09156	1.04891	0.64353
O	-1.23436	3.81007	-1.23210
H	-2.75197	0.13150	0.62009
H	-4.04984	3.33046	-1.54441
H	-0.53322	3.70404	-1.90588
H	-3.12111	3.71376	1.33029
Al	-1.16046	4.98883	0.21641
O	0.14442	6.25690	-0.37250
O	0.44927	4.34058	1.01049
O	-1.51074	6.15536	1.81649
O	-2.55086	6.09704	-0.65549
H	-1.80028	5.62634	2.58072
H	-0.66709	6.58276	2.08413
H	-3.49323	6.03264	-0.30819
H	-2.59630	5.80429	-1.58350
H	0.55950	3.38863	0.78961
H	-0.05936	7.12761	-0.73805
Al	1.69620	5.57027	0.41351
Al	3.74364	3.63203	-0.12925
O	2.48100	4.70286	-1.01685
O	3.31810	4.93815	1.19667
O	2.69566	7.28329	0.08264
O	1.23391	6.58980	2.19305
O	5.12266	4.85814	-0.95037
O	5.40488	2.88392	0.70031
H	2.62562	7.67043	-0.80860
H	3.64513	7.12138	0.24029
H	4.87211	5.20250	-1.82531
H	6.00879	4.46344	-1.02973
H	3.39267	4.72273	2.13662
H	1.98410	4.39143	-1.81126
H	1.37822	6.09056	3.01772
H	1.67064	7.45452	2.30695
H	5.31384	1.89341	0.54640
H	5.56932	2.97591	1.65616
Al	-4.77763	1.40501	-0.05697

Al	-3.49627	-3.36704	-0.02079
O	-6.48791	2.14816	-0.91215
O	-5.83116	0.28445	1.05152
O	-5.04477	2.94533	1.21108
O	-5.05277	-0.08774	-1.18910
H	-5.58826	2.80269	2.00484
H	-5.29406	3.85011	0.83715
H	-7.26488	1.98734	-0.34664
H	-6.63868	1.61733	-1.71559
Al	-5.60902	-1.33085	0.08290
H	-5.61741	0.18697	2.00564
H	-4.47448	-0.29207	-1.96132
O	-5.17706	-2.93944	-0.82353
O	-3.96765	-1.78776	0.88180
O	-7.45628	-1.26015	-0.69528
O	-3.38269	-5.13751	-0.94335
H	-3.84477	-1.64367	1.83606
H	-5.32436	-3.06007	-1.77163
H	-4.02672	-5.87402	-0.72053
H	-3.34733	-5.04206	-1.91043
H	-8.06519	-1.93097	-0.33869
H	-7.54611	-1.26655	-1.66378
O	-4.56062	-4.41235	1.39045
H	-4.87585	-5.34172	1.14391
H	-4.11538	-4.48477	2.25390
O	-6.55526	-2.38045	1.49511
H	-6.32062	-1.98367	2.38543
H	-6.12052	-3.26387	1.50625
Cl	-5.44228	5.74647	0.19807
Cl	1.16773	1.10349	3.23318
Cl	-5.23588	-0.99083	3.87934
Cl	-3.27657	-0.70935	-3.67934
Cl	6.20894	0.29385	3.12783
Cl	-5.34487	-7.08274	0.26992
Cl	2.39486	-2.33832	-3.83433
Cl	1.09082	3.61662	-3.55436
Cl	4.16817	-3.89617	3.57965

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Al13k_Cl.log Energy: -5907594.8417432

Al	0.09306	-0.08481	0.20062
O	-1.15125	-1.38291	-0.21424
O	-0.72417	1.56461	0.25693

O	1.45308	-0.03382	-1.04348
O	0.84657	-0.48046	1.85579
Al	-3.15483	-0.97934	-0.60361
Al	-2.75754	1.85223	-0.13311
Al	3.45590	-0.39997	-0.64425
Al	2.82109	-0.80531	2.14841
Al	-1.59598	-2.93629	0.96227
Al	-1.00958	-2.51910	-1.86282
Al	-0.78329	2.69311	1.90688
Al	-0.21745	3.11329	-0.92396
Al	1.45611	-1.25937	-2.61954
Al	1.88521	1.58011	-2.17067
Al	0.30521	-2.08554	2.95212
Al	0.71408	0.76849	3.43187
O	-3.37889	0.32149	0.72717
O	-2.84521	0.60782	-1.51087
O	3.52256	0.48216	1.00464
O	3.17025	-1.76930	0.60070
O	-3.37852	-2.45797	0.57382
O	-2.79126	-2.06073	-2.09286
O	-2.60817	2.86343	1.48806
O	-2.05906	3.20570	-1.20170
O	3.26062	-1.54014	-2.16279
O	3.62182	1.16489	-1.65093
O	2.16474	-2.31525	3.07802
O	2.55758	0.42324	3.56261
O	-1.51873	-2.03010	2.59071
O	0.12782	-3.31203	1.55898
O	-1.37022	-3.90819	-0.63751
O	0.82956	-2.78388	-1.77074
O	-0.35497	-1.15913	-2.95891
O	1.85474	0.30729	-3.58240
O	1.63536	2.89560	-0.87236
O	0.14192	2.15864	-2.48870
O	-0.26164	4.05526	0.71616
O	0.94610	2.35695	2.49133
O	-1.03638	1.32444	3.14906
O	0.16781	-0.79774	4.31419
O	-5.10055	-1.01746	-0.99050
O	-4.59685	2.54354	-0.44288
O	5.41419	-0.71235	-0.74432
O	4.62485	-1.22897	2.99219
O	-2.30267	-4.61541	1.87740
O	-1.03994	-3.81096	-3.43051

O	-1.01285	4.09829	3.38275
O	-0.06594	4.92850	-1.83645
O	1.65690	-2.37670	-4.36163
O	2.67146	2.88418	-3.52240
O	0.03721	-3.52444	4.35702
O	0.75543	1.72969	5.21557
H	-3.51864	0.17492	1.68733
H	-2.59904	0.73454	-2.44943
H	3.55181	1.45297	1.14167
H	2.96374	-2.71577	0.44285
H	-3.96180	-2.27269	1.32680
H	-3.50908	-2.68384	-2.35213
H	-3.22207	2.58583	2.18653
H	-2.55107	4.05812	-1.22445
H	3.53091	-2.45520	-1.98250
H	4.38735	1.21581	-2.26775
H	2.56639	-2.53068	3.93216
H	2.92997	0.19971	4.42830
H	-2.18367	-1.43760	2.99766
H	0.84584	-3.76146	1.06861
H	-2.07551	-4.51910	-0.89553
H	1.31160	-3.44889	-1.23428
H	-0.86254	-0.50121	-3.47934
H	2.69336	0.28167	-4.06858
H	2.25171	3.12022	-0.14346
H	-0.51534	1.79777	-3.12116
H	-0.82922	4.84023	0.70074
H	1.78578	2.75720	2.17665
H	-1.85522	0.83908	3.38054
H	0.48951	-0.99616	5.20486
H	-5.38413	-0.20444	-1.44386
H	-5.37979	-1.79421	-1.56688
H	-5.24496	2.35489	0.25638
H	-4.63022	3.53388	-0.62788
H	5.82775	-0.29567	-1.56472
H	5.89009	-0.33528	0.01496
H	5.08042	-1.97690	2.56549
H	5.25371	-0.48533	2.98328
H	-3.19672	-4.90280	1.62186
H	-1.72402	-5.39439	1.80164
H	-1.68672	-3.59592	-4.12586
H	-0.15926	-3.72877	-3.84895
H	-1.81852	4.64370	3.34764
H	-0.26342	4.71481	3.45983

H	-0.26019	4.89913	-2.79009
H	0.82805	5.30559	-1.75421
H	1.40200	-1.88128	-5.16091
H	2.53538	-2.75488	-4.54681
H	3.08382	3.66178	-3.10596
H	1.99791	3.23008	-4.13483
H	0.39855	-4.38766	4.08571
H	-0.92038	-3.66684	4.47462
H	-0.11527	2.15552	5.32805
H	1.40589	2.45453	5.24208
Cl	-3.76966	-0.13210	3.77206
Cl	-4.25712	5.46468	-1.13027
Cl	-1.97874	1.02201	-4.55472
Cl	6.34375	0.78771	-3.19928
Cl	2.52350	-4.75985	-0.05834
Cl	-5.51475	-3.49191	-2.69381
Cl	3.64084	3.62390	1.47867

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Al13k-d_Cl.log Energy: -5907598.8077851

Al	-0.11350	-0.02139	0.09099
Al	1.90882	2.56593	0.95064
Al	3.29196	0.04404	0.23142
Al	-1.91637	-0.09921	2.94066
Al	-0.67277	2.47273	2.26899
Al	-2.94136	1.47567	0.65107
Al	-0.57314	-2.56948	2.25067
Al	2.04082	-2.51637	0.86550
Al	-0.44071	-3.17590	-0.61680
Al	-2.73336	-0.90186	-1.82080
Al	-0.15093	-0.84224	-3.14387
Al	-1.47286	1.62337	-2.47515
O	1.43262	0.88751	-0.08354
O	-1.18293	0.80186	1.29778
O	0.15994	-1.74610	0.57480
O	-0.95834	-0.03496	-1.54309
O	1.47131	0.05615	-2.79178
O	0.20479	2.41389	-2.22262
O	2.31492	3.16548	-0.81903
O	0.23242	3.37067	0.92312
O	1.12074	2.01718	2.56340
O	3.52416	1.62861	1.20907
O	2.69487	-0.97266	1.68396

O	2.86631	-1.60588	-0.53311
O	-3.53030	0.60588	2.26096
O	-1.30031	1.48572	3.74535
O	-0.36696	-1.07525	3.36497
O	-2.24895	-1.78232	2.23719
O	-2.38157	3.02547	1.63681
O	-3.36358	-0.11872	-0.25209
O	-2.24112	2.31103	-0.90049
O	1.20608	-3.15469	2.43964
O	-1.10408	-3.90509	1.01360
O	1.32821	-3.83181	-0.29889
O	0.24400	-2.43891	-2.21981
O	-1.92854	-1.53357	-3.43561
O	-3.10588	0.72070	-2.77310
O	-0.72538	0.73748	-4.02536
O	2.81996	4.18759	1.70612
O	5.19688	-0.41907	0.48579
O	-2.84694	-0.51888	4.68999
O	-0.60999	4.08322	3.49953
O	-4.76081	2.19143	0.37011
O	-1.04379	-3.82337	3.77158
O	3.58551	-3.67726	1.28335
O	-0.86531	-4.93329	-1.52275
O	-4.53284	-1.56418	-2.23612
O	0.57736	-1.64709	-4.79897
O	-2.07809	3.16493	-3.57266
O	-2.17024	-2.51370	-0.99066
O	3.59955	0.84183	-1.47523
Al	1.88327	1.62556	-1.82689
O	2.66852	2.48492	-3.48530
H	5.89738	0.21455	0.25955
H	5.50956	-1.32581	0.18051
H	3.89269	-3.58158	2.20178
H	4.40831	-3.55256	0.71167
H	4.31343	2.16895	0.98930
H	4.34698	1.45886	-1.53277
H	2.61068	-0.69026	2.61840
H	3.10478	-1.95333	-1.41248
H	2.29477	4.99808	1.58937
H	3.69558	4.34113	1.25677
H	-0.54296	4.91715	3.00025
H	0.18957	4.04509	4.05592
H	-2.21913	-0.79387	5.38251
H	-3.48657	-1.24864	4.60533

H	-0.73089	-3.48757	4.63109
H	-2.00542	-3.94708	3.86735
H	-0.39183	-5.06893	-2.36315
H	-1.81229	-5.03689	-1.72666
H	-5.25785	-0.93686	-1.92330
H	-4.72109	-1.79172	-3.16246
H	-4.78229	3.04084	-0.10376
H	-5.36829	1.57207	-0.14552
H	-0.12389	4.01253	0.26674
H	1.48721	1.38369	3.21483
H	-1.84850	1.92694	4.40988
H	-3.07669	-2.13342	1.83315
H	0.46532	-0.73404	3.75636
H	1.34261	-4.07782	2.69839
H	-0.93285	-4.83696	1.21091
H	-2.83837	-2.83252	-0.34465
H	-1.90652	-2.50155	-3.48941
H	0.70991	-0.99578	-5.51070
H	1.47463	-2.05427	-4.61641
H	-3.34204	0.51425	-3.68847
H	-1.54509	3.38751	-4.35544
H	-3.01443	3.18539	-3.83570
H	-1.99749	3.24694	-0.74221
H	-2.99989	3.40927	2.27545
H	-4.13507	1.08205	2.84709
H	1.47412	-4.75978	-0.06641
H	1.16297	-2.74927	-2.34701
H	-1.38271	0.53063	-4.70630
H	0.13664	3.32272	-1.85936
H	2.79718	1.83085	-4.19590
H	2.04661	3.14347	-3.84476
H	3.22584	3.51240	-0.90686
H	-3.88306	-0.72819	0.31002
H	2.26006	-0.51478	-2.85555
Cl	-0.89536	5.33842	-1.12065
Cl	5.36203	3.86715	-0.04827
Cl	-6.68675	0.38323	-1.20729
Cl	-4.79254	-2.89693	0.98110
Cl	3.19459	-2.63198	-3.58895
Cl	6.13640	-3.20138	-0.26284
Cl	2.32000	-0.02560	4.69299

Al13k-r_Cl.log Energy: -5907612.1531419

Al	-0.05733	-0.02296	0.02913
Al	-0.50283	3.23339	0.22744
Al	-1.20732	1.65203	2.62937
Al	1.96916	-2.71077	0.67067
Al	0.82606	-1.12837	2.91616
Al	-0.92865	-2.83828	1.29030
Al	2.67901	-1.15692	-1.68783
Al	2.15379	1.78253	-1.47298
Al	0.41105	0.07667	-3.13619
Al	-2.24834	-1.72413	-1.74144
Al	-2.57747	1.14419	-1.77465
Al	-3.28984	-0.43213	0.61839
O	-0.06874	1.47470	1.03405
O	0.39261	-1.42429	1.04224
O	1.09495	0.12697	-1.32578
O	-1.73196	-0.21751	-0.60270
O	-1.99009	2.62831	-0.76817
O	-2.73903	0.91684	1.82580
O	0.93874	3.82714	1.28270
O	-0.62064	-0.00091	3.32072
O	1.92524	0.39546	2.63719
O	-1.66640	3.30332	1.75591
O	2.58282	1.84762	0.37133
O	0.68927	2.94133	-1.19623
O	0.57055	-3.96176	0.92529
O	2.25893	-2.28874	2.49871
O	3.15916	-1.42077	0.08458
O	1.72317	-2.69117	-1.18938
O	-0.42121	-2.60359	3.12703
O	-1.39579	-2.94398	-0.54202
O	-2.40905	-1.74639	1.62808
O	3.52826	0.51796	-1.77665
O	1.87116	-1.11525	-3.40935
O	1.52335	1.65177	-3.30365
O	-1.06197	1.21702	-2.91234
O	-3.16418	-0.36988	-2.76294
O	-3.77491	-1.79015	-0.63431
O	-3.99573	0.93645	-0.53070
O	-0.98679	5.04344	-0.41745
O	-2.33311	1.96252	4.23057
O	3.28510	-4.16951	0.74511
O	1.30497	-1.24655	4.86619
O	-1.97500	-4.50482	1.72172

O	4.24280	-2.07472	-2.44937
O	3.39964	3.26975	-1.84432
O	0.15407	0.05610	-5.13975
O	-2.81122	-3.19801	-2.92283
O	-3.55037	2.45752	-2.90278
O	-4.96912	-0.51097	1.60502
O	-0.72511	-1.43142	-2.86910
O	0.34952	2.44380	3.40652
Al	1.55647	2.11594	1.93800
O	3.09635	2.99066	2.78517
H	-1.82920	2.14902	5.04254
H	-2.87635	1.14223	4.41127
H	3.14537	3.88564	-2.55309
H	3.58089	3.83374	-1.03182
H	-1.72780	4.13694	2.24371
H	0.26440	3.40941	3.45968
H	3.43168	1.39408	0.56608
H	-0.35699	5.76498	-0.24644
H	-1.15775	5.02374	-1.40191
H	2.21406	-0.96447	5.07450
H	0.72029	-0.67268	5.39459
H	4.19232	-3.96700	0.34854
H	2.99167	-4.99399	0.32032
H	4.83075	-2.56479	-1.79009
H	4.02609	-2.72496	-3.13977
H	-0.18926	-0.78980	-5.48020
H	-0.45387	0.74325	-5.46720
H	-2.04910	-3.82335	-3.09715
H	-3.53303	-3.73101	-2.54433
H	-2.64621	-4.39437	2.41898
H	-2.45910	-4.80269	0.92950
H	2.54571	-2.99823	3.09061
H	4.28051	0.69056	-2.35818
H	2.43140	-0.95631	-4.18314
H	-0.24288	-2.25625	-3.07878
H	-2.82390	-0.35934	-3.67098
H	-3.96375	2.13405	-3.72177
H	-2.95100	3.21656	-3.14999
H	-4.63787	-1.58278	-1.04821
H	-4.94267	-0.82955	2.53400
H	-5.76930	-0.81086	1.09993
H	-0.10726	-3.36446	3.63653
H	0.69078	-4.72782	1.50485
H	-4.88788	0.71837	-0.86841

H	-3.35039	1.65625	1.67786
H	2.94837	3.39408	3.65782
H	3.47907	3.69662	2.18512
H	1.65894	4.29937	0.81827
H	-2.76692	2.89850	-0.25045
H	0.37545	3.31750	-2.03950
H	-0.85555	2.13600	-3.17272
H	-1.36531	-0.51242	3.69234
H	-2.62263	-1.66078	2.57986
H	-0.82300	-3.58688	-1.00229
H	1.24591	-3.32432	-1.75614
H	3.78164	-0.88513	0.62556
H	2.87079	0.16491	2.50146
H	2.18761	1.63181	-4.00810
Cl	-1.24537	4.48980	-3.47401
Cl	-6.81304	-0.75856	-0.81844
Cl	3.89260	5.05915	0.62283
Cl	-3.61888	-0.89328	4.53836
Cl	-0.10676	-4.61417	-3.05712
Cl	5.08679	0.27262	1.78645
Cl	5.96376	-3.69822	-0.56801

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Al13p_Cl.log Energy: -8604703.7365019

Al	-0.10893	0.15420	-0.03159
Al	-3.11223	-0.13805	-0.20270
Al	-1.85472	2.59544	0.08953
Al	1.14371	2.87041	0.30187
Al	2.92081	0.41720	0.13873
Al	1.65440	-2.31062	-0.26958
Al	-1.33133	-2.57260	-0.36213
Al	-4.89274	2.08223	1.63068
Al	-0.50960	5.47113	-1.15959
Al	4.10455	2.92889	2.04788
Al	4.77299	-1.77062	-1.66287
Al	0.35245	-5.23308	0.98921
Al	-4.36810	-2.76903	-1.84540
O	-0.21218	1.89353	-0.81122
O	0.04165	-1.59809	0.70866
O	-1.41430	-0.67985	-1.13422
O	-1.62560	0.78510	0.91204
O	1.17297	1.01456	1.09323
O	1.44499	-0.42172	-0.98629

O	-2.96454	1.55008	-0.98661
O	-0.47159	3.31943	1.24481
O	2.55838	2.08030	-0.63731
O	2.78117	-1.30162	0.86607
O	0.23331	-2.83343	-1.37470
O	-2.67712	-1.74648	0.63286
O	-4.40461	0.42447	0.98599
O	-3.26891	2.98609	1.28121
O	-1.81251	4.14765	-0.94529
O	0.94713	4.38168	-0.74519
O	2.35070	3.47970	1.63188
O	3.92378	1.18370	1.47755
O	4.18623	-0.11851	-1.08622
O	3.10825	-2.64271	-1.44416
O	1.63640	-3.90687	0.68633
O	-1.12419	-4.16910	0.59932
O	-2.57423	-3.17931	-1.61878
O	-4.16946	-0.96342	-1.49829
O	-4.31583	1.60991	3.44470
O	-5.68340	2.86283	0.05729
O	-6.62473	1.19560	2.01004
O	-5.58062	3.68233	2.56975
O	-0.38553	5.15336	-3.07319
O	-0.78384	5.93741	0.72722
O	-1.86654	6.82932	-1.58627
O	0.75343	6.95939	-1.28152
O	3.62152	2.45307	3.89633
O	4.89034	3.68989	0.46884
O	4.41742	4.71590	2.85585
O	5.94212	2.39831	2.54671
O	4.35773	-1.28310	-3.55252
O	5.47373	-2.46918	0.00536
O	6.53028	-0.91305	-1.90782
O	5.51777	-3.38103	-2.53238
O	0.21932	-4.90043	2.90183
O	0.47177	-6.02879	-0.78365
O	1.79506	-6.47774	1.49264
O	-0.84785	-6.77875	1.40195
O	-4.07927	-2.58945	-3.80806
O	-4.98173	-3.23676	-0.08482
O	-4.74801	-4.67426	-2.29986
O	-6.25383	-2.41688	-2.32202
H	-0.18033	2.01168	-1.81026
H	0.01001	-1.73170	1.70549

H	-1.40249	-0.57938	-2.10027
H	-1.64171	0.79881	1.89971
H	1.11248	0.91226	2.05963
H	1.49391	-0.30090	-1.94853
H	-3.58381	1.82824	-1.68942
H	-0.56959	2.99350	2.17582
H	2.80478	2.25662	-1.56673
H	2.92982	-1.46130	1.81589
H	0.23705	-3.44602	-2.13394
H	-3.04300	-1.99585	1.50284
H	-4.58450	-0.28460	1.65645
H	-3.14279	3.77580	1.82989
H	-2.72871	4.49415	-1.07444
H	1.82082	4.71134	-1.07469
H	2.11532	4.33671	2.02148
H	4.14293	0.53619	2.19710
H	4.35260	0.59238	-1.75518
H	3.10560	-3.53918	-1.81772
H	2.52131	-4.10368	1.08233
H	-1.98252	-4.64688	0.64981
H	-2.17917	-3.87157	-2.20852
H	-4.75373	-0.31579	-1.96619
H	-3.34485	1.77544	3.61787
H	-4.44352	0.63766	3.63851
H	-5.79687	2.32101	-0.78107
H	-5.29330	3.73086	-0.24116
H	-7.42943	1.72087	2.15667
H	-6.87508	0.41762	1.43638
H	-6.24352	4.29387	2.20483
H	-5.69092	3.63870	3.53599
H	0.32871	5.59414	-3.56634
H	-0.36245	4.17427	-3.34558
H	-0.67928	5.07109	1.21167
H	-0.14570	6.57043	1.10193
H	-2.78573	6.62439	-1.24350
H	-1.97961	6.96240	-2.54561
H	1.73742	6.79701	-1.34969
H	0.54040	7.84595	-1.61747
H	2.69419	2.63556	4.13384
H	3.77302	1.47495	4.09995
H	5.57394	3.13841	-0.00179
H	4.39853	4.25578	-0.18570
H	4.97941	5.36310	2.39441
H	4.52739	4.83594	3.81549

H	6.52075	3.02423	3.01517
H	6.46382	2.04267	1.76869
H	3.51119	-1.63497	-3.88124
H	4.32498	-0.29077	-3.71746
H	6.42135	-2.76414	-0.05058
H	4.99178	-3.19002	0.49278
H	7.31447	-1.50963	-1.79032
H	6.69446	-0.10083	-1.35512
H	6.41788	-3.65060	-2.18212
H	5.60301	-3.30531	-3.50019
H	0.94101	-5.26957	3.44063
H	0.10016	-3.93186	3.19387
H	1.37167	-6.19747	-1.11197
H	-0.07264	-5.74123	-1.58298
H	1.75420	-7.42648	1.28554
H	2.74872	-6.17447	1.50784
H	-1.06593	-6.80246	2.35193
H	-1.72036	-6.80368	0.93190
H	-3.21370	-2.23966	-4.08618
H	-4.76054	-2.10741	-4.31128
H	-5.75392	-2.77440	0.33304
H	-4.74405	-4.07904	0.37135
H	-4.45978	-5.30324	-1.58364
H	-4.37218	-5.00265	-3.13685
H	-6.75993	-3.22304	-2.53199
H	-6.75606	-1.95617	-1.58587
Cl	8.20040	-3.39596	-1.12586
Cl	7.19537	1.71686	-0.19437
Cl	3.58972	5.79387	-1.45225
Cl	-4.59702	5.61919	-0.94496
Cl	-7.45755	-1.37743	0.32959
Cl	-3.74469	-6.05824	0.34904
Cl	4.40215	-4.91621	1.63585
Cl	-0.91783	-5.15339	-3.30733
Cl	4.16003	1.76204	-3.51874
Cl	-0.19478	2.25114	-3.81750
Cl	-5.67227	1.50619	-2.67139
Cl	-0.02467	-2.07195	3.70351
Cl	-4.44159	-1.49544	3.40524
Cl	-1.23693	1.84436	3.86656
Cl	4.03943	-0.55764	3.98835

Al1_Cl.log Energy: -1306420.5997921

Al	-0.12219	-0.27778	0.25217
O	-0.87540	-1.48009	-1.06379
O	1.25206	0.31177	-0.93406
H	-0.62221	-2.41989	-1.05573
H	-1.87269	-1.42520	-1.14040
H	1.38216	1.29573	-0.93840
H	2.14946	-0.14660	-0.90043
O	1.04394	-1.60028	0.94193
H	0.75443	-2.36790	1.46353
H	1.98221	-1.74168	0.56128
O	0.42228	0.97218	1.64240
O	-1.48918	-0.88941	1.48680
H	0.60798	1.89382	1.28305
H	1.17674	0.71076	2.20102
H	-2.40350	-0.93165	1.07205
H	-1.56465	-0.37996	2.31466
O	-1.25150	1.06383	-0.48635
H	-0.96403	2.01478	-0.50215
H	-2.23111	0.93593	-0.53902
Cl	3.61718	-1.48699	-0.45411
Cl	-3.75209	-0.69755	-0.49731
Cl	0.74526	3.31095	-0.21288

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Al2_Cl.log Energy: -1938583.1837712

Al	0.54626	0.31987	1.28822
Al	-0.89551	-0.34537	-1.12289
O	0.76669	0.23558	-0.56105
H	1.62291	0.39984	-1.01782
O	-1.17382	-0.07441	0.70684
H	-1.95950	-0.43010	1.18178
O	-0.52095	-0.55473	-3.04603
H	0.08314	-1.25141	-3.35695
H	-0.36628	0.25333	-3.56616
O	-2.71949	-0.93500	-1.37667
H	-3.24585	-1.18586	-0.53603
H	-2.97926	-1.51936	-2.10885
O	2.41801	0.71817	1.58944
H	2.91103	0.19621	2.24569
H	2.99374	0.80328	0.74795
O	0.18215	0.40197	3.22842
H	-0.40942	1.10441	3.55075

H	0.08607	-0.37502	3.80544
O	-1.53605	1.37505	-1.76084
H	-1.28926	2.26466	-1.34443
H	-2.49950	1.38723	-1.89852
O	-0.37851	-2.22917	-1.11135
H	0.55879	-2.55558	-0.91116
H	-1.00251	-2.91729	-0.82653
O	0.27023	2.22849	1.48629
H	-0.19598	2.81039	0.79873
H	1.07873	2.70388	1.74778
O	0.98430	-1.53455	1.73195
H	0.22031	-2.11423	1.89913
H	1.57559	-2.05610	1.09142
Cl	2.35251	-3.17854	-0.33349
Cl	-3.89177	-1.47435	1.27611
Cl	-0.96901	4.02191	-0.53069
Cl	3.74458	0.96991	-1.04413

46
Al3_Cl.log Energy: -2570771.3750061

Al	-2.04526	-0.09609	0.24413
Al	1.15841	-1.37831	0.38332
Al	1.01039	1.39548	-0.31668
O	-0.85502	1.24869	-0.15114
O	1.49019	0.31728	1.14090
O	-2.23820	0.45458	2.11519
O	0.80336	3.08233	0.67606
O	-0.71551	-1.31158	0.67070
H	-3.05684	0.22354	2.58678
H	-1.47593	0.25014	2.73880
H	-1.02777	-1.99050	1.28785
H	1.14062	0.49018	2.03846
H	-0.07251	3.54457	0.75230
H	1.52148	3.73731	0.68171
H	-1.30212	2.12785	-0.09757
O	1.19680	-0.29012	-1.13132
H	0.82517	-0.48121	-2.01499
O	2.85304	2.00454	-0.52879
H	2.99921	2.37469	-1.41758
H	3.61772	1.36439	-0.36403
O	3.01897	-1.91328	0.15819
H	3.37204	-2.34549	0.95613
H	3.70566	-1.21351	-0.09318

O	0.78595	-3.09737	-0.46239
H	1.43559	-3.47901	-1.07694
H	-0.13845	-3.30248	-0.78638
O	1.34762	-2.24725	2.15412
H	1.11100	-3.18172	2.28656
H	0.95383	-1.70711	2.90543
O	0.80782	2.30875	-2.07012
H	0.39595	1.71111	-2.77011
H	0.33349	3.15740	-2.10803
O	-3.33484	-1.55901	0.61318
H	-3.14033	-2.39401	0.09684
H	-4.29216	-1.39269	0.55417
O	-3.58714	1.10969	-0.00616
H	-3.95053	1.09820	-0.91069
H	-3.39047	2.06383	0.21332
O	-2.25850	-0.61239	-1.61509
H	-2.25569	-1.59875	-1.74991
H	-1.65711	-0.23342	-2.31988
Cl	-2.16810	-3.67763	-1.28467
Cl	-2.24030	3.91083	0.45077
Cl	0.08918	-0.18474	3.98291
Cl	5.16252	0.11325	-0.33046
Cl	-0.35943	0.20557	-3.87359

46
Al3l_Cl.log Energy: -2570755.8712614

Al	-2.53827	-0.84511	-0.04723
Al	2.99279	0.69481	0.11621
Al	0.21423	0.04886	0.09074
O	-1.20806	-0.45986	1.22349
O	-1.16847	-0.23434	-1.16959
O	1.60125	0.50154	-1.11361
O	1.65766	0.21171	1.32589
O	-3.83278	-1.61954	1.24174
O	-3.78923	-1.30805	-1.45026
H	-1.44006	0.13522	1.96560
H	-1.01064	-0.44660	-2.09936
H	1.42862	1.21749	-1.76134
H	1.84392	-0.54894	1.91948
H	-3.55308	-2.45146	1.66465
H	-4.24360	-1.05986	1.92370
H	-3.49970	-1.24440	-2.37730
H	-4.69372	-0.84046	-1.39451

O	3.71442	-1.05626	-0.19911
H	3.62396	-1.66149	0.58901
H	3.35826	-1.58079	-0.98705
O	0.63619	-1.95279	-0.07738
H	1.17188	-2.32497	0.68398
H	1.14004	-2.22729	-0.90988
O	-1.91784	-2.70619	-0.08526
H	-0.92108	-2.70106	-0.08772
H	-2.22495	-3.28238	-0.80660
O	-3.45495	0.80562	0.18948
H	-3.24687	1.39045	0.97642
H	-4.41151	0.89535	-0.09386
O	-0.18991	1.94478	0.35632
H	-0.16881	2.55407	-0.42430
H	-0.89305	2.22328	1.00645
O	2.69131	2.62373	0.29286
H	2.16648	2.84179	1.08549
H	2.17804	3.03377	-0.47686
O	4.30638	0.82625	1.57827
H	4.03021	1.11190	2.46714
H	5.16244	1.24880	1.38489
O	4.43833	1.27015	-1.08189
H	4.84828	0.62021	-1.67984
H	4.46325	2.14203	-1.51432
Cl	0.97244	3.47628	-2.04308
Cl	-2.29545	2.26667	2.55340
Cl	-6.18756	0.38869	-1.02353
Cl	2.59265	-2.66992	2.18247
Cl	2.46637	-2.78525	-2.33854

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Al3r_Cl.log Energy: -2570757.2007846

Al	-2.24012	0.49967	0.00563
O	-1.27943	-0.54066	-1.23589
O	-0.70187	0.18275	1.01697
H	-1.78228	-1.24728	-1.68701
H	-0.79679	-0.11954	1.94077
Al	0.26386	-0.89641	-0.20082
Al	2.69032	0.57268	0.20782
O	1.84916	-0.94120	0.88440
O	1.28424	0.51802	-0.94474
O	4.08281	0.49663	1.60426
O	-0.45820	-2.51424	0.65124

