

AN ABSTRACT OF THE THESIS OF

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Title: A Model for the Prediction of Biologically Mediated Reductive Dechlorination Pathways.

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The environment has been exposed to a number of hazardous chlorinated organic compounds. These compounds may be anaerobically biotransformed by sequential reductive dechlorination reactions in which the chlorine atoms are replaced with hydrogen atoms. Because reductive dechlorination processes may occur very slowly in the environment and chlorine position affects the fate and toxicity of the compound in the environment, it is desirable to develop a model to predict the products of these reactions.

This project was designed to examine the reductive dechlorination pathways of various chlorinated aromatic compounds in relation to additional substituents on the ring and to develop an empirical model to predict these pathways. The model is based on the structural properties of the compound. Molecular structures and properties such as net atomic charges were calculated using the published semi-empirical MNDO (Modified Neglect of Differential Overlap) method, Versions 4.01 and 5.01 at the Cornell National Supercomputer Facility.

Net carbon-chlorine bond charges are compared for chlorinated positions on the ring or aliphatic chain. These data provide a means for correlating charge with the position of dechlorination. The pathways predicted from this model agreed well with experimentally determined pathways for several classes of chlorinated organic compounds including: phenols, dihydroxybenzenes, benzoic acids, and anilines.

**A Model for the Prediction
of Biologically Mediated
Reductive Dechlorination Pathways**

by

Cynthia L. Cozza

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TABLE OF CONTENTS

INTRODUCTION	1
Background on Chlorinated Organic Compounds	1
Objectives	2
Reductive Dechlorination	3
COMPUTATIONAL METHOD	7
MODEL DEVELOPMENT	9
RESULTS AND DISCUSSION	11
Chlorophenols	11
Chlorobenzoic Acids	22
Chlorinated Methoxy and Dihydroxybenzenes	30
Chloroanilines	40
Chlorinated Aliphatic Compounds	44
CONCLUSIONS	46
BIBLIOGRAPHY	47
APPENDICES	54
Appendix A: Accessing the Cornell Supercomputing Facility	54
Appendix B: Output Files	56

LIST OF FIGURES

FIGURE	PAGE
1. Pentachlorophenol Molecule.	16
2. Summary of Predicted Chlorophenol Dechlorination Pathways.	21
3. Summary of Predicted Chlorobenzoic Acid Dechlorination Pathways.	28
4. Degradation of Tetrachloroveratrole.	33
5a. Summary of Predicted Chlorocatechol Dechlorination Pathways.	37
5b. Summary of Predicted Chlororesorcinol Dechlorination Pathways.	38
5c. Summary of Predicted Chlorohydroquinone Dechlorination Pathways.	39

LIST OF TABLES

TABLE	PAGE
1. Chlorinated Compounds and Contaminated Environments.	12
2. Summary of Dechlorination Pathways for Chlorophenols.	14
3. Pentachlorophenol Atomic Charge Pattern.	16
4. Summary of Atomic and Bond Charges for Chlorophenols.	18
5. Summary of Dechlorination Pathways for Chlorobenzoic Acids.	23
6. Summary of Atomic and Bond Charges for Chlorobenzoic Acids.	25
7. Summary of Dechlorination Pathways for Chlorinated Dihydroxybenzenes.	31
8. Summary of Atomic and Bond Charges for Chlorinated Dihydroxybenzenes.	35
9. Summary of Dechlorination Pathways for Chloroanilines.	41
10. Summary of Atomic and Bond Charges for Chloroanilines.	43
11. Summary of Atomic and Bond Charges for Chlorinated Aliphatic Compounds.	45

A Model for the Prediction of Biologically Mediated Reductive Dechlorination Pathways

INTRODUCTION

Background on Chlorinated Organic Compounds

Chlorinated organic compounds such as chlorophenols, chlorobenzoic acids, chloroanilines, polychlorinated biphenyls, and chlorinated dihydroxy, methoxy, and acetylated compounds are used in the manufacture of a variety of products including pesticides, herbicides, wood preservatives, bleaching agents, coolant fluids, solvents, insulating materials, explosives, and pharmaceuticals (Fathepure et al., 1988; Klecka and Gonsior, 1984; Ghosal et al., 1985; Krumme and Boyd, 1988; Moza, et al., 1988; Burttschell, 1959; Quensen et al., 1988). These compounds are released into the environment directly as municipal or industrial effluents or by accidental spillage. Additionally, some chlorinated compounds may form during the chlorination of surface or waste waters, or be produced by the degradation of other more complex chlorinated compounds. Environments which have been exposed to these chlorinated compounds include soils, sediments, surface and groundwaters, and municipal and industrial wastes (Choudhry, 1985).

The presence of chlorinated organic compounds in the environment is of concern because of the potential for surface and groundwater contamination. Some of these compounds have relatively high water solubilities, high mobilities in soil, tend to resist traditional treatment methods, and accumulate in the environment. In addition, many of the chlorinated aromatic and aliphatic compounds are toxic.

To evaluate the potential hazards of these chlorinated organic compounds, it is important to understand their toxicity and fate in the environment. The toxicity of these chlorinated aromatic compounds varies considerably with the position and number of chlorine atoms present on the ring. For example, the ortho and para monochlorophenol isomers are more toxic than the meta isomer (Windholz, 1983). Pentachlorophenol is more toxic than lesser chlorinated congeners. The physical-chemical properties of these compounds also vary with the position and degree of chlorination (Windholz, 1983). Degradation of these chlorinated compounds often produces other chlorinated compounds which may be as or more hazardous than the original contaminant.

Conversion of one type of chlorinated organic compound to another in the environment is believed to occur. Chlorophenols and chlorobenzoic acids are thought to be precursors of chlorinated dibenzo-p-dioxins (Mikesell and Boyd 1985; and Ahonkhai et al., 1988). Understanding the fate of these compounds in the environment is critical for the implementation of remediation or treatment processes which would produce lesser chlorinated, less toxic compounds. Reductive dechlorination reactions of chlorinated organic compounds is one such process.

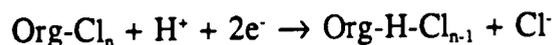
Objectives

Because reductive dechlorination reactions may occur very slowly in the environment, it is desirable to predict the products of reductive dechlorination. The goals of this research were to develop an empirical model to relate the reductive dechlorination pathways to characteristics of the compounds that can be

calculated from first principles, to compare the predicted pathways with experimental pathways published in the literature, and to make predictions for compounds whose pathways have not been determined.

Reductive Dechlorination

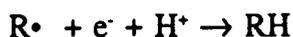
The reductive dechlorination of chlorinated aromatic and aliphatic compounds has been reported in the literature. Reductive dechlorination is important because the dechlorinated products are typically less hazardous and more susceptible to further degradation by aerobic processes. Reductive dechlorination involves the removal of a chlorine from the aromatic ring or aliphatic chain and its replacement with hydrogen. The half reaction for the reductive dechlorination of chlorinated organic compounds has been proposed as follows:



Although biological reductive dechlorination is the initial degradative reaction for most of the chlorinated aromatic and aliphatic compounds under anaerobic conditions (McCarty et al., 1981; DeWeerd et al., 1986; Fathepure et al., 1988; Boyd and Shelton, 1984; Kobayashi and Rittmann, 1982; and Suflita et al., 1982), other reactions may sometimes precede dechlorination. Demethylation has been reported for a number chlorinated compounds under anaerobic conditions (Woods et al., 1989; Gibson and Suflita, 1986; Mikesell and Boyd, 1985; Wise, 1988; DeWeerd et al., 1986; and Boyd et al., 1983). *m*-Hydroxybenzoate and catechol (1,2-dihydroxybenzene) were observed as the metabolites of *m*-anisate (*m*-methoxybenzoic acid) and guaiacol (*o*-methoxyphenol) demethylation (Wise,

1988). Similarly, 2,4-D and 2,4,5-T were converted to their respective chlorophenols (Gibson and Suflita, 1985; and Mikesell and Boyd, 1985). The phenols were then reductively dechlorinated.

The mechanisms of reductive dechlorination are still not clear, however a two step mechanism has been proposed (Macalady et al., 1986) for the reductive dechlorination of chlorinated organic compounds:



Reduced organic substrates are believed to be the source of electrons. Inorganic iron or iron porphyrins are presumed to be the mediator in the electron transfer.

Several groups have proposed mechanisms for abiotic reductive dechlorination reactions. These reactions are catalyzed by reduced iron porphyrins or Fe^{2+} (Klecka and Gonsior, 1984; Esaac and Matsumura, 1980; and Macalady et al., 1986), however they differ in the types of complexes formed and the substance which quenches the reaction. A free radical mechanism coupling redox cycles of organic matter and iron porphyrin mediated dechlorination for anoxic conditions also has been proposed (Glass, 1972). Ferric ions capture electrons from reduced organic compounds in the media yielding ferrous ions. An electron is then transferred to the organic chloride which dissociates into an organic radical and chloride ion. The radical is then quenched by a second electron and abstracts a proton from a donor in the environment (Glass, 1972). The abstraction of a hydrogen atom instead of a proton and electron by the radical intermediate has also been proposed (Ahr et al., 1982). Wade and Castro (1973) proposed a mechanism similar to that of Glass (1972) which included the formation of a

complex between the iron (II) porphyrin and the organic halide prior to dissociation of the chlorinated complex into an organic free radical and iron porphyrin chloride.

Photolysis has been explored as a possible method for degrading chlorinated organic compounds. Dechlorination by direct irradiation presents two disadvantages: low quantum yields and undesirable side reactions (Epling and Florio, 1988). Both of these might produce compounds which are more toxic than the parent compound.

Recent evidence shows that photodechlorination of chlorinated aromatic compounds by sodium borohydride (NaBH_4) may proceed via a radical chain mechanism or a pathway not involving a radical chain reaction. Photodechlorination of chlorobenzene by NaBH_4 via a radical mechanism was reported by Barltrop and Bradbury (1973). The reaction was quenched in the presence of acrylonitrile which is a free radical scavenger.

Photoreduction of chlorotoluenes, chlorobenzenes, and polychlorinated biphenyls is enhanced by the presence of NaBH_4 (Epling and Florio, 1986a,b; and Epling and Florio, 1988a). These reactions were not inhibited when exposed to acrylonitrile or other radical scavengers which suggests that a non-radical mechanism was occurring. The transfer of electrons from BH_4^- to the excited chlorinated organic or direct attack of the aryl chloride by BH_4^- (hydride transfer) were proposed as non-radical mechanisms (Epling and Florio, 1986a,b; and Epling and Florio, 1988a,b). A similar pathway involving a hydride-proton-transfer to the aryl chloride has also been proposed (Tsujimoto et al., 1975).

Excited anionic sensitizers have also been used in photoreduction reactions

instead of irradiating the aryl chloride (Soumillion et al., 1989; and Chaudhary et al., 1985). Naphthol is photolyzed forming the excited naphthoxide ion used as the electron donor (Soumillion et al., 1989). This mechanism is valuable because the chlorinated compounds can be completely reduced and the electron donor is regenerated. Another process involves the formation of an excited complex (exciplex) between the excited donor and the chlorinated compound prior to the transfer of electrons (Chaudhary et al., 1985). This process is also advantageous since the donor is regenerated.

COMPUTATIONAL METHOD

Semiempirical methods are used in many quantum mechanical calculations for molecules of biochemical concern. The MNDO (Modified Neglect of Differential Overlap) method (Dewar, 1977) has recently become one of the methods of choice as a result of its success in providing reasonable enthalpies and geometries for many molecules (Goldblum, 1987). MNDO is commonly used for determining electronic structure, chemical properties, and reactivity of molecular systems.

All semiempirical computations reported here were done using the standard MNDO method. These calculations were performed with MOPAC versions 4.01 and 5.01 on the IBM supercomputer at the Cornell National Supercomputing Facility. The starting coordinates were obtained from PC Model, a program for molecular modeling. Full optimization of all geometrical variables including bond length, bond angle, and dihedral angle was chosen for each structure. The MOPAC program performs geometry optimizations on the starting molecular geometry with the BFGS (Broyden-Fletcher-Goldfarb-Shanno) optimizer.

Certain criteria control the precision of the calculations and termination of the execution. Self consistence is achieved when the change in energy is less than 0.00001 kcal/mole on successive iterations. The heats of formation must differ by less than 0.002 kcal/mole on successive cycles. The gradient norm should be less than 10 kcal/angstrom and the projected changes in geometry and energy must be less than 0.0001 angstroms and 0.001 kcal/mole respectively. When all of the above tests are passed, execution of the program will terminate. If more strict

criteria are desired the "PRECISE" option will increase the thresholds by a factor of 100.

MODEL DEVELOPMENT

Net atomic charges were correlated with observed positions of dechlorination in reductive dechlorination reactions. This correlation was examined for reductive dechlorination pathways for unacclimated bacteria. Bacteria acclimated to specific compounds give significantly different dechlorination patterns than fresh sludge (Boyd, et.al., 1984).

In abiotic organic reactions in solution, substituents on the aromatic ring direct reactions or second substitutions to occur at specific positions on the ring. These substituents are divided into two groups: ortho-para directors and meta directors. In the case of a phenol, the hydroxyl group directs the electrophilic substitution reaction to take place at either the ortho or para position. Carboxylic acid groups are meta directors. o,p-Directors such as -OH and -NH₂ typically have atoms with unshared pairs of electrons attached directly to the aromatic ring. Meta directors such as -COOH do not contain any unshared electron pairs on the atom attached directly to the ring. Delocalization of electrons from the o,p-directing group on to the ring forms resonance structures making the ring more susceptible to electrophilic attack at these positions (Morrison and Boyd, 1981; and Loudon, 1984). Although biological processes are often driven by different mechanisms than abiotic organic reactions in solution, the characteristics of a molecule that direct electrophilic substitutions to occur at a specific location may also make that position more vulnerable to biological processes.

Whereas the mechanism for biological reductive dechlorination reactions is still unknown, a very good correlation of experimental pathways with electrophilic

substitution reactions exists. Chlorophenols are preferentially dechlorinated at the ortho position. Similarly, chlorobenzoic acids are reductively dechlorinated at the meta position. A link between the reductive dechlorination pathway and a mechanism still needs to be established.

Because reductive dechlorination processes may occur very slowly in the environment, it is desirable to develop a model to predict the products of these reactions. An empirical model is proposed correlating the atomic charges of the compounds with the positions of dechlorination.

The net atomic charges for the parent compounds of interest obtained from the MNDO program were examined using two methods. In the first, a comparison of chlorine charges at each position on the aromatic ring or aliphatic chain is made. In Model 1, the chlorine atom with the most negative charge is correlated with the position of dechlorination. In the second model, the charge of the carbon atom as well as that of the chlorine atom is taken into account. The sum of the carbon and chlorine charges was calculated for all carbon-chlorine bonds. The net charges for the bonds were then compared for all chlorinated positions. Both models were tested to evaluate the model's accuracy in predicting reductive dechlorination reactions.

RESULTS AND DISCUSSION

Reductive dechlorination pathways of several chlorinated aromatic and aliphatic compounds were examined. The results are divided into five sections: chlorophenols; chlorobenzoic acids; chlorinated methoxy and dihydroxybenzenes; chloroanilines; and chlorinated aliphatic compounds. Reductive dechlorination for the above compounds has been shown to occur in a number of anaerobic environments including municipal sewage sludge, sediments, and groundwater aquifers (Table 1). Observed and predicted pathways are discussed in each section.