H	1.00103	1.15046	-1.65108
H	2.33745	-1.78866	0.90902
H	-0.13245	-3.40797	0.45590
H	-0.77503	-2.47380	1.60257
H	4.15075	-0.28744	2.17762
H	4.98649	0.78823	1.38805
O	0.91822	-2.22225	-1.51247
H	1.78005	-2.68479	-1.28858
H	0.99904	-1.88774	-2.42303
O	3.94064	-0.38714	-0.96306
H	3.97910	-1.38178	-0.78614
H	3.73502	-0.30941	-1.91272
O	3.63784	2.16997	-0.44203
H	3.21763	3.02439	-0.23682
H	4.07599	2.24674	-1.30757
O	1.87939	1.87598	1.41134
H	2.20331	1.92984	2.32641
H	0.93963	2.20673	1.40320
O	-1.64969	2.15776	-0.79415
H	-1.05620	2.18228	-1.60811
H	-1.26692	2.80097	-0.13856
O	-3.83662	0.70148	-1.10654
H	-4.09565	-0.16940	-1.53691
H	-3.74525	1.36846	-1.81003
O	-3.26740	-0.95491	0.78625
H	-2.89755	-1.36248	1.61880
H	-3.51796	-1.66704	0.14198
O	-2.95565	1.59736	1.45825
H	-3.85265	1.96339	1.36762
H	-2.33962	2.33968	1.72791
Cl	-0.68993	3.63005	1.71801
Cl	-3.97440	-2.21231	-1.92176
Cl	3.54763	-3.31434	-0.40469
Cl	0.26084	2.45436	-3.11687
Cl	-1.73104	-1.88822	3.29307

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Al4b_Cl.log Energy: -3202934.5711897

Al	-2.88084	-0.23029	-0.41065
Al	3.25192	0.53517	-0.40268
Al	0.00576	1.40069	-1.09385
Al	0.35371	-1.11579	0.18468
O	-1.51398	-1.41923	-0.08378

O	0.47804	-0.38266	-1.62517
O	-3.33089	-1.20849	-2.06544
O	0.73513	-2.87639	-0.60660
O	-1.83365	1.02460	-1.32549
H	-3.83672	-0.78377	-2.77898
H	-2.58006	-1.73672	-2.47825
H	-2.15305	1.24846	-2.21308
H	-0.09177	-0.87798	-2.25641
H	0.18737	-3.04467	-1.42732
H	0.76551	-3.69403	-0.08087
H	-1.82357	-2.24734	0.34577
O	-0.06243	0.65867	0.60374
H	0.33376	1.13773	1.35255
O	2.19012	-0.73129	0.45379
H	2.69024	-1.51027	0.80092
O	1.88427	1.70073	-0.94402
H	2.18677	2.60301	-1.12506
O	-0.36570	3.21204	-0.53045
H	0.17192	3.44957	0.28310
H	-1.32513	3.36625	-0.29459
O	-0.01051	2.10171	-2.96203
H	-0.00166	3.07214	-3.05140
H	0.63509	1.74799	-3.59929
O	0.21062	-1.88886	1.95977
H	-0.54725	-2.52624	2.06033
H	-0.01813	-1.16689	2.63126
O	-4.41981	0.93200	-0.83259
H	-4.21642	1.88669	-0.60318
H	-5.25328	0.70799	-0.38064
O	-4.21504	-1.46510	0.41398
H	-3.82957	-2.06912	1.11208
H	-4.60455	-2.06132	-0.25179
O	-2.84802	0.66549	1.30319
H	-2.92809	1.65294	1.22351
H	-2.13236	0.48393	1.97595
O	4.82687	-0.47097	0.07697
H	5.64639	-0.37133	-0.43507
H	4.76066	-1.41240	0.46117
O	3.05600	-0.35620	-2.14079
H	2.05763	-0.49245	-2.17941
H	3.47005	-1.23115	-2.24447
O	3.62812	1.69712	1.09470
H	4.09814	1.31787	1.85724
H	2.87898	2.28672	1.43942

O	4.60569	1.64773	-1.38514
H	4.93609	2.47544	-0.99445
H	4.51106	1.77592	-2.34502
Cl	4.15475	-3.06670	1.27534
Cl	-2.50592	-3.50340	2.00066
Cl	-0.94474	-2.74179	-3.20767
Cl	-3.35861	3.57680	0.34101
Cl	1.37173	3.46856	1.98145
Cl	-0.92921	0.24411	3.74752

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Al4_Cl.log Energy: -3202945.8133231

Al	-1.01560	-1.26704	1.34959
O	-0.96417	0.54254	1.84359
H	-1.82874	0.75320	2.23249
O	-2.85073	-1.36876	2.07520
H	-3.49839	-1.87491	1.49779
H	-2.92821	-1.71136	2.98318
O	-1.72619	-0.89584	-0.35293
H	-2.44353	-1.51788	-0.59853
O	-1.13203	-3.20876	0.93389
H	-0.62383	-3.41829	0.09914
H	-2.06389	-3.48410	0.72155
O	0.77614	-1.35638	0.87371
H	1.19480	-2.20455	1.08539
O	-0.49852	-1.71613	3.21607
H	0.27737	-1.15344	3.51164
H	-0.27062	-2.64252	3.40914
Al	-1.12605	0.20310	-1.73370
O	-1.05511	1.74473	-0.66118
H	-1.91096	2.21756	-0.72343
O	-0.66833	1.39588	-3.27394
H	-0.47039	1.00997	-4.14518
H	0.05355	2.05842	-3.06303
Al	1.92187	-0.34189	-0.19387
O	1.37767	1.28183	0.56186
H	2.08466	1.57941	1.15523
O	3.33462	-0.30883	1.16641
H	3.08469	-0.40692	2.12083
H	4.21945	-0.69663	0.95421
Al	-0.24111	2.06747	0.99848
O	-1.78245	3.17011	1.53118
H	-2.67688	3.04361	1.09191

H	-1.90797	3.40973	2.46512
O	-3.00613	0.55945	-2.24502
H	-3.53098	1.07623	-1.56450
H	-3.10656	1.05508	-3.07823
O	0.55123	3.75318	0.33538
H	-0.05652	4.50809	0.24655
H	0.97064	3.60627	-0.56401
O	2.64771	-2.04611	-0.79389
H	2.04943	-2.63113	-1.33196
H	3.59534	-2.10326	-1.06672
O	0.68010	-0.21887	-1.58332
H	1.16602	0.05090	-2.37795
O	3.16615	0.54038	-1.42069
H	4.13183	0.33049	-1.35420
H	2.99233	1.48744	-1.65676
O	0.46566	2.55675	2.78982
H	0.89437	1.78999	3.27254
H	1.05382	3.32747	2.87405
O	-1.21614	-1.28080	-3.03657
H	-0.70799	-2.08328	-2.70866
H	-2.08673	-1.59590	-3.33588
Cl	1.93977	0.07636	3.96356
Cl	5.61470	-1.17770	-0.71915
Cl	0.27522	-3.73880	-1.86073
Cl	-4.07322	-3.11120	-0.03239
Cl	-4.14445	2.57782	-0.25472
Cl	1.77266	3.16551	-2.46685

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Al4f_Cl.log Energy: -3107006.7621179

Al	0.16151	-1.39589	-0.01948
Al	-0.17127	1.66909	0.12232
Al	2.46364	0.41981	-0.52953
Al	-2.47837	-0.18991	0.64690
O	1.00639	0.20560	0.81858
O	-1.02263	0.07370	-0.69984
O	1.50490	-1.00621	-1.27151
O	1.24125	1.71333	-1.10283
O	-1.55125	1.29241	1.30341
O	-1.22866	-1.45359	1.23872
O	3.60262	0.61815	-2.10046
O	-3.57855	-0.54834	2.21083
H	1.27546	0.07702	1.76531

H	-1.26249	-0.00511	-1.66029
H	2.00483	-1.78946	-1.58694
H	1.57776	2.59226	-1.36987
H	-1.78579	1.81542	2.08244
H	-1.54955	-2.35875	1.44290
H	3.27193	0.30390	-2.96143
H	4.56331	0.45924	-2.07255
H	-3.16248	-0.70980	3.07693
H	-4.38518	-0.02069	2.35201
O	-1.09405	2.99090	-0.89980
H	-1.98243	3.38144	-0.58856
H	-1.09927	2.94670	-1.87141
O	0.49585	3.07431	1.26244
H	1.15364	3.70947	0.83088
H	0.80123	2.90151	2.17051
O	1.14855	-2.70768	0.96829
H	1.55140	-2.37848	1.82234
H	1.87894	-3.15795	0.44956
O	-0.52136	-2.77576	-1.15866
H	-0.97488	-2.45208	-1.98890
H	-1.14502	-3.42111	-0.70958
O	-3.84174	0.99154	0.00941
H	-4.56895	0.68622	-0.55825
H	-3.83720	2.00661	0.04725
O	-3.45430	-1.47290	-0.41937
H	-3.35774	-2.42937	-0.12865
H	-3.24968	-1.44795	-1.39941
O	3.44549	1.78874	0.40716
H	4.36043	1.64356	0.70316
H	3.31504	2.76437	0.18639
O	3.73279	-0.73023	0.35432
H	3.81713	-1.65586	-0.03292
H	3.56311	-0.84523	1.33597
Cl	3.45292	-3.48401	-0.88189
Cl	-2.59641	-4.23164	0.53499
Cl	2.53176	-1.06402	3.15951
Cl	-2.20037	-1.23068	-3.21275
Cl	2.56206	4.54752	-0.33566
Cl	-3.72276	3.95767	0.05547

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Al4l_Cl.log Energy: -3202906.5876497

Al	4.25152	-0.57431	-0.22898

Al	-1.42498	0.25635	0.20679
Al	-4.25443	0.70680	0.28314
Al	1.43636	0.02322	-0.07167
O	2.61931	-1.38815	-0.41839
O	3.12254	0.87832	0.02183
O	0.14405	1.24302	0.56087
O	-0.12224	-0.98070	-0.22941
O	-2.67075	1.59115	0.70971
O	-3.04169	-0.62414	-0.15380
O	5.40880	-2.15832	-0.40283
O	5.80948	0.51888	-0.16516
O	-4.25736	1.50083	-1.50145
O	-5.75021	-0.37524	-0.18554
H	2.28646	-2.31694	-0.48398
H	3.43464	1.75793	0.32659
H	0.10952	2.18511	0.28316
H	-0.09541	-1.95685	-0.37286
H	-2.43786	2.50562	0.44595
H	-3.29152	-1.54925	-0.36951
H	5.34846	-2.79652	0.33157
H	5.48562	-2.66347	-1.23137
H	5.70466	1.47187	0.20565
H	6.69560	0.17517	0.03875
H	-4.85425	1.09275	-2.15386
H	-3.32295	1.40692	-1.83863
H	-6.65270	-0.23082	0.14519
H	-5.58359	-1.37626	-0.34435
O	4.34785	-1.06113	1.66912
H	3.43789	-0.88270	2.04026
H	4.99310	-0.61979	2.24892
O	1.83161	-0.28016	2.02282
H	1.88472	0.63188	2.36584
H	1.23967	-0.73703	2.69940
O	-1.71791	-0.54953	2.09050
H	-1.88203	-1.50353	1.97070
H	-1.06713	-0.52448	2.86420
O	-4.36584	0.24423	2.19468
H	-3.44345	0.02580	2.48226
H	-4.93903	-0.48862	2.48183
O	-1.60126	1.09899	-1.67183
H	-1.22457	2.02437	-1.66030
H	-1.24537	0.61160	-2.47859
O	1.37849	0.71462	-1.90225
H	0.89489	0.25059	-2.65290

H	2.25131	0.99770	-2.22361
O	4.37384	-0.39083	-2.19675
H	5.16678	-0.03943	-2.63890
H	3.92796	-1.01278	-2.79776
O	-5.49725	2.14303	0.75823
H	-5.51718	2.93243	0.18670
H	-5.47829	2.44397	1.68504
Cl	0.85225	-3.91048	-0.59993
Cl	0.13904	-1.07851	4.35669
Cl	-4.84740	-3.12791	-0.65777
Cl	-0.93817	3.91488	-0.71912
Cl	-0.41314	-0.39151	-4.03656
Cl	5.08815	3.17172	0.85558

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Al4r2_Cl.log Energy: -3202928.2846053

Al	-2.80843	-0.51552	-0.08099
O	-2.40500	1.16406	0.73974
H	-2.26889	1.15417	1.71209
O	-1.33787	0.03777	-1.06439
H	-0.99507	-0.40933	-1.87099
Al	-0.87911	1.63849	-0.28211
Al	2.00547	1.02448	-0.29597
O	0.47056	0.95002	0.89320
O	3.12371	-0.02019	0.84846
H	0.45353	1.29843	1.80465
H	4.08582	0.15880	0.76362
O	0.70017	1.95712	-1.26261
H	0.78337	2.21524	-2.19029
Al	2.51365	-1.73416	0.38171
O	1.66712	-0.74631	-0.92812
H	0.99523	-1.07622	-1.55986
O	-0.92067	3.42453	0.45692
H	-0.13253	4.06476	0.41142
H	-1.41446	3.60032	1.27536
O	2.77417	2.60430	0.53279
H	3.02433	2.51739	1.46851
H	2.33961	3.51171	0.42131
O	3.46468	-2.53302	1.91190
H	3.76699	-3.45681	1.85208
H	4.14942	-2.02514	2.38258
O	-4.46306	-0.95289	0.82273
H	-4.41653	-1.19079	1.76343

H	-5.32584	-0.46405	0.63057
O	-3.96438	0.31676	-1.42053
H	-3.57422	1.17524	-1.68770
H	-4.92479	0.48963	-1.18294
O	3.35318	1.30884	-1.70824
H	3.19563	0.76057	-2.49815
H	4.28700	1.09245	-1.41630
O	4.04982	-2.19978	-0.73801
H	4.80446	-1.53110	-0.67935
H	3.83732	-2.25404	-1.68813
O	-2.09416	2.50578	-1.73011
H	-2.28382	3.44823	-1.56325
H	-1.82214	2.43779	-2.66391
O	-2.01100	-1.45214	1.41406
H	-1.66822	-0.94521	2.20970
H	-1.55100	-2.32863	1.32656
O	-2.81204	-2.21757	-1.06095
H	-2.45345	-2.99641	-0.55760
H	-2.22685	-2.17933	-1.86613
O	0.98163	-1.54660	1.56259
H	0.57634	-0.64491	1.38326
H	1.13539	-1.61065	2.52194
O	1.80292	-3.48014	0.01842
H	2.11961	-4.06883	-0.68717
H	0.83165	-3.69477	0.19926
Cl	1.41353	5.26452	0.32944
Cl	-6.75534	0.60464	-0.26470
Cl	5.94669	0.15536	-0.52108
Cl	-1.08313	-4.25952	0.56556
Cl	-1.13511	0.44850	3.60682
Cl	-0.45585	-1.94207	-3.16964

58
Al4r_Cl.log Energy: -3202931.2572934

Al	2.48921	0.60554	0.21805
O	3.98675	-0.16454	-0.72873
O	2.47127	-0.92090	1.46960
O	1.27703	-0.18726	-0.95717
O	0.88097	1.18934	0.94552
Al	-0.34036	0.18028	-0.10647
O	-0.18811	-1.33176	1.18976
O	-1.35171	-1.25760	-1.03676
O	-0.95816	1.47584	-1.36272

O	-1.90024	0.83037	0.73328
Al	-2.55511	1.95690	-0.57539
H	-0.68159	1.53554	-2.28576
H	0.66730	1.23119	1.89904
H	-1.83953	0.97239	1.70279
H	1.37193	-0.63376	-1.82026
H	-0.52687	-1.02301	2.06789
H	1.51714	-1.19571	1.54402
H	2.93704	-1.73314	1.12621
H	-0.98599	-1.44062	-1.93748
H	4.01577	-1.15679	-0.72475
H	4.89807	0.19052	-0.49583
Al	-1.08031	-2.62580	0.20696
O	0.45821	-3.32483	-0.73704
H	1.38833	-3.35824	-0.37725
H	0.56082	-2.99356	-1.68309
O	-0.80251	-3.96421	1.62532
H	-0.86730	-4.90757	1.39115
H	-0.05521	-3.85998	2.24140
O	-4.15031	2.31377	0.47218
H	-4.60448	1.47501	0.78505
H	-4.83433	2.89412	0.09308
O	-3.46143	0.44567	-1.46143
H	-4.21394	0.08116	-0.92244
H	-2.79124	-0.29026	-1.47596
O	-3.32266	2.98583	-2.06546
H	-3.56066	2.49160	-2.87051
H	-2.91987	3.83239	-2.32803
O	-1.87469	3.65903	0.02097
H	-0.90406	3.91381	-0.14397
H	-2.12240	3.98054	0.90464
O	-2.81838	-2.38862	1.05684
H	-3.50418	-1.66765	0.94218
H	-2.93211	-2.76200	1.94770
O	-2.02924	-4.06771	-0.74546
H	-1.64801	-4.48474	-1.53857
H	-2.98949	-3.97378	-0.87743
O	2.73498	2.21592	-0.84673
H	2.10283	2.98164	-0.65983
H	2.70070	2.06358	-1.80697
O	3.64002	1.48696	1.52212
H	3.64919	1.01204	2.37272
H	4.60556	1.57477	1.23461
Cl	3.52622	-3.24671	-0.16187

Cl	6.39408	1.31875	0.33646
Cl	0.92528	4.63933	-0.47502
Cl	-0.79438	0.50989	3.64091
Cl	-5.24928	-0.50772	0.84182
Cl	0.50147	-2.02131	-3.45983

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Al6c_Cl.log Energy: -3792998.1200562

Al	-2.51487	1.43481	-0.40616
Al	-2.40976	-1.42155	-0.32622
Al	0.03302	-2.82300	0.10081
Al	2.51501	-1.43477	0.40630
Al	2.40962	1.42148	0.32622
Al	-0.03297	2.82308	-0.10069
O	-1.02006	-1.50508	0.94566
O	1.01993	1.50499	-0.94548
O	-1.12759	1.63122	0.85641
O	-1.67918	0.00646	-1.30866
O	1.12757	-1.63093	-0.85619
O	1.67933	-0.00647	1.30881
O	-3.38073	0.01349	0.43093
O	-1.44725	-2.84425	-1.09145
O	1.49613	-2.77257	1.28040
O	3.38079	-0.01341	-0.43078
O	1.44720	2.84428	1.09150
O	-1.49604	2.77242	-1.28053
H	-0.55739	-0.65626	1.07784
H	0.55732	0.65615	-1.07773
H	-1.21880	1.75469	1.82042
H	-1.59580	0.06094	-2.28078
H	1.21870	-1.75418	-1.82023
H	1.59560	-0.06096	2.28089
H	-3.65472	-0.07346	1.37172
H	-1.17907	-2.86070	-2.03504
H	1.38696	-2.60820	2.24150
H	3.65516	0.07344	-1.37148
H	1.17908	2.86108	2.03509
H	-1.38649	2.60748	-2.24149
O	3.57210	-2.91014	-0.39960
H	4.08878	-2.75256	-1.20984
H	2.96197	-3.65907	-0.58353
O	3.33289	2.78119	-0.82728
H	3.68038	2.35333	-1.68907

H	4.10037	3.20389	-0.39997
O	0.91754	4.24323	-1.10571
H	0.62886	4.41210	-2.01982
H	1.87270	3.99459	-1.14393
O	-0.98792	4.28845	0.90853
H	-0.86050	4.13804	1.90070
H	-0.70907	5.20105	0.71070
O	-3.57213	2.91031	0.39916
H	-2.96184	3.65918	0.58299
H	-4.08887	2.75298	1.20940
O	-3.90304	1.38811	-1.86590
H	-4.60959	2.05671	-1.81070
H	-3.45371	1.49042	-2.76578
O	-3.94288	-1.61208	-1.60046
H	-3.80537	-2.05658	-2.45577
H	-4.30353	-0.71896	-1.79049
O	3.94306	1.61239	1.60024
H	3.80548	2.05671	2.45564
H	4.30359	0.71920	1.79017
O	3.90290	-1.38863	1.86592
H	3.45344	-1.49017	2.76583
H	4.60894	-2.05781	1.81106
O	-0.91761	-4.24329	1.10571
H	-1.87278	-3.99465	1.14351
H	-0.62937	-4.41194	2.02000
O	0.98733	-4.28826	-0.90893
H	0.70820	-5.20077	-0.71111
H	0.85978	-4.13766	-1.90105
O	-3.33302	-2.78114	0.82716
H	-3.68032	-2.35336	1.68912
H	-4.10056	-3.20385	0.39998
Cl	-4.28531	-1.22341	3.17316
Cl	1.99726	-1.48154	4.17101
Cl	-0.46276	3.18032	3.63672
Cl	4.28585	1.22291	-3.17280
Cl	-1.99741	1.48106	-4.17105
Cl	0.46279	-3.17957	-3.63691

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Al7-1_Cl.log Energy: -5443832.1566197

Al	0.62771	0.04007	0.42501
Al	0.59838	-2.98896	0.30345
Al	-1.99325	-1.45257	0.66965

Al	-2.03915	1.49760	0.70165
Al	0.52700	3.07468	0.20888
Al	3.17618	1.58802	-0.17847
Al	3.21652	-1.45830	-0.15721
Al	-4.48747	0.04249	-1.17604
O	-1.10940	0.04123	-0.31586
O	2.43029	0.08240	1.00390
O	1.27568	-1.38136	-0.74390
O	-0.05414	-1.44895	1.40958
O	-0.07206	1.55561	1.39254
O	1.23902	1.46150	-0.77976
O	-1.16626	-2.83622	-0.25395
O	-2.40414	0.00687	1.73246
O	-1.24111	2.85203	-0.30511
O	2.30874	2.95461	0.71799
O	3.71437	0.07274	-1.04924
O	2.38299	-2.80691	0.79054
O	-3.45434	-1.31710	-0.47458
O	-3.60227	1.44544	-0.29254
O	-3.41624	0.32204	-2.81525
O	-5.86177	-0.17474	0.17521
O	-5.50110	-1.27155	-2.25354
O	-5.72295	1.37226	-1.96157
H	-1.07178	0.02255	-1.31421
H	2.70401	0.09638	1.96148
H	1.01934	-1.26531	-1.69170
H	0.07403	-1.57861	2.40376
H	0.03392	1.69232	2.37147
H	0.99856	1.30901	-1.72361
H	-1.62783	-3.25296	-1.01471
H	-3.19403	-0.02051	2.31735
H	-1.70479	3.23218	-1.08002
H	2.74115	3.54939	1.34831
H	4.12652	0.00391	-1.95870
H	2.83169	-3.36446	1.44269
H	-3.53199	-2.14421	-1.02362
H	-3.67750	2.26928	-0.83271
H	-3.32796	1.28522	-3.03643
H	-2.51696	-0.06088	-2.96606
H	-5.60723	-0.50382	1.09343
H	-6.44884	0.59217	0.30002
H	-6.25711	-1.66039	-1.77572
H	-4.95528	-2.04116	-2.58216
H	-5.31227	2.23052	-2.25038

H	-6.26591	1.04940	-2.70391
O	-2.69736	2.63498	2.11858
H	-3.09645	3.49332	1.88884
H	-2.09069	2.78042	2.90862
O	0.24315	4.41211	1.56540
H	0.05932	4.10235	2.50726
H	-0.36212	5.14803	1.36284
O	4.71763	1.85429	0.94710
H	5.59741	1.75252	0.54148
H	4.73285	1.40161	1.84765
O	4.75811	-1.63442	0.99637
H	4.76407	-1.14818	1.87728
H	5.63926	-1.54265	0.59198
O	3.94824	-2.51856	-1.50886
H	4.27557	-2.10306	-2.36118
H	3.89197	-3.52495	-1.57164
O	0.93434	-4.35737	-0.96081
H	1.85109	-4.78261	-1.13092
H	0.37615	-4.51834	-1.73999
O	0.36356	-4.22210	1.75453
H	-0.26880	-4.95866	1.69254
H	0.32284	-3.81674	2.68615
O	-2.77933	-2.64104	1.96360
H	-3.60256	-2.25831	2.40463
H	-2.98798	-3.55034	1.68512
O	3.88113	2.68305	-1.54813
H	3.79664	3.70033	-1.58297
H	4.10868	2.34356	-2.43169
O	0.81646	4.40051	-1.11330
H	0.32171	4.43950	-1.94944
H	1.71744	4.86615	-1.25456
Cl	3.46616	5.60221	-1.57314
Cl	-3.53226	3.46790	-2.59929
Cl	-0.43513	2.94523	4.10327
Cl	0.38497	-2.50239	4.18102
Cl	-5.09230	-1.01936	2.99821
Cl	4.84629	-0.63395	-3.72591
Cl	-0.27571	-0.10385	-3.19143
Cl	-3.43476	-3.59856	-2.46703
Cl	4.32710	0.14813	3.39840
Cl	3.58902	-5.48502	-1.54454

Al7_Cl.log Energy: -4811650.0760908

Al	-0.10359	-0.07943	-0.05659
Al	-2.40165	1.88410	0.13135
Al	-2.95906	-1.08275	-0.27053
Al	-0.67989	-3.03287	-0.44770
Al	2.21548	-2.04693	-0.18815
Al	2.75569	0.88117	0.13189
Al	0.45902	2.86438	0.24825
O	-1.21486	-1.45979	0.68637
O	1.00436	1.26675	-0.83123
O	-0.68783	1.36522	1.04881
O	-1.74444	0.33409	-1.01410
O	0.46165	-1.55210	-1.18866
O	1.49053	-0.52905	0.89172
O	-3.33903	0.41100	0.77380
O	-2.20161	-2.43545	-1.33299
O	0.96303	-3.30011	0.36716
O	3.11551	-0.61917	-0.89658
O	2.01486	2.29493	1.08540
O	-1.17333	3.05326	-0.63105
H	-1.31806	-1.65464	1.66403
H	1.04698	1.48291	-1.82428
H	-0.73166	1.36502	2.04901
H	-1.81294	0.49079	-1.99526
H	0.51598	-1.42890	-2.15394
H	1.54490	-0.65392	1.88996
H	-4.02492	0.45263	1.45712
H	-2.84931	-3.10526	-1.64373
H	1.13273	-3.96591	1.05126
H	3.75666	-0.56116	-1.65740
H	2.42727	2.72017	1.85197
H	-1.48001	3.95384	-0.85353
O	-0.27747	-4.26554	-1.88240
H	0.09120	-5.15121	-1.71088
H	-0.79213	-4.30417	-2.70887
O	2.88223	-3.22483	-1.56914
H	3.61048	-2.96564	-2.16335
H	2.96756	-4.17970	-1.39325
O	3.86959	1.96049	-0.96460
H	4.46173	2.61206	-0.54948
H	4.36697	1.50212	-1.73232
O	1.24364	4.11440	-0.96826
H	1.28525	3.76351	-1.92355
H	2.10184	4.52294	-0.75620

O	0.12810	4.14863	1.60854
H	-0.14962	3.75953	2.48734
H	-0.56505	4.84456	1.36975
O	-3.05331	3.02045	1.50214
H	-2.94276	4.00638	1.30497
H	-2.65020	2.86162	2.40596
O	-3.72842	2.50798	-1.10951
H	-4.66808	2.48759	-0.85243
H	-3.65473	2.16539	-2.05481
O	-4.35229	-0.88072	-1.57001
H	-4.11679	-0.35526	-2.39992
H	-5.23917	-0.60464	-1.27507
O	4.06055	0.60532	1.49440
H	4.86253	0.02640	1.26759
H	3.71012	0.25584	2.35980
O	3.45577	-2.60726	1.12871
H	3.22227	-2.34670	2.06486
H	4.42736	-2.32871	1.00097
O	-4.05138	-2.20377	0.80296
H	-3.69283	-2.39780	1.71836
H	-4.28900	-3.08970	0.38349
O	-1.51206	-4.35501	0.63111
H	-2.37614	-4.71359	0.25373
H	-1.69547	-4.08195	1.57900
Cl	6.18865	-1.43259	0.91890
Cl	2.53446	-1.05182	3.63586
Cl	-4.18367	-4.82469	-0.70444
Cl	-3.19151	0.95755	-3.63878
Cl	5.04814	0.23690	-3.06033
Cl	-1.14542	2.42617	3.82931
Cl	-2.21822	-2.81987	3.17983
Cl	1.18774	2.54845	-3.50691
Cl	-2.22200	5.80567	0.69113

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Al8_Cl.log Energy: -5635705.2630318

Al	-0.46473	-1.42686	0.02780
Al	0.51586	1.44028	-0.23898
Al	-2.18604	0.81434	0.87618
Al	2.26812	-0.80620	-0.98430
Al	-3.76834	-1.99668	-0.28628
Al	-1.83577	3.79057	-0.78219
Al	3.81471	1.94323	0.45172

Al	1.87648	-3.76908	0.67190
O	-1.06207	0.29487	-0.66640
O	1.09631	-0.28141	0.49001
O	-1.41400	-0.80862	1.54003
O	-0.61033	1.77610	1.21732
O	1.44717	0.74587	-1.70286
O	0.71366	-1.80885	-1.37349
O	0.27608	-2.88595	0.96625
O	-1.97432	-2.30446	-0.65634
O	-0.25310	2.89535	-1.15358
O	2.01566	2.34397	0.44952
O	-3.63063	-0.24139	0.28919
O	-2.83184	2.39983	-0.04571
O	3.70799	0.26192	-0.33340
O	2.89053	-2.37305	-0.03059
O	-3.07415	1.27374	2.50532
O	3.24996	-1.23262	-2.57972
O	-3.45623	4.95879	-0.71374
O	-1.26481	4.59602	0.86195
O	-2.42840	3.42440	-2.61599
O	-1.01090	5.46480	-1.55457
O	4.19107	2.90616	-1.20186
O	3.82392	1.19810	2.27997
O	4.17815	3.71338	1.30800
O	5.80193	1.73094	0.58018
O	2.37224	-3.38158	2.53401
O	1.39817	-4.59504	-0.99833
O	3.52007	-4.90062	0.69241
O	1.04918	-5.44913	1.41820
O	-4.13739	-1.42341	-2.14282
O	-3.71154	-2.78907	1.48616
O	-4.19210	-3.85291	-0.87906
O	-5.74864	-1.86298	-0.04526
H	-1.38978	0.35542	-1.59874
H	1.34830	-0.33837	1.44473
H	-0.88767	-0.70327	2.35108
H	-0.39178	2.18786	2.07042
H	1.92362	1.24859	-2.39202
H	0.47965	-2.07006	-2.27774
H	-0.22827	-3.13292	1.75562
H	-1.76509	-3.26095	-0.72842
H	0.11351	3.04407	-2.03830
H	1.83465	3.31187	0.45536
H	-4.39587	0.28646	-0.03884

H	-3.70145	2.26830	-0.46664
H	4.45575	-0.29962	-0.03248
H	3.71575	-2.20575	0.46952
H	-3.31303	0.49670	3.09683
H	-2.64825	1.99360	3.04976
H	3.42135	-0.43942	-3.15458
H	2.85892	-1.97124	-3.13498
H	-4.07830	4.79610	0.01857
H	-3.24539	5.91064	-0.69775
H	-0.31458	4.88964	0.88712
H	-1.46666	4.22086	1.77186
H	-2.35718	2.47940	-2.95621
H	-3.29503	3.77039	-2.89314
H	-0.11361	5.66620	-1.19060
H	-0.94697	5.52168	-2.52482
H	5.12453	3.17041	-1.28750
H	3.96199	2.45380	-2.07589
H	2.97882	0.85262	2.67260
H	4.44718	0.42926	2.34204
H	3.58594	4.45147	1.01477
H	4.12663	3.69053	2.28146
H	6.29875	2.37794	1.11158
H	6.12163	0.82367	0.83580
H	2.13536	-2.47736	2.89737
H	3.26746	-3.60410	2.84384
H	0.44837	-4.87451	-1.05631
H	1.62645	-4.18990	-1.88901
H	3.33387	-5.85751	0.68115
H	4.16851	-4.73005	-0.01464
H	0.16647	-5.67004	1.02486
H	0.95951	-5.50590	2.38636
H	-3.37397	-0.98954	-2.61301
H	-4.84216	-0.72755	-2.16673
H	-4.48002	-3.34415	1.70724
H	-3.60130	-2.17107	2.27795
H	-3.49278	-4.53745	-0.69804
H	-4.39999	-3.92034	-1.82935
H	-6.31987	-2.58072	-0.36943
H	-6.15788	-0.99861	-0.32134
Cl	-6.02926	0.96055	-1.22262
Cl	1.65753	5.51947	0.35831
Cl	5.74553	-1.20669	1.48767
Cl	3.57701	1.60793	-3.86923
Cl	-1.49517	3.59018	3.72345

Cl	1.55926	-0.56680	3.52045
Cl	-3.81997	-1.21243	4.08284
Cl	-1.55046	-5.53769	-0.47666
Cl	1.82613	-3.58287	-3.85326
Cl	-2.17724	0.52794	-3.57249

Optimized Geometries of Al Clusters with NO_3^- Counterions

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Al10c_NO3.log Energy: -4744202.7180978

Al	-5.38086	0.19164	-0.12831
O	-4.84645	1.47622	1.10234
O	-3.87673	0.91977	-0.93891
Al	-3.24011	2.11225	0.37053
O	-6.43269	1.56988	-1.29071
O	-7.13758	0.00190	0.70029
O	-4.17549	3.67936	-0.42867
O	-2.98216	3.50597	1.83864
O	-5.63163	-1.14623	-1.46764
O	-4.78639	-1.38339	0.75158
O	-1.65092	2.46036	-0.53603
O	-2.02450	1.13367	1.40266
Al	-4.58854	-2.53220	-0.69180
Al	-0.45408	1.25788	0.33658
O	-6.27130	-3.56337	-0.38777
O	-4.66983	-3.46136	-2.58331
O	0.42557	2.66881	1.36046
O	1.10515	1.64888	-0.73311
O	-2.89573	-2.10458	-1.30158
O	-3.58430	-3.94087	0.07498
O	-0.92847	-0.22231	-0.84188
O	0.38949	-0.21938	1.17228
Al	-1.85511	-3.54832	-0.65051
Al	0.23144	-1.56969	-0.13104
O	1.69502	-1.01934	-1.33297
O	1.67741	-2.60532	0.53027
O	-0.28034	-2.90864	-1.53180
O	-1.09924	-2.59040	0.72574
H	-3.42268	0.68731	-1.77296
H	-2.46003	-1.26135	-1.04278
H	-0.92675	0.01210	-1.78616
H	-1.44564	-2.45331	1.63795
H	-4.17461	-1.33663	1.52126