Chlorophenols

Chlorophenols are preferentially dechlorinated by unacclimated microbial consortia at the positions adjacent (ortho) to the hydroxyl group. The dechlorination of pentachlorophenol (PCP) yields 2,3,4,5-tetrachlorophenol (Murthy et al., 1979; Mikesell and Boyd, 1985; and Woods et al., 1989), which is further dechlorinated to yield 3,4,5-TCP. Similarly, dechlorination of 2,4,6-TCP at the ortho positions yielded 2,4-dichlorophenol and 4-chlorophenol (Mikesell and Boyd, 1985; and Woods et al., 1989). Removal of chlorine atoms at the ortho position was also observed for the 2,3-, 2,4-, 2,5-, and 2,6-dichlorophenol isomers (Boyd and Shelton, 1984; Suflita and Miller, 1985; Gibson and Suflita, 1986; and Woods et al., 1989).

Reductive dechlorination also has been observed for compounds without an

TABLE 1. Chlorinated compounds and contaminated environments.

<u>Compound</u>	<u>Environment</u>	<u>Reference</u>
Chlorophenols	Sewage sludge	Horowitz et al., 1982 Boyd et al., 1983 Boyd and Shelton 1984 Mikesell and Boyd, 1985 Gibson and Suflita, 1986 Woods et al., 1989
	Sediments	Horowitz et al. 1982 Murthy et al., 1979
	Aquifers	Suflita and Miller, 1985 Suflita et al., 1988
Chlorobenzoic acids	Sewage sludge	Horowitz et al., 1982
	Aquifer	Suflita et al., 1988
	Sediments	Horowitz et al., 1982 Suflita et al., 1982 Horowitz et al., 1983 Gibson and Suflita, 1986
Chloroanilines	Aquifers	Kuhn and Suflita, 1989
Chlorinated dihydroxybenzenes	Sewage sludge	Woods et al., 1989 Boyd et al., 1983
2,4-D & 2,4,5-T	Sewage sludge	Mikesell and Boyd, 1985 Gibson and Suflita, 1986
	Aquifer	Suflita et al., 1984
	Sediment	Suflita et al., 1984
Chloroaliphatic compounds	Aquifers	Suflita et al., 1988 Bouwer et al., 1988 McCarty et al., 1981

ortho chlorine. Removal of the para chlorine from 3,4,5-trichlorophenol yielded 3,5-dichlorophenol (Mikesell and Boyd, 1985). 4-Chlorophenol was detected for the degradation of 3,4-dichlorophenol by unacclimated bacteria (Mikesell and Boyd, 1985). Experimental dechlorination pathways for chlorophenols are summarized in Table 2.

Dechlorination pathways were predicted for all chlorophenol congeners. Both models described earlier are applied to compounds for which dechlorination pathways are known and results are compared. Predictions are then made for the remaining compounds whose pathways have not been determined experimentally.

The charge pattern for pentachlorophenol (PCP) is presented in Table 3 and corresponds with position numbering shown in Figure 1. Examination of the charges of the chlorine atoms indicates that the most negative value (-0.0602) occurs at a position ortho to the hydroxyl group. Although pentachlorophenol appears to be symmetrical, the hydrogen atom of the hydroxyl group is bent out of the plane of the benzene ring and toward one of the chlorine atoms yielding different charges for the two ortho chlorines. Consideration of the net carbon-chlorine charge also shows the most negative value (-0.1142) at a position ortho to the hydroxyl group. It is suggested that this position will be preferentially dechlorinated to yield 2,3,4,5-tetrachlorophenol which is consistent with the observed degradation pathway (Table 2).

The net atomic charges for the remaining chlorophenol congeners with chlorine atoms in the positions adjacent to the hydroxyl group are presented in Table 4. Comparison of the chlorine and net carbon-chlorine charges indicates that for each of these compounds, the most negative charge occurs at an ortho

TABLE 2. Summary of Dechlorination Pathways for Chlorophenols

PARENT COMPOUND	PREDICTED METABOLITE		EXPERIMENTAL METABOLITE	REFERENCE
	MODEL 1¹	MODEL 2²		
PCP ³	2345-TeCP	2345-TeCP	2345-TeCP	Murthy et al., 1979 Mikesell and Boyd, 1985 Woods et al., 1989
2345-TeCP	345-TCP	345-TCP	345-TCP	Woods et al., 1989
345-TCP	34-DCP	35-DCP	35-DCP	Mikesell and Boyd, 1985
34-DCP	3/4-CP	3-CP	3-CP	Mikesell and Boyd, 1985
35-DCP	3-CP	3-CP	3-CP	Woods et al., 1989 Mikesell and Boyd, 1986
2356-TeCP	235-TCP	235-TCP	236-TCP	Murthy et al., 1979
2346-TeCP	234-TCP	234-TCP	ND ⁴	
246-TCP	24-DCP	24-DCP	24-DCP	Woods et al., 1989 Mikesell and Boyd, 1985
24-DCP	4-CP	4-CP	4-CP	Suflita and Miller, 1985 Boyd and Shelton, 1984 Woods et al., 1989 Gibson and Suflita, 1986
23-DCP	3-CP	3-CP	3-CP	Boyd and Shelton, 1984 Woods et al., 1989

TABLE 2. Continued

26-DCP	2-CP	2-CP	2-CP	Woods et al., 1989 Boyd and Shelton, 1984
25-DCP	3-CP	3-CP	3-CP	Suflita and Miller, 1985 Boyd and Shelton, 1984 Gibson and Suflita, 1986
245-TCP	34-DCP	34-DCP	34-DCP	Mikesell and Boyd, 1985
234-TCP	34-DCP	34-DCP	ND	
235-TCP	35-DCP	35-DCP	ND	
236-TCP	23-DCP	23-DCP	ND	
245-T ⁵ → 245-TCP	34-DCP	34-DCP	34-DCP	Mikesell and Boyd, 1985 Gibson and Suflita, 1985
24-D ⁶ → 24-DCP	4-CP	4-CP	4-CP	Mikesell and Boyd, 1985 Gibson and Suflita, 1985

¹ Model 1: Comparison of Chlorine Charge Densities

² Model 2: Comparison of Carbon-Chlorine Net Charge Densities

³ CP: Chlorophenol

⁴ ND: Not Determined

⁵ 245-T: 2,4,5-Trichlorophenoxyacetic acid converted to 2,4,5-TCP

⁶ 24-D: 2,4-Dichlorophenoxyacetic acid converted to 2,4-DCP

FIGURE 1. Pentachlorophenol Molecule

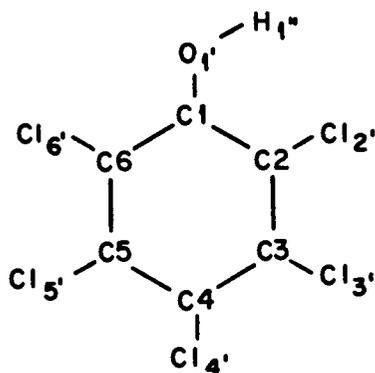


TABLE 3. Pentachlorophenol atomic charge pattern.

Carbon (Cn')	Carbon Charge	Atom (An')	Atom Charge	Atoms Cn-An'	Net Charge ²	Rank ³
C1	0.1795	O-1'	-0.2140	1-1'	-0.0345	
C2	-0.0266	Cl-2'	-0.0334	2-2'	-0.0600	2
C3	0.0670	Cl-3'	-0.0323	3-3'	0.0347	5
C4	-0.0224	Cl-4'	-0.0373	4-4'	-0.0597	3
C5	0.0765	Cl-5'	-0.0330	5-5'	0.0435	4
C6	-0.0840	Cl-6'	-0.0602	6-6'	-0.1442	1
		H-1"	0.2203	1'-1"	0.0063	

¹ "n" is the position on the ring beginning with the hydroxyl group

² Sum of the carbon and atom charges at each position

³ Preference for dechlorination (1-most favorable)

position. In all cases, both models suggested the removal of an ortho chlorine. These predicted removal patterns are supported by observed pathways (Table 2).

Reductive dechlorination pathways for compounds which do not contain an ortho chlorine were also determined (Table 4). The observed pathway for 3,4,5-trichlorophenol by organisms acclimated to a suite of chlorophenols (Woods et al., 1988) and unacclimated bacteria (Mikesell and Boyd, 1985) involves dechlorination at the meta and para positions, respectively. If the carbon-chlorine net charges are compared for 3,4,5-trichlorophenol, the para chlorine is predicted to be removed (Table 4), which is consistent with the results for unacclimated bacteria. However, the removal of a meta chlorine is predicted if only the chlorine charges are compared.

The observed pathways for 3,4-dichlorophenol by organisms acclimated to a suite of chlorophenols and unacclimated bacteria involve dechlorination at the meta position (Woods et al., 1989; and Mikesell and Boyd, 1985). Dechlorination of 3,4-dichlorophenol clearly yields 3-chlorophenol if the net carbon-chlorine charge densities are compared, indicating the removal of the para chlorine. However, the difference in chlorine charges at positions 3 and 4 was less than 5% (Table 4), suggesting that dechlorination could occur at either position.

Predictions of reductive dechlorination pathways were made for several chlorophenols whose dechlorination pathways by unacclimated bacteria have not yet been determined experimentally. Both charge patterns (Model 1 & Model 2) suggested that a chlorine adjacent to the hydroxyl group of 2,3,4,6-tetrachlorophenol (position 6) would be removed yielding 2,3,4-trichlorophenol (Table 4). Attack at this position might be the least sterically hindered since the

TABLE 4. Summary of atomic and bond charges for chlorophenols.

Carbon Atom	Atom	Atom Chg	Net Chg	Atom	Atom Chg	Net Chg	Atom	Atom Chg	Net Chg
<i>Pentachlorophenol</i>									
	<i>PCP</i>								
C1	O	-0.214	-0.035						
C2	Cl	-0.033	-0.060						
C3	Cl	-0.032	-0.035						
C4	Cl	-0.037	-0.060						
C5	Cl	-0.033	+0.044						
C6	Cl	-0.060	-0.144						
<i>Tetrachlorophenols</i>									
	<i>2,3,5,6-TeCP</i>			<i>2,3,4,5-TeCP</i>			<i>2,3,4,6-TeCP</i>		
C1	O	-0.218	-0.047	O	-0.229	-0.071	O	-0.217	-0.040
C2	Cl	-0.067	-0.148	Cl	-0.067	-0.146	Cl	-0.041	-0.072
C3	Cl	-0.057	+0.006	Cl	-0.041	-0.005	Cl	-0.041	+0.028
C4	H	+0.103	+0.038	Cl	-0.044	-0.063	Cl	-0.060	-0.093
C5	Cl	-0.057	-0.002	Cl	-0.058	+0.029	H	+0.100	+0.133
C6	Cl	-0.040	-0.065	H	+0.107	+0.041	Cl	-0.081	-0.174
<i>Trichlorophenols</i>									
	<i>2,3,6-TCP</i>			<i>2,3,5-TCP</i>			<i>3,4,5-TCP</i>		
C1	O	-0.221	-0.054	O	-0.233	-0.083	O	-0.236	-0.105
C2	Cl	-0.050	-0.078	Cl	-0.073	-0.151	H	+0.102	+0.039
C3	Cl	-0.067	-0.012	Cl	-0.069	-0.013	Cl	-0.067	-0.021
C4	H	+0.089	+0.009	H	+0.100	+0.040	Cl	-0.052	-0.068
C5	H	+0.087	+0.103	Cl	-0.083	-0.044	Cl	-0.070	-0.014
C6	Cl	-0.092	-0.182	H	+0.103	+0.038	H	+0.088	-0.036

TABLE 4. Continued.

Carbon	Atom	Atom Chg	Net Chg	Atom	Atom Chg	Net Chg	Atom	Atom Chg	Net Chg
	<i>2,3,4-TCP</i>			<i>2,4,5-TCP</i>			<i>2,4,6-TCP</i>		
C1	O	-0.232	-0.076	O	-0.231	-0.076	O	-0.219	-0.004
C2	Cl	-0.076	-0.160	Cl	-0.092	-0.180	Cl	-0.066	-0.106
C3	Cl	-0.051	+0.018	H	+0.097	+0.122	H	+0.098	+0.122
C4	Cl	-0.069	-0.099	Cl	-0.066	-0.097	Cl	-0.086	-0.130
C5	H	+0.088	+0.092	Cl	-0.069	-0.014	H	+0.098	+0.131
C6	H	+0.092	+0.011	H	+0.104	+0.032	Cl	-0.091	-0.187
	<i>Dichlorophenols</i>								
	<i>2,6-DCP</i>			<i>2,3-DCP</i>			<i>2,5-DCP</i>		
C1	O	-0.224	-0.060	O	-0.237	-0.093	O	-0.236	-0.092
C2	Cl	-0.102	-0.195	Cl	-0.085	-0.165	Cl	-0.103	-0.188
C3	H	+0.081	+0.094	Cl	-0.078	-0.023	H	+0.084	+0.090
C4	H	+0.075	-0.020	H	+0.083	+0.005	H	+0.085	+0.006
C5	H	+0.082	+0.087	H	+0.073	+0.058	Cl	-0.096	-0.055
C6	Cl	-0.079	-0.118	H	+0.087	+0.006	H	+0.099	+0.029
	<i>3,5-DCP</i>			<i>3,4-DCP</i>			<i>2,4-DCP</i>		
C1	O	-0.239	-0.118	O	-0.239	-0.112	O	-0.235	-0.085
C2	H	+0.099	+0.037	H	+0.082	-0.049	Cl	-0.100	-0.193
C3	Cl	-0.095	-0.063	Cl	-0.077	-0.021	H	+0.093	+0.117
C4	H	+0.097	+0.037	Cl	-0.080	-0.106	Cl	-0.097	-0.139
C5	Cl	-0.097	-0.055	H	+0.083	+0.077	H	+0.083	+0.087
C6	H	+0.084	-0.039	H	+0.088	+0.011	H	+0.089	+0.002

chlorine is not crowded by any neighboring chlorine atoms. The product of 2,3,4-trichlorophenol degradation is predicted to be 3,4-dichlorophenol using both models (Tables 2 and 4). The removal of an ortho chlorine was predicted for all chlorophenol congeners containing ortho chlorines. The model predictions are summarized in Table 2 and Figure 2.

Because compounds such as the chlorinated phenoxyacetic acids first degraded to chlorophenols (Mikesell and Boyd, 1985), understanding dechlorination pathways for chlorophenols is also useful in understanding the fate of compounds such as 2,4-D and 2,4,5-T (Table 4). For example, 2,4,5-T would be expected to produce 2,4,5-trichlorophenol which is dechlorination at the ortho position yielding 3,4-dichlorophenol.

Chlorobenzoic Acids

Chlorinated benzoic acids are preferentially dechlorinated at the position meta to the carboxyl group in the presence of unacclimated bacteria. The reductive dechlorination of 2,3,6-trichlorobenzoic acid yielded 2,6-dichlorobenzoic acid as the only degradation product (Horowitz et al., 1983; and Suflita et al., 1982). 2-Chlorobenzoic acid was the only metabolite observed from the dechlorination of 2,5-dichlorobenzoic acid (Suflita et al., 1982; and DeWeerd et al., 1986).

It appears that dechlorination products of chlorobenzoic acids vary with the source of inocula. The initial metabolite detected in replicate analyses of 3,4-dichlorobenzoic acid in aquifer incubations differed. Either 3- or 4-chlorobenzoic acid (Gibson and Suflita, 1986; and Suflita et al., 1982) accumulated, however, 4-chlorobenzoic acid persisted. These results suggest the removal of both meta and para chlorines from chlorobenzoic acids. Observed dechlorination pathways are summarized in Table 5.

The net atomic charge patterns for the chlorobenzoic acids with known dechlorination pathways were examined. The computations indicate that the most negative net carbon-chlorine charge is at the position meta to the carboxylic acid group (Table 6). The experimentally determined pathways show that a meta chlorine is preferentially removed (Table 5). Although the removal of only a meta chlorine was predicted for 3,4-dichlorobenzoic acid, the removal of both meta and para chlorines has been observed (Suflita et al., 1982; and Gibson and Suflita, 1986). The model does not take into account the possibility that

TABLE 5. Summary of Dechlorination Pathways for Chlorobenzoic Acids

PARENT COMPOUND	PREDICTED METABOLITE		EXPERIMENTAL METABOLITE	REFERENCE
	MODEL 1	MODEL 2		
PCZ ¹	2345-TeCZ	2346-TeCZ	ND	
2345-TeCZ	234-TCZ	234-TCZ	ND	
2346-TeCZ	246-TCZ	246-TCZ	ND	
2356-TeCZ	236-TCZ	236-TCZ	ND	
236-TCZ	23-DCZ	26-DCZ	26-DCZ	Suflita et al., 1982 Horowitz et al., 1983
234-TCZ	23/34-DCZ	24-DCZ	ND	
235-TCZ	23-DCZ	23-DCZ	ND	
245-TCZ	34-DCZ	24-DCZ	ND	
246-TCZ	26-DCZ	26-DCZ	ND	
345-TCZ	34-DCZ	34-DCZ	ND	
23-DCZ	2-CZ	2-CZ	ND	
24-DCZ	2-CZ	2-CZ	ND	

TABLE 5. Continued

25-DCZ	2-CZ	2-CZ	2-CZ	Suflita et al., 1982 Deweerd et al., 1986
34-DCZ	3-CZ	4-CZ	3 & 4-CZ	Suflita et al., 1982 Gibson and Suflita, 1986 Deweerd et al., 1986
26-DCZ	2-CZ	2-CZ	ND	

¹ CZ: Chlorobenzoic acid

TABLE 6. Summary of atomic and bond charges for chlorobenzoic acids.

Carbon	Atom	Atom Chg	Net Chg	Atom	Atom Chg	Net Chg	Atom	Atom Chg	Net Chg	
<i>Pentachlorobenzoic Acid</i>										
	<i>PCBz</i>									
C1	C	+0.375	+0.273							
C2	Cl	-0.032	+0.022							
C3	Cl	-0.023	-0.006							
C4	Cl	-0.023	+0.023							
C5	Cl	-0.025	-0.009							
C6	Cl	-0.030	+0.025							
<i>Tetrachlorobenzoic Acids</i>										
	<i>2,3,4,6-TCBz</i>				<i>2,3,5,6-TCBz</i>				<i>2,3,4,5-TCBz</i>	
C1	C	+0.377	+0.273	C	+0.378	+0.273	C	+0.373	+0.258	
C2	Cl	-0.042	+0.010	Cl	-0.042	+0.014	Cl	-0.043	+0.011	
C3	Cl	-0.030	-0.013	Cl	-0.045	-0.040	Cl	-0.029	-0.017	
C4	Cl	-0.043	-0.008	H	+0.106	+0.113	Cl	-0.031	+0.016	
C5	H	+0.105	+0.078	Cl	-0.045	-0.040	Cl	-0.045	-0.041	
C6	Cl	-0.052	-0.008	Cl	-0.042	+0.013	H	+0.099	+0.117	
<i>Trichlorobenzoic Acids</i>										
	<i>3,4,5-TCz</i>				<i>2,3,5-TCz</i>				<i>2,4,6-TCz</i>	
C1	C	+0.373	+0.237	C	+0.376	+0.252	C	+0.379	+0.275	
C2	H	+0.093	+0.109	Cl	-0.051	+0.005	Cl	-0.064	-0.024	
C3	Cl	-0.057	-0.057	Cl	-0.051	-0.049	H	+0.104	+0.079	
C4	Cl	-0.036	+0.012	H	+0.100	+0.103	Cl	-0.068	-0.044	
C5	Cl	-0.055	-0.055	Cl	-0.066	-0.072	H	+0.103	+0.079	
C6	H	+0.094	+0.111	H	+0.095	+0.111	Cl	-0.064	-0.025	

TABLE 6. Continued.

Carbon	Atom	Atom Chg	Net Chg	Atom	Atom Chg	Net Chg	Atom	Atom Chg	Net Chg
<i>Trichlorobenzoic Acids</i>									
	<i>2,3,6-TCz</i>			<i>2,3,4-TCz</i>			<i>2,4,5-TCz</i>		
C1	C	+0.394	+0.348	C	+0.375	+0.255	C	+0.376	+0.257
C2	Cl	-0.054	-0.001	Cl	-0.053	-0.003	Cl	-0.069	-0.025
C3	Cl	-0.059	-0.052	Cl	-0.038	-0.025	H	+0.105	+0.077
C4	H	+0.091	+0.077	Cl	-0.055	-0.020	Cl	-0.055	-0.019
C5	H	+0.094	+0.056	H	+0.093	+0.052	Cl	-0.053	-0.049
C6	Cl	-0.074	-0.027	H	+0.088	+0.092	H	+0.096	+0.109
<i>Dichlorobenzoic Acids</i>									
	<i>3,4-DCz</i>			<i>2,5-DCz</i>			<i>2,3-DCz</i>		
C1	C	+0.370	+0.245	C	+0.377	+0.251	C	+0.393	+0.326
C2	H	+0.105	+0.137	Cl	-0.079	-0.034	Cl	-0.065	-0.009
C3	Cl	-0.061	-0.068	H	+0.091	+0.045	Cl	-0.069	-0.067
C4	Cl	-0.061	-0.018	H	+0.090	+0.081	H	+0.086	+0.071
C5	H	+0.088	+0.035	Cl	-0.083	-0.091	H	+0.079	+0.023
C6	H	+0.066	+0.053	H	+0.093	+0.104	H	+0.077	+0.076
	<i>2,6-DCz</i>			<i>2,4-DCz</i>					
C1	C	+0.397	+0.438	C	+0.376	+0.255			
C2	Cl	-0.083	-0.132	Cl	-0.079	-0.040			
C3	H	+0.088	+0.048	H	+0.101	+0.071			
C4	H	+0.078	+0.048	Cl	-0.080	-0.056			
C5	H	+0.087	+0.047	H	+0.089	+0.047			
C6	Cl	-0.082	-0.040	H	+0.084	+0.081			

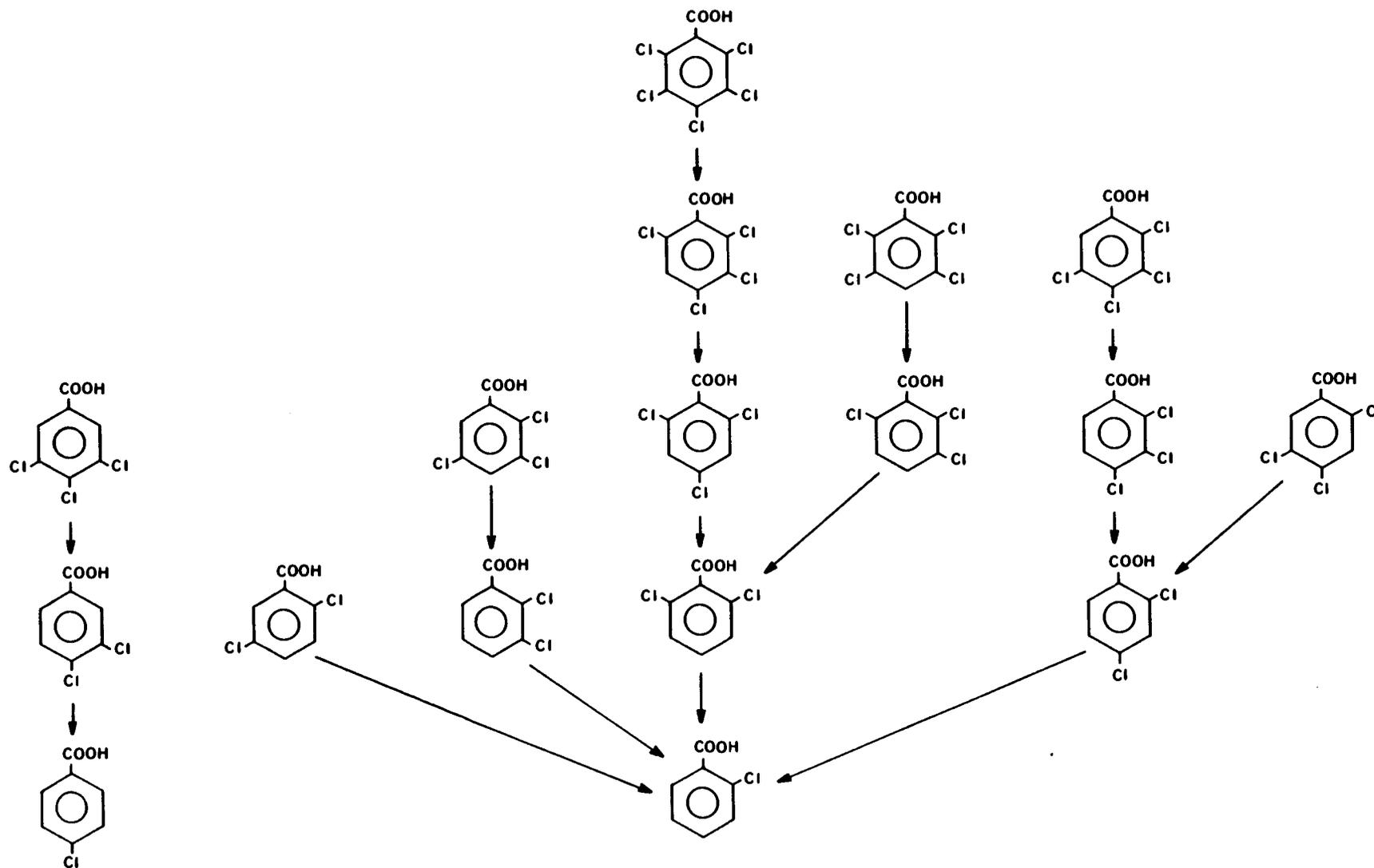
acclimation of the bacterial consortium may have occurred in the sediments where dechlorination was observed, as acclimation may alter the dechlorination pathways.

Consideration of the charges of the chlorine atoms only (Model 1), indicates dechlorination at the ortho position (carbon 6) for 2,3,6-trichlorobenzoic acid and the meta position for 2,5-dichlorobenzoic acid. The difference between the chlorine charges at both the meta and para positions of 3,4-dichlorobenzoic acid was less than 1% (Table 6) suggesting that either position could be dechlorinated.

Reductive dechlorination pathways were predicted for several other chlorobenzoic acid congeners whose pathways have not been reported. The most negative carbon-chlorine net charges occurred at the positions meta to the carboxyl group for the chlorobenzoic acids containing a meta chlorine. The carboxyl group is a meta director in electrophilic reactions, and may also direct dechlorination reactions for the chlorobenzoic acids at this position. However, comparison of the chlorine charges indicates that the meta position is not preferentially dechlorinated for all the chlorobenzoic acids tested. The removal of an ortho chlorine is predicted for 2,4,5-trichlorobenzoic acid and a para chlorine for 2,3,4-trichlorobenzoic acid. The chlorobenzoic acid pathways are summarized in Table 5 and Figure 3.

It appears that the comparison of the net carbon-chlorine charges provides a better means for predicting dechlorination reactions for the chlorobenzoic acids because a larger difference in charges between the chlorines is obtained. The net carbon-chlorine charge (Model 2) also provided a better correlation with position of dechlorination than the chlorine charge (Model 1) for the chlorophenols,

FIGURE 3. Summary of Predicted Chlorobenzoic Acid Dechlorination Pathways.



therefore only Model 2 will be used for predicting dechlorination of the remaining compounds.

Chlorinated Methoxy and Dihydroxybenzenes

Unlike the biodegradation of chlorophenols, biodegradation of most chlorinated veratroles (dimethoxybenzenes) and guaiacols (methoxyphenols) does not proceed via an initial reductive dechlorination reaction. Sequential demethylation of these compounds to their respective hydroxy derivatives prior to dechlorination has been reported (Woods et al., 1989).

Tetrachloroguaiacol (a chlorinated methoxyphenol) and tetrachlorocatechol (a chlorinated dihydroxybenzene) were observed during the degradation of tetrachloroveratrole (Woods, et al., 1989) indicating the initial reaction was cleavage of the ether linkage and conversion to a hydroxyl (Fig. 4). The appearance of 3,4,5-trichlorocatechol, 4,5-dichlorocatechol, and 4-chlorocatechol suggests the reductive dechlorination of tetrachlorocatechol (Woods et al., 1989). It appears that the chlorocatechols were dechlorinated in a manner similar to that of the chlorophenols with the removal of ortho chlorines. In the absence of an ortho chlorine, a chlorine meta to one hydroxyl group was removed. The experimental dechlorination pathways are presented in Table 7.

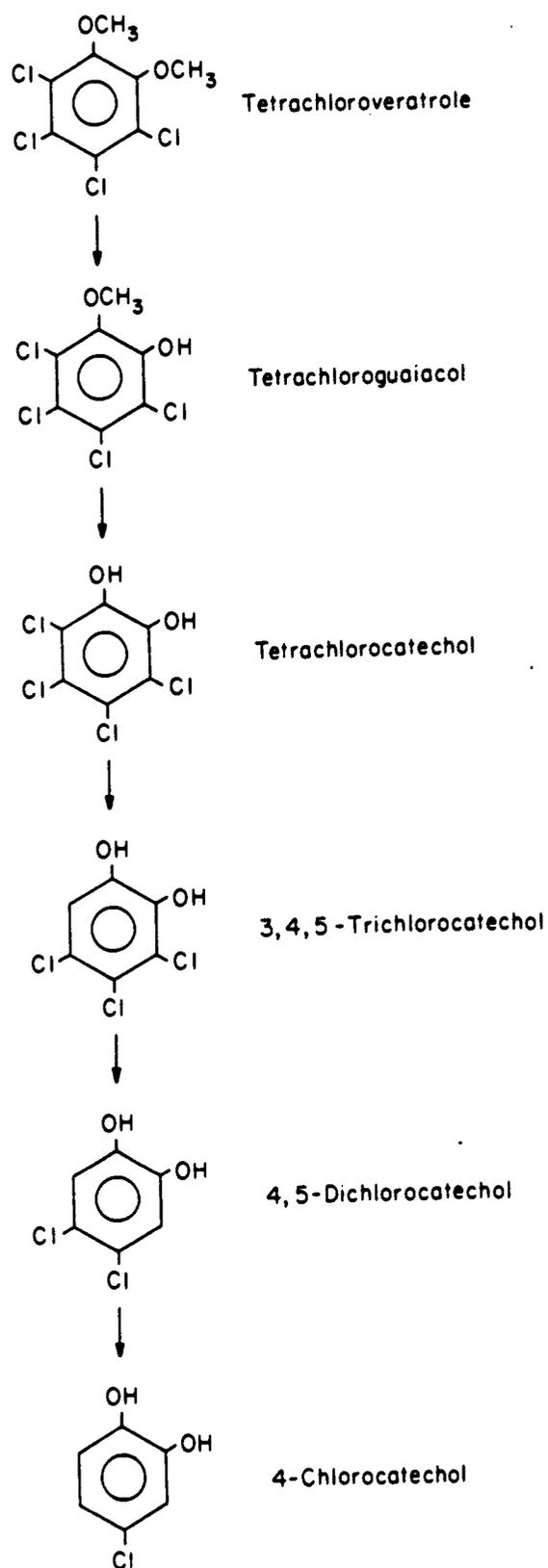
Reductive dechlorination pathways were predicted for the chlorinated methoxybenzenes and methoxyphenols. Because these compounds undergo demethylation reactions prior to dechlorination, the charges on the demethylated intermediates, dihydroxybenzenes, were examined. The net carbon-chlorine charges for the chlorocatechols (chlorinated dihydroxybenzenes) are presented in Table 8. Comparison of the net carbon-chlorine charges for tetrachlorocatechol indicates the most negative position to be adjacent to the hydroxyl groups.