H	-2.27369	0.33113	1.90209
H	-3.89923	-4.82628	0.30323
H	1.06945	-0.15408	1.87125
H	-5.30625	1.65558	1.95375
H	-5.32742	-0.91600	-2.36808
H	-1.41364	3.33393	-0.88903
H	-0.54444	-2.53405	-2.39228
H	-7.15160	-0.79245	1.26124
H	-0.14826	3.33097	1.77087
H	-7.45341	0.78460	1.28869
H	-2.78458	3.05687	2.67900
H	-6.47021	-3.84216	0.52447
H	-3.71806	4.12301	1.99404
H	1.89859	-2.47815	1.47485
H	-7.05595	-3.08270	-0.71058
H	-6.15388	1.56703	-2.22294
H	1.60322	0.82615	-0.89871
H	-7.40128	1.46651	-1.30017
H	-3.58933	4.28849	-0.96930
H	-4.45270	-2.74553	-3.26256
H	-4.94809	3.41459	-0.95734
H	-5.48486	-3.91201	-2.86691
H	1.57714	-0.71053	-2.25143
Al	3.04207	-2.16679	-0.67918
O	4.53244	-1.60307	-1.70073
O	3.75078	-0.80158	0.40619
H	3.14897	-0.12870	0.75241
H	5.06726	-2.20987	-2.23027
Al	5.26986	-0.29209	-0.53790
Al	1.80783	3.11036	0.16332
O	7.00932	-0.45937	-1.40078
O	5.77319	1.15638	0.58105
O	6.10198	-1.58264	0.84715
O	4.58683	1.18267	-1.46140
H	5.65160	-1.34742	1.69729
H	7.07923	-1.47096	0.97752
H	7.79086	-0.43954	-0.76072
H	7.20534	0.09853	-2.17155
Al	4.67408	2.49248	-0.10298
H	6.69598	1.24065	0.90845
H	3.89046	1.18922	-2.15097
O	3.35574	3.58337	-0.87391
O	3.23184	2.22307	1.07065
O	6.10658	3.42766	-1.19962

O	0.77538	4.19764	-1.10514
H	3.17396	1.63554	1.85136
H	3.19177	3.42098	-1.82619
H	0.25091	5.04686	-1.01694
H	0.67317	3.80216	-2.00590
H	5.86772	4.33511	-1.46360
H	6.23213	2.93355	-2.02994
O	2.07688	4.83563	1.16134
H	2.86736	5.30335	0.83473
H	2.17431	4.75948	2.12677
O	5.31434	3.89215	1.20024
H	6.25931	4.12802	1.19516
H	5.08311	3.67211	2.11987
O	-2.27563	-4.62632	-2.29022
H	-2.25832	-5.58471	-2.12457
H	-3.18754	-4.40103	-2.60027
O	-1.06665	-5.26119	-0.08028
H	-0.95282	-5.35271	0.88854
H	-0.12348	-5.42183	-0.37669
O	2.36224	-3.60987	-1.85139
H	1.38668	-3.42053	-1.93358
H	2.36311	-4.45368	-1.33356
O	4.23875	-3.56993	0.04819
H	3.83896	-4.28477	0.61861
H	5.03764	-3.20333	0.48144
N	3.36932	-0.91577	3.08234
N	-2.70597	-1.70041	3.76341
N	-2.86239	-0.96779	-3.77935
N	1.52037	1.86163	-3.46345
N	1.79609	-5.64059	1.06162
N	-1.90425	6.11739	-0.95866
N	-7.46394	2.34806	3.12176
N	9.13132	0.18808	1.26189
O	10.22080	0.09340	1.82527
O	8.42746	1.22516	1.35220
O	8.70467	-0.81264	0.55122
O	2.95363	-5.42942	1.50136
O	0.84831	-5.84172	1.84221
O	1.59550	-5.66838	-0.20446
O	1.19259	0.66787	-3.65246
O	2.73489	2.15632	-3.22932
O	0.66307	2.77897	-3.52642
O	-4.11214	-1.23841	-3.89557
O	-2.52787	0.14354	-3.28884

O	-2.01138	-1.78574	-4.15740
O	-3.23553	-0.86331	2.94885
O	-3.00894	-1.66502	4.96224
O	-1.87870	-2.54988	3.32910
O	2.66079	0.12737	2.86743
O	2.81020	-2.03560	3.11832
O	4.60395	-0.80059	3.25512
O	-2.80508	6.88377	-0.60706
O	-0.68647	6.40121	-0.76140
O	-2.18120	5.01069	-1.54567
O	-8.03014	3.11333	3.91002
O	-8.06369	1.99883	2.04422
O	-6.30499	1.90161	3.36495

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Al13c_NO3.log Energy: -5853539.9449602

Al	-3.18101	-5.02543	-0.18107
O	-1.72593	-5.55157	-1.20013
O	-1.74807	-4.30072	0.89212
Al	-0.27355	-4.81860	-0.21247
O	-3.01282	-6.57516	1.13845
O	-4.33164	-6.35340	-1.14285
O	-0.17440	-6.64848	0.61268
O	0.93184	-5.46164	-1.72695
O	-4.67583	-4.34784	0.72162
O	-3.60454	-3.52897	-1.19977
O	1.15352	-4.25760	0.83229
O	-0.02808	-3.14474	-0.97442
Al	-4.61191	-2.57239	0.08258
Al	1.50722	-2.51446	0.00308
O	-6.32748	-2.75168	-0.89949
O	-5.68799	-1.86350	1.63842
O	2.76335	-3.16852	-1.27909
O	3.17518	-2.28558	0.88540
O	-3.14488	-1.94534	1.12833
O	-4.44483	-0.85537	-0.61692
O	0.50813	-1.59473	1.30619
O	1.37701	-0.73043	-0.73979
Al	-2.90397	-0.19604	0.43715
Al	0.04461	0.03388	0.43881
O	-4.26508	0.56629	1.66736
O	-3.20005	1.50132	-0.33547
O	1.24225	1.04182	1.53159

O	0.00581	1.73798	-0.44000
O	-1.46575	0.31503	1.51841
O	-1.43641	-0.69797	-0.68437
H	-1.78118	-4.44588	1.85847
H	-2.37831	-2.54468	1.04560
H	-0.03925	-2.06632	1.94476
H	-1.47047	-0.47647	-1.62729
H	-3.03801	-3.19382	-1.92676
H	-0.73089	-2.46222	-0.96314
H	-4.61967	-0.67778	-1.55876
H	1.30910	-0.59585	-1.70217
H	-1.68148	-5.27510	-2.14886
H	-4.79715	-4.46706	1.69402
H	1.90559	-4.79651	1.11062
H	-1.36309	0.14366	2.46961
H	-3.17480	1.72294	-1.28318
H	-5.29303	-6.21040	-1.10062
H	2.58000	-4.03752	-1.66771
H	-4.10863	-6.56961	-2.06509
H	0.47954	-5.16550	-2.56909
H	-6.49073	-2.06352	-1.60724
H	1.05303	-6.42527	-1.79426
H	0.24528	1.70538	-1.38316
H	-6.50394	-3.62165	-1.29158
H	-3.12658	-6.21511	2.06497
H	-3.94640	0.70371	2.58636
H	3.33153	-1.67376	1.62850
H	-3.64316	-7.30776	1.01513
H	0.31355	-6.73038	1.45067
H	-5.31754	-0.95576	1.81205
H	-1.08354	-6.98063	0.78509
H	-5.46868	-2.39796	2.43566
H	1.89841	0.63056	2.10907
Al	1.45447	2.62341	0.52475
O	3.18673	3.18125	1.19492
O	1.14688	4.27758	-0.44270
O	2.65809	1.80131	-0.73249
O	0.30384	3.59954	1.72733
H	2.49767	0.83677	-0.73316
H	3.33689	4.11772	1.40103
H	-0.25372	3.13174	2.37794
H	1.94707	4.83619	-0.45370
Al	-0.28514	4.95425	0.58069
O	-1.83363	5.62644	1.46407

O	-1.66448	4.00328	-0.28866
O	-0.44863	6.44245	-0.76710
O	0.77419	6.29011	1.62932
H	-0.02440	6.17401	-1.60133
H	-1.40973	6.55187	-0.97018
H	1.68986	6.45054	1.25261
H	0.92183	5.90810	2.51305
H	-1.49468	3.03882	-0.33991
H	-1.86587	6.50488	1.86592
Al	-3.18731	4.70595	0.53866
Al	-4.56018	2.22357	0.74610
O	-3.55109	3.39777	1.81198
O	-4.63874	3.81166	-0.28470
O	-4.57924	5.97613	1.27101
O	-3.14827	6.02269	-1.01593
O	-6.09390	2.76677	1.93676
O	-6.00956	1.28496	-0.18556
H	-4.54814	6.14032	2.23036
H	-5.45194	5.57948	1.08851
H	-5.83201	2.93024	2.85955
H	-6.83522	2.13640	1.94303
H	-4.50352	3.66154	-1.24935
H	-2.91996	3.18733	2.53660
H	-3.17040	5.54890	-1.92302
H	-3.83774	6.70970	-1.01667
H	-5.64712	0.36490	-0.28244
H	-6.36701	1.49789	-1.09565
Al	4.30043	2.36304	-0.10182
Al	4.38620	-2.67689	-0.48237
O	5.94018	3.21596	0.69038
O	5.51470	1.48111	-1.33804
O	4.26158	3.81739	-1.42721
O	4.68276	0.76991	0.79540
H	3.69510	3.58296	-2.20126
H	4.30420	4.80783	-1.29252
H	6.43371	3.74297	0.03712
H	6.54174	2.47496	0.94053
Al	5.77831	-0.12494	-0.41739
H	5.08652	1.36996	-2.21310
H	4.31947	0.40692	1.63013
O	5.87279	-1.81498	0.38970
O	4.62266	-1.11889	-1.50289
O	7.19104	0.66856	0.98505
O	4.81024	-4.37210	0.53486

H	4.00649	-0.70164	-2.13640
H	5.88750	-1.78181	1.36844
H	5.77421	-4.60142	0.50024
H	4.57061	-4.24883	1.46955
H	8.13087	0.44849	0.85545
H	6.91869	0.31082	1.86261
O	5.41493	-3.65237	-1.87469
H	6.23894	-4.12116	-1.55084
H	5.69537	-3.02463	-2.56225
O	7.45310	-0.47245	-1.38676
H	7.50583	-0.16462	-2.30676
H	7.82377	-1.40305	-1.34467
N	-0.91631	-3.34653	-3.71777
N	-3.06765	3.66426	-3.52980
N	2.58190	1.43170	-3.36854
N	4.89472	-0.71977	3.69709
N	-2.06111	1.60665	4.09326
N	-3.63514	-4.14369	3.81086
N	3.84806	6.89455	-0.15019
N	8.14322	-3.67477	-0.34303
N	-7.25841	0.11334	-2.92131
O	3.63553	0.72067	-3.32599
O	2.67738	2.66827	-3.56181
O	1.45922	0.88607	-3.23527
O	8.28712	-3.00415	-1.40984
O	7.34460	-4.68316	-0.39343
O	8.74323	-3.40086	0.69320
O	-0.87098	-4.62724	-3.56553
O	0.02051	-2.76857	-4.27696
O	-1.92815	-2.71689	-3.31239
O	-6.30871	-0.68002	-2.58182
O	-7.16794	1.33608	-2.60641
O	-8.22820	-0.31297	-3.55390
O	4.61401	6.45203	-1.04882
O	3.80204	8.08898	0.13758
O	3.10340	6.04490	0.47156
O	-3.77733	2.98587	-2.71974
O	-2.95513	4.92265	-3.36424
O	-2.50602	3.11470	-4.48117
O	-1.67484	2.76016	3.72567
O	-3.29688	1.37444	4.19066
O	-1.22356	0.70939	4.33423
O	3.82124	-0.48783	3.03240
O	4.86801	-0.73336	4.92618

O	5.97936	-0.93836	3.06563
O	-2.85473	-5.05315	3.35707
O	-3.23713	-3.35960	4.66979
O	-4.82751	-4.07809	3.36419

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Al13k-d_NO3.log Energy: -5117298.4679379

Al	0.12138	-0.09010	0.24720
Al	-1.93092	-1.57536	-2.03714
Al	-3.22759	0.27352	-0.11433
Al	1.34720	-2.90662	1.63892
Al	0.33758	-3.13891	-1.10247
Al	2.83108	-1.64151	-0.58793
Al	0.10384	-1.06978	3.48841
Al	-2.15930	0.59058	2.56975
Al	0.52662	1.77159	2.91851
Al	3.00262	1.57402	0.58135
Al	0.74150	3.17622	-0.23949
Al	1.96580	1.35091	-2.12157
O	-1.32860	-0.01446	-0.82710
O	0.96457	-1.67850	0.12103
O	-0.26275	0.24095	1.99136
O	1.22523	1.28190	-0.26195
O	-0.95075	2.76588	-0.98227
O	0.28553	1.10913	-2.91717
O	-1.95124	-0.14287	-3.29093
O	-0.17941	-2.01971	-2.51179
O	-1.48406	-2.92828	-0.80449
O	-3.57310	-1.13957	-1.26601
O	-2.92892	-0.69219	1.45393
O	-2.66211	1.62064	1.07113
O	3.08729	-2.83148	0.90226
O	0.61960	-4.17876	0.44407
O	-0.27385	-2.60995	2.51831
O	1.78669	-1.64979	2.94953
O	2.15943	-3.09723	-1.61999
O	3.39408	-0.25115	0.52357
O	2.36323	-0.47230	-1.99947
O	-1.69572	-0.69400	3.88700
O	0.81792	0.49418	4.29065
O	-1.30597	2.05422	3.42697
O	0.17883	3.05884	1.57453
O	2.52266	3.43751	0.46536

O	3.55284	1.74537	-1.20913
O	1.47962	3.21001	-1.99874
O	-2.78162	-2.82027	-3.29163
O	-5.11630	0.57410	0.32241
O	1.91875	-4.46468	2.80050
O	0.16986	-4.74601	-2.29181
O	4.61382	-1.94300	-1.35906
O	0.24479	-1.99307	5.28648
O	-3.85114	0.96287	3.49049
O	1.05704	3.20701	4.25056
O	4.92237	1.80720	1.09651
O	0.29116	5.07930	-0.21286
O	2.96552	1.41904	-3.82964
O	2.29809	1.57067	2.32165
O	-3.23499	1.55808	-1.54239
Al	-1.46241	1.35506	-2.19209
O	-1.88697	2.58961	-3.68358
H	-5.78418	0.36195	-0.34987
H	-5.34277	1.48570	0.69583
H	-4.46495	0.21395	3.39969
H	-4.35196	1.78774	3.17987
H	-4.30785	-1.79970	-1.23251
H	-3.93220	1.39924	-2.19541
H	-2.99613	-1.66421	1.54577
H	-2.09638	2.27358	0.62220
H	-2.42081	-2.82556	-4.19361
H	-3.79992	-2.79082	-3.36995
H	0.69467	-4.57195	-3.11803
H	-0.75550	-4.87767	-2.56571
H	1.17058	-4.89153	3.25554
H	2.53351	-4.18539	3.50257
H	-0.23730	-2.83823	5.33003
H	1.17083	-2.20156	5.50552
H	0.86540	4.11942	3.96902
H	1.99868	3.19418	4.49929
H	5.46208	1.35803	0.39106
H	5.27390	2.70787	1.20497
H	4.52092	-2.13438	-2.31803
H	5.19020	-1.12386	-1.28757
H	0.32511	-2.00936	-3.35006
H	-1.99227	-3.13623	0.00538
H	1.02734	-5.05194	0.35668
H	2.66778	-1.23178	3.05211
H	-1.08806	-3.16712	2.53073

H	-1.96009	-0.53483	4.80430
H	0.52005	0.71744	5.18431
H	2.91580	1.21629	3.01516
H	2.47142	3.81077	1.35959
H	-0.03465	5.57767	-1.03671
H	0.91096	5.66332	0.25483
H	4.01454	2.57324	-1.40458
H	2.93445	2.21607	-4.38541
H	3.92186	1.16930	-3.68698
H	2.25968	-0.96948	-2.84071
H	2.65943	-3.92501	-1.58513
H	3.61648	-3.63318	0.79112
H	-1.53779	2.24437	4.34718
H	-0.65492	3.50812	1.78294
H	2.22171	3.83172	-2.03519
H	0.21306	0.26744	-3.39526
H	-2.07055	3.53238	-3.39581
H	-1.12947	2.62563	-4.29466
H	-2.73331	-0.05254	-3.85349
H	3.77987	-0.58216	1.36245
H	-1.38528	3.59424	-1.28317
N	-3.32051	-4.28837	2.11452
N	4.88945	-0.06599	3.87598
N	2.52583	-3.01278	-4.26935
N	5.92034	1.01085	-2.12263
N	-1.40152	5.86938	-2.97592
N	-5.67821	3.69844	2.03653
N	-6.10510	-2.94781	-2.62477
O	6.16629	2.22601	-2.11893
O	5.46173	0.43004	-3.14570
O	6.12364	0.31697	-1.06588
O	-5.35843	-2.71409	-3.63674
O	-7.30528	-3.19238	-2.79561
O	-6.08762	4.86530	2.06536
O	-5.87370	2.98789	1.00140
O	-5.07398	3.21912	3.04776
O	-2.03696	4.89422	-2.42801
O	-1.71091	6.25690	-4.10095
O	-0.46397	6.42013	-2.32766
O	1.94819	-4.12474	-4.37716
O	1.83970	-1.93859	-4.34524
O	3.76052	-2.94727	-4.10204
O	-3.36291	-3.39591	1.19553
O	-4.25476	-5.08724	2.24020

O	-2.31680	-4.33558	2.88233
O	4.17219	0.93602	4.16294
O	4.43557	-0.94948	3.06560
O	6.01135	-0.20673	4.37347
O	-5.60553	-2.93010	-1.46012

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Al13k_NO3.log Energy: -5117279.3314342

Al	0.08630	-0.19711	0.24000
O	-1.27457	-1.19730	-0.50012
O	-0.53015	1.47992	0.69983
O	1.47300	0.02501	-0.94834
O	0.72485	-1.10553	1.73398
Al	-3.15403	-0.48552	-0.72443
Al	-2.45776	2.05779	0.40629
Al	3.38020	-0.69783	-0.66421
Al	2.62911	-1.69809	1.94388
Al	-1.93427	-2.99398	0.20336
Al	-1.24113	-1.85211	-2.39213
Al	-0.53576	2.10904	2.57275
Al	0.19074	3.22934	-0.00407
Al	1.36764	-0.72800	-2.79427
Al	2.14515	1.82171	-1.59228
Al	-0.00924	-2.86420	2.35880
Al	0.68147	-0.28081	3.57335
O	-3.15933	0.40105	0.90863
O	-2.63127	1.21381	-1.23689
O	3.50403	-0.27595	1.15713
O	2.78414	-2.28053	0.17610
O	-3.62738	-2.17061	-0.04174
O	-3.01991	-1.19812	-2.47056
O	-2.32769	2.61245	2.24254
O	-1.62151	3.56726	-0.25977
O	3.11140	-1.32562	-2.44659
O	3.79600	1.05459	-1.20329
O	1.81499	-3.32883	2.45808
O	2.47148	-0.86184	3.63838
O	-1.81594	-2.55401	2.02527
O	-0.26205	-3.68505	0.69722
O	-1.76823	-3.46686	-1.60706
O	0.54453	-2.34280	-2.41936
O	-0.42219	-0.32532	-3.07652
O	1.97115	0.99021	-3.29508

O	1.98643	2.74478	0.01876
O	0.51743	2.71904	-1.76961
O	0.14850	3.70411	1.84568
O	1.14550	1.41522	2.95565
O	-0.98863	0.50827	3.39972
O	-0.04952	-1.95199	4.00661
O	-5.09223	0.08196	-0.93862
O	-4.30131	2.81897	0.20516
O	5.25474	-1.26510	-0.84780
O	4.36403	-2.51444	2.64737
O	-2.89807	-4.69990	0.53956
O	-1.40614	-2.60039	-4.27874
O	-0.56010	2.97645	4.47407
O	0.58172	5.19009	-0.37353
O	1.46076	-1.32548	-4.79140
O	3.14779	3.31857	-2.54824
O	-0.45093	-4.57624	3.35486
O	0.69908	0.33067	5.49664
H	-3.67275	0.29782	1.73631
H	-2.33602	1.53587	-2.11364
H	3.84684	0.53799	1.57508
H	3.15698	-3.16871	0.01986
H	-4.26519	-2.19983	0.68580
H	-3.64581	-1.94256	-2.61557
H	-2.96252	2.12030	2.80035
H	-2.07289	4.44322	-0.18552
H	3.25493	-2.28774	-2.56286
H	4.58172	1.13740	-1.78223
H	2.11879	-3.74742	3.27698
H	2.77930	-1.38590	4.39254
H	-2.37246	-1.93319	2.52802
H	0.43861	-3.97150	0.08169
H	-2.60639	-3.82302	-1.98361
H	0.87484	-3.21492	-2.11927
H	-0.82830	0.53531	-3.31737
H	2.80178	0.99178	-3.79475
H	2.67725	2.97787	0.66991
H	-0.15166	2.62371	-2.48010
H	-0.41045	4.48311	1.99125
H	1.91271	1.93154	3.27699
H	-1.83522	0.02117	3.49758
H	0.11511	-2.39194	4.85163
H	-5.10080	1.02475	-0.66125
H	-5.42345	0.06504	-1.85400

H	-4.73858	3.06500	1.03860
H	-4.35604	3.64668	-0.39924
H	5.67642	-0.71221	-1.58524
H	5.80391	-1.01148	-0.08297
H	4.72479	-3.30058	2.20067
H	5.09796	-1.87936	2.72357
H	-3.68442	-4.81751	-0.07766
H	-2.33124	-5.48375	0.44317
H	-2.00938	-2.08351	-4.84168
H	-0.51421	-2.48400	-4.66488
H	-1.43727	3.25427	4.79486
H	0.01783	3.75520	4.57167
H	0.47872	5.41858	-1.31459
H	1.49256	5.43959	-0.13638
H	1.30171	-0.59348	-5.41427
H	2.28342	-1.75628	-5.08574
H	3.63572	3.91032	-1.94830
H	2.53030	3.88690	-3.04241
H	-0.22056	-5.36943	2.83802
H	-1.41361	-4.62594	3.50028
H	0.19214	1.16904	5.51586
H	1.56428	0.52443	5.89876
N	-1.98799	2.44129	-4.65902
N	-4.26316	-0.24478	4.07904
N	2.70327	-4.61242	-1.59116
N	4.03424	2.76821	2.66243
N	-5.24275	-4.01278	-1.89579
N	-3.94034	5.93455	-0.99244
N	7.20117	1.05490	-1.75566
O	3.15604	-4.20439	-2.68932
O	1.44662	-4.73172	-1.43539
O	-4.24724	-3.76189	-2.65600
O	-6.33359	-3.46897	-2.10328
O	-5.10635	-4.83947	-0.94456
O	3.47563	-4.86765	-0.63430
O	7.38881	0.60556	-0.60220
O	6.23673	0.55576	-2.47256
O	7.90062	1.95218	-2.24021
O	3.91838	3.64503	1.76280
O	4.79631	1.78112	2.48473
O	3.37232	2.87218	3.73247
O	-3.04328	5.87508	-0.09825
O	-4.51794	4.85895	-1.37815
O	-4.26610	7.01584	-1.49336

O	-3.22633	-0.98001	3.95204
O	-4.41073	0.74811	3.29226
O	-5.10121	-0.49017	4.94623
O	-2.83945	1.68191	-5.14443
O	-1.60983	3.48339	-5.20599
O	-1.46253	2.12134	-3.50420

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Al13k-r_NO3.log Energy: -5117300.7547518

Al	0.17164	-0.23204	-0.05029
Al	-1.05067	-3.21580	0.61434
Al	0.75838	-2.03256	2.65605
Al	-0.06343	3.14017	0.31253
Al	0.48280	1.41265	2.66951
Al	2.59044	1.83431	0.63696
Al	-1.87466	1.99707	-1.65180
Al	-2.86574	-0.75324	-1.02159
Al	-0.80910	-0.32209	-3.10923
Al	2.57694	-0.05342	-2.26531
Al	1.40543	-2.66443	-1.90600
Al	3.21073	-1.53608	0.15208
O	-0.38647	-1.42905	1.17803
O	0.66554	1.28584	0.74307
O	-1.10949	0.12394	-1.25122
O	1.57649	-1.00659	-0.86935
O	0.32949	-3.53752	-0.62775
O	2.30001	-2.31559	1.59251
O	-2.39502	-2.88806	1.88434
O	1.20637	-0.27047	3.12937
O	-1.26827	0.66123	2.76970
O	0.16237	-3.75345	1.99672
O	-2.91553	-0.43224	0.83645
O	-2.15116	-2.46976	-0.71346
O	1.77802	3.50116	0.37688
O	-0.26876	3.11217	2.21779
O	-1.83603	2.66249	0.06258
O	-0.11003	2.70869	-1.58279
O	2.29047	2.04497	2.54412
O	2.70845	1.50394	-1.22936
O	3.24930	0.12603	1.00890
O	-3.45185	1.01300	-1.37667
O	-1.54665	1.40144	-3.43065
O	-2.56248	-1.12764	-2.90652

O	-0.08786	-2.03124	-2.88345
O	2.49274	-1.74091	-3.18339
O	4.05515	-0.78939	-1.33675
O	2.89327	-3.17619	-0.83903
O	-1.65279	-5.04959	0.14575
O	1.84761	-2.80322	4.11062
O	-0.36777	5.04377	0.06462
O	0.43712	1.93439	4.61733
O	4.36790	2.67059	0.63302
O	-2.78670	3.55949	-2.37689
O	-4.72372	-1.40515	-0.98325
O	-0.84705	-0.56380	-5.10080
O	3.89226	0.77027	-3.51097
O	1.32209	-4.37820	-2.90808
O	4.92024	-2.14696	0.87926
O	0.95463	0.47927	-3.11668
O	-0.83247	-1.83584	3.69565
Al	-1.93860	-1.05574	2.32228
O	-3.56709	-0.91794	3.40712
H	1.62537	-2.54564	5.02174
H	2.82328	-2.62861	3.96654
H	-4.94357	-2.14245	-1.57767
H	-4.97024	-1.70133	-0.04762
H	-0.11072	-4.45445	2.60581
H	-1.22928	-2.69587	3.90761
H	-3.35870	0.42218	1.05376
H	-2.52659	-5.33792	0.46047
H	-1.64914	-5.11460	-0.85291
H	-0.44053	2.21095	4.93664
H	0.69033	1.16895	5.16521
H	-1.31467	5.38810	0.15085
H	0.01951	5.38295	-0.78036
H	-3.00893	4.35539	-1.79635
H	-2.49485	3.90222	-3.23764
H	-0.24024	0.03655	-5.57111
H	-0.65305	-1.46229	-5.42261
H	4.74795	0.83011	-3.01279
H	4.07998	0.31534	-4.35045
H	4.63999	3.14155	1.43840
H	5.13225	2.05569	0.38519
H	0.04093	3.90589	2.67824
H	-4.28156	1.20682	-1.83267
H	-2.28419	1.42701	-4.05802
H	0.77136	1.40341	-2.84182

H	2.04338	-1.69920	-4.04178
H	1.64993	-4.40643	-3.82330
H	0.36261	-4.66371	-2.91783
H	4.61261	-1.38051	-1.86208
H	4.93645	-2.20157	1.86761
H	5.70550	-1.64740	0.53263
H	2.40375	2.95125	2.86595
H	2.22350	4.28434	0.00719
H	3.64434	-3.62050	-1.25769
H	2.31050	-3.27415	1.43440
H	-3.54429	-1.29122	4.30446
H	-4.31313	-1.36245	2.89942
H	-3.31076	-2.90846	1.54556
H	0.93105	-4.16491	-0.19441
H	-2.16414	-3.01558	-1.51920
H	-0.76597	-2.72692	-2.97121
H	2.15627	-0.18071	3.35118
H	3.57919	0.07479	1.92939
H	2.63116	2.33620	-1.73843
H	0.09207	3.47445	-2.16033
H	-2.54449	2.54190	0.74037
H	-1.95808	1.34447	2.69141
H	-3.24760	-0.87043	-3.54072
N	2.03238	4.86249	-2.24450
N	-4.90733	2.42242	1.63287
N	-2.16785	-5.17096	-3.43082
N	4.76285	-1.04788	4.14049
N	-3.68043	6.24080	-0.10687
N	-6.15277	-2.84295	1.85078
N	6.46465	0.36591	-0.81766
O	6.34580	0.98353	0.28284
O	6.76199	-0.85665	-0.79232
O	6.30919	0.97181	-1.90437
O	-4.63850	6.92154	0.27771
O	-3.68440	5.74465	-1.27688
O	-2.68518	6.05797	0.66172
O	2.51686	3.90126	-2.88677
O	0.80724	5.17829	-2.42500
O	2.71299	5.49278	-1.40166
O	4.01924	-0.09055	3.76134
O	4.52954	-2.23251	3.68945
O	5.69365	-0.85594	4.91941
O	-5.05753	3.56056	1.16112
O	-3.69713	1.98310	1.82993

O	-5.86100	1.68385	1.92481
O	-5.11795	-2.08629	1.56566
O	-6.82886	-3.27770	0.91038
O	-6.39143	-3.07438	3.04196
O	-1.78439	-5.20730	-4.60400
O	-1.35979	-4.63473	-2.53352
O	-3.25809	-5.59924	-3.04050

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Al13p_NO3.log Energy: -6911240.5608404

Al	-0.30248	0.25639	-0.02132
Al	-2.96752	-1.13011	-0.11073
Al	-2.84387	1.88132	0.00889
Al	-0.17056	3.26538	0.19983
Al	2.36214	1.64785	0.10998
Al	2.24697	-1.35023	-0.33799
Al	-0.44163	-2.71385	-0.43911
Al	-5.54423	0.36685	1.53190
Al	-2.65641	5.09843	-1.18271
Al	2.31486	4.33641	2.30640
Al	4.77756	0.41045	-1.97021
Al	2.10989	-4.55129	0.98904
Al	-3.10606	-3.85111	-2.23404
O	-1.06418	1.80652	-0.88084
O	0.50159	-1.31629	0.71016
O	-1.21473	-1.00003	-1.11925
O	-1.95237	0.30159	0.91495
O	0.55594	1.56529	1.06417
O	1.33892	0.31382	-0.98697
O	-3.46688	0.46884	-1.00123
O	-1.82263	3.07083	1.12694
O	1.39315	2.99298	-0.75309
O	2.94548	0.00396	0.79597
O	1.11302	-2.34358	-1.47957
O	-1.95663	-2.50157	0.66329
O	-4.41174	-1.02480	1.06503
O	-4.32974	1.75979	1.14819
O	-3.39560	3.37266	-1.01386
O	-0.89823	4.53165	-0.96250
O	0.66456	4.38905	1.43174
O	2.94872	2.75201	1.49794
O	3.74757	1.74394	-1.13167
O	3.59830	-1.01996	-1.61382

O	2.85830	-2.87059	0.49633
O	0.38432	-4.11343	0.41724
O	-1.35019	-3.75588	-1.67603
O	-3.63328	-2.25777	-1.43173
O	-4.98095	0.50645	3.40857
O	-6.44935	0.34474	-0.18769
O	-6.85765	-0.89114	2.26133
O	-6.92109	1.71575	1.97767
O	-2.60426	4.95869	-3.14690
O	-2.87421	5.43380	0.72240
O	-4.42627	5.89507	-1.43029
O	-1.92748	6.90124	-1.38750
O	1.53768	3.40221	3.83538
O	3.18228	5.54256	1.05601
O	1.87143	5.96234	3.32961
O	4.00710	4.33702	3.32497
O	3.84047	0.69663	-3.71468
O	5.86098	0.11687	-0.41674
O	5.96548	1.84345	-2.51178
O	5.89577	-0.83585	-2.94528
O	1.69154	-4.03219	2.75951
O	2.43600	-5.39978	-0.76835
O	3.82531	-5.17658	1.54172
O	1.37358	-6.32032	1.54776
O	-2.43290	-3.06812	-3.91650
O	-3.67964	-5.00173	-0.82442
O	-2.86549	-5.61120	-3.14100
O	-4.87881	-3.86071	-3.11023
H	-0.98076	1.91116	-1.85676
H	0.56267	-1.45052	1.68661
H	-1.32627	-0.85253	-2.08520
H	-1.99654	0.36279	1.90460
H	0.61088	1.40173	2.04015
H	1.39713	0.35833	-1.96919
H	-4.10506	0.54603	-1.74161
H	-1.68966	2.84858	2.09018
H	1.38272	3.09945	-1.72071
H	3.24878	-0.13807	1.71149
H	1.00483	-2.01365	-2.38827
H	-1.90929	-2.83014	1.58424
H	-4.68971	-1.91754	1.38995
H	-4.54375	2.57740	1.62290
H	-4.37391	3.41040	-0.97791
H	-0.23059	4.84004	-1.62341