TABLE 7. Summary of Dechlorination Pathways for Chlorinated Dihydroxybenzenes

PARENT COMPOUND	PREDICTED METABOLITE		EXPERIMENTAL METABOLITE	REFERENCE
	MODEL 1	MODEL 2		
TeCC ¹	345-TCC	345-TCC	345-TCC	Woods et al., 1989
345-TCC	45-DCC	45-DCC	45-DCC	Woods et al., 1989
45-DCC	4-CC	4-CC	4-CC	Woods et al., 1989
34-DCC	4-CC	4-CC	ND	
TeCR ²	456-TCR	456-TCR	ND	
456-TCR	45-DCR	45-DCR	ND	
246-TCR	26-DCR	26-DCR	ND	
245-TCR	45-DCR	45-DCR	ND	
25-DCR	5-CR	5-CR	ND	
24-DCR	4-CR	4-CR	ND	
45-DCR	5-CR	5-CR	ND	
TeCHQ ³	236-TCHQ	236-TCHQ	ND	
236-TCHQ	23-DCHQ	23-DCHQ	ND	

TABLE 7. Continued

- ¹ CC: chlorocatechol
- ² CR: chlororesorcinol
- ³ CHQ: chlorohydroquinol

FIGURE 4. Degradation of Tetrachloroveratrole.

Dechlorination at these positions yields 3,4,5-trichlorocatechol which is consistent with the observed degradation pathway. The chlorine adjacent to the other hydroxyl group is removed leaving 4,5-dichlorocatechol. The remaining chlorinated positions have approximately equal charges. Removal of either chlorine yields the same product, 4-chlorocatechol. These results are consistent with the observed reductive dechlorination pathways for chlorocatechols.

Reductive dechlorination pathways were also predicted for the chlorinated resorcinols and hydroquinones (dihydroxy compounds). Examination of the charges (Table 8) for the resorcinols indicates that the most likely chlorine to be removed is in a position ortho to both of the hydroxyl groups or ortho to one and para to the other. This dechlorination pattern is similar to the chlorophenols and chlorocatechols, which are preferentially dechlorinated at the ortho position. It seems that the charges at each chlorinated position of tetrachlorohydroquinone should be equal since the molecule appears symmetrical, however the hydrogen atoms of the hydroxyl group are bent out of the plane of the ring and towards the chlorine atoms yielding different charges for the chlorines. All the chlorines are in positions ortho to a hydroxyl group, but the two with the highest charges would be predicted to be removed. Dechlorination of 2,3,6-trichlorohydroquinone is predicted at position 6. These pathways are summarized in Table 7 and Figures 5a,b, and c.

TABLE 8. Summary of atomic and bond charges for chlorinated dihydroxybenzenes.

Carbon	Atom	Atom Chg	Net Chg	Atom	Atom Chg	Net Chg	Atom	Atom Chg	Net Chg
<i>Chlorocatechols</i>									
	<i>TeCC</i>			<i>3,4,5-TCC</i>			<i>4,5-DCC</i>		
C1	O	-0.213	-0.082	O	-0.236	-0.122	O	-0.240	-0.128
C2	O	-0.213	-0.083	O	-0.254	-0.186	O	-0.259	-0.217
C3	Cl	-0.066	-0.117	Cl	-0.074	-0.108	H	+0.083	+0.001
C4	Cl	-0.042	-0.013	Cl	-0.064	-0.039	Cl	-0.078	-0.067
C5	Cl	-0.044	-0.015	Cl	-0.052	-0.039	Cl	-0.076	-0.062
C6	Cl	-0.065	-0.117	H	+0.101	+0.059	H	+0.100	+0.053
	<i>3,4-DCC</i>								
C1	O	-0.223	-0.124						
C2	O	-0.220	-0.100						
C3	Cl	-0.081	-0.131						
C4	Cl	-0.080	-0.064						
C5	H	+0.085	+0.052						
C6	H	+0.073	-0.036						
<i>Chlororesorcinols</i>									
	<i>TeCR</i>			<i>2,4,6-TCR</i>			<i>4,5,6-TCR</i>		
C1	O	-0.214	+0.007	O	-0.218	-0.007	O	-0.231	-0.042
C2	Cl	-0.092	-0.280	Cl	-0.073	-0.212	H	+0.108	-0.014
C3	O	-0.214	+0.007	O	-0.219	-0.002	O	-0.232	-0.044
C4	Cl	-0.047	-0.122	Cl	-0.091	-0.230	Cl	-0.077	-0.198
C5	Cl	-0.036	+0.069	H	+0.097	+0.166	Cl	-0.046	+0.067
C6	Cl	-0.045	-0.119	Cl	-0.069	-0.151	Cl	-0.078	-0.201

TABLE 8. Continued.

Carbon	Atom	Atom Chg	Net Chg	Atom	Atom Chg	Net Chg	Atom	Atom Chg	Net Chg
	<i>2,4-DCR</i>			<i>4,5-DCR</i>			<i>2,5-DCR</i>		
C1	O	-0.234	-0.041	O	-0.237	-0.075	O	-0.234	-0.049
C2	Cl	-0.107	-0.290	H	+0.087	-0.088	Cl	-0.106	-0.282
C3	O	-0.222	-0.017	O	-0.237	-0.051	O	-0.234	-0.047
C4	Cl	-0.079	-0.159	Cl	-0.083	-0.203	H	+0.099	-0.014
C5	H	+0.083	+0.121	Cl	-0.077	+0.011	Cl	-0.090	-0.015
C6	H	+0.090	-0.039	H	+0.100	-0.011	H	+0.099	-0.016
	<i>2,4,5-TCR</i>								
C1	O	-0.229	-0.032						
C2	Cl	-0.099	-0.281						
C3	O	-0.219	-0.010						
C4	Cl	-0.050	-0.121						
C5	Cl	-0.065	+0.024						
C6	H	+0.104	-0.011						
	<i>Chlorohydroquinones</i>								
	<i>TeCH</i>			<i>2,3,6-TCH</i>					
C1	O	-0.220	-0.090	O	-0.235	-0.127			
C2	Cl	-0.038	-0.023	Cl	-0.073	-0.110			
C3	Cl	-0.038	-0.023	Cl	-0.047	-0.034			
C4	O	-0.220	+0.090	O	-0.222	-0.095			
C5	Cl	-0.066	-0.102	H	+0.103	+0.083			
C6	Cl	-0.066	-0.102	Cl	-0.090	-0.140			

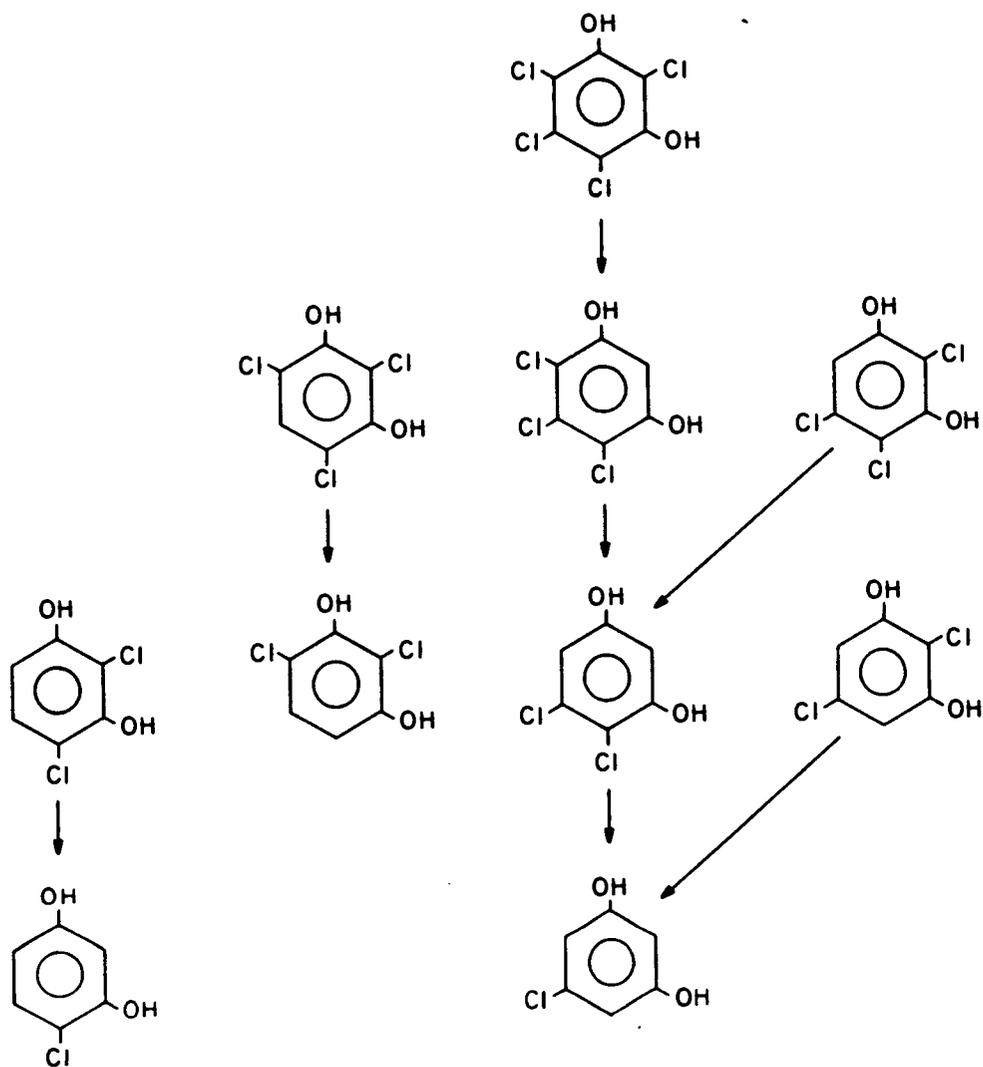
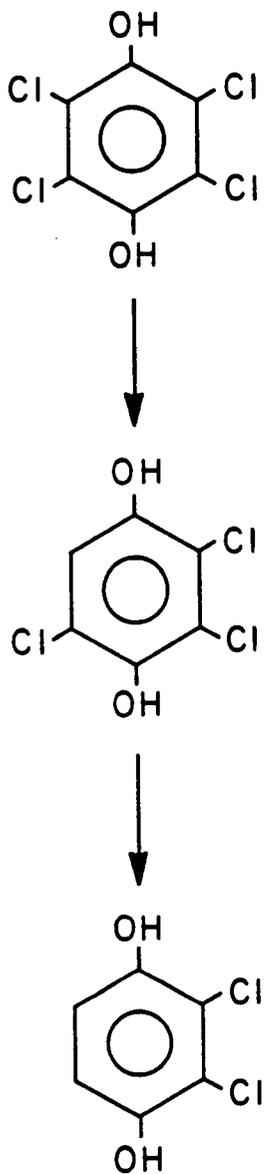
FIGURE 5b. Summary of Predicted Chlororesorcinol Dechlorination Pathways.

FIGURE 5c. Summary of Predicted Chlorohydroquinone Dechlorination Pathways.

Chloroanilines

Experimental results indicate that chlorinated anilines are preferentially dechlorinated by unacclimated bacteria at the positions ortho and para to the amino group (Table 9). The sequential dechlorination of 2,3,4,5-tetrachloroaniline yielded 2,3,5-trichloroaniline and 3,5-dichloroaniline (Kuhn and Suflita, 1989). 3,4-Dichloroaniline was converted to 3-chloroaniline. Reductive dechlorination of chloroanilines was observed only if the parent compound had "at least two halogens in adjacent positions on the aromatic ring" (Kuhn and Suflita, 1989).

Net carbon-chlorine charges for the chloroanilines with known dechlorination pathways were examined. Consideration of the carbon-chlorine charges for 2,3,4,5-tetrachloroaniline indicates that the most negative value is at the position ortho to the amino group (Table 10). However, dechlorination for this compound was observed at the para position. The amine group is an o,p-directing substituent and may have some effect on the position to be dechlorinated. It is possible that steric effects in enzymic processes would inhibit dechlorination at the ortho position, and the model does not take enzymic reactions into account. 3,5-dichloroaniline was correctly predicted as the metabolic product of 2,3,5-trichloroaniline showing ortho chlorine removal. Removal of a para chlorine from 3,4-dichloroaniline was predicted, which is consistent with the observed pathway.

Predictions were made for some chloroanilines whose reductive dechlorination pathways have not been determined yet (Table 9). Although, reductive dechlorination has not been observed for those chloroanilines which do

TABLE 9. Summary of Dechlorination Pathways for Chloroanilines

PARENT COMPOUND	PREDICTED METABOLITE		EXPERIMENTAL METABOLITE	REFERENCE
	MODEL 1	MODEL 2		
2345-TeCA ¹	345-TCA	345-TCA	235-TCA	Kuhn and Suflita, 1989
235-TCA	23-DCA	35-DCA	35-DCA	Kuhn and Suflita, 1989
34-DCA	3-CA	3-CA	3-CA	Kuhn and Suflita, 1989
234-TCA	23/34-DCA	34-DCA	ND	
245-TCA	34-DCA	24-DCA	ND	
345-TCA	34-DCA	34-DCA	ND	
23-DCA	3-CA	3-CA	ND	
25-DCA	3-CA	2-CA	ND	
24-DCA	4-CA	4-CA	ND	

¹ CA: Chloroaniline

not contain chlorines in adjacent positions on the aromatic ring, dechlorination pathways were predicted. Examination of the charges (Table 10), indicates the removal of chlorines from ortho, meta, and para positions. Meta dechlorination would not be expected if the directing character of the amino group has any effect on the position of dechlorination since the amino group is an o,p-director. The model does not predict preferential dechlorination of the ortho position over the para position and vice versa. Because the pathways for very few chloroanilines have been experimentally determined, it is difficult to state whether there is preferential dechlorination of one of these two positions.

TABLE 10. Summary of atomic and bond charges for chloroanilines.

Carbon	Atom	Atom Chg	Net Chg	Atom	Atom Chg	Net Chg	Atom	Atom Chg	Net Chg
	<i>2,3,4,5-TeCA</i>			<i>2,3,5-TCA</i>			<i>2,3,4-TCA</i>		
C1	N	-0.234	-0.134	N	-0.232	-0.144	N	-0.235	-0.141
C2	Cl	-0.066	-0.103	Cl	-0.073	-0.105	Cl	-0.073	-0.113
C3	Cl	-0.044	+0.015	Cl	-0.071	-0.026	Cl	-0.053	+0.006
C4	Cl	-0.046	-0.060	H	+0.099	+0.044	Cl	-0.073	-0.098
C5	Cl	-0.064	-0.012	Cl	-0.088	-0.051	H	+0.085	+0.086
C6	H	+0.092	+0.009	H	+0.088	+0.099	H	+0.080	-0.053
	<i>2,4,5-TCA</i>			<i>3,4,5-TCA</i>			<i>2,3-DCA</i>		
C1	N	-0.233	-0.320	N	-0.232	-0.309	N	-0.231	-0.152
C2	Cl	-0.091	+0.003	H	+0.088	+0.156	Cl	-0.083	-0.116
C3	H	+0.097	+0.053	Cl	-0.072	-0.147	Cl	-0.081	-0.038
C4	Cl	-0.071	-0.057	Cl	-0.054	-0.011	H	+0.083	+0.011
C5	Cl	-0.071	-0.096	Cl	-0.071	-0.080	H	+0.071	+0.052
C6	H	+0.089	+0.140	H	+0.088	+0.131	H	+0.072	-0.020
	<i>3,4-DCA</i>			<i>2,4-DCA</i>			<i>2,5-DCA</i>		
C1	N	-0.231	-0.170	N	-0.232	-0.144	N	-0.231	-0.313
C2	H	+0.083	+0.009	Cl	-0.101	-0.147	Cl	-0.102	-0.022
C3	Cl	-0.079	-0.037	H	+0.093	+0.104	H	+0.083	+0.043
C4	Cl	-0.082	-0.101	Cl	-0.099	-0.134	H	+0.084	+0.078
C5	H	+0.081	+0.071	H	+0.081	+0.080	Cl	-0.101	-0.173
C6	H	+0.074	-0.015	H	+0.074	-0.025	H	+0.085	+0.122

Chlorinated Aliphatic Compounds

The reductive dechlorination of chlorinated aliphatic compounds has been reported (Vogel et al., 1987; Bouwer and Wright, 1988). 1,1,2-Trichloroethylene (1,1,2-TCE) is reductively dechlorinated to 1,1-dichloroethylene (1,1-DCE). The models suggest the removal of a chlorine from carbon 2, yielding 1,1-DCE (Table 11). The observed reductive dechlorination of 1,1,2-trichloroethane (1,1,2-TCA) yields 1,2-DCA (Vogel, 1990). Both models predict 1,1-DCA (Table 11) as the dechlorination product of 1,1,2-TCA. It seems that a reaction at the predicted position would be less sterically hindered than at the carbon with two chlorines. With the results from only two compounds it is difficult to state whether these models are accurate at predicting dechlorination reactions for chlorinated aliphatic compounds.

TABLE 11. Summary of atomic and bond charges for chlorinated aliphatic compounds.

Carbon	Atom	Atom Chg	Net Chg	Atom	Atom Chg	Net Chg
	<i>1,1,2-Trichloroethane</i>			<i>1,1,2-Trichloroethylene</i>		
C1	H	+0.080	+0.240	Cl	-0.035	-0.006
C1	Cl	-0.151	+0.028	Cl	-0.054	-0.025
C1	Cl	-0.131	+0.009			
C2	H	+0.063	+0.157	Cl	-0.072	-0.049
C2	H	+0.056	+0.150	H	+0.109	+0.132
C2	Cl	-0.171	-0.077			

CONCLUSIONS

Although this model does not consider a mechanism for the electron transfer and factors such as enzyme interactions or thermodynamics which influence dechlorination reactions, it seems to provide a satisfactory means for predicting reductive dechlorination reactions for a variety of compounds. Predictions have been made for compounds whose pathways are still unknown. Further research might involve the identification of a mechanism for the transfer of electrons and alteration of the model to take this into account. Tests to confirm the accuracy of this model to predict dechlorination reactions will provide a useful tool for determining the fate of a number of compounds in the environment.

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APPENDICES

Appendix A: Accessing the Cornell Supercomputing Facility

1. Log on to PANACEA via CELAN.
2. Exit to DOS permanently.
3. Type: NCSA 128.84.252.21
4. At CNSF prompt, enter appropriate logon name
5. Enter password.

Accessing MOPAC

Prior to running the MOPAC program enter the following:

1. DEFINE STORAGE 50M
2. SET MACHINE XA
3. IPL CMSXA
4. OBTAIN VERSION TEST
5. OBTAIN MOPAC

File Transfer to and from Cornell (Must be logged onto Cornell)

1. <ALT-T>
2. At the user prompt, enter: your name
3. At the password prompt, enter: <ALT-W>
4. To FTP to Cornell GET a: fname lname.input

fname=foreign name (name on disk)
lname=local name (name at Cornell)

To FTP from Cornell PUT a: lname.extension fname.extension

extensions: input
 archive
 moout
 ortep

5. To exit FTP, enter BYE.

File Management

1. To list files in storage at Cornell, enter: FILEL
2. Files must be in the following format to be run by MOPAC:

```
FILETYPE: INPUT
FORMAT:   F
LRECL:   80
```

3. To meet the above requirements, enter the edit mode:
At the prompt, enter:

```
RECFM F <RETURN>
LRECL 80 <RETURN>
FILE
```

4. The file is now ready to be executed.
5. To run MOPAC:

F3
MOPAC filename (without extension)
6. Output files are automatically created with appropriate extensions.

Appendix B: Output Files

The archive files for most of the compounds presented in the body of the thesis are included in this appendix. These output files contain the important details of the calculations and the optimized geometries. The information includes: heat of formation, dipole moment, total energy, execution time, and the gradient norm. Error messages will also be printed if the criteria which control the precision are not met. From this file, one can determine whether the output is reasonable.

The optimized geometry is printed in the following manner:

Column 1: Chemical symbols for the atoms (numbered consecutively I=1-n)

2: Bond length (angstroms) NA:I

3: Bond angle (degrees) NB:NA:I

4: Twist angle (degrees) NC:NB:NA:I

5,6,7: Connection of the atoms- NA, NB, NC

8: Atomic charge

SUMMARY OF MNDO CALCULATION

VERSION 5.01

C6 H 0 Cl5

20- 3-1990

2,3,4,5,6-pentachlorophenol

HERBERTS TEST WAS SATISFIED IN BFGS
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION = -46.311369 KCAL
ELECTRONIC ENERGY = -11498.801563 EV
CORE-CORE REPULSION = 8622.837031 EV
GRADIENT NORM = 2.169483
DIPOLE = 1.80879 DEBYE
NO. OF FILLED LEVELS = 33
IONIZATION POTENTIAL = 9.962710 EV
MOLECULAR WEIGHT = 266.338
SCF CALCULATIONS = 94
COMPUTATION TIME = 23.438 SECONDS

FINAL GEOMETRY OBTAINED

CHARGE

2,3,4,5,6-pentachlorophenol

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.0840
C	1.411227	1	0.000000	0	0.000000	0	1	0	0	0.0765
C	1.411400	1	119.962344	1	0.000000	0	2	1	0	-0.0224
C	1.416398	1	120.119084	1	-0.013274	1	3	2	1	0.0670
C	1.425086	1	120.551639	1	0.024323	1	1	2	3	0.1795
C	1.407903	1	120.314681	1	0.063147	1	4	3	2	-0.0266
O	1.347094	1	124.210856	1	179.877545	1	5	1	2	-0.2140
Cl	1.743239	1	120.217387	1	179.991990	1	6	4	3	-0.0334
Cl	1.742421	1	119.747788	1	180.071239	1	4	3	2	-0.0323
Cl	1.742586	1	119.947526	1	180.018471	1	3	2	1	-0.0373
Cl	1.742149	1	120.105720	1	180.019852	1	2	3	1	-0.0330
Cl	1.747539	1	119.798871	1	179.839932	1	1	2	3	-0.0602
H	0.949437	1	114.634823	1	-0.304282	1	7	5	1	0.2203
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MNDO CALCULATION

VERSION 5.01

C6 H2 O C14

20- 3-1990

2,3,5,6-tetrachlorophenol

HERBERTS TEST WAS SATISFIED IN BFGS
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION = -45.529126 KCAL
ELECTRONIC ENERGY = -9860.345872 EV
CORE-CORE REPULSION = 7324.624441 EV
GRADIENT NORM = 3.699800
DIPOLE = 1.04953 DEBYE
NO. OF FILLED LEVELS = 30
IONIZATION POTENTIAL = 9.871091 EV
MOLECULAR WEIGHT = 231.893
SCF CALCULATIONS = 23
COMPUTATION TIME = 7.879 SECONDS

FINAL GEOMETRY OBTAINED

CHARGE

2,3,5,6-tetrachlorophenol

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.0807
C	1.409735	1	0.000000	0	0.000000	0	1	0	0	0.0634
C	1.404871	1	120.292200	1	0.000000	0	2	1	0	-0.0646
C	1.408274	1	120.080769	1	0.215315	1	3	2	1	0.0547
C	1.427091	1	120.116247	1	-0.282361	1	1	2	3	0.1708
C	1.407969	1	120.762098	1	-0.063886	1	4	3	2	-0.0244
O	1.348707	1	124.072051	1	-179.802353	1	5	1	2	-0.2181
Cl	1.742861	1	120.289564	1	179.940965	1	6	4	3	-0.0403
Cl	1.744796	1	117.792926	1	179.940657	1	4	3	2	-0.0570
H	1.091624	1	119.997369	1	-179.841936	1	3	2	1	0.1026
Cl	1.744233	1	118.173433	1	179.905089	1	2	3	1	-0.0571
Cl	1.747626	1	119.967296	1	179.805558	1	1	2	3	-0.0671
H	0.949114	1	114.542859	1	0.018557	1	7	5	1	0.2178
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MNDO CALCULATION

VERSION 5.01

C6 H2 O C14

20- 3-1990

2,3,4,6-tetrachlorophenol

HERBERTS TEST WAS SATISFIED IN BFGS
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION = -45.726800 KCAL
ELECTRONIC ENERGY = -9859.039281 EV
CORE-CORE REPULSION = 7323.309278 EV
GRADIENT NORM = 5.144361
DIPOLE = 2.28863 DEBYE
NO. OF FILLED LEVELS = 30
IONIZATION POTENTIAL = 9.801316 EV
MOLECULAR WEIGHT = 231.893
SCF CALCULATIONS = 69
COMPUTATION TIME = 16.033 SECONDS

FINAL GEOMETRY OBTAINED

CHARGE

2,3,4,6-tetrachlorophenol

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.0923
C	1.404745	1	0.000000	0	0.000000	0	1	0	0	0.0334
C	1.406716	1	120.263683	1	0.000000	0	2	1	0	-0.0335
C	1.414877	1	120.159087	1	0.030541	1	3	2	1	0.0681
C	1.424978	1	120.676275	1	-0.012113	1	1	2	3	0.1765
C	1.410066	1	119.929788	1	0.029996	1	4	3	2	-0.0313
O	1.347489	1	124.340235	1	179.895269	1	5	1	2	-0.2167
Cl	1.744414	1	119.896879	1	179.893865	1	6	4	3	-0.0411
Cl	1.742736	1	119.822246	1	-179.906130	1	4	3	2	-0.0401
Cl	1.743830	1	118.163328	1	179.942158	1	3	2	1	-0.0596
H	1.092312	1	119.866376	1	179.979765	1	2	3	1	0.1000
Cl	1.748731	1	118.037359	1	179.970565	1	1	2	3	-0.0814
H	0.949154	1	114.464281	1	-0.138886	1	7	5	1	0.2177
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MNDO CALCULATION

VERSION 4.01

C6 H2 O CL4
2,3,4,5-tetrachlorophenol

HERBERTS TEST WAS SATISFIED IN BFGS
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	-45.510808	KCAL/MOL
HEAT OF FORMATION	=	-190.690266	KJ/MOL
ELECTRONIC ENERGY	=	-9861.841013	EV
CORE-CORE REPULSION	=	7326.120375	EV
GRADIENT NORM	=	3.429128	
DIPOLE	=	2.19845	DEBYE
NO. OF FILLED LEVELS	=	30	
IONIZATION POTENTIAL	=	9.823983	EV
MOLECULAR WEIGHT	=	231.893	
SCF CALCULATIONS	=	123	

FINAL GEOMETRY OBTAINED

CHARGE

2,3,4,5-tetrachlorophenol

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.0656
C	1.402192	1	0.000000	0	0.000000	0	1	0	0	0.0529
C	1.414267	1	120.947899	1	0.000000	0	2	1	0	-0.0192
C	1.410942	1	119.573172	1	-0.028063	1	3	2	1	0.0697
C	1.425916	1	119.712666	1	0.013120	1	1	2	3	0.1583
C	1.412598	1	120.271029	1	0.004032	1	4	3	2	-0.0798
O	1.350531	1	115.641414	1	180.001888	1	5	1	2	-0.2292
CL	1.747088	1	120.127623	1	180.033809	1	6	4	3	-0.0666
CL	1.743609	1	119.931448	1	180.010739	1	4	3	2	-0.0412
CL	1.742803	1	120.030851	1	179.974857	1	3	2	1	-0.0441
CL	1.745346	1	121.261763	1	-179.973684	1	2	3	1	-0.0582
H	1.091541	1	120.351959	1	180.008099	1	1	2	3	0.1069
H	0.948780	1	114.571476	1	179.835182	1	7	5	1	0.2161
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MNDO CALCULATION

VERSION 5.01

C6 H3 O C13

20- 3-1990

2,3,5-trichlorophenol

HERBERTS TEST WAS SATISFIED IN BFGS
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION = -44.038613 KCAL
ELECTRONIC ENERGY = -8318.662246 EV
CORE-CORE REPULSION = 6123.214628 EV
GRADIENT NORM = 4.045255
DIPOLE = 0.92455 DEBYE
NO. OF FILLED LEVELS = 27
IONIZATION POTENTIAL = 9.719463 EV
MOLECULAR WEIGHT = 197.448
SCF CALCULATIONS = 149
COMPUTATION TIME = 29.924 SECONDS

FINAL GEOMETRY OBTAINED										CHARGE
GEO-OK										
2,3,5-trichlorophenol										
C	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.0649
C	1.401837	1	0.000000	0	0.000000	0	1	0	0	0.0392
C	1.412832	1	121.624095	1	0.000000	0	2	1	0	-0.0608
C	1.404613	1	118.715663	1	-0.812436	1	3	2	1	0.0560
C	1.426654	1	119.364808	1	0.973012	1	1	2	3	0.1497
C	1.424336	1	119.511269	1	-0.400108	1	5	1	2	-0.0778
O	1.351763	1	115.663853	1	179.560756	1	5	1	2	-0.2327
Cl	1.746445	1	120.185862	1	179.921593	1	6	5	1	-0.0731
Cl	1.747718	1	117.607941	1	179.991878	1	4	3	2	-0.0688
H	1.090197	1	120.414353	1	179.275911	1	3	2	1	0.1004
Cl	1.747761	1	119.027328	1	-179.510708	1	2	3	1	-0.0834
H	1.091137	1	120.591788	1	-179.417545	1	1	2	3	0.1027
H	0.948571	1	114.384193	1	179.837738	1	7	5	1	0.2135
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MNDO CALCULATION

VERSION 4.01

C6 H3 O CL3
2,3,6-trichlorophenol

HERBERTS TEST WAS SATISFIED IN BFGS
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	-42.219412	KCAL/MOL
HEAT OF FORMATION	=	-176.899321	KJ/MOL
ELECTRONIC ENERGY	=	-8375.971853	EV
CORE-CORE REPULSION	=	6180.603121	EV
GRADIENT NORM	=	3.901967	
DIPOLE	=	2.35381	DEBYE
NO. OF FILLED LEVELS	=	27	
IONIZATION POTENTIAL	=	9.664329	EV
MOLECULAR WEIGHT	=	197.448	
SCF CALCULATIONS	=	98	

FINAL GEOMETRY OBTAINED

CHARGE

2,3,6-trichlorophenol

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.0285
C	1.408700	1	0.000000	0	0.000000	0	1	0	0	0.0552
C	1.407972	1	120.530831	1	0.000000	0	2	1	0	-0.0805
C	1.404388	1	120.221967	1	-0.074983	1	3	2	1	0.0155
C	1.404674	1	119.996597	1	0.167476	1	4	3	2	-0.0892
C	1.426382	1	120.746469	1	0.036084	1	5	4	3	0.1668
O	1.349845	1	124.153785	1	179.599683	1	6	5	4	-0.2212
CL	1.744951	1	120.117836	1	-179.952268	1	1	2	3	-0.0496
CL	1.746001	1	117.993046	1	179.928512	1	2	3	1	-0.0668
H	1.090765	1	120.557854	1	179.990074	1	3	2	1	0.0890
H	1.091215	1	119.430093	1	-179.876933	1	4	3	2	0.0872
CL	1.750666	1	118.112162	1	180.037847	1	5	4	3	-0.0924
H	0.948372	1	114.328483	1	0.315679	1	7	6	5	0.2148
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MNDO CALCULATION