H	0.29863	5.30215	1.34377
H	3.89492	2.55735	1.67325
H	3.72392	2.60007	-1.60274
H	3.86266	-1.82297	-2.09087
H	3.80738	-2.76075	0.74595
H	-0.23554	-4.87197	0.46620
H	-0.68968	-4.30540	-2.17566
H	-4.48682	-1.89411	-1.76056
H	-4.00838	0.62894	3.59519
H	-5.30992	-0.20655	3.98353
H	-6.26709	-0.29039	-0.92992
H	-6.86730	1.16222	-0.54320
H	-7.72566	-0.46678	2.37948
H	-7.02413	-1.78491	1.81009
H	-7.23046	2.31335	1.23278
H	-6.85407	2.22983	2.80019
H	-1.99468	5.51473	-3.66541
H	-2.58785	4.06223	-3.52891
H	-2.57128	4.57962	1.14936
H	-2.27394	6.13479	1.06756
H	-5.16543	5.41316	-0.94332
H	-4.71929	5.99419	-2.35411
H	-1.29362	7.10301	-0.63949
H	-2.54699	7.64962	-1.45548
H	0.55104	3.38485	3.89356
H	1.76586	2.43399	3.89487
H	4.14120	5.39040	0.91027
H	2.77879	5.79095	0.16161
H	1.46499	6.75476	2.86164
H	1.39008	5.84324	4.16608
H	4.08291	5.05846	3.97420
H	4.83660	4.34702	2.76722
H	2.85955	0.57212	-3.77223
H	4.06457	1.51171	-4.19693
H	5.87863	0.86677	0.23064
H	5.76982	-0.74915	0.08564
H	6.79453	1.60993	-3.04580
H	6.24847	2.42768	-1.76737
H	6.91784	-0.71262	-2.91269
H	5.64701	-0.96787	-3.87622
H	2.33096	-3.95696	3.52756
H	0.73752	-3.89824	3.01792
H	3.34528	-5.47662	-1.10029
H	1.84260	-5.20873	-1.54860

H	3.91740	-5.43123	2.51676
H	4.68905	-4.77227	1.23931
H	0.69901	-6.20683	2.26830
H	0.94465	-6.88828	0.85564
H	-1.46101	-3.17352	-4.09431
H	-2.92270	-3.07236	-4.75543
H	-4.54558	-4.93886	-0.33237
H	-2.97670	-5.47581	-0.30455
H	-2.58170	-6.35499	-2.54056
H	-2.34393	-5.68111	-3.95835
H	-5.33537	-4.70202	-3.27811
H	-5.54557	-3.14667	-2.95235
N	1.69774	-0.26167	3.59091
N	0.00457	0.52683	-3.67246
O	2.94046	-0.29865	3.65857
O	1.00892	-1.29479	3.43583
O	1.08842	0.86434	3.66058
O	1.15099	-0.05428	-3.65191
O	-1.02170	-0.16892	-3.80837
O	-0.05972	1.76439	-3.48475
N	-1.45987	-4.99871	3.27859
N	4.06381	-4.99387	4.94322
N	-1.69687	1.66706	4.28410
O	-0.66572	-5.97458	3.40173
O	-2.68167	-5.15101	3.38432
O	-0.98072	-3.82809	3.05384
O	-1.18061	2.65737	3.66790
O	-2.31401	0.78228	3.58494
O	-1.61441	1.56078	5.49732
O	3.48657	-3.88843	4.69269
O	4.59153	-5.18642	6.04387
O	4.09733	-5.90562	4.05227
N	2.24779	5.24398	-2.03437
N	1.12428	-4.22740	-3.74270
N	-5.79786	-0.57309	-3.37157
O	2.05513	6.19534	-1.21755
O	3.36405	4.69425	-2.11648
O	1.27543	4.84576	-2.74195
O	-6.08770	-0.95019	-4.50113
O	-6.00179	-1.38391	-2.35785
O	-5.31452	0.55574	-3.12735
O	0.32244	-3.43801	-4.31497
O	2.32909	-4.21993	-4.00358
O	0.66959	-5.04874	-2.85909

N	-0.09956	8.04834	1.31299
N	6.06224	3.44884	0.72472
N	6.41604	-3.07581	0.50639
N	-1.10338	-7.18259	-0.58300
N	-6.24399	-3.80493	0.89328
N	-7.08131	3.84634	-0.74265
O	-0.59075	9.05151	0.80172
O	0.79616	8.11792	2.18919
O	-0.50958	6.87825	0.92530
O	5.79408	4.52671	1.34295
O	6.66370	3.49548	-0.36006
O	5.70981	2.34815	1.24446
O	-5.96732	4.14646	-0.18613
O	-7.53864	4.52355	-1.65442
O	-7.70430	2.81819	-0.30903
O	-6.17453	-4.77040	0.09505
O	-7.30698	-3.12691	0.95590
O	-5.26087	-3.51871	1.62897
O	-1.82314	-7.55598	-1.53960
O	-1.48862	-6.23231	0.17747
O	-0.01053	-7.74704	-0.36007
O	5.49557	-2.23183	0.82677
O	6.18862	-4.30569	0.66029
O	7.49311	-2.67148	0.06603
N	8.88238	0.41951	-3.58196
O	8.07684	1.32490	-3.97137
O	10.06957	0.45660	-3.90574
O	8.44762	-0.53640	-2.85242

31
Al1_NO3.log Energy: -967722.0593314

Al	0.01752	-0.37814	1.04037
O	1.34839	0.86029	0.55828
O	-1.40308	0.83202	0.74905
H	1.12351	1.85216	0.42314
H	1.92573	0.53561	-0.18662
H	-2.22925	0.39600	0.39012
H	-1.20695	1.64306	0.16263
O	-0.00952	0.17717	2.91403
H	0.81286	0.08336	3.42720
H	-0.41653	1.03233	3.14180
O	-1.22673	-1.77094	1.50901
O	1.43220	-1.57047	1.54410

H	-1.85950	-2.03649	0.75373
H	-1.72162	-1.70065	2.34326
H	2.29045	-1.58603	0.98527
H	1.15647	-2.49242	1.68945
O	-0.05719	-1.02257	-0.77381
H	-0.79408	-1.60032	-1.08814
H	0.79219	-1.15968	-1.25957
N	-3.45137	-1.46463	-0.95407
N	3.51313	-1.26936	-1.06955
N	-0.09211	3.71320	-0.46591
O	-0.95892	2.85269	-0.82894
O	-0.13759	4.86439	-0.89874
O	0.82673	3.37099	0.35218
O	-4.25887	-1.77664	-1.82151
O	-3.57036	-0.40098	-0.28737
O	-2.45396	-2.25998	-0.70158
O	4.38302	-1.53726	-1.89052
O	2.49774	-0.55510	-1.41432
O	3.60204	-1.67682	0.13008

46
Al2_NO3.log Energy: -1486978.5465924

Al	-0.31258	-0.45766	1.35210
Al	0.35542	0.33650	-1.31583
O	-0.88640	-0.68892	-0.39655
H	-1.54627	-1.36889	-0.68973
O	0.95324	0.53702	0.44046
H	1.55900	1.26407	0.73649
O	-0.25432	0.02119	-3.17735
H	-1.11581	0.38567	-3.44399
H	-0.12911	-0.84133	-3.60854
O	1.68267	1.54778	-1.96498
H	2.50662	1.81176	-1.39503
H	1.94423	1.50504	-2.89927
O	-1.70280	-1.59657	2.02315
H	-1.99798	-1.45671	2.93835
H	-2.53813	-1.78461	1.43930
O	0.34123	-0.21551	3.20779
H	1.19653	-0.61590	3.44211
H	0.21832	0.59164	3.73547
O	1.50755	-1.16684	-1.75743
H	1.16934	-2.04173	-1.49654
H	2.45910	-1.15679	-1.38057

O	-0.89762	1.80962	-1.48312
H	-1.79956	1.80634	-1.00685
H	-0.54444	2.71336	-1.51436
O	0.83305	-2.03301	1.50832
H	1.60756	-2.28305	0.91762
H	0.34962	-2.84998	1.71938
O	-1.40077	1.09844	1.82298
H	-0.90052	1.93385	1.83389
H	-2.19068	1.27673	1.19671
N	3.62933	2.71590	0.49921
N	-3.74189	-2.58769	-0.45365
N	-3.84581	2.63968	0.02379
N	3.87823	-2.47320	-0.14553
O	-4.44852	2.80868	1.08779
O	-3.95669	3.37344	-0.96370
O	-3.03979	1.60015	-0.07091
O	-4.74133	-3.08879	-0.97451
O	-3.84409	-2.01705	0.68915
O	-2.61449	-2.63093	-1.03129
O	4.93002	-2.99384	0.22297
O	3.88559	-1.34728	-0.74180
O	2.75730	-3.06065	0.04719
O	3.78277	2.18671	-0.65723
O	2.51031	2.62134	1.08672
O	4.57262	3.31285	1.02455

61
Al3l_NO3.log Energy: -2006249.0775468

Al	1.99271	0.22400	-1.26025
Al	-3.05367	0.24345	1.40381
Al	-0.59802	0.27720	-0.08492
O	0.43302	1.29700	-1.30280
O	0.98796	-0.66061	0.01287
O	-1.50352	-0.71761	1.22559
O	-2.23081	1.18893	0.01845
O	2.91448	1.19270	-2.76406
O	3.48486	-0.96779	-1.16690
H	0.58052	2.25650	-1.16601
H	1.07626	-1.54208	0.46326
H	-0.98536	-1.27667	1.86994
H	-2.64859	1.80372	-0.60883
H	2.53807	1.05976	-3.65232
H	3.15015	2.13318	-2.67999

H	4.10872	-0.90848	-0.34801
H	4.04394	-1.01854	-1.96088
O	-4.00750	-1.17048	0.43118
H	-4.57153	-0.94064	-0.35979
H	-3.42017	-1.90705	0.18358
O	-1.23803	-0.74463	-1.66071
H	-2.06331	-0.44777	-2.10565
H	-1.16982	-1.75986	-1.67988
O	1.29472	-0.81621	-2.75767
H	0.37145	-0.50615	-2.87341
H	1.18471	-1.80462	-2.55528
O	2.87416	1.44304	-0.08268
H	2.56998	2.38694	-0.11097
H	3.86535	1.38001	0.12094
O	0.04156	1.54343	1.46414
H	0.84819	1.18703	1.87940
H	0.23348	2.51962	1.24357
O	-2.30578	1.41778	2.77828
H	-2.73922	2.28102	2.90403
H	-1.36011	1.59098	2.51497
O	-4.62603	1.35595	1.21409
H	-4.82404	1.65097	0.27345
H	-5.45833	1.11912	1.65922
O	-3.87760	-0.60829	2.96174
H	-4.22978	-1.51287	2.88362
H	-3.44290	-0.51459	3.82823
N	1.07309	4.55382	0.13331
N	-4.41603	0.79512	-1.96071
N	0.01202	-3.97488	-1.80477
N	0.71179	-3.04076	2.49247
N	5.73482	0.15132	1.03531
O	-5.25509	-0.09652	-1.65670
O	-3.51498	0.57948	-2.79603
O	-4.47782	1.92927	-1.38038
O	1.06495	-3.03213	1.27184
O	1.08375	-3.95371	3.24241
O	-0.02660	-2.10688	2.94609
O	6.73912	0.10266	1.74469
O	5.42695	1.22302	0.42082
O	4.98974	-0.88093	0.90979
O	-1.07491	-3.33362	-1.62114
O	0.04695	-5.18936	-1.58913
O	1.05406	-3.37553	-2.21917
O	0.36201	4.10220	1.08260

O	1.22971	5.76295	-0.01370
O	1.62310	3.72809	-0.68286

61
Al3_NO3.log Energy: -2006264.6441302

Al	1.64160	0.54138	1.15578
Al	-1.35026	1.17840	-0.47564
Al	-0.63816	-1.59097	-0.26514
O	0.83729	-1.07855	0.78673
O	-1.87426	-0.36708	0.45578
O	1.14817	0.38133	3.04359
O	-0.97327	-2.96747	1.16195
O	0.12162	1.50628	0.68734
H	1.47268	1.06953	3.64940
H	0.16286	0.26893	3.21162
H	-0.01954	2.27681	1.25717
H	-1.87880	-0.25043	1.43407
H	-0.89926	-2.69421	2.09322
H	-1.83597	-3.40662	1.05298
H	1.38677	-1.84502	1.09410
O	-0.51290	-0.16309	-1.47927
H	0.05318	-0.00915	-2.25926
O	-2.09253	-2.55989	-1.14308
H	-1.80873	-3.22539	-1.79153
H	-2.87927	-2.04968	-1.53070
O	-2.84207	1.25491	-1.72086
H	-3.63416	1.66131	-1.32181
H	-3.19141	0.34986	-2.01916
O	-0.73148	2.75195	-1.43083
H	-1.01299	2.89351	-2.34944
H	0.22135	3.06227	-1.30489
O	-2.48894	2.30812	0.67018
H	-2.41464	3.27669	0.64332
H	-2.70847	2.02628	1.61445
O	0.45384	-2.94413	-1.15173
H	0.82499	-2.76863	-2.06068
H	1.18862	-3.36829	-0.61957
O	2.40686	2.32738	1.60935
H	2.32476	2.93039	0.81149
H	3.31679	2.39986	1.94546
O	3.34585	-0.27317	1.73935
H	4.05474	-0.14678	1.08324
H	3.29176	-1.25934	1.91142

O	2.55206	0.78795	-0.53429
H	2.38792	1.66145	-0.96330
H	2.70437	0.07990	-1.23411
N	3.17344	-3.68492	1.01575
N	2.38193	4.37021	-1.33577
N	-5.01608	-0.96348	-1.39843
N	1.93727	-1.05906	-3.07467
N	-2.18412	0.98062	3.78238
O	4.32851	-4.03554	1.24750
O	2.60432	-2.80867	1.77740
O	2.51116	-4.17777	0.06327
O	-5.54459	-2.00218	-0.99737
O	-3.94175	-1.05724	-2.14937
O	-5.44586	0.17409	-1.13891
O	1.76078	3.34557	-0.77446
O	1.83642	4.91264	-2.29902
O	3.46229	4.71751	-0.85267
O	1.37014	-2.09168	-3.52571
O	1.53344	0.08331	-3.39945
O	2.88689	-1.18535	-2.24646
O	-3.06866	1.64540	3.17128
O	-1.47624	0.13931	3.10740
O	-1.99784	1.11214	4.98897

61
Al3r_NO3.log Energy: -2006252.6619875

Al	2.26884	0.99343	-1.10551
O	0.55110	1.61904	-0.88818
O	1.70081	-0.09457	0.29291
H	0.15243	2.51703	-1.05192
H	2.17522	-0.48776	1.04576
Al	-0.12559	0.42800	0.39175
Al	-1.34970	-2.19053	0.10956
O	-0.63320	-1.09251	1.42035
O	-0.70094	-0.84374	-1.02638
O	-1.80529	-3.62582	1.40889
O	0.17306	1.50664	1.98611
H	-1.30634	-0.49320	-1.71701
H	-1.19983	-0.89312	2.19759
H	-0.57364	1.59955	2.62012
H	1.05554	1.57261	2.45517
H	-1.74088	-3.48738	2.37048
H	-2.63544	-4.10572	1.23754

O	-1.88004	1.22563	0.36568
H	-2.24220	1.46832	1.25648
H	-2.05491	1.98436	-0.28538
O	-3.16269	-1.50168	0.44454
H	-3.21759	-1.02768	1.31257
H	-3.63650	-0.93211	-0.22315
O	-2.20399	-3.30860	-1.22788
H	-1.56989	-3.83858	-1.74219
H	-2.89698	-2.94314	-1.86023
O	0.19444	-3.30893	-0.21882
H	0.46833	-3.93920	0.46872
H	1.02513	-3.05124	-0.73222
O	1.64719	-0.33363	-2.40886
H	0.72542	-0.57183	-2.12898
H	2.14659	-1.17992	-2.26729
O	2.74456	2.05946	-2.69195
H	2.86006	3.02209	-2.60140
H	2.23192	1.88933	-3.50251
O	3.12303	2.43342	-0.10540
H	3.79445	2.12107	0.57842
H	2.50941	3.01371	0.37976
O	4.02552	0.21219	-1.21678
H	4.59635	0.47767	-1.95766
H	4.18326	-0.76908	-1.01812
N	3.39901	0.99576	2.49496
N	-3.55788	-0.82542	-2.49740
N	3.35626	-2.99390	-0.57665
N	-2.95747	0.59674	3.54364
N	-1.70805	4.11331	-1.51791
O	-0.49286	4.04858	-1.15055
O	-2.46895	3.10196	-1.36302
O	-2.15387	5.14886	-2.02432
O	-2.80422	-0.55719	3.01264
O	-2.39744	1.61090	2.99873
O	-3.62632	0.72911	4.56144
O	3.19375	-3.95531	0.17381
O	2.44175	-2.69813	-1.43657
O	4.39969	-2.28690	-0.53109
O	-3.98125	-2.00899	-2.67935
O	-4.13283	-0.08811	-1.65023
O	-2.54790	-0.41466	-3.11580
O	3.09554	-0.17121	2.81590
O	4.45816	1.23190	1.84252
O	2.63202	1.96816	2.77335

76
Al4b_NO3.logEnergy: -2525531.0221642

Al	2.09218	2.51053	-0.05557
Al	-1.65292	-2.32870	-0.13833
Al	-0.69504	0.79057	0.84659
Al	1.43142	-0.81704	-0.20556
O	2.52275	0.72326	-0.34019
O	0.70832	-0.30151	1.43495
O	3.23533	2.55942	1.54105
O	2.80715	-1.85053	0.72585
O	0.52431	2.26429	0.92958
H	3.46266	3.41545	1.94515
H	4.05944	2.01399	1.47499
H	0.45356	2.78597	1.74367
H	1.33566	0.06606	2.07485
H	2.60391	-1.94413	1.69644
H	3.75184	-1.54885	0.64509
H	3.49249	0.59167	-0.20202
O	0.03539	0.34008	-0.90662
H	-0.59400	-0.12258	-1.49399
O	0.20935	-2.26759	-0.26001
H	0.59131	-3.06392	-0.66795
O	-1.84462	-0.68567	0.67151
H	-2.53255	-0.74458	1.38206
O	-2.03811	2.01890	0.21942
H	-2.68575	1.63757	-0.44397
H	-1.68928	2.88758	-0.12684
O	-1.26451	0.99790	2.71906
H	-2.25661	0.95096	2.87532
H	-0.85651	0.27268	3.24791
O	2.13462	-1.45704	-1.91736
H	2.33311	-0.79108	-2.59657
H	1.66606	-2.23706	-2.34546
O	1.76893	4.42500	0.16620
H	0.81873	4.63459	-0.10460
H	2.36252	5.05196	-0.28269
O	3.73201	3.06059	-1.07531
H	3.61622	3.00481	-2.04173
H	4.53765	2.53855	-0.85267
O	1.11192	2.56136	-1.72619
H	0.38695	3.23631	-1.67450
H	0.64365	1.67030	-1.70233

O	-1.56497	-3.99070	-1.16372
H	-2.35390	-4.44336	-1.50523
H	-0.81618	-4.04453	-1.84003
O	-1.63397	-3.30847	1.53289
H	-0.81671	-3.20745	2.13042
H	-1.83136	-4.25876	1.47587
O	-2.00068	-1.38007	-1.82631
H	-2.03581	-1.81268	-2.69568
H	-2.69245	-0.59763	-1.79850
O	-3.62478	-2.66491	0.03315
H	-4.19096	-2.36075	-0.69763
H	-3.99036	-2.25158	0.86217
N	1.21515	-4.61491	-3.14539
N	5.90016	0.08525	0.44745
N	-1.34702	5.30050	-1.21038
N	-4.56175	-0.17263	2.66842
N	-4.02375	1.11683	-2.61022
N	0.84089	-2.06898	3.45348
O	-3.95717	0.89246	2.98755
O	-5.78841	-0.24938	2.71126
O	-3.85847	-1.19079	2.31248
O	-0.67761	6.31063	-1.45099
O	-2.55823	5.20025	-1.41481
O	-0.72046	4.26021	-0.68931
O	5.06161	1.06715	0.30173
O	7.09985	0.32454	0.53364
O	5.44727	-1.08606	0.48649
O	-4.48215	2.26082	-2.56808
O	-4.02920	0.39924	-3.61920
O	-3.50168	0.61920	-1.50995
O	0.63192	-3.59099	-2.56114
O	0.58674	-5.67826	-3.20317
O	2.34970	-4.45052	-3.60490
O	-0.05628	-1.41164	4.02219
O	0.57691	-3.18397	2.90794
O	2.02942	-1.64615	3.41061

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Al4f_NO3.log Energy: -2429598.2334094

Al	-1.55237	0.19042	0.30358
Al	1.49365	-0.29244	0.04844
Al	0.43653	2.45716	0.79618
Al	-0.44034	-2.51246	-0.45414

O	0.10005	1.02366	-0.58184
O	-0.12269	-1.08695	0.90512
O	-1.12387	1.61672	1.40668
O	1.66329	1.12024	1.24228
O	1.03036	-1.58973	-1.19772
O	-1.73945	-1.24130	-0.84993
O	0.79649	3.27375	2.53703
O	-0.90207	-3.38385	-2.13941
H	0.04352	1.18578	-1.55427
H	-0.01635	-1.27240	1.87311
H	-1.34583	1.59268	2.35427
H	2.12912	1.05928	2.09151
H	0.99044	-1.38966	-2.15256
H	-2.30265	-1.22283	-1.64332
H	0.82206	2.63573	3.29949
H	0.26975	4.05097	2.79401
H	-0.85367	-2.74614	-2.90436
H	-0.46563	-4.21347	-2.40183
O	2.58863	-1.37328	1.19146
H	3.13921	-2.19135	0.92957
H	2.30116	-1.45359	2.12371
O	2.91186	0.29591	-1.06358
H	3.54806	1.03092	-0.72027
H	3.40731	-0.34714	-1.59721
O	-2.82131	1.11756	-0.77669
H	-2.76002	0.96139	-1.74858
H	-3.05588	2.09101	-0.59853
O	-2.75063	-0.43174	1.65991
H	-2.38561	-0.45783	2.56927
H	-3.42115	-1.18657	1.54935
O	0.80624	-3.81004	0.14515
H	0.51137	-4.67966	0.46147
H	1.75401	-3.90059	-0.25752
O	-1.72123	-3.55243	0.52114
H	-2.71948	-3.38887	0.29855
H	-1.64218	-3.72187	1.47466
O	1.83007	3.42177	-0.11134
H	1.69557	3.77763	-1.00586
H	2.79594	3.07447	-0.06309
O	-0.65482	3.91590	0.27342
H	-1.68108	3.83778	0.14549
H	-0.35628	4.72946	-0.16346
N	-3.47679	4.44301	-1.12799
N	-5.01589	-2.86782	0.60195

N	4.15533	-4.07013	-0.33824
N	5.07316	2.86521	-0.83895
N	-0.98443	-0.12407	-3.41592
N	0.29802	0.11679	3.78211
O	-3.12525	3.60264	-0.16884
O	-4.45727	4.15862	-1.81525
O	-2.79712	5.46777	-1.26358
O	-4.13768	-3.28259	-0.22956
O	-6.20592	-3.11702	0.41360
O	-4.64676	-2.20674	1.62361
O	5.82363	2.12451	-1.47853
O	4.12899	2.29667	-0.10535
O	5.14711	4.09569	-0.82426
O	5.16141	-4.66729	-0.71923
O	3.05636	-4.20245	-0.97671
O	4.20341	-3.32087	0.68843
O	0.70389	-1.03459	3.44034
O	-0.93420	0.35371	3.84605
O	1.14029	1.01853	4.03529
O	-0.36051	-1.20140	-3.65877
O	-2.23811	-0.14301	-3.26959
O	-0.34501	0.94776	-3.30148

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Al4l_NO3.log Energy: -2525527.4940989

Al	-4.01874	-0.14547	0.36788
Al	1.73418	-0.28879	0.09460
Al	4.59333	-0.26925	-0.25864
Al	-1.10540	-0.25612	0.49538
O	-2.52553	0.98822	0.44005
O	-2.61551	-1.40043	0.38966
O	0.33285	-1.44327	0.58909
O	0.31796	0.92642	0.09411
O	3.20168	-1.45651	0.14587
O	3.14333	0.86304	-0.34430
O	-5.29134	1.33329	0.63546
O	-5.39347	-1.45940	0.22839
O	4.47393	-0.52152	-2.21432
O	5.90083	1.09940	-0.47274
H	-2.44424	1.66887	-0.25784
H	-2.66725	-2.34430	0.59124
H	0.42946	-2.08339	1.33506
H	0.20946	1.65691	-0.55371

H	3.22600	-2.40815	0.33369
H	3.21815	1.84211	-0.21614
H	-4.97400	1.98715	1.32738
H	-5.53945	1.84583	-0.15309
H	-5.64768	-1.90871	-0.66323
H	-6.19737	-1.31599	0.75517
H	3.61573	-0.17506	-2.52627
H	4.55075	-1.46729	-2.52467
H	6.71033	0.85603	-0.95363
H	5.57210	2.01459	-0.84845
O	-4.26837	-0.28456	2.30298
H	-3.87694	0.49350	2.82810
H	-3.87917	-1.09129	2.68213
O	-1.10884	-0.04319	2.41241
H	-0.49192	-0.50654	3.04065
H	-1.59768	0.69683	2.85716
O	2.16525	0.13690	2.08471
H	1.91266	1.05387	2.29960
H	1.70912	-0.44000	2.77409
O	4.90017	-0.11923	1.68177
H	4.01327	-0.04295	2.11454
H	5.44340	0.63337	1.97606
O	1.50165	-0.80604	-1.82553
H	1.77867	-1.73830	-1.99464
H	0.53797	-0.75010	-2.04571
O	-1.14227	-0.44619	-1.61346
H	-1.44268	0.44452	-1.97577
H	-1.81163	-1.09948	-1.88757
O	-4.17234	0.10078	-1.54491
H	-4.97102	-0.23403	-2.08676
H	-3.76955	0.87245	-1.99641
O	5.96623	-1.64544	-0.32335
H	5.70815	-2.42620	-0.90167
H	6.27371	-1.98441	0.53631
N	-3.10806	2.80449	2.92817
N	3.66745	-3.55806	-1.75648
N	4.32670	4.02377	-0.84220
N	-1.36569	2.89789	-2.39934
N	-6.40259	-1.96243	-2.91763
N	0.79499	-2.51804	3.86049
O	3.60414	-4.17022	-0.67818
O	2.65515	-3.31428	-2.44973
O	4.81478	-3.13252	-2.17468
O	-2.94999	1.62761	3.44411

O	-4.20182	3.07856	2.36505
O	-2.20461	3.63038	3.02458
O	0.66192	-3.09232	2.74910
O	0.78248	-1.21658	3.90682
O	0.93461	-3.14826	4.90400
O	-6.22070	-0.70072	-2.90666
O	-5.93496	-2.66996	-1.96142
O	-7.02123	-2.49612	-3.83629
O	5.17813	3.31825	-1.49391
O	3.62356	3.47655	0.05806
O	4.20796	5.22298	-1.10238
O	-1.76297	3.79405	-3.13686
O	-2.16763	1.91123	-2.10537
O	-0.21402	2.88561	-1.90542

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Al4_NO3.log Energy: -2525543.1710675

Al	-1.45152	-0.79879	1.00621
O	-1.19116	1.00150	1.47493
H	-1.96430	1.34235	1.95079
O	-3.39224	-0.53959	1.19057
H	-3.82977	0.02567	0.50663
H	-3.93079	-1.38439	1.25001
O	-1.56630	-0.38870	-0.83200
H	-1.68580	-1.25062	-1.28305
O	-1.75085	-2.68662	0.77530
H	-1.15707	-3.16608	0.13687
H	-2.69481	-3.04747	0.76800
O	0.39693	-1.17192	0.89592
H	0.71982	-1.71867	1.63090
O	-1.49422	-1.19744	2.95217
H	-0.97794	-0.60476	3.56219
H	-1.36005	-2.11584	3.23958
Al	-0.68614	0.75229	-2.01711
O	-0.38099	2.21592	-0.87309
H	0.06862	2.92707	-1.36833
O	0.13330	1.80008	-3.51021
H	0.09185	1.33030	-4.36254
H	1.07997	2.12510	-3.41120
Al	1.86629	-0.40178	0.01831
O	1.53556	1.30665	0.81506
H	2.05307	1.38881	1.63594
O	2.98076	-0.95730	1.55432

H	2.99222	-0.48034	2.42185
H	3.88216	-1.31326	1.32526
Al	-0.02268	2.36800	0.95435
O	-1.51966	3.68355	1.04897
H	-2.30225	3.52695	0.43903
H	-1.84840	4.00296	1.90610
O	-2.37744	1.57709	-2.59904
H	-2.87411	2.00937	-1.82766
H	-2.25169	2.28718	-3.25352
O	1.08039	4.00314	0.73478
H	0.54558	4.81620	0.78457
H	1.58847	4.05857	-0.12670
O	2.38736	-2.16714	-0.72450
H	1.71850	-2.89407	-0.68145
H	3.28512	-2.50906	-0.51793
O	0.96377	-0.04887	-1.60612
H	1.64736	0.00979	-2.29312
O	3.50605	0.18795	-0.88220
H	4.31093	-0.37505	-0.69945
H	3.75023	1.14550	-0.91695
O	0.24227	2.74827	2.85851
H	0.24387	1.96370	3.48778
H	0.95748	3.35353	3.11811
O	-1.06652	-0.50473	-3.53661
H	-1.04987	-1.48319	-3.31370
H	-1.94753	-0.33806	-3.91920
N	1.27408	-0.12270	3.98887
N	-0.14189	-3.36257	-2.12291
N	-4.45803	2.38800	-0.02033
N	2.73607	3.01913	-1.97653
N	6.18051	-2.16377	0.11741
N	-5.01214	-3.33495	0.07200
O	1.30766	-1.35622	4.04259
O	0.18352	0.49708	4.26438
O	2.27944	0.56062	3.63907
O	-4.51176	-4.08178	-0.78273
O	-4.28454	-3.01538	1.11345
O	-6.16259	-2.88569	-0.00101
O	6.96393	-1.73951	-0.73842
O	6.49864	-2.94074	1.02319
O	4.93031	-1.76455	0.05774
O	-1.27763	-2.81688	-2.34517
O	0.67225	-3.52402	-3.02731
O	0.12015	-3.72357	-0.92701

O	-3.45570	2.94789	-0.62608
O	-4.80049	1.23763	-0.39661
O	-5.02617	2.99125	0.88734
O	2.67684	2.27489	-2.99142
O	1.81695	3.87561	-1.78436
O	3.67110	2.90773	-1.15704

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Al4r2_NO3.log Energy: -2525538.8316136

Al	3.23521	-0.95682	0.83344
O	2.85692	-0.03248	-0.76319
H	3.02982	-0.36004	-1.66714
O	1.51018	-0.31513	1.15853
H	1.00125	-0.28859	1.99662
Al	1.24806	0.81270	-0.27253
Al	-1.60458	0.80370	-0.76254
O	0.08369	0.36947	-1.59069
O	-2.62285	-0.33989	-1.86798
H	0.19919	-0.25917	-2.33298
H	-2.82966	-0.20997	-2.80273
O	-0.31172	1.62336	0.33225
H	-0.44231	2.08242	1.18166
Al	-2.79735	-1.88044	-0.83838
O	-1.82236	-0.79370	0.30147
H	-1.97954	-0.67888	1.25818
O	2.12257	2.46726	-0.35549
H	1.57001	3.25310	-0.70634
H	3.04838	2.49643	-0.71522
O	-1.80841	2.29311	-2.02140
H	-1.05737	2.30968	-2.64102
H	-1.79488	3.20286	-1.58068
O	-3.66453	-2.92663	-2.26040
H	-3.23618	-3.69802	-2.66934
H	-4.62943	-3.04863	-2.26556
O	5.08209	-1.37777	0.42013
H	5.26725	-2.13867	-0.15652
H	5.58707	-0.57218	0.07855
O	3.99574	0.57567	1.73171
H	3.36506	1.22157	2.18236
H	4.66081	1.07590	1.18832
O	-2.99030	1.71726	0.25586
H	-2.90210	1.53459	1.21960
H	-3.95335	1.56375	-0.00901

O	-4.61909	-1.46817	-0.35703
H	-5.00005	-0.51770	-0.45709
H	-4.93042	-1.83588	0.48677
O	2.35577	2.34979	2.85670
H	2.26493	3.07084	2.21108
H	1.43031	2.10071	3.07650
O	2.79146	-2.69367	0.08246
H	2.68324	-2.80938	-0.89879
H	1.94932	-3.08488	0.45617
O	3.23825	-1.88382	2.54794
H	4.05750	-2.32422	2.83352
H	2.47527	-2.50379	2.70522
O	-1.22415	-2.84608	-1.46137
H	-0.64088	-3.11329	-0.71206
H	-0.63410	-2.50782	-2.19657
O	-2.98037	-3.30024	0.48633
H	-3.28249	-4.18303	0.21315
H	-2.25334	-3.42153	1.17618
N	0.03891	-3.38956	2.04776
N	5.36094	1.49577	-1.23386
N	-0.31055	4.57814	-0.46956
N	-6.41500	1.26987	0.15962
N	1.61389	-2.06934	-2.97632
N	-0.95188	0.78278	3.05325
O	5.82552	1.06588	-0.10424
O	5.57975	0.85367	-2.26227
O	4.71334	2.57326	-1.23847
O	0.47412	4.14020	-1.38155
O	0.13400	4.96652	0.61601
O	-1.55352	4.59251	-0.71561
O	-5.34572	0.97276	-0.55007
O	-6.54847	2.43395	0.54646
O	-7.22532	0.36323	0.38693
O	0.91763	-3.25093	2.92349
O	0.36085	-3.47213	0.81828
O	-1.16586	-3.46686	2.38357
O	-0.21185	-0.18595	3.34041
O	-0.49615	1.96433	3.05953
O	-2.15540	0.58245	2.72226
O	1.81040	-3.14854	-2.36445
O	0.41648	-1.75675	-3.30114
O	2.54794	-1.29072	-3.24984

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Al4r_NO3.log Energy: -2525528.2553431

Al	-2.45866	-0.60668	0.33029
O	-4.00101	-0.09351	-0.71160
O	-2.68869	0.95942	1.49520
O	-1.26282	0.27517	-0.80569
O	-0.83056	-1.01114	1.14221
Al	0.33016	0.09703	0.15846
O	0.00884	1.64440	1.34399
O	1.32838	1.50419	-0.76818
O	1.07499	-1.23307	-0.96290
O	2.00374	-0.33274	1.10816
Al	2.68269	-1.60201	-0.12335
H	0.92054	-1.19844	-1.91641
H	-0.75639	-1.28683	2.07699
H	1.95609	-0.61269	2.05543
H	-1.42623	0.95726	-1.48739
H	0.13437	1.46558	2.30863
H	-1.82185	1.43330	1.53488
H	-3.35498	1.63439	1.17620
H	1.09718	1.67230	-1.72399
H	-4.20997	0.87240	-0.69719
H	-4.86732	-0.58321	-0.52212
Al	1.08072	2.88152	0.45744
O	-0.28423	3.75167	-0.55778
H	-1.15907	3.95120	-0.10189
H	-0.55451	3.27858	-1.40848
O	0.90497	4.18771	1.90985
H	1.18665	5.10882	1.76502
H	0.13298	4.19753	2.50322
O	4.29032	-1.90961	0.86629
H	4.93289	-1.10425	0.81790
H	4.85107	-2.64451	0.55356
O	3.55143	-0.16318	-1.12841
H	4.43898	0.13077	-0.78304
H	2.93654	0.61466	-1.12589
O	3.25764	-2.86810	-1.49883
H	3.60046	-2.47977	-2.32382
H	2.53394	-3.51342	-1.74063
O	1.85409	-3.09286	0.78076
H	1.03906	-3.49825	0.34099
H	2.35127	-3.78216	1.25022
O	2.71660	2.23948	1.33714
H	2.67383	1.23714	1.34198

H	2.90049	2.53869	2.24499
O	2.29465	4.20339	-0.34083
H	1.99385	4.68940	-1.12965
H	3.22367	3.94306	-0.47567
O	-2.45730	-2.28126	-0.67088
H	-1.68152	-2.88904	-0.48935
H	-2.48397	-2.20371	-1.64081
O	-3.53356	-1.55792	1.61777
H	-3.81234	-1.01646	2.37565
H	-4.34198	-2.09572	1.28703
N	-3.56376	3.49315	-0.22552
N	6.87469	-0.47526	-0.20628
N	-0.02034	-4.09262	-1.75735
N	0.45619	-0.38425	3.90060
N	-0.45287	2.14844	-3.61280
N	-6.47896	-2.38898	0.20729
O	-7.55590	-2.97007	0.05658
O	-6.33210	-1.19380	-0.20137
O	-5.50780	-2.98840	0.77959
O	-0.90846	-3.91844	-2.59731
O	-0.29198	-3.91633	-0.50793
O	1.14001	-4.45410	-2.08366
O	5.80053	0.08668	0.30550
O	6.93528	-1.71943	-0.22212
O	7.76822	0.25455	-0.63474
O	-4.33620	2.52120	0.10474
O	-2.65295	3.81215	0.60319
O	-3.71143	4.08325	-1.29236
O	-0.40508	-1.29980	3.91125
O	1.68285	-0.67007	3.79733
O	0.09632	0.82599	3.96454
O	-0.89330	2.11445	-4.75833
O	0.76937	1.93697	-3.36746
O	-1.24891	2.40717	-2.62679

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Al5r_NO3.log Energy: -3044807.9944342

Al	-2.74351	-0.89694	-0.97652
O	-2.75055	0.94885	-0.53667
O	-1.41163	-1.03547	-2.30761
H	-2.04545	1.57071	-0.76320
H	-1.60501	-0.93651	-3.24766
O	-1.20920	-1.46104	-0.03746

H	-1.23373	-1.73861	0.90040
Al	-3.75398	0.96763	1.06623
O	-3.87248	-0.81334	0.53022
H	-4.54657	-1.47081	0.77235
Al	0.02459	-1.78292	-1.37547
Al	2.72117	-1.01557	-0.52618
O	1.21304	-0.34535	-1.42908
O	3.87871	0.44830	-0.78118
H	1.29197	0.33925	-2.12139
H	4.84428	0.27419	-0.87774
O	1.47847	-2.41566	-0.36380
H	1.47846	-3.04698	0.36904
Al	3.47492	1.48375	0.72140
O	2.46980	-0.04820	1.08540
H	1.91889	-0.26318	1.85292
O	0.83605	-2.56449	-3.04598
H	1.80589	-2.35821	-3.04901
H	0.48425	-2.29065	-3.91038
O	3.29706	-1.60156	-2.49094
H	3.44436	-0.77932	-3.03756
H	4.09754	-2.15131	-2.57174
O	4.67011	2.85732	-0.05431
H	4.60651	3.75212	0.32317
H	4.52188	2.93303	-1.03270
O	-5.51544	1.39125	0.34875
H	-6.04662	0.66484	-0.07038
H	-5.52319	2.18221	-0.26458
O	-4.02330	-0.45331	-2.42509
H	-4.24413	0.50749	-2.54210
H	-4.85703	-0.98164	-2.49192
O	-3.37649	-2.76444	-1.20613
H	-4.31215	-2.90963	-1.50086
H	-2.76569	-3.35413	-1.68786
O	4.11453	-2.22622	0.01273
H	3.97003	-2.61547	0.92490
H	5.09035	-2.01358	-0.10928
O	4.99805	0.92011	1.78501
H	5.76233	0.70479	1.18835
H	4.83641	0.09373	2.33259
O	-4.68349	0.61889	2.76367
H	-5.65045	0.52276	2.71857
H	-4.31147	-0.19804	3.20014
O	-0.79109	-3.71962	-1.44056
H	-0.27524	-4.30668	-2.02362

H	-0.86818	-4.17194	-0.58142
O	-2.21326	0.80510	2.20547
H	-1.39987	1.25767	1.87019
H	-1.97038	-0.13551	2.49231
O	-3.60159	2.87776	1.29730
H	-3.86213	3.38912	0.48448
H	-2.76126	3.25950	1.67232
O	3.03838	2.59793	2.22157
H	3.40149	2.42050	3.10490
H	2.17144	3.09966	2.30113
O	2.04716	2.45044	-0.15241
H	1.14158	2.35809	0.24034
H	1.99738	2.36551	-1.14709
N	-0.26316	3.47449	2.04672
N	3.33837	1.78252	-3.12074
N	-4.19384	3.01914	-2.03330
N	-2.69811	-2.36552	3.05408
N	3.48050	-1.85379	3.05066
N	-6.39625	-1.70401	-0.83938
N	7.27221	-0.80301	-0.43940
O	8.49931	-0.73276	-0.49382
O	6.68208	-1.92137	-0.50628
O	6.57160	0.26937	-0.32927
O	0.80226	4.02785	2.39905
O	-0.22395	2.41830	1.32260
O	-1.36159	3.94694	2.39842
O	-5.93389	-2.27816	-1.88784
O	-6.91381	-0.56554	-0.96395
O	-6.29703	-2.26355	0.26933
O	-3.67039	-1.77063	3.59592
O	-2.70984	-3.58435	2.87792
O	-1.66213	-1.68450	2.69764
O	4.15763	2.67263	-2.80254
O	3.69783	0.79678	-3.80512
O	2.11638	1.89036	-2.76647
O	-4.78809	3.52469	-1.00324
O	-4.82105	2.15456	-2.70013
O	-3.05587	3.39013	-2.32986
O	2.60989	-1.25848	3.70795
O	3.18579	-2.89815	2.38748
O	4.67631	-1.43252	3.00691

Al6c_NO3.log Energy: -3115590.5021024

Al	2.20904	0.43931	1.80079
Al	2.26093	-1.96263	0.23192
Al	0.06787	-2.54006	-1.57873
Al	-2.13354	-0.67700	-1.57209
Al	-2.20123	1.71698	0.07362
Al	0.05913	2.38177	1.69988
O	1.32953	-1.16694	-1.19350
O	-1.34569	1.12663	1.63604
O	1.21155	1.43933	0.53061
O	1.16758	-1.11383	1.55177
O	-1.33061	-1.95818	-0.47366
O	-1.00074	0.80095	-1.14011
O	3.35012	-0.57645	0.76830
O	1.21945	-3.38267	-0.37145
O	-1.07076	-1.64992	-2.76672
O	-3.18616	0.22652	-0.36576
O	-1.17691	3.19055	0.55894
O	1.22636	1.57840	2.91330
H	1.72080	-0.56167	-1.84673
H	-1.33267	0.26551	2.08441
H	0.69729	0.86928	-0.07766
H	0.63264	-1.51685	2.25621
H	-1.49366	-2.16952	0.45900
H	-0.54289	1.24773	-1.87395
H	4.15452	-0.20873	0.32216
H	0.95272	-4.19658	0.10063
H	-0.77869	-1.36859	-3.65454
H	-4.17354	0.18449	-0.27229
H	-0.95641	3.89069	-0.10506
H	1.28094	1.61796	3.87908
O	-3.73209	-1.71595	-2.07136
H	-4.48666	-1.71173	-1.40846
H	-3.53981	-2.63956	-2.30760
O	-3.84020	2.39921	1.05170
H	-4.64313	1.83861	0.96288
H	-4.10424	3.30093	0.79897
O	-0.75763	3.28344	3.28683
H	-0.97127	2.57896	3.95170
H	-1.60570	3.69324	3.03825
O	1.30175	3.93933	1.45006
H	1.25218	4.29413	0.51128
H	1.18420	4.69273	2.05507
O	3.63709	1.86356	1.81036

H	3.19532	2.73479	1.74864
H	4.27983	1.80511	1.06627
O	2.91011	-0.44211	3.49742
H	3.67214	-0.02275	3.93483
H	2.17451	-0.48036	4.17200
O	2.96843	-3.18041	1.65905
H	2.19840	-3.66995	2.04596
H	3.31068	-2.61321	2.37778
O	-2.87716	2.79897	-1.50281
H	-2.25751	3.51016	-1.79655
H	-3.02026	2.19886	-2.26824
O	-2.68342	0.54112	-3.19481
H	-1.87917	0.73632	-3.74505
H	-3.36226	0.16014	-3.78079
O	1.20267	-3.08998	-3.14287
H	2.11984	-3.20540	-2.82448
H	1.22954	-2.37809	-3.82945
O	-0.91049	-4.29520	-1.74376
H	-0.49868	-4.96819	-2.31388
H	-1.00251	-4.69904	-0.84339
O	3.73055	-2.54030	-1.02846
H	4.33252	-1.78877	-1.30369
H	4.29551	-3.26740	-0.71438
N	-0.53434	-4.19975	1.81837
N	-6.25930	-0.73462	0.28828
N	-0.37049	0.04147	4.58229
N	5.49287	0.65248	-1.46130
N	0.33804	4.76534	-1.97037
N	0.80499	0.30433	-4.01545
O	-5.74909	0.41829	0.04816
O	-5.72077	-1.76145	-0.22581
O	-7.26075	-0.83420	0.99826
O	-1.61451	-3.58794	1.91900
O	-0.37951	-5.08743	0.91040
O	0.42794	-3.94457	2.59192
O	-1.15182	0.98457	4.87236
O	-0.70310	-0.82886	3.74373
O	0.76708	-0.01188	5.14847
O	-0.11999	1.16199	-3.88651
O	0.57931	-0.75609	-4.68086
O	1.91131	0.49002	-3.47685
O	6.00634	1.55852	-2.12053
O	5.09220	-0.41137	-2.02114
O	5.37361	0.76913	-0.18922

O	-0.86208	4.76933	-1.51126
O	1.30626	4.66839	-1.15952
O	0.53603	4.87541	-3.18117

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Al7-1_NO3.log Energy: -4314831.7243553

Al	-0.40917	-0.06788	0.24918
Al	0.03605	2.89378	-0.04720
Al	2.37693	1.05218	0.48070
Al	1.98514	-1.88777	0.59694
Al	-0.74631	-3.07432	0.18826
Al	-3.15220	-1.28209	-0.29929
Al	-2.76710	1.77202	-0.24984
Al	4.68820	-0.85767	-1.30609
O	1.32907	-0.33953	-0.49364
O	-2.18545	0.15294	0.89822
O	-0.90926	1.36644	-0.95033
O	0.44511	1.34531	1.17439
O	0.04986	-1.63013	1.26364
O	-1.21827	-1.40452	-0.89700
O	1.76111	2.42576	-0.58358
O	2.52744	-0.42678	1.57246
O	1.03244	-3.19064	-0.33684
O	-2.51457	-2.70901	0.68865
O	-3.55374	0.31927	-1.06768
O	-1.71112	3.03782	0.59423
O	3.92058	0.66762	-0.55103
O	3.52870	-2.03964	-0.45427
O	3.64405	-0.82448	-2.95384
O	6.15194	-0.91713	-0.02969
O	5.97049	0.25559	-2.33979
O	5.64193	-2.37517	-2.13900
H	1.32856	-0.38565	-1.48388
H	-2.32590	0.20198	1.88173
H	-0.78708	1.32255	-1.93397
H	0.28904	1.55653	2.15139
H	-0.10807	-1.69773	2.27022
H	-1.02744	-1.35053	-1.85354
H	2.40547	3.13089	-0.84645
H	2.70500	-0.43972	2.53305
H	1.38175	-3.51226	-1.20014
H	-3.10134	-3.48624	0.79680
H	-4.03065	0.33686	-1.95104

H	-1.85817	3.35807	1.50716
H	4.39658	1.47949	-0.79361
H	3.37124	-2.77844	-1.09275
H	3.21116	-1.67899	-3.17490
H	3.08046	-0.08000	-3.31385
H	5.97547	-1.04244	0.95434
H	6.78224	-1.62185	-0.26861
H	6.72371	0.71430	-1.92806
H	5.75538	0.69571	-3.18064
H	5.19265	-3.24084	-2.41681
H	6.21694	-2.11107	-2.87863
O	2.54605	-3.03465	2.05794
H	2.93409	-3.90327	1.84889
H	3.13972	-2.58774	2.73013
O	-0.61847	-4.33196	1.60564
H	-0.89763	-4.00544	2.55178
H	0.16575	-4.90115	1.67796
O	-4.82167	-1.45134	0.66707
H	-5.57292	-0.89976	0.38613
H	-4.85222	-1.53427	1.66623
O	-4.26907	2.29951	0.84931
H	-4.57115	1.81513	1.68273
H	-5.07040	2.50959	0.33738
O	-3.28772	2.85524	-1.68302
H	-3.49257	2.45989	-2.57728
H	-3.24494	3.86845	-1.71188
O	-0.15218	3.99124	-1.57793
H	-0.80927	4.77468	-1.65195
H	0.00146	3.57671	-2.45097
O	0.58828	4.28055	1.12178
H	1.55448	4.51577	1.18914
H	0.16489	4.21356	2.03237
O	3.21908	2.13040	1.79153
H	3.92998	1.71684	2.33422
H	3.38556	3.11248	1.62454
O	-3.75205	-2.23328	-1.82501
H	-4.20304	-3.14423	-1.77480
H	-4.11472	-1.71044	-2.58303
O	-1.34837	-4.30889	-1.14315
H	-0.77123	-5.02079	-1.46988
H	-2.25878	-4.70589	-0.92522
N	3.24397	-4.59654	-2.89666
N	3.86057	5.00578	0.12596
N	0.93413	0.91932	-3.47204

N	4.88983	-0.82613	3.05870
N	-1.03601	-2.52796	4.45017
N	-0.72762	2.93205	4.03058
N	-4.24110	0.01289	3.18410
N	-4.11137	0.53361	-4.32841
N	-4.69155	-5.31768	-0.77032
N	-2.73451	6.38288	-1.64463
O	-5.00545	-4.51342	-1.69747
O	-5.42344	-6.25345	-0.46936
O	-3.58182	-5.14194	-0.13551
O	2.55898	-5.56020	-3.20881
O	2.67384	-3.49428	-2.50700
O	4.50404	-4.62564	-2.93700
O	3.26947	4.68249	1.24120
O	4.51811	6.03708	0.07685
O	3.74370	4.24282	-0.87270
O	-3.14702	7.54439	-1.62486
O	-1.47954	6.16094	-1.67413
O	-3.55945	5.41618	-1.63629
O	-5.17734	0.76415	2.78875
O	-4.44749	-1.22543	3.29068
O	-3.09903	0.49133	3.41469
O	-0.23834	-1.74833	3.83340
O	-1.48700	-3.57157	3.86752
O	-1.36878	-2.28312	5.60734
O	5.12500	0.39847	3.02653
O	5.62926	-1.64324	2.44925
O	3.87576	-1.27202	3.68927
O	-0.98707	3.85764	3.17527
O	-1.20488	2.99646	5.16010
O	0.02787	1.96624	3.70077
O	2.07910	1.20002	-3.88374
O	0.68347	-0.25585	-3.05053
O	0.01932	1.78356	-3.45281
O	-4.65637	-0.10877	-3.34902
O	-4.10319	0.03870	-5.45328
O	-3.61201	1.67180	-4.10581

103
Al7_NO3.log Energy: -3795546.8615805

Al	0.08236	-0.13441	0.09623
Al	1.41854	-2.86305	0.49916
Al	-1.49921	-2.61830	-0.45412

Al	-2.88874	0.12230	-0.71841
Al	-1.20448	2.56947	-0.26585
Al	1.63366	2.39033	0.65801
Al	3.00322	-0.29931	0.97101
O	-0.96504	-0.90394	-1.27463
O	1.19026	0.57327	1.48248
O	1.69640	-1.06520	-0.40137
O	-0.29908	-1.80448	0.98484
O	-1.52835	0.73239	0.60541
O	0.49175	1.53471	-0.73838
O	0.11317	-3.52949	-0.62274
O	-3.00785	-1.62223	-0.07103
O	-2.21542	1.66994	-1.50237
O	-0.02155	3.13203	1.05701
O	3.13639	1.39936	0.33797
O	2.58052	-1.97593	1.62684
H	-0.76219	-0.80052	-2.23607
H	0.90636	0.48074	2.42773
H	1.94728	-1.14962	-1.35576
H	-0.53831	-1.83460	1.93948
H	-1.81352	0.81371	1.57552
H	0.72408	1.55555	-1.70708
H	0.34595	-4.11051	-1.37540
H	-3.89886	-2.04972	-0.19784
H	-2.47767	2.05563	-2.35679
H	-0.41443	3.22302	1.95640
H	3.91973	1.66360	-0.24241
H	2.83309	-2.29529	2.51249
O	-4.26210	0.92880	0.16216
H	-5.06210	1.08441	-0.36675
H	-4.90613	0.35806	1.47051
O	-2.76294	3.20024	0.65024
H	-2.60926	3.25235	1.64128
H	-3.50323	2.54403	0.49732
O	2.44675	3.08005	2.32547
H	3.22217	3.64990	2.15995
H	1.91355	3.53224	3.00574
O	3.72135	0.12685	2.73353
H	3.33004	-0.33706	3.52138
H	3.82242	1.07162	2.95176
O	4.53929	-0.84125	0.05670
H	5.03829	-0.18488	-0.47783
H	5.16058	-1.59032	0.43210
O	2.73899	-3.77801	-0.46522

H	3.73437	-3.75938	-0.28098
H	2.57285	-3.93515	-1.43514
O	1.15433	-4.12061	1.93979
H	0.64484	-4.93943	1.80768
H	0.87549	-3.69759	2.79872
O	-2.15157	-4.02851	0.72698
H	-2.98080	-3.93805	1.23009
H	-2.05816	-4.96204	0.46392
O	2.29132	3.77616	-0.40342
H	1.86082	4.66822	-0.59328
H	2.96842	3.54904	-1.10993
O	-0.81034	3.93992	-1.46537
H	-0.87818	3.78330	-2.43219
H	-0.63790	4.94198	-1.21737
O	-2.09180	-3.44105	-2.06441
H	-1.45626	-3.35666	-2.82099
H	-3.03422	-3.27782	-2.38303
O	-3.62739	-0.29614	-2.44507
H	-4.04725	-1.19694	-2.60709
H	-3.01525	-0.08450	-3.19109
N	1.19193	-2.84369	-3.18135
N	-0.66109	1.41257	-3.74061
N	4.95318	2.23476	-2.27034
N	-2.04396	2.04393	3.76497
N	1.08923	-1.36429	4.03091
N	-6.66165	-0.19729	2.01718
N	0.53127	6.91115	-0.68324
N	-5.48248	-3.11518	-1.91074
N	6.12283	-3.72523	0.66651
O	-6.46070	-3.72039	-2.32434
O	-5.34736	-2.81765	-0.69311
O	-4.55043	-2.76187	-2.75511
O	7.02790	-4.46589	1.04760
O	6.01095	-2.55225	1.17106
O	5.30773	-4.10450	-0.22817
O	0.28077	-2.28369	3.69966
O	2.28887	-1.65169	4.30224
O	0.70093	-0.17416	4.05388
O	5.67568	1.99733	-3.23516
O	3.96582	3.02082	-2.36883
O	5.20461	1.68874	-1.12998
O	1.59425	6.24812	-0.86878
O	0.57479	8.12207	-0.46919
O	-0.60685	6.32125	-0.72742

O	-2.04612	2.03592	4.99006
O	-2.28069	0.98432	3.10560
O	-1.81492	3.14465	3.13155
O	-7.33967	-0.66100	2.91355
O	-7.03838	0.12432	0.89519
O	-5.34595	-0.02356	2.32017
O	-1.32826	2.46648	-3.91631
O	0.56027	1.47653	-3.43554
O	-1.22268	0.28429	-3.83885
O	2.01073	-1.90591	-3.03036
O	1.52245	-4.03172	-2.85776
O	0.03774	-2.62187	-3.62160

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Al8_NO3.log Energy: -4506715.1807204

Al	-0.24988	1.48625	0.06492
Al	0.80496	-1.44244	0.13587
Al	-1.92351	-0.83795	-0.77531
Al	2.44259	0.87048	1.09636
Al	-3.63159	1.86102	0.51689
Al	-1.42087	-3.98068	0.56978
Al	4.20067	-1.74416	-0.30405
Al	2.07961	3.97144	-0.29316
O	-0.75122	-0.35961	0.71556
O	1.30687	0.39671	-0.44045
O	-1.28123	0.89420	-1.45297
O	-0.32320	-1.62349	-1.34016
O	1.83947	-0.89109	1.65182
O	0.80454	1.64227	1.58663
O	0.52865	3.04287	-0.72072
O	-1.80922	2.34982	0.65540
O	0.22019	-3.10429	0.81832
O	2.39291	-2.12647	-0.63509
O	-3.31122	0.07969	0.12422
O	-2.36455	-2.47391	0.09814
O	3.89829	0.00231	0.23666
O	3.02211	2.54283	0.42843
O	-2.95099	-1.24336	-2.32154
O	3.26367	1.13789	2.81402
O	-3.20358	-4.91601	0.47959
O	-1.09443	-4.58258	-1.24931
O	-1.68920	-3.82513	2.50225
O	-0.67141	-5.72083	1.01940

O	3.98387	-2.39125	1.52703
O	4.42477	-1.38665	-2.20061
O	4.71614	-3.60053	-0.67600
O	6.12573	-1.42528	-0.02367
O	2.86780	3.76970	-2.09367
O	1.48402	4.68459	1.39695
O	3.72553	5.07374	0.09915
O	1.38054	5.64234	-1.07731
O	-3.77717	1.63903	2.43107
O	-3.63509	2.31191	-1.35480
O	-4.14075	3.73438	0.90365
O	-5.57143	1.44126	0.37422
H	-1.15288	-0.45906	1.60363
H	1.65918	0.37685	-1.36024
H	-0.76261	0.78806	-2.26785
H	-0.07835	-1.91922	-2.24611
H	1.48926	-0.93679	2.57544
H	0.57193	2.19308	2.35288
H	-0.14090	3.64366	-1.11020
H	-1.73991	3.27823	0.34738
H	0.95856	-3.74169	0.88325
H	2.26098	-3.04873	-0.91634
H	-3.88184	-0.53416	0.64099
H	-3.19423	-2.39643	0.62142
H	4.69125	0.57881	0.14494
H	3.93211	2.54137	0.05244
H	-3.28117	-0.51825	-2.93805
H	-2.61486	-2.01079	-2.86082
H	3.43930	0.30397	3.38263
H	4.01788	1.74484	2.88993
H	-4.05575	-4.42645	0.34381
H	-3.39468	-5.78357	0.87240
H	-1.49664	-5.44625	-1.44809
H	-1.31805	-3.99672	-2.03912
H	-1.57643	-2.87894	2.82746
H	-2.52530	-4.10360	2.91829
H	0.14510	-6.06634	0.52012
H	-0.51674	-5.84791	1.97152
H	4.65869	-2.15567	2.18966
H	3.14987	-1.89897	1.80609
H	3.61818	-0.91616	-2.59869
H	5.21233	-0.92853	-2.54002
H	4.02628	-4.24380	-0.33431
H	4.85817	-3.81902	-1.61451

H	6.79717	-2.09131	-0.24852
H	6.51110	-0.51957	-0.12626
H	2.37551	3.18940	-2.74529
H	3.80939	3.49086	-2.12443
H	2.12091	4.67201	2.12985
H	0.54552	4.68950	1.76846
H	3.70733	5.98786	-0.23415
H	4.60048	4.69014	-0.12216
H	0.46629	6.02202	-0.88045
H	1.53154	5.72372	-2.03487
H	-3.28748	2.32681	2.95131
H	-3.68257	0.77296	2.93377
H	-4.35604	1.88580	-1.92492
H	-2.77265	1.96721	-1.69747
H	-3.89753	4.43832	0.24668
H	-3.75709	4.05456	1.75879
H	-6.15508	1.85123	1.03500
H	-5.85279	0.49650	0.26679
N	2.62047	1.04228	-3.47469
N	-3.02559	-1.41399	3.87606
N	2.66114	-1.46659	4.76719
N	-1.42376	3.97841	3.00351
N	-0.89279	-3.14303	-4.31788
N	-4.98833	0.90142	-4.00214
N	-5.55269	-2.20624	0.36599
N	6.28920	2.21730	-0.94905
N	2.37985	-6.02057	-0.47530
N	-1.93717	5.78886	-0.56813
O	1.33025	-6.70766	-0.33757
O	3.33792	-6.44097	-1.12614
O	2.44739	-4.86200	0.08123
O	5.30432	3.03788	-0.97680
O	6.25429	1.29572	-0.06529
O	7.22553	2.32679	-1.72624
O	-3.09420	6.06074	-0.18575
O	-1.67172	4.61110	-0.95937
O	-1.04093	6.67201	-0.57246
O	-6.31937	-1.32876	-0.08281
O	-5.57166	-3.37837	-0.06761
O	-4.71299	-1.89444	1.28803
O	-5.49451	1.25252	-2.88803
O	-3.75385	0.57715	-4.04783
O	-5.67734	0.88409	-5.02504
O	2.28459	-0.09725	-2.98545

O	1.71441	1.91318	-3.59536
O	3.79728	1.27037	-3.77397
O	-2.67101	3.92372	3.25312
O	-1.01980	4.85203	2.18356
O	-0.63739	3.19397	3.55747
O	-3.79223	-0.42802	4.01643
O	-1.96435	-1.29324	3.16307
O	-3.27966	-2.49761	4.42083
O	1.51719	-1.12719	4.34977
O	2.79616	-2.20585	5.74427
O	3.70880	-1.02939	4.15463
O	0.12970	-2.55551	-3.88563
O	-1.86295	-3.40554	-3.48723
O	-1.00691	-3.47912	-5.49355

Optimized Geometries of Al Clusters with ClO_4^- Counterions

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Al10c_ClO4.log Energy: -7156046.2996768

Al	-5.14445	-1.16635	0.47380
O	-4.85777	0.59755	0.97810
O	-3.84837	-0.55473	-0.81915
Al	-3.57732	1.25002	-0.24103
O	-6.67174	-0.88898	-0.74005
O	-6.59060	-1.34213	1.85536
O	-5.00593	2.05672	-1.40191
O	-3.82735	2.99362	0.72090
O	-5.19115	-2.97925	-0.04360
O	-3.94810	-2.00306	1.66254
O	-2.33878	1.88524	-1.48025
O	-1.98108	0.94174	0.68927
Al	-3.59085	-3.58337	0.71740
Al	-0.66596	1.57719	-0.56651
O	-4.67673	-4.77613	1.90153
O	-3.56204	-5.22161	-0.49197
O	-0.42929	3.30606	0.27630
O	0.39073	2.56234	-1.81306
O	-2.35994	-2.96435	-0.55385
O	-2.01602	-4.07637	1.59135
O	-0.36689	-0.10481	-1.41437
O	0.80314	0.83220	0.47121
Al	-0.75501	-3.33216	0.36542
Al	0.83775	-0.94668	-0.24829

O	2.44247	-0.81102	-1.24718
O	2.20964	-1.51391	1.04543
O	0.48396	-2.70426	-0.85524
O	-0.60314	-1.52550	0.97438
H	-3.93406	-0.81590	-1.75518
H	-2.49558	-2.01880	-0.75921
H	-0.23762	-0.14010	-2.37748
H	-0.41630	-1.45373	1.92866
H	-3.35482	-1.59544	2.31745
H	-1.76568	0.00946	0.90464
H	-1.94181	-4.03741	2.56579
H	0.79319	0.98151	1.42946
H	-5.43098	1.13611	1.54410
H	-5.56042	-3.23315	-0.90920
H	-2.47968	2.53385	-2.18042
H	1.11745	-3.27323	-1.32177
H	-6.21582	-1.50777	2.73844
H	-1.05694	3.79802	0.82645
H	-7.16526	-0.54550	1.93088
H	-3.30982	3.11501	1.53486
H	-4.38994	-4.92596	2.81980
H	-3.80638	3.85506	0.24230
H	2.19229	-1.04293	1.89968
H	-5.60747	-4.48981	1.93463
H	-6.62760	-1.32307	-1.61915
H	0.99735	2.15029	-2.45591
H	-7.12944	-0.01549	-0.80921
H	-5.03317	1.80827	-2.34140
H	-3.72756	-4.94616	-1.42633
H	-5.93673	2.03056	-1.06718
H	-4.18524	-5.93925	-0.28037
H	2.55147	-0.77080	-2.21575
Al	3.77381	-0.98470	0.03474
O	5.24548	-0.23693	-0.91308
O	3.69914	0.81486	0.60601
H	2.81161	1.19465	0.45354
H	6.07573	-0.73044	-1.05577
Al	5.17755	1.53229	-0.28467
Al	0.87008	4.04777	-0.81686
O	6.93710	1.92823	-1.15676
O	5.10959	3.36260	0.29980
O	6.31008	1.25042	1.31073
O	4.24959	2.38430	-1.69983
H	5.81198	1.10389	2.14894

H	7.09805	0.65205	1.28661
H	7.22045	2.83730	-0.94719
H	6.92544	1.86125	-2.12829
Al	3.81729	4.01881	-0.87800
H	5.00313	3.47544	1.25711
H	3.66169	1.92932	-2.32935
O	2.34423	4.58624	-1.87291
O	2.36062	3.54674	0.20479
O	5.15465	4.84459	-2.10456
O	-0.30071	5.18028	-1.96360
H	2.40301	3.23504	1.12214
H	2.30064	4.83663	-2.80399
H	-0.98141	5.76216	-1.54747
H	-0.73072	4.64654	-2.65334
H	5.10872	5.80563	-2.25125
H	5.26733	4.41038	-2.96814
O	0.95461	5.79183	0.31803
H	1.03131	5.56822	1.26359
H	0.18352	6.40627	0.25184
O	3.86167	5.88611	-0.10544
H	4.35848	6.06131	0.71254
H	2.94347	6.20208	0.03710
O	-0.67203	-5.08995	-0.51987
H	0.12690	-5.66763	-0.45465
H	-1.48157	-5.62465	-0.41511
O	0.76160	-3.80068	1.60444
H	0.53095	-3.65677	2.54616
H	1.47483	-3.12790	1.41907
O	4.25371	-2.78717	-0.58463
H	3.73549	-3.10299	-1.35508
H	4.18288	-3.54227	0.04263
O	4.80936	-1.51937	1.63109
H	4.73099	-0.89585	2.38918
H	5.74779	-1.83067	1.56567
O	2.52155	-4.62459	-1.82880
O	3.78037	-6.72417	-1.76294
O	1.64828	-6.56207	-0.59301
O	3.59738	-5.34519	0.25473
O	7.34423	-2.51897	1.35821
O	8.52302	-0.38335	1.11918
O	9.62325	-2.46826	0.48204
O	7.78504	-1.60693	-0.87827
O	-6.14917	-2.89579	-2.65884
O	-5.37775	-3.18009	-4.96569