VERSION 5.01

C6 H3 O Cl3

20- 3-1990

2,4,5-trichlorophenol

HERBERTS TEST WAS SATISFIED IN BFGS
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION = -44.520900 KCAL
ELECTRONIC ENERGY = -8302.711112 EV
CORE-CORE REPULSION = 6107.242580 EV
GRADIENT NORM = 3.639556
DIPOLE = 1.88418 DEBYE
NO. OF FILLED LEVELS = 27
IONIZATION POTENTIAL = 9.641590 EV
MOLECULAR WEIGHT = 197.448
SCF CALCULATIONS = 74
COMPUTATION TIME = 17.322 SECONDS

FINAL GEOMETRY OBTAINED

CHARGE

2,4,5-trichlorophenol

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.0717
C	1.403197	1	0.000000	0	0.000000	0	1	0	0	0.0541
C	1.412968	1	121.052663	1	0.000000	0	2	1	0	-0.0308
C	1.407147	1	119.438509	1	0.086955	1	3	2	1	0.0251
C	1.406789	1	120.185068	1	-0.008413	1	4	3	2	-0.0885
C	1.422505	1	120.783421	1	-0.028003	1	5	4	3	0.1548
O	1.350647	1	125.151803	1	179.956965	1	6	5	4	-0.2310
H	1.091032	1	120.317177	1	179.875600	1	1	2	3	0.1036
Cl	1.746849	1	121.074339	1	180.031597	1	2	3	1	-0.0685
Cl	1.743802	1	121.996129	1	180.042792	1	3	2	1	-0.0662
H	1.091959	1	119.969896	1	179.972683	1	4	3	2	0.0970
Cl	1.750420	1	118.002960	1	179.990396	1	5	4	3	-0.0915
H	0.948681	1	114.258006	1	0.642798	1	7	6	5	0.2135
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MNDO CALCULATION

VERSION 4.01

C6 H3 O CL3
2,4,6-trichlorophenol

HERBERTS TEST WAS SATISFIED IN BFSS
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION = -44.566953 KCAL/MOL
HEAT OF FORMATION = -186.733513 KJ/MOL
ELECTRONIC ENERGY = -8317.143036 EV
CORE-CORE REPULSION = 6121.672507 EV
DIPOLE = 1.08882 DEBYE
NO. OF FILLED LEVELS = 27
IONIZATION POTENTIAL = 9.628510 EV
MOLECULAR WEIGHT = 197.448
SCF CALCULATIONS = 136

FINAL GEOMETRY OBTAINED

CHARGE

2,4,6-trichlorophenol

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.0405
C	1.405474	1	0.000000	0	0.000000	0	1	0	0	0.0243
C	1.407884	1	119.574403	1	0.000000	0	2	1	0	-0.0442
C	1.405481	1	121.192964	1	0.020404	1	3	2	1	0.0337
C	1.428928	1	120.780463	1	0.272647	1	1	2	3	0.1733
C	1.406285	1	119.051023	1	-0.277368	1	4	3	2	-0.0954
O	1.348295	1	117.451204	1	179.762335	1	5	1	2	-0.2193
CL	1.750759	1	117.737221	1	-179.784192	1	6	4	3	-0.0911
H	1.091244	1	120.612466	1	179.812500	1	4	3	2	0.0977
CL	1.747569	1	119.381832	1	179.986470	1	3	2	1	-0.0859
H	1.091636	1	120.278219	1	180.058157	1	2	3	1	0.0979
CL	1.746415	1	117.961702	1	-179.837786	1	1	2	3	-0.0658
H	0.949059	1	114.320208	1	-179.962146	1	7	5	1	0.2154
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MNDO CALCULATION

VERSION 4.01

C6 H3 O CL3
3,4,5-trichlorophenol

HERBERTS TEST WAS SATISFIED IN BFGS
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	-42.920780	KCAL/MOL
HEAT OF FORMATION	=	-179.838052	KJ/MOL
ELECTRONIC ENERGY	=	-8316.854104	EV
CORE-CORE REPULSION	=	6121.454958	EV
GRADIENT NORM	=	4.202809	
DIPOLE	=	3.12525	DEBYE
NO. OF FILLED LEVELS	=	27	
IONIZATION POTENTIAL	=	9.646699	EV
MOLECULAR WEIGHT	=	197.448	
SCF CALCULATIONS	=	142	

FINAL GEOMETRY OBTAINED

CHARGE

3,4,5-trichlorophenol

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.0632
C	1.405152	1	0.000000	0	0.000000	0	1	0	0	0.0460
C	1.413284	1	121.135524	1	0.000000	0	2	1	0	-0.0163
C	1.410478	1	119.000348	1	-0.081495	1	3	2	1	0.0559
C	1.422812	1	119.213887	1	-0.146255	1	1	2	3	0.1309
C	1.406121	1	121.136696	1	0.226312	1	4	3	2	-0.1232
O	1.354586	1	116.744207	1	180.011638	1	5	1	2	-0.2357
H	1.090731	1	119.845439	1	-179.830639	1	6	4	3	0.0875
CL	1.747246	1	121.283019	1	-179.793926	1	4	3	2	-0.0696
CL	1.742950	1	120.486526	1	179.992559	1	3	2	1	-0.0515
CL	1.746703	1	121.177622	1	179.958924	1	2	3	1	-0.0669
H	1.090985	1	120.459717	1	179.916515	1	1	2	3	0.1024
H	0.948358	1	113.376501	1	179.534116	1	7	5	1	0.2035
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MNDO CALCULATION

VERSION 4.01

C6 H4 O CL2
2,4-dichlorophenol

HERBERTS TEST WAS SATISFIED IN BFGS
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	-40.564827	KCAL/MOL
HEAT OF FORMATION	=	-169.966606	KJ/MOL
ELECTRONIC ENERGY	=	-6915.446077	EV
CORE-CORE REPULSION	=	5060.358272	EV
GRADIENT NORM	=	5.102643	
DIPOLE	=	1.05256	DEBYE
NO. OF FILLED LEVELS	=	24	
IONIZATION POTENTIAL	=	9.409768	EV
MOLECULAR WEIGHT	=	163.003	
SCF CALCULATIONS	=	152	

FINAL GEOMETRY OBTAINED

CHARGE

2,4-dichlorophenol

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.0866
C	1.398769	1	0.000000	0	0.000000	0	1	0	0	0.0037
C	1.409626	1	119.906736	1	0.000000	0	2	1	0	-0.0413
C	1.403275	1	121.088265	1	-0.184635	1	3	2	1	0.0237
C	1.409757	1	119.156971	1	-0.070020	1	4	3	2	-0.0932
C	1.422043	1	120.756513	1	0.257618	1	5	4	3	0.1508
O	1.351192	1	124.969830	1	179.870219	1	6	5	4	-0.2354
H	1.090869	1	119.592073	1	-179.814121	1	1	2	3	0.0886
H	1.091246	1	120.586585	1	-179.892686	1	2	3	1	0.0831
CL	1.749335	1	119.485204	1	179.905736	1	3	2	1	-0.0974
H	1.091041	1	120.693328	1	-179.990128	1	4	3	2	0.0934
CL	1.751680	1	117.940201	1	-179.800060	1	5	4	3	-0.1002
H	0.948507	1	114.171738	1	-0.724975	1	7	6	5	0.2107
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MINDO CALCULATION

VERSION 4.01

06 H4 0 0L2
2,5-dichlorocobenzol

HERBERTS TEST WAS SATISFIED IN EFGS
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION = -40.298313 KCAL/MOL
HEAT OF FORMATION = -168.649314 KJ/MOL
ELECTRONIC ENERGY = -6915.197511 EV
CORE-CORE REPAUSION = 5060.121263 EV
GRADIENT NORM. = 3.387418
DIPOLE = 1.07234 DEBYE
NO. OF FILLED LEVELS = 24
IONIZATION POTENTIAL = 9.485213 EV
MOLECULAR WEIGHT = 163.003
SCF CALCULATIONS = 135

FINAL GEOMETRY OBTAINED

CHARGE

2,5-dichlorocobenzol

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	0.0403
C	1.403069	1	0.000000	0	0.000000	0	1	0	0	-0.0730
C	1.403192	1	119.436087	1	0.000000	0	2	1	0	0.0062
C	1.408030	1	119.974506	1	-0.027917	1	3	2	1	-0.0857
C	1.403118	1	121.722419	1	0.023407	1	1	2	3	-0.0705
C	1.427174	1	119.035454	1	-0.002562	1	5	1	2	0.1442
O	1.352574	1	115.988089	1	179.984318	1	6	5	1	-0.2359
Cl	1.752356	1	118.014574	1	180.009246	1	4	3	2	-0.1027
H	1.090866	1	119.554669	1	179.977323	1	3	2	1	0.0837
H	1.090089	1	119.699680	1	180.012063	1	2	3	1	0.0652
Cl	1.750123	1	119.163095	1	-179.978011	1	1	2	3	-0.0957
H	1.090537	1	120.711899	1	179.967280	1	5	1	2	0.0993
H	0.948443	1	114.104939	1	-179.976154	1	7	6	5	0.2104
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MNDO CALCULATION

VERSION 4.01

C6 H4 O CL2
2,6-dichlorophenol

HERBERTS TEST WAS SATISFIED IN BFGS
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	-38.353624	KCAL/MOL
HEAT OF FORMATION	=	-160.701667	KJ/MOL
ELECTRONIC ENERGY	=	-6984.101720	EV
CORE-CORE REPULSION	=	5129.109801	EV
GRADIENT NORM	=	3.969592	
DIPOLE	=	1.90228	DEBYE
NO. OF FILLED LEVELS	=	24	
IONIZATION POTENTIAL	=	9.429094	EV
MOLECULAR WEIGHT	=	163.003	
SCF CALCULATIONS	=	126	

FINAL GEOMETRY OBTAINED

CHARGE

2,6-dichlorophenol

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	0.0048
C	1.406215	1	0.000000	0	0.000000	0	1	0	0	-0.0958
C	1.404333	1	120.012110	1	0.000000	0	2	1	0	0.0127
C	1.407134	1	120.078671	1	-0.271691	1	3	2	1	-0.0928
C	1.404515	1	120.248141	1	-0.051478	1	1	2	3	-0.0387
C	1.428785	1	120.890044	1	0.417743	1	5	1	2	0.1638
O	1.349546	1	117.633529	1	179.491707	1	6	5	1	-0.2239
CL	1.752319	1	117.944577	1	-179.913108	1	4	3	2	-0.1024
H	1.091142	1	119.654532	1	179.814405	1	3	2	1	0.0812
H	1.089834	1	120.024663	1	180.060929	1	2	3	1	0.0754
H	1.091359	1	119.403762	1	-179.924601	1	1	2	3	0.0821
CL	1.748692	1	117.923497	1	-179.763857	1	5	1	2	-0.0789
H	0.948789	1	114.265801	1	179.077060	1	7	6	5	0.2124
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MNDO CALCULATION

VERSION 4.01

C6 H4 O CL2
3,4-dichlorophenol

HERBERTS TEST WAS SATISFIED IN BFGS
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	-39.167747 KCAL/MOL
HEAT OF FORMATION	=	-164.112843 KJ/MOL
ELECTRONIC ENERGY	=	-6911.799295 EV
CORE-CORE REPULSION	=	5056.772072 EV
GRADIENT NORM	=	5.124131
DIPOLE	=	2.34331 DEBYE
NO. OF FILLED LEVELS	=	24
IONIZATION POTENTIAL	=	9.397232 EV
MOLECULAR WEIGHT	=	163.003
SCF CALCULATIONS	=	126

FINAL GEOMETRY OBTAINED

CHARGE

3,4-dichlorophenol

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.1311
C	1.407508	1	0.000000	0	0.000000	0	1	0	0	0.0562
C	1.407522	1	120.122293	1	0.000000	0	2	1	0	-0.0265
C	1.412123	1	119.868771	1	-0.030221	1	3	2	1	-0.0057
C	1.418595	1	120.046351	1	-0.060423	1	1	2	3	0.1270
C	1.400086	1	120.820042	1	0.088462	1	4	3	2	-0.0771
O	1.355467	1	123.189998	1	-179.744713	1	5	1	2	-0.2389
H	1.090199	1	120.079392	1	-179.898245	1	6	4	3	0.0876
H	1.091728	1	120.095930	1	-179.837299	1	4	3	2	0.0830
CL	1.746422	1	121.800652	1	179.999470	1	3	2	1	-0.0797
CL	1.746961	1	121.806670	1	179.981743	1	2	3	1	-0.0773
H	1.091213	1	119.436147	1	-179.911742	1	1	2	3	0.0819
H	0.948495	1	113.236952	1	-1.415172	1	7	5	1	0.2006
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MNDO CALCULATION

VERSION 4.01

C6 H4 O CL2
3,5-dichlorophenol

HERBERTS TEST WAS SATISFIED IN BFGS
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	-40.752238 KCAL/MOL
HEAT OF FORMATION	=	-170.751859 KJ/MOL
ELECTRONIC ENERGY	=	-6869.154482 EV
CORE-CORE REPULSION	=	5014.058551 EV
GRADIENT NORM	=	2.603424
DIPOLE	=	1.95952 DEBYE
NO. OF FILLED LEVELS	=	24
IONIZATION POTENTIAL	=	9.528483 EV
MOLECULAR WEIGHT	=	163.003
SCF CALCULATIONS	=	147

FINAL GEOMETRY OBTAINED

CHARGE

3,5-dichlorophenol

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.1227
C	1.407039	1	0.000000	0	0.000000	0	1	0	0	0.0419
C	1.404662	1	121.998959	1	0.000000	0	2	1	0	-0.0595
C	1.409602	1	118.038330	1	-0.005713	1	3	2	1	0.0323
C	1.420315	1	118.867814	1	-0.099500	1	1	2	3	0.1212
C	1.403095	1	122.228758	1	0.121024	1	4	3	2	-0.0617
O	1.356061	1	123.144996	1	180.037865	1	5	1	2	-0.2391
H	1.090577	1	120.847972	1	179.919240	1	6	4	3	0.0986
CL	1.750790	1	118.805536	1	180.062174	1	4	3	2	-0.0950
H	1.089724	1	121.066792	1	179.983632	1	3	2	1	0.0966
CL	1.750687	1	119.182870	1	179.974607	1	2	3	1	-0.0967
H	1.090158	1	120.082262	1	179.935992	1	1	2	3	0.0836
H	0.948136	1	113.203810	1	0.005164	1	7	5	1	0.2005
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MNDO CALCULATION

VERSION 4.01

C7 H O2 CL5
pentachlorobenzoate

HERBERTS TEST WAS SATISFIED IN BFGS
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	-80.151215	KCAL/MOL
HEAT OF FORMATION	=	-335.833555	KJ/MOL
ELECTRONIC ENERGY	=	-14415.910040	EV
CORE-CORE REPULSION	=	11090.115972	EV
GRADIENT NORM	=	5.326455	
DIPOLE	=	3.39085	DEBYE
NO. OF FILLED LEVELS	=	38	
IONIZATION POTENTIAL	=	10.745647	EV
MOLECULAR WEIGHT	=	294.349	
SCF CALCULATIONS	=	80	

FINAL GEOMETRY OBTAINED

CHARGE

pentachlorobenzoate

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	0.0548
C	1.414772	1	0.000000	0	0.000000	0	1	0	0	0.0160
C	1.412249	1	120.176154	1	0.000000	0	2	1	0	0.0453
C	1.413933	1	120.143894	1	0.118260	1	3	2	1	0.0168
C	1.416017	1	119.983958	1	0.236734	1	1	2	3	-0.1025
C	1.416212	1	119.494059	1	-0.539855	1	5	1	2	0.0546
C	1.515876	1	120.151674	1	176.912155	1	5	1	2	0.3751
O	1.357570	1	119.456891	1	91.054001	1	7	5	1	-0.2630
CL	1.743350	1	119.374896	1	-179.252527	1	6	5	1	-0.0323
CL	1.740584	1	120.219502	1	179.963595	1	4	3	2	-0.0227
CL	1.741050	1	120.011701	1	180.062879	1	3	2	1	-0.0228
CL	1.741398	1	120.052297	1	-179.912781	1	2	3	1	-0.0249
CL	1.741802	1	120.148320	1	-179.592575	1	1	2	3	-0.0296
O	1.223912	1	123.970493	1	-88.942543	1	7	5	1	-0.2723
H	0.947307	1	114.723850	1	0.170090	1	8	7	5	0.2074
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MNDO CALCULATION

VERSION 4.01

C7 H2 O2 CL4
2,3,4,5-tetrachlorobenzoate

HERBERTS TEST WAS SATISFIED IN BFGS
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	-79.818962	KCAL/MOL
HEAT OF FORMATION	=	-334.441418	KJ/MOL
ELECTRONIC ENERGY	=	-12555.713419	EV
CORE-CORE REPULSION	=	9570.142938	EV
GRADIENT NORM	=	6.157515	
DIPOLE	=	3.05621	DEBYE
NO. OF FILLED LEVELS	=	35	
IONIZATION POTENTIAL	=	10.641757	EV
MOLECULAR WEIGHT	=	259.904	
SCF CALCULATIONS	=	94	

FINAL GEOMETRY OBTAINED

CHARGE

2,3,4,5-tetrachlorobenzoate

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	0.0182
C	1.411877	1	0.000000	0	0.000000	0	1	0	0	0.0039
C	1.410579	1	120.028485	1	0.000000	0	2	1	0	0.0464
C	1.416235	1	119.767383	1	-0.121354	1	3	2	1	0.0120
C	1.409437	1	120.797240	1	-0.355879	1	1	2	3	-0.1170
C	1.416670	1	118.951031	1	0.716031	1	5	1	2	0.0542
C	1.510639	1	118.618956	1	178.128113	1	5	1	2	0.3747
O	1.358472	1	119.439049	1	94.890176	1	7	5	1	-0.2692
CL	1.743788	1	119.251013	1	179.584664	1	6	5	1	-0.0433
CL	1.740769	1	119.926135	1	-179.621384	1	4	3	2	-0.0293
CL	1.741231	1	119.936618	1	179.920772	1	3	2	1	-0.0305
CL	1.741834	1	121.782232	1	-179.990000	1	2	3	1	-0.0453
H	1.092791	1	119.270352	1	179.441090	1	1	2	3	0.0992
O	1.224616	1	124.265004	1	-83.003212	1	7	5	1	-0.2811
H	0.947433	1	114.659416	1	5.269610	1	8	7	5	0.2073
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MINDO CALCULATION

VERSION 5.01

07 FEB 02 014

2- 4-1960

2,3,4,6-tetrachlorobenzoic acid

HERBERT'S TEST WAS SATISFIED IN 6405
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION = -75.894755 kcal
ELEC HEAT ENERGY = -12636.921505 eV
CORE-CORE REPULSION = 9553.347737 eV
GRAVITEN. EN. = 12.221655
SCF FIELDS = 3.955500 Debye
NO. OF FILLED LEVELS = 35
IONIZATION POTENTIAL = 10.657557 eV
MOLECULAR WEIGHT = 286.904
SCF CALCULATIONS = 60
COMPUTATION TIME = 16.041 SECONDS

FINAL GEOMETRY OBTAINED

D=4932

2,3,4,6-TETRACHLOROBENZOIC ACID

C	0.000000	0	0.000000	0	0.000000	0	0	0	0.0441	
C	1.406665	1	0.000000	0	0.000000	0	1	0	-0.0257	
C	1.407542	1	120.672620	1	0.000000	0	2	1	0.0212	
C	1.412418	1	119.768609	1	-0.034291	1	3	2	0.0172	
C	1.416223	1	120.125551	1	0.243353	1	1	2	3	-0.1005
C	1.412388	1	119.183606	1	-0.211452	1	4	3	2	0.0517
C	1.514051	1	120.357535	1	-177.418177	1	5	1	2	0.3755
O	1.358150	1	119.185439	1	-90.221762	1	7	5	1	-0.2642
Cl	1.745145	1	119.495213	1	-179.308554	1	6	4	3	-0.0421
Cl	1.741045	1	120.142517	1	179.667344	1	4	3	2	-0.0255
Cl	1.740905	1	118.383822	1	179.933475	1	3	2	1	-0.0430
H	1.093231	1	115.417939	1	-179.625210	1	2	3	1	0.1043
Cl	1.742921	1	118.405557	1	179.851219	1	1	2	3	-0.0515
O	1.223504	1	124.065082	1	89.229655	1	7	5	1	-0.2753
H	0.946965	1	114.423249	1	-1.456290	1	8	7	5	0.2053
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MASC CALCULATION

VERSION 5.01

E7 H2 O2 C14

3- 4-1990

2356-tetrachlorobenzoic acid

HERBERT'S TEST WAS SATISFIED IN RFGS
SCF FIELD WAS PERTURBED

HEAT OF FORMATION = -80.095767 KCAL
ELECTRONIC ENERGY = -10256.888862 EV
CORE-CORE REPELSION = 9571.307444 EV
GRADIENT NORM = 7.19E-222
DIPOLE = 4.27905 DEBYE
NO. OF FILLED LEVELS = 36
IONIZATION POTENTIAL = 10.551264 EV
MOLECULAR WEIGHT = 269.514
SCF CALCULATIONS = 102
COMPUTATION TIME = 34.612 SECONDS

FINAL GEOMETRY OBTAINED

2-4933

2356-tetrachlorobenzoic acid

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	0.0024
C	1.407848	1	0.000000	0	0.000000	0	1	0	0	0.0022
C	1.408714	1	119.882253	1	0.000000	0	2	1	0	0.0050
C	1.413200	1	119.941079	1	0.443229	1	3	2	1	0.0559
C	1.410247	1	120.018158	1	-0.209150	1	1	2	3	0.0552
C	1.417100	1	120.923688	1	-0.243213	1	5	1	2	-0.1052
C	1.512988	1	120.760369	1	-177.217826	1	6	5	1	0.3763
O	1.358209	1	119.358076	1	-90.749382	1	7	6	5	-0.2647
Cl	1.745406	1	119.801017	1	-179.893099	1	4	3	2	-0.0420
Cl	1.741676	1	118.241542	1	-179.593802	1	3	2	1	-0.0445
H	1.092327	1	120.029693	1	179.985508	1	2	3	1	0.1064
Cl	1.742545	1	118.079682	1	179.506586	1	1	2	3	-0.0453
Cl	1.745023	1	119.635337	1	179.531572	1	5	1	2	-0.0422
O	1.224353	1	124.145571	1	89.124029	1	7	6	5	-0.2749
H	0.947414	1	114.684763	1	-0.135638	1	8	7	6	0.2068
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MNDO CALCULATION

VERSION 4.01

C7 H3 O2 CL3
2,3,4-trichlorobenzoate

HERBERTS TEST WAS SATISFIED IN BFGS
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	-77.004832	KCAL/MOL
HEAT OF FORMATION	=	-322.650213	KJ/MOL
ELECTRONIC ENERGY	=	-10939.140667	EV
CORE-CORE REPULSION	=	8293.901396	EV
GRADIENT NORM	=	4.487103	
DIPOLE	=	3.85569	DEBYE
NO. OF FILLED LEVELS	=	32	
IONIZATION POTENTIAL	=	10.550055	EV
MOLECULAR WEIGHT	=	225.458	
SCF CALCULATIONS	=	81	

FINAL GEOMETRY OBTAINED

CHARGE

2,3,4-trichlorobenzoate

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	0.0042
C	1.406662	1	0.000000	0	0.000000	0	1	0	0	-0.0409
C	1.406488	1	120.322918	1	0.000000	0	2	1	0	0.0353
C	1.412977	1	120.136235	1	-0.245230	1	3	2	1	0.0124
C	1.412559	1	120.291055	1	-0.156562	1	1	2	3	-0.1197
C	1.414779	1	119.152152	1	0.502423	1	5	1	2	0.0498
C	1.510165	1	118.565816	1	178.082473	1	5	1	2	0.3748
O	1.358840	1	119.432520	1	96.147477	1	7	5	1	-0.2713
CL	1.746747	1	119.195517	1	179.367692	1	6	5	1	-0.0525
CL	1.741181	1	120.232157	1	-179.503165	1	4	3	2	-0.0377
CL	1.743768	1	118.427836	1	179.856249	1	3	2	1	-0.0552
H	1.091563	1	120.092471	1	179.834663	1	2	3	1	0.0932
H	1.091535	1	119.066400	1	179.506931	1	1	2	3	0.0876
O	1.224969	1	124.290782	1	-81.560715	1	7	5	1	-0.2863
H	0.947280	1	114.502293	1	6.341979	1	8	7	5	0.2064
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF SCF CALCULATION

VERSION 5.01

07 H3 02 013

1- 4-1990

2,3,5-trichlorobenzoic acid

HERBERT'S TEST WAS SATISFIED IN 8765
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION = -75.830946 KCAL
ELECTRONIC ENERGY = -10854.049968 EV
CORE-CORE REPELSION = 8248.731208 EV
GRADIENT NORM = 10.210871
DIPOLE = 3.87058 DEBYE
NO. OF FILLED LEVELS = 32
IONIZATION POTENTIAL = 10.475841 EV
MOLECULAR WEIGHT = 220.455
SCF CALCULATIONS = 85
COMPUTATION TIME = 22.798 SECONDS

FINAL GEOMETRY OBTAINED

1-4-90

2,3,5-trichlorobenzoic acid

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.0083
C	1.402216	1	0.000000	0	0.000000	0	1	0	0	0.0001
C	1.408847	1	120.653445	1	0.000000	0	2	1	0	0.0020
C	1.411034	1	119.723812	1	-0.077502	1	3	2	1	0.0562
C	1.410282	1	119.695746	1	-0.101389	1	1	2	3	0.0157
C	1.414881	1	120.429966	1	0.210119	1	2	1	2	-0.1240
C	1.510577	1	118.472726	1	-178.269045	1	6	5	1	0.3755
C	1.359594	1	119.217162	1	-92.533217	1	7	6	5	-0.2718
Cl	1.745435	1	120.419513	1	-179.245753	1	4	3	2	-0.0512
Cl	1.742462	1	118.363988	1	-175.899951	1	3	2	1	-0.0514
H	1.093104	1	119.432793	1	180.036554	1	2	3	1	0.0938
Cl	1.742622	1	120.250927	1	179.674578	1	1	2	3	-0.0620
H	1.092444	1	119.624486	1	-179.568894	1	5	1	2	0.0945
O	1.224695	1	124.536897	1	85.638014	1	7	6	5	-0.2839
H	0.947413	1	114.558409	1	-5.430859	1	8	7	6	0.2053
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MNDO CALCULATION

VERSION 4.01

C7 H3 O2 CL3
2,3,6-trichlorobenzoate

HERBERTS TEST WAS SATISFIED IN BFGS
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	-80.813127	KCAL/MOL
HEAT OF FORMATION	=	-338.606968	KJ/MOL
ELECTRONIC ENERGY	=	-11029.551821	EV
CORE-CORE REPULSION	=	8384.147410	EV
GRADIENT NORM	=	4.148364	
DIPOLE	=	2.58369	DEBYE
NO. OF FILLED LEVELS	=	32	
IONIZATION POTENTIAL	=	10.277962	EV
MOLECULAR WEIGHT	=	225.458	
SCF CALCULATIONS	=	90	

FINAL GEOMETRY OBTAINED

CHARGE

2,3,6-trichlorobenzoate

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	0.0532
C	1.410874	1	0.000000	0	0.000000	0	1	0	0	0.0071
C	1.410046	1	119.995502	1	0.000000	0	2	1	0	-0.0141
C	1.402418	1	120.351125	1	-0.025324	1	3	2	1	-0.0376
C	1.419375	1	120.516194	1	0.058882	1	1	2	3	-0.0468
C	1.409761	1	119.326574	1	-0.043981	1	4	3	2	0.0466
C	1.505635	1	120.863849	1	-179.093983	1	5	1	2	0.3943
O	1.355659	1	113.840289	1	-90.639130	1	7	5	1	-0.2881
CL	1.748739	1	117.695567	1	180.036845	1	6	4	3	-0.0735
H	1.090611	1	119.777758	1	179.970303	1	4	3	2	0.0939
H	1.091623	1	120.286131	1	179.949386	1	3	2	1	0.0910
CL	1.743944	1	118.220319	1	179.999085	1	2	3	1	-0.0587
CL	1.746040	1	119.910883	1	-179.899604	1	1	2	3	-0.0538
O	1.227738	1	125.946222	1	89.499151	1	7	5	1	-0.3347
H	0.950027	1	115.307831	1	-179.976124	1	8	7	5	0.2212
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MNDO CALCULATION

VERSION 4.01

C7 H3 O2 CL3
2,4,5-trichlorobenzoate

HERBERTS TEST WAS SATISFIED IN BFGS
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	-79.274769	KCAL/MOL
HEAT OF FORMATION	=	-332.161249	KJ/MOL
ELECTRONIC ENERGY	=	-10862.838881	EV
CORE-CORE REPULSION	=	8217.501178	EV
GRADIENT NORM	=	6.357673	
DIPOLE	=	3.35291	DEBYE
NO. OF FILLED LEVELS	=	32	
IONIZATION POTENTIAL	=	10.514971	EV
MOLECULAR WEIGHT	=	225.458	
SCF CALCULATIONS	=	108	

FINAL GEOMETRY OBTAINED

CHARGE

2,4,5-trichlorobenzoate

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	0.0128
C	1.409554	1	0.000000	0	0.000000	0	1	0	0	0.0040
C	1.410079	1	119.752670	1	0.000000	0	2	1	0	0.0361
C	1.409167	1	120.243826	1	-0.253534	1	3	2	1	-0.0288
C	1.414121	1	120.950584	1	-0.505060	1	1	2	3	-0.1185
C	1.414945	1	118.209243	1	0.892292	1	5	1	2	0.0438
C	1.508410	1	119.050033	1	178.324433	1	5	1	2	0.3759
O	1.359073	1	119.361128	1	95.365765	1	7	5	1	-0.2711
CL	1.747526	1	120.677207	1	179.585081	1	6	5	1	-0.0691
H	1.091259	1	120.154360	1	-179.376850	1	4	3	2	0.1053
CL	1.743752	1	121.507719	1	179.899572	1	3	2	1	-0.0548
CL	1.742697	1	121.798820	1	179.991485	1	2	3	1	-0.0533
H	1.092621	1	119.161030	1	179.463547	1	1	2	3	0.0959
O	1.224795	1	124.403063	1	-83.059539	1	7	5	1	-0.2346
H	0.947316	1	114.531157	1	4.451398	1	8	7	5	0.2063
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MNDO CALCULATION

VERSION 4.01

C7 H3 O2 CL3
3,4,5-trichlorobenzoate

HERBERTS TEST WAS SATISFIED IN BFGS
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	-78.537676	KCAL/MOL
HEAT OF FORMATION	=	-329.072829	KJ/MOL
ELECTRONIC ENERGY	=	-10798.832705	EV
CORE-CORE REPULSION	=	8153.526964	EV
GRADIENT NORM	=	11.123899	
DIPOLE	=	2.61440	DEBYE
NO. OF FILLED LEVELS	=	32	
IONIZATION POTENTIAL	=	10.563539	EV
MOLECULAR WEIGHT	=	225.458	
SCF CALCULATIONS	=	98	