O	-4.21381	-4.31005	-3.14571
O	-4.04291	-1.86783	-3.39753
O	0.43120	0.18529	-4.27495
O	2.12628	0.70400	-5.96119
O	2.28422	1.68635	-3.72234
O	2.70450	-0.70388	-4.04632
O	2.21117	0.56390	3.22773
O	3.42750	2.67922	2.90788
O	4.66088	0.62143	3.48470
O	3.22878	1.69870	5.13446
O	-1.15922	-1.89733	5.94749
O	-2.32510	-1.17676	3.92191
O	-0.08469	-2.14472	3.75731
O	-1.97670	-3.57108	4.36142
O	-7.62198	1.65542	-0.59845
O	-7.51269	1.31318	1.84543
O	-8.01901	3.51808	0.93126
O	-9.66366	1.70473	0.74266
O	-1.55166	6.87375	-0.24833
O	-3.63425	5.59465	-0.30047
O	-3.34898	7.42345	1.31499
O	-2.10009	5.33284	1.58850
Cl	-8.23312	2.06851	0.75009
Cl	-2.68325	6.31437	0.61169
Cl	8.33223	-1.75173	0.51148
Cl	2.89967	-5.82759	-0.98566
Cl	1.88254	0.46052	-4.52352
Cl	-4.93461	-3.05963	-3.56167
Cl	3.36437	1.40243	3.69207
Cl	-1.39484	-2.19056	4.51909

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Al13c_ClO4.log Energy: -8566851.0203280

Al	-2.04945	5.00958	-1.08144
O	-0.60613	5.68887	-0.12718
O	-0.61138	4.07378	-1.80241
Al	0.75899	4.45817	-0.55321
O	-1.87379	6.37414	-2.56010
O	-3.17562	6.48414	-0.28386
O	1.54534	5.86302	-1.73335
O	1.98462	5.22592	0.86768
O	-3.49666	4.17073	-1.95948
O	-2.68084	3.79126	0.22030

O	1.99779	3.19149	-1.11046
O	0.40803	3.14963	0.75215
Al	-3.86120	2.72236	-0.78515
Al	1.68077	1.81031	0.20608
O	-5.51164	3.70169	-0.21289
O	-4.98803	1.80655	-2.12013
O	3.09051	2.50069	1.34304
O	3.17825	0.73665	-0.37292
O	-2.57096	1.48231	-1.32527
O	-4.28266	1.37264	0.51432
O	0.36765	0.94187	-0.84720
O	1.14485	0.46146	1.42060
Al	-2.89925	0.04102	-0.12992
Al	-0.12559	-0.46334	0.36577
O	-4.27938	-0.65749	-1.36427
O	-3.65563	-1.32642	0.91309
O	1.15025	-1.70357	-0.34542
O	-0.39464	-1.96810	1.50878
O	-1.52880	-1.02155	-0.82304
O	-1.59234	0.56386	1.09358
H	-0.58056	3.38140	-2.49182
H	-1.62341	1.71093	-1.28236
H	0.59689	0.74453	-1.77539
H	-1.76728	0.50134	2.05131
H	-2.61300	3.98376	1.17103
H	-0.49421	2.78950	0.78602
H	-4.09192	1.64829	1.42626
H	1.01286	0.67299	2.36149
H	-0.66992	6.30416	0.62133
H	-3.53707	4.02692	-2.91561
H	2.92340	3.35472	-1.35013
H	-1.38912	-0.96595	-1.78034
H	-3.71789	-1.32363	1.88897
H	-4.12191	6.28313	-0.18518
H	3.08954	3.46777	1.42755
H	-2.85014	6.74541	0.61289
H	1.48730	5.53366	1.65573
H	-6.30138	3.16039	0.03168
H	2.65435	5.90076	0.61448
H	-0.58073	-1.90163	2.46149
H	-5.81723	4.36098	-0.85999
H	-1.79310	6.06616	-3.47950
H	-3.83399	-1.02991	-2.15307
H	2.99316	-0.21022	-0.23436

H	-2.52996	7.09324	-2.55136
H	2.47055	5.76228	-2.07060
H	-4.83013	0.82515	-2.00992
H	0.96354	6.06779	-2.48443
H	-5.96385	1.92719	-2.15842
H	1.16365	-1.88036	-1.29620
Al	0.87003	-3.19228	0.80147
O	2.43005	-4.09083	0.13754
O	0.16480	-4.66840	1.85751
O	2.21826	-2.72836	2.10443
O	-0.34893	-4.08752	-0.41453
H	2.17756	-1.87208	2.56272
H	2.39053	-5.03320	-0.11042
H	-0.76280	-3.59086	-1.14089
H	0.81195	-5.27353	2.24460
Al	-1.23084	-5.23579	0.73321
O	-2.79912	-5.79032	-0.20001
O	-2.57138	-4.03497	1.37163
O	-1.73121	-6.58061	2.16122
O	-0.30454	-6.82027	-0.04316
H	-1.37646	-6.32854	3.03221
H	-2.70999	-6.60494	2.25686
H	-0.34194	-7.61491	0.51679
H	0.61523	-6.76082	-0.40228
H	-2.31747	-3.09275	1.31246
H	-2.84403	-6.53122	-0.81798
Al	-4.08734	-4.60043	0.44242
Al	-5.03666	-1.95127	-0.17453
O	-4.22750	-3.43593	-0.98766
O	-5.43900	-3.39508	1.01693
O	-5.58270	-5.78810	-0.20103
O	-4.39508	-5.80140	2.13402
O	-6.64791	-2.24361	-1.31784
O	-6.15426	-0.60828	0.71272
H	-5.50949	-6.17074	-1.09364
H	-6.41925	-5.28680	-0.18092
H	-6.47809	-2.75299	-2.12912
H	-7.21815	-1.48048	-1.55124
H	-5.63597	-3.18964	1.94167
H	-3.71711	-3.50421	-1.81982
H	-4.46551	-5.33536	2.98746
H	-5.15948	-6.40474	2.07442
H	-5.62453	0.23723	0.74053
H	-7.04551	-0.37816	0.36353

Al	3.72696	-3.40691	1.26250
Al	4.51060	1.48169	0.70476
O	5.14698	-4.57055	0.50334
O	5.07170	-2.58877	2.36644
O	3.57589	-4.95179	2.57576
O	4.27805	-1.93379	0.21495
H	3.18515	-4.68663	3.42677
H	4.39073	-5.44872	2.76642
H	5.93243	-4.02637	0.27521
H	4.90380	-5.11162	-0.28729
Al	5.56814	-1.12865	1.30468
H	4.93243	-2.51037	3.32098
H	4.29099	-1.91399	-0.75878
O	6.01167	0.36431	0.27573
O	4.57275	0.22135	2.11022
O	6.89930	-2.32694	0.23132
O	4.89575	2.61880	-0.89158
H	3.82970	0.04980	2.72209
H	6.41408	0.26192	-0.60572
H	5.42482	3.45466	-0.86962
H	5.10795	2.10233	-1.69948
H	7.79621	-2.37189	0.61060
H	6.99557	-2.00828	-0.70155
O	5.75119	2.75590	1.66361
H	6.69721	2.60817	1.48775
H	5.64301	2.71466	2.63077
O	7.21202	-0.87740	2.43295
H	7.13350	-0.97638	3.39831
H	7.66787	-0.03219	2.27317
O	-1.76458	6.68224	4.44590
O	-1.69581	7.06246	2.02813
O	0.12460	5.86622	3.13113
O	-2.08213	4.80090	2.92251
O	1.56969	-0.35385	6.15403
O	3.16061	1.34771	5.39560
O	2.76842	-0.65225	4.04680
O	1.02357	1.06381	4.23770
O	-2.36446	0.41142	3.85050
O	-2.93717	-0.82993	5.87723
O	-3.79515	-1.56808	3.71077
O	-1.41203	-1.81594	4.24262
O	5.83137	7.26419	-1.82855
O	6.01903	5.12227	-0.67022
O	4.19324	5.48591	-2.24819

O	4.20896	6.68782	-0.10290
O	6.95643	-0.78689	-2.08448
O	5.41790	0.79288	-3.13314
O	4.67181	-1.50145	-2.64425
O	6.29122	-1.08485	-4.42409
O	-2.51492	-1.37835	-3.58585
O	-0.74494	-3.00587	-3.11085
O	-3.04538	-3.76593	-3.47758
O	-1.73354	-2.88908	-5.34543
O	1.52840	2.44402	-4.78095
O	-0.03239	0.86574	-5.81385
O	-0.74610	2.20350	-3.90304
O	0.88605	0.39571	-3.60120
O	2.39686	-6.78277	-0.57536
O	3.49912	-8.36197	-2.08608
O	2.38020	-6.38358	-2.99913
O	4.45576	-6.13998	-1.72431
O	-9.89510	1.88847	-1.00720
O	-7.78252	2.10090	0.22254
O	-8.38179	-0.02043	-0.82234
O	-7.77675	1.91091	-2.22445
Cl	3.18480	-6.93091	-1.88206
Cl	-8.47784	1.48822	-0.96619
Cl	-1.99938	-2.76353	-3.89501
Cl	5.81872	-0.65065	-3.09356
Cl	-1.35723	6.08952	3.15442
Cl	0.41809	1.48162	-4.53833
Cl	-2.62360	-0.95084	4.43435
Cl	2.12639	0.36368	4.98026
Cl	5.06989	6.15816	-1.21275

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Al13k_ClO4.log Energy: -7227650.8276247

Al	0.01690	-0.12943	-0.36600
O	-0.43278	1.59104	0.10965
O	-1.24351	-1.32936	0.24931
O	1.66251	-0.55545	0.32897
O	0.08662	-0.25016	-2.22319
Al	-2.10484	2.02731	1.18771
Al	-2.85608	-0.75455	1.36365
Al	3.29093	-1.00188	-0.79780
Al	1.76410	-0.75851	-3.23993
Al	-0.78641	3.10191	-1.21498

Al	0.69178	2.76471	1.30577
Al	-2.38964	-2.53616	-0.93651
Al	-0.80508	-2.82325	1.52469
Al	2.73592	0.73059	1.53735
Al	1.98064	-2.08844	1.59140
Al	-0.27807	1.32897	-3.45355
Al	-1.08070	-1.49107	-3.29898
O	-3.25587	0.79578	0.39318
O	-1.98360	0.55371	2.33013
O	2.43535	-2.05148	-2.08493
O	2.95473	0.20108	-2.18996
O	-2.30079	3.34106	-0.13486
O	-0.94171	3.09013	2.19683
O	-3.76985	-1.88414	0.16543
O	-2.30460	-2.18168	2.45919
O	4.11268	0.23358	0.34289
O	3.41030	-2.43383	0.43006
O	1.31604	0.76007	-4.26052
O	0.56931	-1.93755	-4.08765
O	-1.67724	2.08035	-2.50775
O	0.55500	2.66554	-2.44947
O	0.38843	4.00584	-0.05784
O	2.38484	2.32474	0.64999
O	1.21853	1.36502	2.41875
O	2.91065	-0.80330	2.59521
O	0.83177	-3.32470	0.79193
O	0.41938	-1.91247	2.58250
O	-1.83062	-3.83262	0.31140
O	-1.08591	-2.98689	-2.18446
O	-2.63849	-1.27040	-2.29825
O	-1.39288	0.06523	-4.30263
O	-3.70881	2.77556	2.18812
O	-4.56858	-0.63628	2.42576
O	5.15059	-1.43820	-1.44158
O	3.13592	-1.20283	-4.66766
O	-1.24489	4.84600	-2.09588
O	1.46682	4.26227	2.44125
O	-3.74872	-3.80434	-1.67122
O	-0.86416	-4.44672	2.75839
O	4.11150	1.57129	2.75527
O	2.79323	-3.48511	2.83644
O	-0.57753	2.53415	-5.05839
O	-1.99796	-2.53788	-4.77523
H	-3.60445	0.84605	-0.51575

H	-1.69872	0.54845	3.26287
H	2.11071	-2.96554	-1.97826
H	3.16802	1.14285	-2.32318
H	-3.16904	3.44517	-0.56635
H	-1.19548	4.03732	2.18840
H	-4.57518	-1.54894	-0.25556
H	-2.99074	-2.86685	2.57368
H	4.59987	0.96326	-0.07867
H	4.28761	-2.51861	0.84688
H	1.35419	0.68945	-5.22544
H	0.60976	-2.05525	-5.04799
H	-2.59203	1.74430	-2.47492
H	1.50669	2.85629	-2.39766
H	0.12537	4.91449	0.18548
H	2.92297	2.70879	-0.06093
H	1.04280	1.27778	3.37482
H	3.83467	-1.02848	2.81357
H	0.98516	-3.83859	-0.02340
H	0.28061	-1.43475	3.41973
H	-2.56190	-4.31065	0.74450
H	-0.33846	-3.60108	-2.04738
H	-3.33533	-0.61200	-2.43869
H	-1.38065	0.02010	-5.26976
H	-4.43726	2.12938	2.14415
H	-3.56320	2.96404	3.13200
H	-5.13066	-1.44410	2.31707
H	-4.44105	-0.51477	3.38276
H	5.74511	-1.58428	-0.66683
H	5.21013	-2.23386	-1.99818
H	3.92724	-0.63679	-4.61073
H	3.46050	-2.11881	-4.59809
H	-1.29505	5.57515	-1.42745
H	-0.60418	5.12959	-2.77044
H	1.43042	4.13519	3.40541
H	2.39052	4.47750	2.22454
H	-4.43379	-4.07934	-1.01164
H	-3.39491	-4.61124	-2.08252
H	-0.62705	-4.24531	3.68087
H	-0.26744	-5.16097	2.47308
H	4.88025	0.96234	2.87427
H	4.47106	2.42691	2.46630
H	2.70391	-4.39604	2.50442
H	2.41215	-3.48311	3.73231
H	0.09400	3.23214	-5.16047

H	-1.43613	2.99169	-5.00614
H	-2.95160	-2.35059	-4.84387
H	-1.92620	-3.49681	-4.61810
O	-3.27323	6.54376	0.54933
O	-1.79678	8.21312	1.56305
O	-1.65662	5.88575	2.27652
O	-0.87300	6.54188	0.04119
O	-6.56465	1.55092	-1.58922
O	-4.23901	1.07414	-2.19012
O	-4.89496	3.34533	-1.57138
O	-5.64574	2.39288	-3.69955
O	2.81305	-6.28775	-1.39518
O	1.65230	-6.00108	-3.53488
O	0.42364	-6.80627	-1.57263
O	1.18446	-4.48477	-1.67445
O	7.17980	0.15542	1.21555
O	5.74963	-0.68118	3.02649
O	6.22480	-2.10035	1.06574
O	7.97340	-1.62611	2.69931
O	4.41318	5.00574	-2.11841
O	3.39353	2.89875	-2.83840
O	5.82443	3.17304	-2.92914
O	4.68468	2.97992	-0.76966
O	0.82608	1.27785	5.20219
O	0.16008	-1.07897	5.24690
O	-1.54619	0.67010	5.09700
O	-0.29234	0.35982	7.17352
O	-4.11096	-4.42773	2.06782
O	-6.08843	-2.96394	2.10960
O	-5.70609	-4.45555	0.19648
O	-6.34577	-5.37225	2.36016
Cl	-0.21377	0.30695	5.69715
Cl	-5.56728	-4.31030	1.68762
Cl	-5.37857	2.11205	-2.27253
Cl	-1.92709	6.80513	1.11764
Cl	4.60483	3.53860	-2.17399
Cl	6.80675	-1.04864	1.99575
Cl	1.53067	-5.94559	-2.05759

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Al13k-d_ClO4.log Energy: -7227658.4760238

Al	-0.37246	0.10296	0.22863
Al	1.86494	2.64478	0.60905

Al	3.00805	0.01456	-0.12470
Al	-1.68746	0.30447	3.33426
Al	-0.47812	2.78811	2.32145
Al	-2.99548	1.77380	1.15461
Al	-0.61202	-2.30931	2.53252
Al	1.78101	-2.45559	0.83264
Al	-0.92095	-3.10154	-0.26953
Al	-3.29701	-0.76215	-1.16917
Al	-0.96590	-0.89580	-2.91294
Al	-2.05937	1.67145	-2.17763
O	1.15928	0.91435	-0.23243
O	-1.18902	1.04670	1.55554
O	-0.09691	-1.61126	0.75416
O	-1.45199	0.03862	-1.24752
O	0.73664	-0.10276	-2.84355
O	-0.31024	2.36921	-2.24622
O	2.01504	3.08756	-1.22332
O	0.24036	3.54138	0.77404
O	1.30847	2.27440	2.36405
O	3.43459	1.65198	0.68888
O	2.52146	-0.86259	1.48912
O	2.50413	-1.68541	-0.70023
O	-3.36610	1.06510	2.91621
O	-0.86862	1.87636	3.92648
O	-0.17940	-0.78708	3.54895
O	-2.27402	-1.36328	2.61066
O	-2.22423	3.34859	1.92792
O	-3.57383	0.10354	0.47434
O	-2.52457	2.46807	-0.52592
O	1.15224	-2.96278	2.53729
O	-1.36609	-3.69703	1.50489
O	0.85278	-3.76717	-0.14548
O	-0.47884	-2.48676	-2.01300
O	-2.78520	-1.48837	-2.85774
O	-3.77938	0.82680	-2.09116
O	-1.62565	0.68068	-3.75662
O	3.00755	4.21662	1.10930
O	4.92024	-0.36428	-0.01745
O	-2.33247	-0.00663	5.20562
O	-0.16044	4.45458	3.40841
O	-4.77781	2.57286	1.06404
O	-0.94973	-3.42210	4.17386
O	3.34304	-3.64271	1.03170
O	-1.50999	-4.85857	-0.97724

O	-5.10863	-1.44589	-1.29115
O	-0.68981	-1.70218	-4.69690
O	-2.88273	3.12457	-3.22804
O	-2.63161	-2.33508	-0.35786
O	3.07731	0.68093	-1.89831
Al	1.38007	1.49990	-2.06811
O	1.83320	2.25840	-3.88214
H	5.54157	0.37673	-0.19356
H	5.31779	-1.24104	-0.24173
H	3.84630	-3.68044	1.86822
H	4.04859	-3.45733	0.36035
H	3.87041	1.60838	1.56132
H	3.87835	1.19210	-2.13004
H	3.10592	-0.90468	2.27005
H	2.44498	-2.03466	-1.60410
H	2.59840	5.09550	1.03073
H	3.82545	4.22089	0.55951
H	-0.19798	5.26833	2.87364
H	0.73014	4.43980	3.80489
H	-1.67788	-0.35934	5.83408
H	-3.17270	-0.46721	5.37715
H	-0.63142	-3.05691	5.01806
H	-1.81698	-3.82997	4.34344
H	-1.37616	-4.94658	-1.93696
H	-2.43723	-5.16202	-0.78416
H	-5.81295	-1.05091	-0.71824
H	-5.26690	-2.42207	-1.33041
H	-5.09603	2.64621	0.14355
H	-5.49133	2.04072	1.51019
H	-0.14469	4.13482	0.10827
H	1.69023	1.65840	3.01500
H	-1.21255	2.35240	4.69571
H	-3.06261	-1.81415	2.94561
H	0.72926	-0.46738	3.68965
H	1.29584	-3.86312	2.86324
H	-1.11819	-4.60714	1.72550
H	-3.23587	-2.79012	0.26227
H	-2.85083	-2.45382	-2.90267
H	-0.62687	-1.03489	-5.40207
H	-0.01695	-2.40420	-4.90351
H	-4.20963	0.56820	-2.92015
H	-2.50746	4.04248	-3.29278
H	-3.82992	3.22425	-3.02792
H	-2.48874	3.44329	-0.48150

H	-2.73417	3.88020	2.55510
H	-3.73328	1.67649	3.57170
H	1.03574	-4.70696	-0.00866
H	0.40442	-2.84030	-2.23595
H	-2.40448	0.49351	-4.30163
H	-0.19871	3.29509	-1.95779
H	2.39011	1.72831	-4.47912
H	0.99426	2.41948	-4.35202
H	2.88707	3.42341	-1.49360
H	-3.40835	-0.53417	1.19527
H	1.45850	-0.55463	-3.32085
O	-9.06287	0.88625	0.75256
O	-7.09169	1.66693	-0.48286
O	-7.27028	-0.67682	0.22082
O	-6.90634	1.08918	1.88717
O	-2.63255	5.38100	-0.76101
O	-2.01552	5.70690	-3.11216
O	-0.29687	5.19907	-1.44825
O	-1.40269	7.39020	-1.44892
O	4.87617	4.00791	-0.99415
O	5.37525	2.20466	-2.56719
O	7.12316	3.78701	-1.91661
O	6.32910	2.12556	-0.31282
O	7.65753	-2.21831	0.94207
O	5.99272	-3.60970	2.08135
O	7.42244	-4.58402	0.34680
O	5.67334	-2.98412	-0.27031
O	-4.72644	-3.86264	0.89463
O	-5.49140	-4.16988	-1.41054
O	-3.99655	-5.82339	-0.39230
O	-6.30710	-5.65403	0.36119
O	4.35869	0.62439	5.75953
O	4.35479	1.55696	3.49684
O	4.11441	-0.85744	3.82527
O	2.28816	0.64946	4.45179
O	1.32699	-3.43944	-5.26566
O	2.67056	-1.52887	-4.52214
O	3.71733	-3.72566	-4.83777
O	2.16842	-3.34750	-2.97196
Cl	5.94161	3.03165	-1.44490
Cl	6.72186	-3.35937	0.79707
Cl	3.79674	0.49541	4.39904
Cl	2.49828	-3.01418	-4.41231
Cl	-7.59908	0.74916	0.58357

Cl	-5.14570	-4.88223	-0.12545
Cl	-1.59392	5.94708	-1.68265

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Al13k-r_ClO4.log Energy: -7227664.1608831

Al	0.00948	-0.12080	-0.05374
Al	2.40322	-2.32613	0.50584
Al	0.85979	-2.66228	-1.99857
Al	-0.89650	2.78826	-1.61804
Al	-0.20262	0.38415	-3.20402
Al	-2.73612	0.45222	-1.68133
Al	0.63651	3.12203	0.84763
Al	2.68574	1.01084	1.38413
Al	0.15533	1.05571	2.90794
Al	-2.77264	-0.45161	1.67949
Al	-0.61978	-2.27124	2.36631
Al	-2.17245	-2.64083	-0.12990
O	1.27797	-1.22657	-0.69158
O	-0.82360	0.73180	-1.38411
O	0.73921	1.07265	1.05389
O	-1.17366	-1.18624	0.78877
O	0.97980	-2.91247	1.60670
O	-0.71528	-3.29653	-1.13658
O	3.79107	-1.79252	-0.65028
O	-0.19474	-1.50790	-3.04223
O	1.62526	0.51267	-2.76573
O	1.87139	-3.68566	-0.74218
O	3.16633	0.81216	-0.43982
O	2.78665	-0.85884	1.61786
O	-2.71432	2.34581	-1.81359
O	-0.29169	2.27533	-3.33667
O	0.82670	3.17651	-1.01469
O	-1.11350	3.15322	0.20235
O	-2.10814	0.22700	-3.50028
O	-3.23774	0.58378	0.14653
O	-2.63296	-1.45053	-1.56154
O	2.47477	2.87602	1.12790
O	0.04282	2.93418	2.63711
O	2.05635	1.11317	3.20955
O	0.24537	-0.80302	3.19248
O	-2.23060	-1.61906	3.12740
O	-3.56998	-1.97769	0.93893
O	-1.53831	-3.62973	1.38347

O	3.52926	-3.60007	1.51910
O	0.83034	-4.18867	-3.25046
O	-1.26668	4.60745	-2.28634
O	0.12209	0.20686	-5.16709
O	-4.59192	0.42790	-2.33859
O	0.82775	5.06608	1.11146
O	4.57498	1.26744	1.90675
O	-0.16602	1.40645	4.86403
O	-4.42697	0.04213	2.61582
O	-0.25427	-3.50785	3.87125
O	-3.33942	-4.07100	-0.78232
O	-1.70107	0.90507	2.50290
O	2.41549	-2.00550	-2.87673
Al	2.80623	-0.53558	-1.72341
O	4.35575	0.04451	-2.75260
H	0.44496	-3.99903	-4.12345
H	0.38533	-4.99955	-2.88530
H	4.78860	1.14095	2.84753
H	5.19444	0.68038	1.39351
H	2.58426	-4.26527	-1.04818
H	3.13182	-2.65854	-2.85526
H	3.32009	1.68371	-0.85383
H	4.49755	-3.51596	1.53190
H	3.21951	-3.79493	2.44046
H	0.88852	0.67303	-5.54652
H	0.23054	-0.73578	-5.39237
H	-0.46470	5.16172	-2.31486
H	-1.89886	5.13719	-1.73128
H	1.08137	5.52636	0.28883
H	-0.00414	5.53478	1.38392
H	-1.07229	1.68584	5.08742
H	0.04777	0.66949	5.46396
H	-4.69404	0.97318	2.83978
H	-4.61303	-0.51352	3.39227
H	-4.72158	0.24104	-3.28393
H	-5.35069	-0.00251	-1.86264
H	-0.68873	2.72239	-4.09795
H	3.02205	3.53188	1.58070
H	0.40242	3.52393	3.31576
H	-2.09827	1.79131	2.40393
H	-2.00678	-1.09199	3.91058
H	-0.66797	-3.37274	4.74027
H	0.70101	-3.73334	4.01056
H	-4.49797	-1.94071	0.64671

H	-2.99159	-4.75408	-1.41421
H	-4.22985	-3.79737	-1.10873
H	-2.43632	0.81089	-4.19942
H	-3.28849	2.79388	-2.45008
H	-2.27237	-4.02282	1.88082
H	-0.53694	-4.22035	-0.87961
H	4.52360	-0.36830	-3.61582
H	5.22643	0.21627	-2.30308
H	4.55039	-1.38050	-0.19211
H	0.73456	-3.77856	1.23623
H	2.89545	-1.07757	2.56265
H	1.08662	-1.03425	3.63054
H	-1.13208	-1.74018	-2.88500
H	-3.33617	-1.83433	-2.11255
H	-3.49793	1.49934	0.35697
H	-1.93721	3.31691	0.68935
H	1.67240	3.12115	-1.49604
H	2.05594	1.27640	-3.20469
H	2.37228	1.84163	3.76380
O	2.80033	-1.50826	4.45551
O	4.57197	-3.06439	5.11438
O	2.46497	-2.98904	6.37456
O	2.51019	-3.92550	4.11429
O	-5.48857	-2.82808	-1.98936
O	-6.81674	-0.83412	-1.48443
O	-6.29436	-2.44494	0.28866
O	-7.88205	-3.03069	-1.47955
O	-1.92496	-7.64782	-0.84714
O	-0.21374	-6.14101	-1.71127
O	-2.51406	-5.98102	-2.54904
O	-1.13230	-7.89685	-3.15498
O	8.27042	0.53789	0.35478
O	6.09346	-0.56016	0.58231
O	6.65542	0.69164	-1.46169
O	7.73965	-1.45454	-0.97761
O	-2.69881	6.29035	-0.67248
O	-0.35659	6.99522	-0.75994
O	-2.08091	8.53691	0.07014
O	-1.42575	6.59735	1.40684
O	3.43823	3.27288	-1.98140
O	2.97768	2.51110	-4.26712
O	5.22882	3.25687	-3.64950
O	3.40227	4.87766	-3.82313
O	-5.25228	2.57414	3.25665

O	-5.38947	4.47265	1.71248
O	-3.45155	2.97274	1.67043
O	-3.77393	4.50652	3.55334
Cl	-4.48359	3.67060	2.56072
Cl	-1.64089	7.12784	0.00881
Cl	3.77813	3.49098	-3.45100
Cl	7.22486	-0.20103	-0.38377
Cl	3.10952	-2.86700	5.05093
Cl	-6.64224	-2.29694	-1.16087
Cl	-1.45739	-6.94970	-2.06623

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Al13p_ClO4.log Energy: -11433399.2498560

Al	-0.68534	-0.05680	0.38616
Al	-3.25041	-1.61280	0.08992
Al	-3.29422	1.41038	0.05295
Al	-0.70512	2.95318	0.17947
Al	1.93386	1.45833	0.51111
Al	1.93528	-1.56006	0.75156
Al	-0.66058	-3.08775	0.41953
Al	-5.82175	-0.14537	1.78207
Al	-3.14907	4.20719	-1.87654
Al	1.75085	4.54917	1.96121
Al	4.64117	-0.18063	-0.85623
Al	1.67192	-4.49802	2.51652
Al	-2.81325	-4.36780	-1.90484
O	-1.40735	1.31690	-0.70961
O	0.02889	-1.43578	1.49252
O	-1.35449	-1.52541	-0.61056
O	-2.42759	-0.04508	1.15958
O	0.04193	1.44409	1.30057
O	1.04297	-0.11373	-0.41176
O	-3.72035	-0.12491	-0.89457
O	-2.37721	2.73909	0.99346
O	1.02700	2.72549	-0.60487
O	2.43382	0.02316	1.63289
O	1.07062	-2.88761	-0.22393
O	-2.36635	-2.86107	1.12271
O	-4.80357	-1.55802	1.12593
O	-4.82320	1.30838	1.13875
O	-3.82062	2.58238	-1.29304
O	-1.41419	4.06688	-1.16447
O	-0.00849	4.24150	1.35753

O	2.40082	2.82193	1.68089
O	3.42488	1.24460	-0.56964
O	3.48826	-1.54339	-0.24721
O	2.38086	-2.80890	2.09282
O	-0.04095	-4.20897	1.80854
O	-1.24490	-4.27550	-0.89713
O	-3.69106	-2.85119	-1.25474
O	-4.85798	-0.12152	3.47206
O	-7.02580	-0.09348	0.23898
O	-7.04384	-1.49373	2.56765
O	-7.10273	1.07924	2.67014
O	-2.67367	3.44833	-3.61589
O	-3.84459	5.10333	-0.31071
O	-4.90060	4.57782	-2.78401
O	-2.61789	5.91866	-2.66565
O	1.31273	4.14066	3.82652
O	2.19686	5.07735	0.14948
O	1.34606	6.41804	2.41833
O	3.53081	5.03724	2.58795
O	4.00510	-0.43730	-2.68998
O	5.39981	-0.06211	0.91584
O	5.87026	1.12549	-1.56807
O	5.96211	-1.51230	-1.30340
O	1.11043	-3.94644	4.30197
O	2.30913	-5.39201	0.94401
O	3.37141	-4.92533	3.39312
O	1.14057	-6.30511	3.13798
O	-1.97382	-3.51755	-3.41994
O	-3.61044	-5.50606	-0.53456
O	-2.21459	-6.04603	-2.78730
O	-4.44341	-4.58504	-3.01533
H	-1.45347	1.20397	-1.69808
H	-0.17039	-1.48888	2.44740
H	-1.14565	-1.44085	-1.57631
H	-2.45244	0.05465	2.13060
H	-0.16032	1.48740	2.26125
H	1.04410	-0.21689	-1.38599
H	-4.05361	-0.18477	-1.81386
H	-2.75315	3.33000	1.66016
H	1.04540	2.60806	-1.59217
H	2.28728	0.09066	2.60302
H	1.33870	-3.01277	-1.15829
H	-2.66111	-3.18111	1.99764
H	-5.23131	-2.43847	1.16034

H	-5.27078	2.17111	1.24696
H	-4.47133	2.18630	-1.91626
H	-0.71572	4.43304	-1.74546
H	-0.55098	5.05499	1.33155
H	2.94488	2.53079	2.44577
H	3.36092	1.78807	-1.38566
H	3.90092	-2.42811	-0.30859
H	2.92992	-2.42661	2.79661
H	-0.77316	-4.54350	2.35657
H	-0.66332	-5.06047	-0.95964
H	-4.34335	-2.48837	-1.88113
H	-4.32246	0.66232	3.75884
H	-4.42648	-0.92637	3.83791
H	-7.02168	-0.87260	-0.36191
H	-7.06313	0.70357	-0.33459
H	-7.94876	-1.17052	2.72567
H	-7.11483	-2.38999	2.16147
H	-7.25052	1.97485	2.27342
H	-6.97319	1.20683	3.62756
H	-2.18376	4.01373	-4.23744
H	-2.30099	2.52298	-3.67469
H	-4.80985	5.01980	-0.12646
H	-3.56386	6.02909	-0.09626
H	-5.68332	4.68200	-2.19208
H	-5.15122	3.92750	-3.46938
H	-2.01103	6.53530	-2.17615
H	-3.31509	6.44527	-3.09529
H	0.40386	3.79275	4.00921
H	1.95872	3.54070	4.26713
H	3.15022	5.19707	-0.09759
H	1.85303	4.32677	-0.40077
H	0.64845	6.88723	1.89320
H	1.13700	6.57091	3.35823
H	3.69581	5.96951	2.81140
H	4.33841	4.68716	2.11511
H	3.38118	-1.18906	-2.83192
H	3.63777	0.38153	-3.11643
H	6.21587	0.47004	1.15541
H	4.77333	0.00231	1.66490
H	6.66208	0.84219	-2.09349
H	6.03663	2.02469	-1.20044
H	6.38665	-2.14415	-0.68009
H	6.30277	-1.66947	-2.22569
H	1.78880	-3.80274	4.98490

H	0.38734	-3.26954	4.41631
H	3.11185	-5.04680	0.47797
H	1.68523	-5.78856	0.29061
H	3.47055	-5.86176	3.64249
H	4.22652	-4.63829	2.96704
H	0.66998	-6.34769	3.98954
H	0.66807	-6.90199	2.50791
H	-0.98645	-3.62219	-3.48949
H	-2.18543	-2.63498	-3.82004
H	-4.58514	-5.54900	-0.41711
H	-3.18671	-6.33997	-0.24337
H	-2.00492	-6.83437	-2.22885
H	-1.59709	-6.02965	-3.53970
H	-4.39910	-5.26620	-3.70979
H	-5.28895	-4.71530	-2.52329
O	-1.13722	9.25759	0.39480
O	-2.98668	7.68348	0.08440
O	-0.88660	7.36209	-1.13534
O	-0.99101	6.98564	1.29374
O	-6.57063	4.88664	-0.56667
O	-8.77547	4.30167	0.30962
O	-7.41921	2.59870	-0.82411
O	-6.74737	3.43419	1.38508
O	-6.92278	-2.67467	-1.09611
O	-8.52900	-4.33563	-0.25990
O	-6.55229	-3.77100	1.07581
O	-6.30586	-5.03952	-0.99918
O	2.90202	-4.41389	-4.39593
O	2.30857	-2.69952	-2.74958
O	1.49299	-2.52490	-5.06069
O	0.61841	-4.26356	-3.55765
O	-4.98843	-0.67310	-3.27219
O	-6.52237	0.21293	-4.95835
O	-7.19614	0.16331	-2.60756
O	-5.45740	1.72261	-3.36086
O	3.27884	2.11285	-3.23190
O	0.86992	2.76738	-3.28707
O	0.54929	5.95796	-3.58426
O	1.79100	1.24771	-5.01215
O	-0.19902	-0.81669	-2.91039
O	-1.86318	-1.11029	-4.71278
O	0.84635	5.16391	-2.70529
O	-1.86943	0.93598	-3.31135
O	6.97040	-1.87462	-3.78005

O	6.69771	0.05044	-5.27062
O	7.94382	0.29365	-3.17150
O	8.89292	-1.00058	-5.00756
O	6.26440	-5.88112	0.70061
O	5.61553	-4.04320	2.19238
O	4.61246	-4.23643	-0.04938
O	6.95701	-3.58457	0.21371
O	0.35870	-6.59276	-0.65046
O	-0.51997	-7.67461	1.38559
O	0.25441	-9.03446	-0.50331
O	-1.80975	-7.72504	-0.67810
O	-1.69092	1.65386	5.95953
O	-1.33632	3.35065	4.22166
O	-3.40168	2.08244	4.25059
O	-1.30820	0.96103	3.64569
O	4.78491	5.32862	-0.71817
O	5.58824	4.03239	1.21055
O	6.98474	5.79839	0.23428
O	6.61245	3.71989	-0.98144
O	-2.59170	-3.92148	3.64881
O	-3.31376	-1.94243	4.91609
O	-1.98202	-3.67181	6.00199
O	-0.94870	-2.22184	4.32369
O	9.74818	2.19674	1.56049
O	9.39854	-0.18763	1.98576
O	7.48491	1.33420	1.80289
O	8.79754	0.76655	-0.18538
O	2.40619	0.23037	4.38742
O	4.02680	0.93775	6.08137
O	3.52355	2.40504	4.18377
O	4.78823	0.34566	3.82635
Cl	7.62908	-0.62405	-4.33164
Cl	5.88006	-4.46087	0.76754
Cl	-0.40861	-7.78715	-0.10070
Cl	1.83986	-3.47317	-3.97831
Cl	3.70219	0.96086	4.64317
Cl	6.00467	4.73489	-0.06303
Cl	8.88175	1.01949	1.28241
Cl	-1.49480	7.85173	0.15467
Cl	-1.92685	2.00885	4.54844
Cl	-7.41718	3.79450	0.06555
Cl	-6.06550	0.34938	-3.56006
Cl	-7.11363	-3.94567	-0.32774
Cl	-0.94995	-0.09158	-4.05080

Cl	2.10898	2.47331	-4.19299
Cl	-2.22561	-2.94710	4.74231

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Al1_ClO4.log Energy: -1872151.6071265

Al	-0.25296	-0.36016	0.63149
O	-0.93332	-1.62777	-0.64131
O	1.15414	0.12925	-0.53237
H	-0.79048	-2.58240	-0.51848
H	-1.83350	-1.47573	-1.03983
H	1.52849	1.04851	-0.53377
H	1.83349	-0.52101	-0.87279
O	0.85212	-1.68783	1.41059
H	0.54134	-2.23521	2.15146
H	1.84646	-1.80283	1.27758
O	0.24808	0.96542	1.94983
O	-1.61105	-0.94027	1.89084
H	0.20488	1.92268	1.67142
H	1.05420	0.82999	2.47875
H	-2.49184	-1.25824	1.54503
H	-1.78147	-0.33972	2.63863
O	-1.40969	0.95195	-0.11812
H	-1.20896	1.91987	-0.11283
H	-2.24711	0.72588	-0.59139
O	4.11615	-3.64807	-0.44305
O	5.17876	-1.45054	-0.63102
O	3.44460	-1.80869	1.04226
O	2.84782	-1.76814	-1.33831
O	2.02139	2.70490	-0.31532
O	0.45899	4.11053	-1.58860
O	1.52533	4.96793	0.44692
O	-0.19717	3.23222	0.59762
O	-5.33739	-1.94427	-1.21375
O	-3.30773	-0.57244	-1.27389
O	-3.89109	-1.84302	0.74642
O	-5.21052	0.12608	0.09593
Cl	-4.48395	-1.05810	-0.40269
Cl	3.92580	-2.18443	-0.35373
Cl	0.97213	3.78795	-0.24245

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Al2_ClO4.log Energy: -2692894.5492220

Al	0.43205	-0.98453	1.63167
Al	0.16704	0.42512	-0.86791
O	-0.71108	-0.84008	0.16594
H	-1.64029	-1.14635	0.17286
O	1.41948	0.08801	0.48015
H	2.20522	0.63445	0.69198
O	-1.22477	0.76759	-2.14379
H	-2.16052	1.05445	-1.90190
H	-1.27610	0.14898	-2.89380
O	1.37346	1.63093	-1.81234
H	1.72739	2.39988	-1.28685
H	1.06654	1.97611	-2.67016
O	-0.80116	-2.13155	2.55942
H	-0.80768	-2.28844	3.51866
H	-1.72626	-2.23211	2.17318
O	1.61727	-0.98138	3.17878
H	2.44934	-1.48580	3.13698
H	1.77732	-0.14808	3.65700
O	0.79409	-0.88834	-2.15096
H	0.57645	-1.81303	-1.93268
H	1.77631	-0.89164	-2.34247
O	-0.50053	1.98800	0.19985
H	-1.39587	2.42513	0.06235
H	0.17969	2.71261	0.26664
O	1.38907	-2.59478	1.16404
H	1.90299	-2.69291	0.30983
H	0.92498	-3.43310	1.33308
O	-0.31197	0.60097	2.53978
H	-0.50060	1.29994	1.86540
H	-1.10897	0.50464	3.09035
O	-4.80469	-3.03760	-0.17639
O	-3.57735	-4.40529	1.44609
O	-3.00624	-2.04234	1.14091
O	-2.47967	-3.67049	-0.61745
O	4.68556	-3.26755	-2.34371
O	4.50971	-1.85803	-0.34602
O	2.53698	-3.04427	-1.19490
O	3.45645	-1.15512	-2.44834
O	1.72442	3.52943	0.03280
O	2.15518	3.46014	2.43985
O	3.83961	4.39062	0.91767
O	3.41226	1.98584	0.93140
O	-3.66826	1.45522	-1.42119
O	-2.85844	3.21913	0.07931

O	-3.67614	3.79665	-2.15767
O	-5.23783	3.03517	-0.42944
Cl	-3.88026	2.90161	-0.99601
Cl	-3.48301	-3.33070	0.42678
Cl	2.81096	3.35264	1.11849
Cl	3.83459	-2.33528	-1.57570

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Al3_ClO4.log Energy: -3513652.0509116

Al	1.53335	0.68883	-1.31727
Al	-1.11265	-1.44762	-0.83291
Al	-1.09612	0.81227	0.90997
O	0.46944	1.40789	-0.00051
O	-2.07635	0.11993	-0.53636
O	0.98257	2.08762	-2.54083
O	-1.72703	2.65517	0.66511
O	0.25798	-0.57723	-1.81430
H	1.09998	2.00186	-3.50202
H	0.12804	2.56914	-2.36573
H	0.03222	-0.55915	-2.75818
H	-2.44106	0.70181	-1.23334
H	-1.66783	3.02544	-0.25490
H	-2.61525	2.84072	1.01634
H	0.80520	2.22798	0.42252
O	-0.53941	-0.98102	0.87851
H	0.18854	-1.36865	1.40353
O	-2.67238	0.63240	2.05247
H	-2.57756	0.61393	3.01853
H	-3.51908	0.17489	1.80065
O	-2.39673	-2.69794	-0.04915
H	-3.34786	-2.66595	-0.31873
H	-2.45464	-2.63033	0.92890
O	-0.09556	-3.06655	-1.15831
H	-0.24286	-3.87619	-0.64163
H	0.85073	-3.02065	-1.46334
O	-2.00653	-1.79429	-2.57258
H	-1.96088	-2.68819	-2.95602
H	-2.85951	-1.40085	-2.82802
O	-0.26689	1.33558	2.60398
H	0.22047	0.64966	3.13661
H	0.30767	2.13535	2.55495
O	2.59721	-0.00642	-2.83743
H	2.67097	-0.99423	-2.84964

H	3.48957	0.36181	-2.96598
O	3.09746	1.82411	-0.94861
H	3.71288	1.41519	-0.31335
H	3.02989	2.78576	-0.69673
O	2.51901	-0.58195	-0.20640
H	2.69631	-1.44422	-0.66116
H	2.30055	-0.79567	0.73655
O	-6.40743	-2.39026	2.19242
O	-3.95414	-2.45641	2.26715
O	-5.11925	-2.43013	0.11273
O	-5.10733	-0.42777	1.53387
O	-3.28143	1.89126	-2.34387
O	-3.24552	4.13340	-3.31077
O	-1.72511	2.40895	-4.17224
O	-1.34782	3.35823	-1.95893
O	1.12758	3.55077	1.65284
O	3.45074	2.93486	2.15548
O	2.92911	4.28582	0.18027
O	2.70548	5.26101	2.41197
O	1.81339	-1.74146	2.12862
O	2.32619	-2.54844	4.37730
O	3.30819	-0.44911	3.57379
O	0.91275	-0.58435	4.09806
O	2.46073	-2.59948	-1.98783
O	2.80659	-4.96555	-1.48082
O	4.71342	-3.42045	-1.45916
O	3.65546	-4.03102	-3.58401
Cl	-5.16242	-1.93881	1.53851
Cl	2.11880	-1.32820	3.57308
Cl	2.58185	4.01641	1.62892
Cl	-2.42847	2.94921	-2.98447
Cl	3.45606	-3.80755	-2.13644

66
Al3l_ClO4.logEnergy: -3513638.5375453

Al	1.09860	-2.48084	1.50433
Al	-1.45111	1.58591	-1.70741
Al	-0.07662	-0.39062	-0.13099
O	0.33191	-2.23453	-0.17208
O	0.75835	-0.64877	1.52642
O	-0.61882	1.40717	-0.05467
O	-0.96561	-0.22183	-1.78739
O	1.25212	-4.42359	1.53839

O	1.88153	-2.38472	3.27988
H	0.04251	-2.90137	-0.80810
H	1.23688	-0.00405	2.07620
H	-0.20237	2.15789	0.40607
H	-1.62459	-0.88310	-2.06567
H	0.45207	-4.97922	1.54138
H	1.94405	-4.86484	1.01400
H	2.34825	-1.53526	3.49355
H	2.40009	-3.12745	3.63678
O	-3.25685	1.30377	-1.07452
H	-3.61906	0.40877	-1.30634
H	-3.37475	1.39083	-0.08495
O	-1.83071	-0.95378	0.80396
H	-2.50901	-1.31473	0.17269
H	-2.28781	-0.20127	1.27464
O	-0.64866	-2.86888	2.30663
H	-1.29982	-2.23155	1.90677
H	-0.70629	-2.77750	3.27472
O	2.87212	-2.55836	0.75941
H	2.92908	-2.46245	-0.23463
H	3.58818	-1.99400	1.14895
O	1.62751	0.15594	-0.95734
H	2.26671	0.55926	-0.32915
H	2.11827	-0.56866	-1.43280
O	0.16284	2.19445	-2.61543
H	0.07235	2.88204	-3.29814
H	0.94580	2.44964	-2.05439
O	-2.26407	1.50867	-3.48810
H	-1.78283	1.15086	-4.25513
H	-2.91921	2.15219	-3.81078
O	-1.84732	3.49173	-1.50684
H	-2.73671	3.75760	-1.21206
H	-1.17811	3.96672	-0.94088
O	5.27890	-2.03073	-1.41437
O	4.36458	-0.63001	-3.20781
O	2.87463	-2.05300	-1.88414
O	4.44014	-3.06482	-3.47221
O	-5.66608	1.62492	1.75141
O	-3.25731	1.20083	1.61366
O	-4.37258	1.21730	3.79266
O	-4.78722	-0.61587	2.22089
O	2.40605	4.79844	0.85036
O	1.43403	5.60653	-1.25153
O	2.08446	3.25243	-1.01202

O	0.14311	4.12588	0.21075
O	4.96188	1.34487	3.02332
O	2.80806	0.19401	3.22834
O	3.47855	1.17835	1.08817
O	4.63370	-0.81933	1.94016
O	-3.43321	-1.36516	-1.33692
O	-4.52111	-3.37637	-0.46876
O	-4.56415	-2.90292	-2.87300
O	-5.87715	-1.52467	-1.33105
Cl	-4.64509	-2.32903	-1.51014
Cl	1.54274	4.47603	-0.30283
Cl	3.99316	0.49222	2.31423
Cl	-4.56709	0.84655	2.37166
Cl	4.28840	-1.94117	-2.51878

66
Al3r_ClO4.log Energy: -3513651.7571744

Al	-1.54577	-0.64701	-0.80692
O	0.27908	-0.92147	-0.95165
O	-0.93928	-0.30508	0.97922
H	0.79254	-1.28989	-1.69412
H	-1.53304	-0.59597	1.70128
Al	0.90309	-0.91921	0.81583
Al	1.83976	1.32404	2.39438
O	1.38617	-0.46877	2.59338
O	1.74509	0.76701	0.64868
O	1.82116	1.71063	4.31005
O	0.30025	-2.70826	1.38609
H	1.58742	1.34860	-0.12174
H	1.22154	-1.00697	3.37818
H	0.99739	-3.36255	1.56604
H	-0.45487	-2.86877	2.00486
H	1.33013	1.17870	4.96100
H	1.84499	2.63161	4.62763
O	2.49031	-1.93903	0.32619
H	3.36902	-1.47509	0.42800
H	2.46753	-2.35278	-0.56581
O	3.75511	1.06052	2.58440
H	4.08327	0.77101	3.45336
H	4.20084	0.49376	1.88465
O	2.30892	3.17920	2.12152
H	1.91879	3.64981	1.33229
H	3.27198	3.32603	2.08658

O	-0.02176	1.94726	2.23115
H	-0.54363	2.22430	3.00407
H	-0.55716	1.28189	1.72009
O	-1.50671	1.18620	-1.36966
H	-0.63164	1.65078	-1.43367
H	-2.18244	1.83587	-1.03062
O	-1.91245	-1.03095	-2.69709
H	-1.47031	-1.84030	-3.05154
H	-1.72555	-0.29718	-3.30930
O	-1.85220	-2.56393	-0.59868
H	-2.54908	-2.95238	-0.01790
H	-1.11093	-3.20793	-0.70095
O	-3.39586	-0.48934	-0.34381
H	-4.03415	0.15960	-0.76482
H	-3.64064	-0.63488	0.59786
O	1.72553	4.41554	-0.19122
O	1.02550	4.66890	-2.50668
O	-0.65032	4.20454	-0.77478
O	0.92352	2.46164	-1.45222
O	1.80169	-2.73082	-2.38299
O	1.42843	-4.92673	-3.40148
O	-0.30208	-3.20616	-3.54117
O	0.18171	-4.29352	-1.39524
O	5.17040	1.53146	-0.38906
O	4.54018	-0.47286	-1.65910
O	6.76436	-0.31013	-0.64242
O	4.78241	-0.59677	0.77055
O	-1.86356	-3.09404	3.07812
O	-3.60269	-3.40614	1.36828
O	-4.22489	-2.98591	3.69578
O	-3.22158	-1.19417	2.35261
O	-3.47368	2.76120	-0.38302
O	-4.99520	1.24434	-1.56119
O	-4.80774	3.56945	-2.28182
O	-5.88409	3.04399	-0.14714
Cl	0.73713	3.96880	-1.23956
Cl	5.33703	0.06323	-0.52549
Cl	-4.80845	2.68165	-1.09720
Cl	-3.24525	-2.68852	2.64009
Cl	0.77836	-3.81231	-2.68977

82
Al4b_ClO4.log Energy: -4334408.4326661

Al	1.43310	2.79188	-0.29163
Al	-1.34403	-2.63790	0.86886
Al	-1.08479	0.75268	0.78328
Al	1.30453	-0.62817	0.00369
O	2.16193	1.08717	-0.16684
O	0.42793	-0.08932	1.62606
O	2.49256	3.45546	1.16274
O	2.78933	-1.35689	1.01389
O	-0.12042	2.37633	0.67267
H	2.26813	4.27708	1.63094
H	3.03060	2.86137	1.76643
H	-0.37192	3.02501	1.34885
H	1.01079	0.41935	2.22474
H	2.93163	-0.90596	1.88437
H	3.67572	-1.46524	0.57705
H	3.06158	1.00930	-0.54711
O	-0.21862	0.18427	-0.81642
H	-0.69461	-0.36591	-1.47418
O	0.29948	-2.24379	0.06381
H	0.81408	-3.03581	-0.18689
O	-1.99840	-0.89320	0.90295
H	-2.86971	-0.81752	1.34464
O	-2.61766	1.50152	-0.14264
H	-3.04176	0.86452	-0.77073
H	-2.45376	2.35481	-0.62141
O	-1.88359	1.40560	2.45982
H	-2.78468	1.02512	2.64788
H	-1.36317	1.30509	3.27650
O	2.10068	-1.19965	-1.65179
H	2.98329	-0.85067	-1.92756
H	1.86530	-2.02108	-2.14660
O	0.68998	4.61831	-0.39211
H	-0.25794	4.62306	-0.68946
H	1.17208	5.27610	-0.92435
O	2.89608	3.47709	-1.43996
H	2.95762	3.18826	-2.36762
H	3.79297	3.64528	-1.10194
O	0.57905	2.38215	-1.98826
H	-0.23609	2.91729	-2.14947
H	0.25150	1.44984	-1.82831
O	-0.77923	-4.51448	0.95052
H	-1.42238	-5.18516	1.23795
H	-0.18954	-4.89973	0.25638
O	-0.59782	-2.34731	2.65228

H	-0.09644	-1.48951	2.54366
H	0.03120	-3.01965	2.96992
O	-2.30374	-2.97739	-0.78050
H	-1.81745	-3.44647	-1.50189
H	-2.74816	-2.17671	-1.16627
O	-2.93689	-3.32800	1.78189
H	-3.69389	-3.56723	1.21879
H	-3.29025	-2.88324	2.60342
O	4.69856	0.50676	4.50647
O	4.10098	1.94987	2.64014
O	2.59604	0.12192	3.31718
O	2.83508	2.08885	4.73654
O	-1.42739	-0.86171	-3.14982
O	-2.92598	1.05435	-3.50281
O	-3.44494	-0.62861	-1.80819
O	-3.61651	-1.19584	-4.19641
O	4.37796	0.24499	-1.68153
O	6.52750	-0.82877	-2.16278
O	6.27586	0.58828	-0.17844
O	5.17773	-1.60656	-0.28474
O	-4.61761	0.11876	4.87912
O	-4.16015	-0.04070	2.47776
O	-6.09533	-1.18888	3.42075
O	-3.83782	-1.99263	3.94349
O	1.08094	-4.72271	-1.01032
O	1.34909	-3.45463	-3.08600
O	1.10631	-5.88330	-3.16951
O	-0.81123	-4.50367	-2.56666
O	-2.26928	4.47377	-3.71426
O	-2.35806	6.11228	-1.89474
O	-4.01416	4.30433	-1.99856
O	-1.68904	3.80621	-1.41969
Cl	5.62995	-0.39735	-1.07210
Cl	0.67997	-4.65388	-2.48233
Cl	3.56841	1.17700	3.83120
Cl	-2.62175	4.71036	-2.29586
Cl	-4.70643	-0.77660	3.70759
Cl	-2.85855	-0.39681	-3.21220

82
Al4_ClO4.log Energy: -4334418.9078762

Al	0.68372	1.39994	1.74175
O	0.94009	-0.38846	2.22782

H	1.80751	-0.41682	2.66716
O	2.49061	1.67373	2.57691
H	3.28084	1.82757	2.00165
H	2.61163	2.14095	3.42034
O	1.52744	1.23296	0.08624
H	1.78946	2.08862	-0.30435
O	0.66261	3.36788	1.56613
H	0.10183	3.77128	0.85213
H	1.53900	3.81966	1.54236
O	-1.02217	1.24828	0.98079
H	-1.40450	2.10631	0.72184
O	0.00138	1.70432	3.55616
H	-0.49435	0.93774	3.94232
H	-0.52239	2.50999	3.70893
Al	1.49908	-0.05708	-1.26206
O	1.54117	-1.58039	-0.18142
H	2.34739	-2.12351	-0.30973
O	1.82277	-1.23307	-2.79710
H	1.74086	-0.86121	-3.69179
H	1.48050	-2.16371	-2.80434
Al	-1.78659	-0.05389	-0.15521
O	-1.10008	-1.47460	0.87135
H	-1.75537	-1.70816	1.55720
O	-3.39361	0.02605	0.96087
H	-3.39384	0.28790	1.91135
H	-4.28015	-0.29690	0.67962
Al	0.60880	-2.02237	1.37874
O	2.30354	-2.75598	2.08184
H	3.05900	-3.01082	1.49104
H	2.28764	-3.32970	2.86624
O	3.45835	0.19079	-1.31905
H	3.84546	0.74704	-0.60742
H	4.08401	-0.55815	-1.49483
O	0.10557	-3.81909	0.74243
H	0.74152	-4.55423	0.71775
H	-0.39957	-3.82764	-0.11176
O	-2.62140	1.39151	-1.16806
H	-2.05130	1.88078	-1.81047
H	-3.53382	1.29711	-1.53576
O	-0.37644	-0.13475	-1.40540
H	-0.65037	-0.68154	-2.16756
O	-2.79938	-1.31660	-1.27150
H	-3.78553	-1.34550	-1.20778
H	-2.45152	-2.23941	-1.30910

O	-0.03162	-2.67527	3.14694
H	-0.37586	-1.96716	3.74775
H	-0.66364	-3.41439	3.17831
O	1.46730	1.38624	-2.63866
H	0.67622	1.98396	-2.62384
H	2.26194	1.94845	-2.69643
O	-1.43046	-3.72287	-1.56457
O	-1.21844	-4.67619	-3.81261
O	-0.99597	-2.25529	-3.47776
O	0.75464	-3.76330	-2.67965
O	-1.23699	-0.59632	4.56654
O	-3.26263	0.47284	3.68619
O	-2.86452	-1.91915	3.31333
O	-3.42586	-1.09846	5.55660
O	-5.14243	0.90955	-2.20370
O	-5.41372	-0.92701	-0.59486
O	-7.09363	-0.54853	-2.33486
O	-6.87709	1.02895	-0.47123
O	5.21937	4.27248	-0.37289
O	4.38787	2.18793	0.62775
O	3.03579	3.36946	-1.03760
O	3.33214	4.32363	1.19148
O	5.19523	-1.91334	-1.56021
O	6.12162	-3.91670	-0.52016
O	5.65379	-1.93763	0.85178
O	3.80833	-3.26789	-0.06443
O	-0.82759	2.96576	-2.49105
O	-1.14884	4.07137	-0.31096
O	0.44457	4.98268	-1.94145
O	-1.97344	5.11903	-2.34841
Cl	-0.72524	-3.61514	-2.91904
Cl	5.23381	-2.75619	-0.30937
Cl	4.01395	3.56673	0.08767
Cl	-6.16594	0.13572	-1.41134
Cl	-0.86684	4.32502	-1.78145
Cl	-2.73095	-0.79440	4.29462

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Al4f_ClO4.log Energy: -4238466.3954948

Al	1.31780	0.58892	0.41565
Al	-1.61623	0.05240	-0.36988
Al	-0.51654	2.80055	-0.34502
Al	0.16194	-2.20599	0.54810

O	-0.50898	1.21927	0.84499
O	0.23330	-0.63526	-0.74071
O	1.13843	2.03743	-0.75226
O	-1.46761	1.58637	-1.39447
O	-1.51812	-1.43100	0.71855
O	1.13094	-0.90966	1.48775
O	-0.58634	4.08583	-1.80564
O	-0.02362	-3.19301	2.20526
H	-0.80330	1.15075	1.79080
H	0.59336	-0.73160	-1.65542
H	1.91656	2.59528	-0.93875
H	-2.21526	1.85878	-1.97188
H	-2.30854	-1.88461	1.07772
H	1.54705	-1.02583	2.35346
H	-0.34545	3.78468	-2.70089
H	-0.29256	5.00990	-1.71331
H	-0.52295	-2.68080	2.89299
H	-0.34267	-4.11277	2.21347
O	-2.54826	-0.83806	-1.79091
H	-2.89990	-1.76517	-1.65139
H	-2.29691	-0.73169	-2.72469
O	-3.21644	0.60324	0.52788
H	-4.02822	0.95054	0.07534
H	-3.41665	0.25974	1.43341
O	2.25797	1.52896	1.80428
H	1.85769	1.82032	2.64085
H	3.05846	2.10411	1.61225
O	2.99944	0.14720	-0.37351
H	2.93187	-0.09884	-1.33085
H	3.52634	-0.56762	0.09112
O	-0.63331	-3.55455	-0.57032
H	-0.21193	-4.40234	-0.79029
H	-1.61149	-3.60048	-0.77524
O	1.76620	-3.08734	0.00003
H	2.61620	-2.78417	0.43207
H	1.94575	-3.15626	-0.97792
O	-2.09188	3.64191	0.41483
H	-2.38591	3.42273	1.31664
H	-2.91540	3.78121	-0.13736
O	0.40236	4.04767	0.80723
H	1.36110	4.25418	0.62046
H	-0.03728	4.83148	1.18020
O	4.00113	-1.99283	-3.40590
O	2.02487	-2.01633	-4.86115

O	2.02618	-0.68587	-2.80736
O	-1.34571	0.90395	3.43356
O	-3.23412	-0.61244	3.00138
O	-2.65437	0.02970	5.28910
O	-5.53936	-3.01352	-0.61898
O	-6.05816	3.26197	-2.60016
O	-4.34527	3.98746	-1.02072
O	-3.81793	-3.02666	1.12576
O	-3.19808	-3.36656	-1.23312
O	-5.27852	1.71766	-0.87842
O	-3.80267	2.32791	-2.74462
O	-4.41340	-5.10820	-0.01645
O	1.95060	-3.14488	-2.70349
O	-1.19121	-1.47312	4.05950
O	4.98874	-3.81224	-0.19360
O	6.08592	-1.61797	-0.20413
O	6.02090	-2.94700	1.85410
O	3.96850	-1.92631	0.98973
O	4.08858	5.38261	1.57024
O	5.26647	4.55639	-0.41617
O	2.85545	4.22814	-0.19931
O	4.41190	2.97472	1.23328
Cl	-2.11134	-0.28921	3.95478
Cl	2.52386	-1.97499	-3.47275
Cl	4.18427	4.31205	0.55594
Cl	5.31848	-2.60046	0.59820
Cl	-4.88557	2.82427	-1.82452
Cl	-4.28775	-3.64535	-0.15789

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Al4l_ClO4.logEnergy: -4334383.0814969

Al	3.69982	-0.10046	-1.20522
Al	-2.00141	0.62356	-0.64179
Al	-4.77858	1.04388	-0.20861
Al	0.85596	0.28019	-0.86112
O	2.39863	1.20775	-1.42093
O	2.19492	-1.00385	-0.61932
O	-0.67675	-0.63994	-0.33209
O	-0.51981	1.45559	-1.40832
O	-3.47518	-0.20307	0.14456
O	-3.35574	1.90045	-1.03987
O	5.17989	1.00578	-1.86415
O	4.91564	-1.57627	-1.05048

O	-4.48391	1.88266	1.52426
O	-6.04317	2.46926	-0.62497
H	2.50317	2.16896	-1.54539
H	2.13234	-1.92575	-0.29105
H	-0.78678	-1.46346	0.18869
H	-0.42777	2.41931	-1.55943
H	-3.54399	-1.16370	0.35661
H	-3.16329	2.85817	-0.94305
H	5.16999	1.17079	-2.82457
H	5.30198	1.87725	-1.40660
H	4.79331	-2.37166	-0.44024
H	5.86537	-1.45330	-1.21950
H	-4.84076	2.77601	1.67741
H	-3.49880	1.91818	1.65702
H	-7.00352	2.37692	-0.49177
H	-5.88819	3.12538	-1.32754
O	3.48169	-0.58556	-3.09753
H	2.50778	-0.53460	-3.28681
H	3.78798	-1.47289	-3.35558
O	0.79859	-0.40901	-2.85319
H	0.41611	-1.30381	-3.08683
H	0.34344	0.24771	-3.40999
O	-2.61685	-0.24362	-2.42040
H	-2.41141	0.27299	-3.22033
H	-2.40269	-1.20344	-2.61890
O	-5.28871	0.05841	-1.81660
H	-4.44305	-0.20331	-2.26261
H	-5.86501	0.45918	-2.49174
O	-1.80399	1.62453	1.14438
H	-1.42637	1.11440	1.91204
H	-1.29063	2.47200	1.07943
O	1.04982	1.15061	0.89740
H	1.70925	1.87384	0.95962
H	1.12325	0.59560	1.72335
O	4.26302	0.47336	0.57089
H	5.11574	0.19857	0.94722
H	4.03928	1.38162	0.90581
O	-6.28599	0.15080	0.64585
H	-6.25012	0.02908	1.61273
H	-6.61618	-0.67645	0.24913
O	-1.32124	-4.84728	-3.86965
O	-0.05991	-2.76323	-3.78260
O	-2.39663	-2.82813	-3.03345
O	-0.64614	-3.91986	-1.70405

O	-0.47278	4.24641	-1.64159
O	-2.64689	4.57527	-0.56580
O	-0.66305	4.11475	0.79948
O	-0.89800	6.26889	-0.33175
O	3.34382	2.93960	1.11313
O	2.94349	3.95845	-1.08602
O	4.06587	5.23906	0.67485
O	5.22340	3.37067	-0.39658
O	4.72407	-3.68801	0.51225
O	2.29204	-3.65293	0.19042
O	3.24252	-3.21741	2.40801
O	3.34327	-5.46675	1.44200
O	-1.15836	-2.79182	1.39995
O	-2.42031	-4.88254	1.50681
O	-3.00132	-3.02245	2.98792
O	-3.47770	-2.88790	0.58810
O	-1.23813	0.30595	3.43065
O	0.49216	1.34159	4.81862
O	1.11877	-0.32435	3.13437
O	-0.09705	-1.01571	5.13116
Cl	3.38662	-4.01363	1.16456
Cl	-1.10008	-3.61469	-3.08202
Cl	-2.51372	-3.40713	1.63743
Cl	-1.16623	4.82127	-0.43619
Cl	0.07201	0.08360	4.15453
Cl	3.89624	3.91072	0.06666

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Al4r2_ClO4.log Energy: -4334395.5400762

Al	-3.47587	0.96272	0.54464
O	-3.22873	0.15485	-1.12514
H	-4.01789	-0.19917	-1.57620
O	-2.04581	-0.13050	0.97323
H	-1.99539	-0.65578	1.79506
Al	-1.77389	-1.01100	-0.68716
Al	1.16945	-0.94295	-0.80352
O	-0.37807	0.17124	-1.17112
O	2.27503	0.48853	-1.25198
H	-0.37123	0.72340	-1.97705
H	2.65041	0.69415	-2.12521
O	-0.23572	-2.04996	-0.35394
H	-0.17430	-2.78006	0.29396
Al	2.42740	1.35315	0.38733

O	1.60552	-0.24138	0.88482
H	1.15406	-0.49950	1.70762
O	-1.83124	-1.73498	-2.54956
H	-0.92116	-1.83240	-2.90250
H	-2.32370	-1.21414	-3.20875
O	1.12365	-1.60470	-2.74589
H	1.75604	-1.13291	-3.34151
H	1.36013	-2.54955	-2.80868
O	3.09318	2.96787	-0.53234
H	3.55111	3.65159	-0.01221
H	2.48035	3.42190	-1.15562
O	-5.00416	2.11537	0.03075
H	-4.90573	2.85335	-0.59520
H	-5.92108	1.79299	-0.01325
O	-4.95888	-0.20804	1.06589
H	-4.93769	-0.73129	1.88564
H	-5.36244	-0.76070	0.33881
O	2.51888	-2.33578	-0.63938
H	2.85358	-2.51909	0.28054
H	3.31224	-2.25288	-1.22486
O	4.27795	0.84022	0.56191
H	4.64183	0.56055	-0.31020
H	4.52646	0.12815	1.22197
O	-2.83725	-2.54183	-0.13121
H	-3.63983	-2.91657	-0.58085
H	-2.81811	-2.77655	0.81988
O	-2.41121	2.50697	0.08880
H	-2.23237	2.90021	-0.80022
H	-2.04450	3.08771	0.80166
O	-3.60363	1.61752	2.37753
H	-4.45955	1.99671	2.64678
H	-2.89959	2.24645	2.69180
O	0.64432	2.15215	0.34953
H	0.03480	1.45415	-0.01625
H	0.53773	2.94534	-0.22855
O	2.55679	2.19639	2.11004
H	3.25194	1.99775	2.75961
H	1.70304	2.38332	2.59304
O	-2.02384	-2.36933	2.61982
O	-0.65825	-3.52110	4.29737
O	0.22309	-1.55512	3.14296
O	-0.06956	-3.67606	1.92955
O	4.96368	-0.98814	2.40128
O	5.60525	-2.49039	0.57786

O	3.54699	-2.91495	1.82340
O	5.70599	-3.25222	2.91341
O	3.39124	-0.12694	-3.68756
O	4.42407	-2.07753	-2.61562
O	5.25859	0.18240	-2.12189
O	5.65410	-0.82322	-4.31165
O	-4.94513	-3.48502	-1.52915
O	-6.70591	-2.62730	-2.98649
O	-5.75292	-1.17832	-1.26681
O	-7.17947	-3.05456	-0.61843
O	0.20497	2.57908	3.42907
O	0.32043	4.75945	2.31136
O	-0.79573	4.53968	4.48707
O	-1.82767	3.61033	2.48354
O	0.02360	2.19159	-3.18761
O	-1.63933	3.75444	-2.28701
O	0.70969	3.99898	-1.65775
O	-0.00756	4.51830	-3.93887
Cl	-6.17499	-2.61065	-1.60892
Cl	4.70504	-0.71377	-3.18878
Cl	4.97647	-2.42959	1.92408
Cl	-0.49503	3.89526	3.19317
Cl	-0.23121	3.61410	-2.79856
Cl	-0.61538	-2.78979	3.01462

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Al4r_ClO4.log Energy: -4334405.8134980

Al	-1.99045	1.35971	0.06553
O	-3.40071	1.72901	1.35427
O	-2.74739	-0.38041	-0.29693
O	-0.83821	0.66009	1.41987
O	-0.52806	0.97258	-0.96698
Al	0.62850	0.03011	0.20642
O	-0.38752	-1.65639	-0.06727
O	1.31046	-1.08114	1.59243
O	1.85026	1.45597	0.43104
O	1.93718	-0.40990	-1.08174
Al	3.09457	1.01339	-0.87030
H	2.06774	1.88586	1.28249
H	-0.56822	0.75137	-1.92038
H	1.68018	-0.87238	-1.90030
H	-0.56089	1.27159	2.12147
H	-0.21017	-2.02586	-0.96218

H	-2.00875	-1.04916	-0.30283
H	-3.50374	-0.77048	0.20719
H	1.66287	-0.71705	2.43067
H	-3.43261	1.24377	2.19609
H	-4.33854	1.95080	1.07308
Al	0.25033	-2.57566	1.44462
O	-1.06974	-1.76602	2.60954
H	-1.97583	-2.15528	2.70878
H	-1.15924	-0.80863	2.35030
O	-0.88684	-4.10274	1.09604
H	-0.86752	-4.84002	1.73140
H	-1.83452	-3.96765	0.81293
O	4.23591	0.42070	-2.34341
H	4.28674	-0.56390	-2.47839
H	5.14239	0.77318	-2.38375
O	4.31855	0.06901	0.31681
H	4.30477	-0.91350	0.19096
H	4.30035	0.25004	1.29370
O	4.27538	2.54612	-0.58720
H	4.97779	2.49687	0.08438
H	3.84630	3.44069	-0.51973
O	2.24372	2.11605	-2.23405
H	1.72465	2.93948	-2.03438
H	2.70555	2.23732	-3.08034
O	1.65807	-3.58121	0.58459
H	2.51203	-3.13946	0.32211
H	1.47372	-4.27946	-0.06731
O	0.83426	-3.50231	3.08242
H	0.62106	-3.08410	3.93609
H	1.73997	-3.85676	3.13150
O	-1.47439	3.21983	0.38157
H	-0.54646	3.57397	0.37177
H	-1.95023	3.67243	1.09976
O	-3.09197	2.04055	-1.36070
H	-4.02694	1.70502	-1.48850
H	-3.07498	2.99860	-1.52596
O	-7.35597	0.67826	0.15502
O	-5.77476	2.53147	0.47976
O	-7.41426	2.63265	-1.31787
O	-5.55688	1.03449	-1.45453
O	-5.50871	-3.92662	1.70414
O	-4.74450	-1.68073	1.12067
O	-3.50880	-3.01789	2.77120
O	-3.45530	-3.62575	0.39487

O	0.91249	4.50096	0.71459
O	3.03356	4.98656	-0.40773
O	1.02199	4.47978	-1.72931
O	1.21010	6.59718	-0.52563
O	5.87404	-3.57062	-1.56504
O	3.59111	-4.47142	-1.69579
O	4.08629	-2.63493	-0.17855
O	4.08687	-2.27330	-2.62406
O	2.31209	0.07990	3.94405
O	4.47576	0.70139	2.96927
O	3.75552	1.68978	5.08096
O	2.63319	2.32296	3.00411
O	0.38522	-2.07916	-2.73183
O	-0.48978	0.03032	-3.63532
O	-0.10086	-1.86707	-5.11993
O	-1.93518	-1.94629	-3.49460
Cl	-6.55772	1.71453	-0.53599
Cl	-4.32514	-3.07270	1.50448
Cl	1.54002	5.16105	-0.48477
Cl	-0.55604	-1.46939	-3.76762
Cl	4.43174	-3.26146	-1.53877
Cl	3.29399	1.20569	3.76431

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Al5r_ClO4.log Energy: -5155156.5555740

Al	-2.58673	1.13531	0.72987
O	-2.73780	-0.71072	0.40897
O	-1.48188	1.08601	2.27323
H	-2.67383	-1.43313	1.05234
H	-1.82689	1.04167	3.17371
O	-0.87136	1.45654	0.04683
H	-0.70398	1.96754	-0.76845
Al	-3.58278	-0.77599	-1.24711
O	-3.40771	1.05369	-0.98928
H	-3.95790	1.76704	-1.35547
Al	0.16711	1.57650	1.56470
Al	2.75309	0.51952	0.65317
O	1.06729	-0.11674	1.41361
O	3.55676	-1.15293	0.55734
H	1.10308	-0.73146	2.17478
H	3.91696	-1.62027	1.33325
O	1.77660	2.07520	0.77960
H	2.02686	2.87035	0.26784

Al	2.80222	-1.81458	-1.02267
O	2.42877	0.00421	-1.13639
H	1.67641	0.33499	-1.67103
O	0.97063	1.82836	3.37683
H	1.91893	1.55589	3.37244
H	0.56016	1.42005	4.15883
O	3.38105	0.67922	2.63300
H	3.55731	-0.19448	3.06852
H	4.20681	1.19609	2.69315
O	3.31812	-3.61313	-0.45723
H	3.04233	-4.38665	-0.98020
H	3.15186	-3.81336	0.49781
O	-5.46301	-0.73663	-0.69063
H	-5.91327	0.13363	-0.57047
H	-5.81827	-1.38120	-0.02884
O	-4.17185	1.05790	1.90201
H	-4.53426	0.18848	2.18751
H	-4.90710	1.70552	1.78694
O	-2.93122	3.08031	0.88246
H	-3.53623	3.50884	0.23769
H	-2.10482	3.60015	0.97873
O	4.35485	1.57015	0.30527
H	4.21126	2.51754	0.07532
H	5.05214	1.19242	-0.29813
O	4.45652	-1.69759	-2.03690
H	5.22749	-2.16887	-1.64537
H	4.80238	-0.77310	-2.08817
O	-4.41092	-0.77260	-3.03309
H	-5.36167	-0.59037	-3.12806
H	-3.93387	-0.38038	-3.78461
O	-0.31484	3.58232	1.75863
H	-0.43012	3.83593	2.69310
H	0.36027	4.21813	1.39875
O	-1.97578	-0.92489	-2.31482
H	-1.51148	-1.77584	-2.50416
H	-1.28097	-0.21747	-2.32886
O	-3.79632	-2.69863	-1.13410
H	-3.81920	-3.05064	-0.20928
H	-3.32943	-3.36944	-1.69110
O	2.10883	-2.47739	-2.68599
H	2.64229	-2.50890	-3.49698
H	1.16447	-2.72247	-2.86837
O	0.99694	-2.08517	-0.37005
H	0.71619	-1.40695	0.30240

H	0.47308	-2.91392	-0.30575
O	-5.47160	-3.79106	3.23243
O	-6.14977	-2.58148	1.22012
O	-3.78407	-3.10474	1.59464
O	-4.90107	-1.42939	2.99449
O	1.43962	-2.21633	3.33923
O	2.88662	-3.64275	4.69429
O	2.77028	-3.99562	2.28491
O	3.88033	-1.99997	3.16992
O	6.07043	0.43619	-1.44882
O	7.37697	0.06949	0.59288
O	6.99388	-1.78752	-0.96105
O	8.48451	0.04731	-1.59314
O	3.22122	4.10518	-0.31495
O	3.60516	4.95731	1.95762
O	3.57188	6.49980	0.05194
O	1.50059	5.44491	0.79021
O	0.21527	0.64306	-2.75154
O	-0.35902	2.97501	-2.27677
O	-0.96245	1.97741	-4.43165
O	1.38839	2.44745	-3.91109
O	-5.02954	3.38826	-0.93676
O	-6.79421	1.69331	-0.78934
O	-6.11270	2.93075	1.21788
O	-7.35454	4.05851	-0.55908
O	-2.35387	-4.67993	-2.37770
O	-0.16955	-5.61930	-2.94166
O	-0.50620	-3.18935	-2.93855
O	-0.47650	-4.43254	-0.81829
Cl	-6.34278	3.02866	-0.26528
Cl	7.26863	-0.31549	-0.83420
Cl	-0.86797	-4.51840	-2.26154
Cl	2.99467	5.27501	0.64361
Cl	0.07170	2.03883	-3.37335
Cl	-5.08925	-2.73522	2.27944
Cl	2.72824	-2.97791	3.38903

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Al6c_ClO4.log Energy: -4924468.9243127

Al	-2.04954	0.55794	2.20149
Al	-1.92993	1.59506	-0.49824
Al	0.26441	1.29529	-2.38444
Al	2.27762	-0.56871	-1.45150

Al	2.25636	-1.52906	1.30777
Al	0.11883	-1.07083	3.23147
O	-0.97324	0.22844	-1.34916
O	1.50444	-0.16647	2.34910
O	-1.31712	-1.16519	2.03180
O	-0.94960	1.55655	1.08091
O	1.75116	1.22507	-1.24028
O	1.11898	-1.36541	-0.20735
O	-3.04209	0.59353	0.63054
O	-0.75291	2.61417	-1.53790
O	1.16504	-0.24890	-2.97177
O	3.35363	-0.62241	0.10323
O	1.12140	-2.48140	2.48870
O	-0.91585	0.43995	3.70921
H	-1.45405	-0.52458	-1.74013
H	1.62275	0.79641	2.26693
H	-1.39522	-1.76985	1.27345
H	-0.11879	2.01778	1.29244
H	1.86815	1.70457	-0.40966
H	0.24541	-0.93492	-0.17762
H	-3.98990	0.36904	0.52769
H	-0.42741	3.51631	-1.32850
H	0.67450	-0.96511	-3.40310
H	4.30945	-0.44524	0.11414
H	0.68229	-3.27197	2.12654
H	-0.49545	1.26057	4.02723
O	3.90238	-0.23522	-2.53372
H	4.76809	-0.39797	-2.08764
H	3.94717	0.62626	-2.98358
O	3.79546	-1.69999	2.58492
H	4.67634	-1.84210	2.15906
H	3.65767	-2.46121	3.17656
O	1.23260	-0.96781	4.89511
H	0.82435	-0.63736	5.71501
H	2.05004	-0.45744	4.75300
O	-0.90099	-2.31625	4.42897
H	-1.66599	-2.71990	3.98154
H	-0.40226	-3.03934	4.84961
O	-3.60782	0.04023	3.26189
H	-3.39882	-0.22289	4.17492
H	-4.22342	-0.64943	2.87397
O	-2.67588	2.49242	2.77377
H	-3.37662	2.54890	3.44844
H	-1.90293	3.00742	3.10507

O	-2.96104	3.22243	0.03515
H	-2.60850	4.09573	-0.21212
H	-3.05135	3.20985	1.01680
O	2.89380	-3.31120	0.66614
H	2.15756	-3.90563	0.39273
H	3.58287	-3.30543	-0.03413
O	2.55403	-2.44441	-2.06242
H	1.73768	-2.99920	-1.97983
H	2.95311	-2.60123	-2.93524
O	-0.97634	1.32927	-3.93637
H	-1.81014	1.76482	-3.66882
H	-1.21972	0.44001	-4.30911
O	1.28214	2.55438	-3.50625
H	0.81413	2.83675	-4.31100
H	1.63507	3.37360	-3.06040
O	-3.25364	1.48334	-2.03375
H	-3.46701	0.56155	-2.32336
H	-4.08923	1.97490	-1.94217
O	-7.46960	-1.39117	1.65938
O	-5.10105	-1.84776	2.10240
O	-6.04573	-2.33849	-0.09206
O	-5.75150	-0.00699	0.61676
O	-1.38661	-3.06813	-0.22367
O	-1.39883	-5.44701	-0.75869
O	0.43720	-4.52438	0.56143
O	0.23500	-3.99367	-1.82718
O	-3.05733	-1.19133	-2.66570
O	-2.72991	-3.25826	-3.92856
O	-1.45000	-1.26477	-4.52229
O	-3.85724	-1.34787	-4.97468
O	5.37746	-3.15092	-0.80481
O	6.01370	-0.77293	-0.74606
O	6.24094	-2.14445	1.26046
O	7.73287	-2.51443	-0.63909
O	0.36647	6.15606	-3.17239
O	2.13587	4.76984	-2.19733
O	1.68450	6.98269	-1.27680
O	0.06775	5.18595	-0.94256
O	1.42332	2.66221	1.98730
O	-0.12887	3.16216	3.83447
O	2.27339	3.48687	4.12533
O	1.00170	4.98063	2.65037
Cl	6.35609	-2.16711	-0.23970
Cl	1.05716	5.79856	-1.90725

Cl	1.16004	3.60443	3.16172
Cl	-6.11495	-1.40521	1.05762
Cl	-2.79610	-1.78740	-4.04312
Cl	-0.54439	-4.25632	-0.56725

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Al7-1_ClO4.log Energy: -7329609.1060569

Al	0.20021	-0.08205	0.43462
Al	0.68539	-2.81756	-0.72938
Al	-2.17228	-1.92786	-0.13092
Al	-2.68088	0.80604	0.90353
Al	-0.35506	2.70232	1.46916
Al	2.49996	1.87648	0.78399
Al	3.03331	-0.98147	-0.21908
Al	-4.78250	-0.26271	-1.61032
O	-1.47719	-0.05417	-0.45446
O	1.91151	-0.06008	1.26779
O	1.17178	-0.87421	-1.01652
O	-0.27472	-1.91449	0.77431
O	-0.79603	0.79027	1.83012
O	0.64616	1.75489	-0.01634
O	-1.04392	-2.70872	-1.37161
O	-2.86754	-0.97788	1.29121
O	-2.00717	2.52345	0.66475
O	1.41315	2.67251	2.05439
O	3.39514	0.81121	-0.41300
O	2.36985	-2.68917	0.03142
O	-3.63979	-1.70912	-1.25959
O	-3.99015	0.92009	-0.41992
O	-3.60437	0.25702	-3.08137
O	-6.12272	-0.84010	-0.32165
O	-5.82564	-1.29697	-2.91810
O	-5.92932	1.23170	-2.13827
H	-1.47500	0.37793	-1.34308
H	1.98086	-0.28990	2.22632
H	1.06548	-0.51539	-1.94219
H	-0.18252	-2.27427	1.69929
H	-0.71013	0.51153	2.77593
H	0.43006	1.98093	-0.95733
H	-1.31177	-3.00137	-2.27087
H	-3.39743	-1.36950	2.02205
H	-2.54419	3.22112	0.23718
H	1.63358	2.65276	3.01136

H	3.99947	1.21860	-1.07993
H	2.95937	-3.47339	0.10070
H	-3.73490	-2.42067	-1.92897
H	-4.07534	1.85815	-0.70478
H	-3.76241	1.07980	-3.57625
H	-3.15339	-0.37953	-3.69237
H	-6.07217	-1.74945	0.04846
H	-6.24830	-0.28785	0.48567
H	-6.67311	-1.68059	-2.62715
H	-5.35768	-1.97850	-3.46038
H	-6.22323	1.94277	-1.51118
H	-6.61340	1.11144	-2.81960
O	-3.80420	1.36572	2.35760
H	-4.19207	2.26651	2.22312
H	-4.57554	0.76746	2.55135
O	-0.92174	3.20289	3.25054
H	-0.84366	2.52908	3.97139
H	-1.70235	3.76229	3.40977
O	3.95844	1.92541	2.02074
H	4.11606	2.70305	2.58359
H	4.84842	1.49764	1.82448
O	4.52208	-1.36702	0.90702
H	4.46289	-1.91728	1.70796
H	5.23180	-0.67545	1.07395
O	3.96380	-1.35415	-1.82466
H	4.16794	-0.67368	-2.51836
H	4.11933	-2.27634	-2.15938
O	1.31212	-3.38619	-2.44109
H	2.24219	-3.72575	-2.59363
H	0.78227	-3.45722	-3.25501
O	0.56445	-4.63276	-0.09362
H	0.02704	-5.26842	-0.59840
H	0.50723	-4.87921	0.87321
O	-2.76823	-3.58590	0.65762
H	-2.47246	-3.91208	1.55593
H	-2.86769	-4.36757	0.08576
O	2.97602	3.42539	-0.20192
H	2.67110	4.37007	-0.07237
H	3.55468	3.35260	-0.99601
O	-0.24065	4.52441	0.94855
H	-0.44975	4.87454	0.04438
H	0.59935	4.99777	1.15993
O	8.36455	0.15739	2.55963
O	6.59806	1.29451	3.82533

O	6.18880	0.59595	1.51338
O	6.38083	-1.08985	3.28382
O	1.29079	7.99887	-0.75470
O	2.37531	6.30470	-2.15797
O	0.10175	5.93286	-1.32864
O	2.00607	5.87510	0.22834
O	-6.51333	3.15723	-0.23352
O	-5.04850	3.79169	1.63294
O	-4.16310	3.66974	-0.65696
O	-5.70922	5.46418	-0.01629
O	-3.99770	-3.19793	-3.61887
O	-1.61578	-3.64576	-3.89122
O	-3.10202	-3.80510	-5.82336
O	-2.59483	-1.61237	-4.86161
O	3.89953	-3.93805	-2.59145
O	4.23815	-4.72740	-0.27930
O	5.94490	-5.13445	-1.98148
O	3.80287	-6.32717	-2.08348
O	-0.05463	-2.98071	3.25837
O	-0.29876	-4.83759	4.82687
O	-1.93460	-4.54464	3.04078
O	0.35246	-5.28727	2.51933
O	-0.31700	0.84566	4.51018
O	1.76843	-0.37718	4.08091
O	1.83576	1.99560	4.73245
O	1.19301	0.28568	6.36039
O	-4.49814	-1.87542	3.32947
O	-6.81092	-1.80828	4.12072
O	-6.32645	-2.58486	1.84795
O	-6.04606	-0.21869	2.40536
O	4.23431	0.68386	-3.62209
O	4.46957	3.00641	-4.32807
O	6.45679	1.71943	-3.69562
O	4.86036	2.40225	-1.98165
O	0.76645	0.02921	-3.55286
O	-0.62386	1.67766	-2.38257
O	-1.11804	1.08865	-4.70463
O	0.88189	2.40014	-4.17155
Cl	4.49516	-5.07493	-1.71988
Cl	-0.48148	-4.41913	3.42942
Cl	6.91855	0.22696	2.84975
Cl	1.14483	0.67948	4.94523
Cl	-5.93642	-1.64928	2.94796
Cl	1.44315	6.55885	-1.03945

Cl	-0.01609	1.30997	-3.74333
Cl	-5.37598	4.04690	0.19051
Cl	5.02098	1.96144	-3.44240
Cl	-2.82197	-3.06841	-4.58391

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Al7_ClO4.log Energy: -6508842.3447122

Al	-0.24006	-0.02162	-0.25723
Al	-2.95878	-1.19383	-0.92368
Al	-2.37069	1.73985	-1.55172
Al	0.29752	2.93235	-0.71904
Al	2.42926	1.17102	0.55288
Al	1.85563	-1.74622	1.07442
Al	-0.76199	-2.97308	0.17351
O	-0.38857	1.24617	-1.70189
O	-0.13288	-1.31491	1.15747
O	-0.95834	-1.52124	-1.22438
O	-2.09605	0.41974	-0.01218
O	0.39581	1.49893	0.69423
O	1.62166	-0.40353	-0.44497
O	-3.06409	0.15005	-2.18361
O	-1.53109	3.14605	-0.74220
O	2.07287	2.46776	-0.70098
O	2.42236	-0.16874	1.80945
O	1.07130	-3.11530	0.09240
O	-2.54433	-2.48536	0.32854
H	-0.07893	1.02519	-2.60661
H	-0.62304	-1.15017	2.00752
H	-0.69511	-1.67974	-2.16953
H	-2.38172	0.79749	0.86000
H	0.00638	1.78629	1.56644
H	2.01423	-0.70620	-1.31077
H	-3.24462	-0.04589	-3.12509
H	-1.96088	3.99872	-0.46708
H	2.72296	2.91267	-1.29529
H	2.79953	-0.02907	2.71164
H	1.58465	-3.55898	-0.61417
H	-3.22448	-3.12628	0.64299
O	0.37625	4.35929	0.57723
H	1.18512	4.87981	0.72746
H	-0.04451	4.15229	1.45538
O	2.86756	2.41795	1.97229
H	3.01599	2.07630	2.89015

H	3.47457	3.16299	1.81440
O	1.78803	-2.65583	2.77706
H	2.39693	-3.41177	2.87439
H	1.85395	-2.11697	3.61581
O	-0.94938	-4.00620	1.77131
H	-1.62440	-3.70483	2.44506
H	-0.15898	-4.33509	2.23497
O	-1.02187	-4.48972	-0.95283
H	-0.65042	-4.60783	-1.84451
H	-1.81322	-5.09923	-0.85117
O	-3.61820	-2.40469	-2.23237
H	-4.06096	-3.28078	-2.04618
H	-3.42578	-2.30386	-3.18867
O	-4.60153	-0.93944	0.02029
H	-5.28215	-0.28981	-0.22955
H	-4.52577	-0.97258	1.00984
O	-4.10279	2.33509	-1.06003
H	-4.32438	3.20460	-0.58493
H	-4.82971	2.13475	-1.67590
O	3.56419	-2.40466	0.65316
H	4.42561	-2.12914	1.08645
H	3.71630	-2.85700	-0.21799
O	4.15342	0.91285	-0.15221
H	4.40290	1.24536	-1.05067
H	4.98111	0.72723	0.38931
O	-2.44584	2.43486	-3.35381
H	-1.97863	1.92532	-4.06033
H	-2.40942	3.38516	-3.56339
O	0.62847	3.98782	-2.27877
H	0.12782	4.79155	-2.50309
H	1.54590	4.04148	-2.66288
O	4.87360	3.47791	-4.52571
O	3.30841	3.79272	-2.66787
O	2.94886	1.97783	-4.28638
O	4.81501	1.86563	-2.69446
O	-0.85111	0.53409	-4.47383
O	-0.50714	-1.82567	-3.92827
O	-2.72998	-1.04662	-4.62615
O	-0.89782	-1.15937	-6.24758
O	3.17149	-3.55442	-1.70229
O	2.75876	-3.42401	-4.10445
O	4.79991	-2.45294	-3.15330
O	2.63473	-1.38608	-2.76543
O	-2.55155	5.54887	-0.06100

O	-4.36446	6.19926	-1.57270
O	-4.77442	4.53460	0.18313
O	-4.42368	6.86867	0.78472
O	-0.64732	2.96164	2.65390
O	-2.86537	2.06974	2.05063
O	-2.67495	4.22217	3.18785
O	-2.16532	2.15516	4.39644
O	3.30694	0.71762	4.15447
O	1.07573	0.94844	5.16340
O	3.02868	0.48889	6.57383
O	2.17495	-1.24443	5.08865
O	-2.98448	-3.07028	3.25093
O	-3.41945	-1.44601	5.02688
O	-4.03954	-0.91356	2.73782
O	-1.66530	-1.00046	3.39938
O	7.15291	-1.39578	0.01260
O	8.02982	-0.93476	2.26026
O	5.76800	-1.79938	1.99151
O	6.30811	0.50312	1.31251
O	-3.12788	-6.09976	-0.61672
O	-4.38960	-4.51355	0.77202
O	-4.88216	-4.70523	-1.62771
O	-5.47534	-6.51991	-0.10755
Cl	6.84364	-0.91882	1.38068
Cl	2.36934	0.24141	5.27825
Cl	-4.03623	5.81787	-0.17843
Cl	-1.23828	-0.88650	-4.84668
Cl	3.99399	2.75835	-3.58595
Cl	3.35531	-2.70112	-2.96418
Cl	-2.12312	2.85575	3.09894
Cl	-3.03257	-1.60216	3.61438
Cl	-4.48422	-5.46954	-0.38670

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Al8_ClO4.log Energy: -7521503.7293985

Al	0.69864	1.68085	-0.06640
Al	-0.64777	-1.12819	0.23546
Al	-2.22829	1.28557	-0.41311
Al	2.28516	-0.76963	0.56084
Al	-1.28406	4.37828	0.75559
Al	-3.87185	-1.16740	1.32407
Al	1.20181	-3.75609	-0.84013
Al	3.98820	1.78757	-1.00158

O	-0.82694	0.77553	0.84278
O	0.90368	-0.15069	-0.67311
O	-0.69112	2.04171	-1.36136
O	-1.81971	-0.41713	-1.05331
O	0.75789	-1.42193	1.41884
O	1.90800	1.05843	1.28494
O	2.16506	2.25582	-1.10922
O	0.27864	3.33708	0.72939
O	-2.09455	-1.73694	1.29795
O	-0.33703	-2.73091	-0.63248
O	-2.43569	2.95561	0.45266
O	-3.56610	0.56023	0.70824
O	2.41744	-2.40191	-0.43708
O	3.67966	0.05141	-0.39588
O	-3.51437	1.69786	-1.80363
O	3.47758	-1.30919	1.94294
O	-5.76482	-0.63411	1.56501
O	-4.38395	-1.89691	-0.38321
O	-3.68871	-0.57083	3.21232
O	-4.49976	-2.85008	2.10970
O	1.24750	-4.49406	0.92860
O	1.14540	-3.41340	-2.80513
O	0.14889	-5.36280	-1.28720
O	2.78413	-4.91445	-1.27218
O	4.12278	1.27229	-2.86704
O	4.02429	2.54518	0.78446
O	5.91686	1.39200	-0.90883
O	4.60908	3.53632	-1.62027
O	-1.22890	4.30523	2.70427
O	-1.13466	4.68626	-1.16526
O	-0.29585	6.03854	0.92399
O	-2.86486	5.53547	0.86640
H	-0.96849	0.84684	1.81276
H	0.95844	-0.27694	-1.64294
H	-0.48113	1.61464	-2.21584
H	-1.90214	-0.73510	-1.96734
H	0.66035	-1.68890	2.35314
H	1.54421	1.09290	2.18809
H	2.01260	3.12518	-1.53597
H	1.06832	3.82474	1.01128
H	-2.01468	-2.71161	1.40630
H	-1.09631	-2.95499	-1.21960
H	-3.38041	3.21098	0.49174
H	-3.81181	1.20732	1.40143

H	3.18056	-2.42202	-1.04568
H	4.41990	-0.56279	-0.59130
H	-3.24740	1.58287	-2.74011
H	-4.37358	1.19187	-1.71132
H	3.28824	-2.12076	2.48339
H	4.20550	-0.77574	2.34747
H	-6.13400	0.24543	1.31638
H	-6.47385	-1.29828	1.55563
H	-4.92957	-1.26288	-0.92428
H	-3.72510	-2.30951	-0.99954
H	-2.78126	-0.28331	3.49218
H	-4.31401	0.11584	3.51181
H	-3.99076	-3.64880	1.78088
H	-4.43015	-2.85241	3.08163
H	1.73808	-4.10159	1.69088
H	0.46793	-5.01842	1.26146
H	0.27625	-3.61130	-3.23407
H	1.49720	-2.59476	-3.22743
H	-0.37373	-5.74151	-0.53346
H	-0.47262	-5.26884	-2.06338
H	2.52368	-5.74472	-1.70892
H	3.47324	-4.49273	-1.83328
H	3.29787	1.24014	-3.41709
H	4.64206	0.45564	-3.07124
H	4.83589	2.45064	1.34398
H	3.27641	2.07102	1.24905
H	6.50831	2.14161	-1.09405
H	6.30485	0.87565	-0.15203
H	4.24158	4.37852	-1.23160
H	4.70094	3.65776	-2.58124
H	-0.61090	3.62369	3.08189
H	-2.04843	4.24846	3.22798
H	-1.92382	5.03698	-1.61533
H	-0.94383	3.78402	-1.54872
H	0.31467	6.34105	0.19371
H	0.06280	6.32016	1.78292
H	-2.78121	6.46292	1.14622
H	-3.77137	5.20795	1.07393
O	-2.55405	-2.87970	-2.22732
O	-3.47729	-5.17309	-2.54586
O	-1.24236	-4.58844	-3.44319
O	-3.03277	0.41282	-4.38134
O	-7.45259	-1.19300	-2.70657
O	2.01606	-1.21412	-4.31388

O	-5.69092	0.11477	-1.63020
O	0.33480	-0.13883	-5.75474
O	-7.20365	1.19285	-3.21935
O	-5.54276	-0.41827	-4.02613
O	0.19805	0.07185	-3.31991
O	1.98236	1.21564	-4.56842
O	5.45660	0.05467	3.26217
O	6.84122	0.00086	1.23991
O	6.29884	2.14627	2.29477
O	2.63924	-3.56413	3.12664
O	1.39177	-4.64522	4.93354
O	2.69937	-2.62020	5.38026
O	-2.68515	-4.48215	1.11352
O	-1.82157	-5.34030	3.27990
O	-0.82401	-6.12196	1.15452
O	-2.40004	-0.57220	-4.05036
O	0.63995	-2.48426	4.06067
O	7.83282	0.59864	3.39826
O	0.30678	2.27343	3.77978
O	-1.14413	0.33451	3.57260
O	-1.86877	2.27269	4.90119
O	-0.06863	0.81925	5.72393
O	-4.63322	2.25586	2.70305
O	-5.07795	3.87794	0.92214
O	-6.46585	3.87169	2.94556
O	-6.64236	2.04519	1.31823
O	5.71141	-1.76261	-1.12028
O	6.60688	-3.19250	-2.89656
O	4.18099	-2.92440	-2.62961
O	5.54132	-1.07145	-3.46974
O	3.39729	5.77505	-0.72116
O	1.76683	4.87318	-2.30523
O	1.27792	6.94984	-1.06173
O	2.93933	6.95007	-2.83172
Cl	-5.73053	3.01953	1.99804
Cl	-6.50361	-0.08062	-2.93829
Cl	-2.15767	-5.74178	1.87243
Cl	-2.70583	-4.08071	-3.22344
Cl	-0.70060	1.43030	4.54303
Cl	6.62268	0.69840	2.56215
Cl	2.34661	6.14088	-1.74812
Cl	1.12855	-0.02105	-4.51880
Cl	5.53618	-2.24657	-2.53560
Cl	1.82680	-3.33004	4.41983