FINAL GEOMETRY OBTAINED

CHARGE

3,4,5-trichlorobenzoate

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.0008
C	1.412592	1	0.000000	0	0.000000	0	1	0	0	0.0484
C	1.409671	1	118.901476	1	0.000000	0	2	1	0	-0.0001
C	1.409590	1	120.787824	1	0.285228	1	3	2	1	0.0155
C	1.410317	1	120.401338	1	-0.189741	1	1	2	3	0.0173
C	1.410869	1	120.603043	1	-0.255601	1	5	1	2	-0.1351
C	1.507535	1	120.337305	1	178.361551	1	6	5	1	0.3725
O	1.359773	1	119.092659	1	98.952000	1	7	6	5	-0.2761
H	1.088668	1	120.218085	1	-179.439934	1	4	3	2	0.0934
CL	1.745479	1	121.466921	1	-179.805606	1	3	2	1	-0.0567
CL	1.740409	1	120.513465	1	-179.977019	1	2	3	1	-0.0363
CL	1.743826	1	121.324101	1	179.836408	1	1	2	3	-0.0545
H	1.093168	1	119.396250	1	179.587110	1	5	1	2	0.0940
O	1.224858	1	124.673770	1	-81.334358	1	7	6	5	-0.2876
H	0.947201	1	114.486872	1	-7.460785	1	8	7	6	0.2062
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MNDO CALCULATION

VERSION 5.01

C7 H4 O2 Cl2

22- 3-1990

2,5-dichlorobenzoate

HERBERTS TEST WAS SATISFIED IN BFGS
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION = -75.866070 KCAL
ELECTRONIC ENERGY = -9357.165451 EV
CORE-CORE REPULSION = 7052.184740 EV
DIPOLE = 4.47325 DEBYE
NO. OF FILLED LEVELS = 29
IONIZATION POTENTIAL = 10.307464 EV
MOLECULAR WEIGHT = 191.013
SCF CALCULATIONS = 45
COMPUTATION TIME = 16.742 SECONDS

FINAL GEOMETRY OBTAINED CHARGE
PRECISE
2,5-dichlorobenzoate

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	0.0446
C	1.408495	1	0.000000	0	0.000000	0	1	0	0	-0.0459
C	1.406198	1	119.885007	1	0.000000	0	2	1	0	-0.0086
C	1.407350	1	119.121086	1	-0.027710	1	3	2	1	-0.0073
C	1.414459	1	121.280900	1	0.156142	1	1	2	3	-0.1255
C	1.407474	1	121.249144	1	-0.269809	1	4	3	2	0.0113
C	1.508046	1	122.546522	1	177.697401	1	5	1	2	0.3766
O	1.359676	1	119.305650	1	88.531962	1	7	5	1	-0.2735
H	1.091795	1	119.969791	1	-179.328216	1	6	4	3	0.0926
Cl	1.747595	1	119.438788	1	179.785192	1	4	3	2	-0.0832
H	1.090597	1	119.779225	1	180.040369	1	3	2	1	0.0899
H	1.090888	1	119.454296	1	179.905996	1	2	3	1	0.0909
Cl	1.748832	1	118.010216	1	-179.642306	1	1	2	3	-0.0786
O	1.225104	1	124.563435	1	-93.244199	1	7	5	1	-0.2887
H	0.947217	1	114.441869	1	-4.863546	1	8	7	5	0.2053
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MNDO CALCULATION

VERSION 4.01

C7 H4 O2 CL2
2,3-dichlorobenzoate

HERBERTS TEST WAS SATISFIED IN BFGS
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	-76.955231	KCAL/MOL
HEAT OF FORMATION	=	-322.442386	KJ/MOL
ELECTRONIC ENERGY	=	-9420.158905	EV
CORE-CORE REPULSION	=	7115.130964	EV
GRADIENT NORM	=	6.377407	
DIPOLE	=	3.09221	DEBYE
NO. OF FILLED LEVELS	=	29	
IONIZATION POTENTIAL	=	10.130790	EV
MOLECULAR WEIGHT	=	191.013	
SCF CALCULATIONS	=	74	

FINAL GEOMETRY OBTAINED

CHARGE

2,3-dichlorobenzoate

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.0013
C	1.408642	1	0.000000	0	0.000000	0	1	0	0	-0.0562
C	1.403429	1	119.794467	1	0.000000	0	2	1	0	-0.0149
C	1.413007	1	120.068329	1	-0.094699	1	3	2	1	0.0019
C	1.407927	1	120.170451	1	0.039319	1	4	3	2	0.0560
C	1.419128	1	120.086792	1	0.104953	1	5	4	3	-0.0674
C	1.501965	1	122.111377	1	-179.266567	1	6	5	4	0.3932
O	1.356093	1	114.140453	1	-88.018950	1	7	6	5	-0.2926
H	1.091758	1	118.922050	1	179.990315	1	1	2	3	0.0774
H	1.089972	1	120.077180	1	179.699529	1	2	3	1	0.0788
H	1.091040	1	119.632257	1	-179.907691	1	3	2	1	0.0857
CL	1.745482	1	117.769028	1	-179.913249	1	4	3	2	-0.0688
CL	1.747092	1	120.418497	1	-179.778839	1	5	4	3	-0.0647
O	1.228849	1	125.988372	1	93.584803	1	7	6	5	-0.3462
H	0.949792	1	115.438440	1	178.256196	1	8	7	6	0.2191
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MNDO CALCULATION

VERSION 4.01

C7 H4 O2 CL2
2,6-dichlorobenzoate

HERBERTS TEST WAS SATISFIED IN BFGS
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	-77.335148	KCAL/MOL
HEAT OF FORMATION	=	-324.034236	KJ/MOL
ELECTRONIC ENERGY	=	-9501.388847	EV
CORE-CORE REPULSION	=	7196.344432	EV
GRADIENT NORM	=	3.843622	
DIPOLE	=	3.14172	DEBYE
NO. OF FILLED LEVELS	=	29	
IONIZATION POTENTIAL	=	10.152753	EV
MOLECULAR WEIGHT	=	191.013	
SCF CALCULATIONS	=	92	

FINAL GEOMETRY OBTAINED

CHARGE

2,6-dichlorobenzoate

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	0.0422
C	1.408422	1	0.000000	0	0.000000	0	1	0	0	-0.0410
C	1.404333	1	119.863816	1	0.000000	0	2	1	0	-0.0297
C	1.406072	1	120.011675	1	-0.005555	1	3	2	1	-0.0401
C	1.415741	1	121.481669	1	0.053721	1	1	2	3	-0.0485
C	1.407352	1	119.533640	1	-0.039033	1	4	3	2	0.0416
C	1.504200	1	121.330948	1	-178.972035	1	5	1	2	0.3968
O	1.355785	1	113.810619	1	-90.405761	1	7	5	1	-0.2899
CL	1.750179	1	117.762059	1	179.991684	1	6	4	3	-0.0831
H	1.090734	1	119.757539	1	179.954320	1	4	3	2	0.0880
H	1.090586	1	120.003259	1	179.973577	1	3	2	1	0.0781
H	1.091123	1	119.639355	1	-179.952695	1	2	3	1	0.0873
CL	1.750057	1	117.805065	1	-179.762100	1	1	2	3	-0.0820
O	1.228012	1	126.158120	1	89.465433	1	7	5	1	-0.3393
H	0.949789	1	115.393106	1	-179.992221	1	8	7	5	0.2195
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MNDO CALCULATION

VERSION 4.01

C7 H4 O2 CL2
3,4-dichlorobenzoate

HERBERTS TEST WAS SATISFIED IN BFGS
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	-70.685933	KCAL/MOL
HEAT OF FORMATION	=	-296.174030	KJ/MOL
ELECTRONIC ENERGY	=	-9261.829549	EV
CORE-CORE REPULSION	=	6957.073465	EV
GRADIENT NORM	=	5.390804	
DIPOLE	=	3.97671	DEBYE
NO. OF FILLED LEVELS	=	29	
IONIZATION POTENTIAL	=	10.403617	EV
MOLECULAR WEIGHT	=	191.013	
SCF CALCULATIONS	=	57	

FINAL GEOMETRY OBTAINED

CHARGE

3,4-dichlorobenzoate

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.0126
C	1.402713	1	0.000000	0	0.000000	0	1	0	0	-0.0527
C	1.409218	1	120.843835	1	0.000000	0	2	1	0	0.0436
C	1.407847	1	119.242454	1	0.000598	1	3	2	1	-0.0076
C	1.418119	1	120.736346	1	0.119873	1	1	2	3	-0.1255
C	1.409390	1	119.876948	1	0.078626	1	4	3	2	0.0325
C	1.507336	1	123.663228	1	179.581504	1	5	1	2	0.3701
O	1.360754	1	122.428315	1	-2.525412	1	7	5	1	-0.2784
H	1.094179	1	118.007599	1	179.742110	1	6	4	3	0.1045
CL	1.744570	1	121.721577	1	179.931266	1	4	3	2	-0.0608
CL	1.743339	1	118.762727	1	-179.459921	1	3	2	1	-0.0613
H	1.091677	1	120.009971	1	179.999145	1	2	3	1	0.0877
H	1.090451	1	117.255892	1	-179.787949	1	1	2	3	0.0657
O	1.229651	1	124.194240	1	177.365954	1	7	5	1	-0.3071
H	0.944545	1	115.921033	1	-2.758717	1	8	7	5	0.2018
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MNDO CALCULATION

VERSION 4.01

C7 H4 O2 CL2
2,4-dichlorobenzoate

HERBERTS TEST WAS SATISFIED IN BFGS
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	-75.794563	KCAL/MOL
HEAT OF FORMATION	=	-317.579187	KJ/MOL
ELECTRONIC ENERGY	=	-9337.739385	EV
CORE-CORE REPULSION	=	7032.761775	EV
GRADIENT NORM	=	4.656049	
DIPOLE	=	3.93274	DEBYE
NO. OF FILLED LEVELS	=	29	
IONIZATION POTENTIAL	=	10.429085	EV
MOLECULAR WEIGHT	=	191.013	
SCF CALCULATIONS	=	82	

FINAL GEOMETRY OBTAINED

CHARGE

2,4-dichlorobenzoate

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.0022
C	1.408481	1	0.000000	0	0.000000	0	1	0	0	-0.0426
C	1.405008	1	119.957405	1	0.000000	0	2	1	0	0.0243
C	1.408743	1	120.670483	1	-0.220054	1	3	2	1	-0.0297
C	1.413674	1	120.621853	1	-0.231415	1	1	2	3	-0.1211
C	1.416215	1	118.301205	1	0.445661	1	5	1	2	0.0386
C	1.507817	1	119.039834	1	178.139489	1	5	1	2	0.3764
O	1.359868	1	119.385576	1	96.106497	1	7	5	1	-0.2739
CL	1.749528	1	120.631748	1	179.958037	1	6	5	1	-0.0787
H	1.091240	1	120.607720	1	-179.358091	1	4	3	2	0.1010
CL	1.746363	1	119.821280	1	179.909671	1	3	2	1	-0.0801
H	1.091118	1	120.828478	1	179.844793	1	2	3	1	0.0891
H	1.091441	1	118.858128	1	179.531129	1	1	2	3	0.0835
O	1.225245	1	124.505610	1	-82.023785	1	7	5	1	-0.2900
H	0.947353	1	114.478012	1	5.276109	1	8	7	5	0.2055
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MNDO CALCULATION

VERSION 4.01

06 H2 O2 CL4
3,4,5,6-tetrachlorocatechol

HERBERTS TEST WAS SATISFIED IN RFOBS
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION = -89.651770 KCAL/MOL
HEAT OF FORMATION = -375.640880 KJ/MOL
ELECTRONIC ENERGY = -11667.013491 EV
CORE-CORE REPULSION = 8808.927581 EV
DIPOLE = 1.58474 DEBYE
NO. OF FILLED LEVELS = 33
IONIZATION POTENTIAL = 9.498460 EV
MOLECULAR WEIGHT = 247.893
SCF CALCULATIONS = 155

FINAL GEOMETRY OBTAINED

CHARGE

3,4,5,6-tetrachlorocatechol

C1	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.0516
C	1.416988	1	0.000000	0	0.000000	0	1	0	0	0.0284
C	1.404910	1	119.802520	1	0.000000	0	2	1	0	0.0283
C	1.416785	1	120.314654	1	0.108536	1	3	2	1	-0.0519
C	1.414383	1	120.987322	1	0.039551	1	1	2	3	0.1304
C	1.450113	1	119.122764	1	-0.163291	1	5	1	2	0.1308
O	1.350432	1	124.841713	1	179.817649	1	5	1	2	-0.2133
O	1.349866	1	116.085646	1	-179.820300	1	6	5	1	-0.2125
CL	1.748506	1	119.619087	1	179.930081	1	4	3	2	-0.0646
CL	1.743987	1	120.043252	1	-179.919425	1	3	2	1	-0.0436
CL	1.742968	1	120.320164	1	179.991905	1	2	3	1	-0.0415
CL	1.749080	1	119.478213	1	180.030716	1	1	2	3	-0.0656
H	0.949145	1	114.313459	1	0.372984	1	7	5	1	0.2135
H	0.949250	1	114.231372	1	-179.801141	1	8	6	5	0.2134
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MNDO CALCULATION

VERSION 4.01

C6 H3 O2 CL3
3,4,5-trichlorocatechol

HERBERTS TEST WAS SATISFIED IN BFGS
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	-88.763064	KCAL/MOL
HEAT OF FORMATION	=	-371.917201	KJ/MOL
ELECTRONIC ENERGY	=	-10020.450939	EV
CORE-CORE REPULSION	=	7502.612745	EV
GRADIENT NORM	=	10.316257	
DIPOLE	=	2.65874	DEBYE
NO. OF FILLED LEVELS	=	30	
IONIZATION POTENTIAL	=	9.382755	EV
MOLECULAR WEIGHT	=	213.447	
SCF CALCULATIONS	=	129	

FINAL GEOMETRY OBTAINED

CHARGE

3,4,5-trichlorocatechol

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.0424
C	1.409763	1	0.000000	0	0.000000	0	1	0	0	0.0125
C	1.407796	1	120.113788	1	0.000000	0	2	1	0	0.0241
C	1.413389	1	119.810813	1	-0.549913	1	3	2	1	-0.0347
C	1.415379	1	121.097308	1	0.804085	1	1	2	3	0.1140
C	1.440961	1	118.939913	1	-0.616699	1	5	1	2	0.0684
O	1.352879	1	116.311142	1	179.593593	1	5	1	2	-0.2356
O	1.356076	1	116.044658	1	-179.954167	1	6	5	1	-0.2544
CL	1.750254	1	119.605405	1	179.870199	1	4	3	2	-0.0737
CL	1.744292	1	120.037003	1	179.687861	1	3	2	1	-0.0515
CL	1.744483	1	121.862099	1	-179.814217	1	2	3	1	-0.0635
H	1.092681	1	119.332037	1	-179.557070	1	1	2	3	0.1011
H	0.947912	1	114.787828	1	-179.486809	1	7	5	1	0.2168
H	0.948371	1	114.310581	1	178.118657	1	8	6	5	0.2191
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MNDO CALCULATION

VERSION 5.01

C6 H4 O2 C12

21- 3-1990

4,5-dichlorocatechol

HERBERTS TEST WAS SATISFIED IN BFGS
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION = -86.177374 KCAL
ELECTRONIC ENERGY = -8459.528860 EV
CORE-CORE REPULSION = 6282.011970 EV
DIPOLE = 3.22033 DEBYE
NO. OF FILLED LEVELS = 27
IONIZATION POTENTIAL = 9.170313 EV
MOLECULAR WEIGHT = 179.002
SCF CALCULATIONS = 46
COMPUTATION TIME = 14.055 SECONDS

FINAL GEOMETRY OBTAINED									CHARGE
PRECISE									
4,5-dichlorocatechol									
C	0.000000	0	0.000000	0	0.000000	0	0	0	-0.0466
C	1.408016	1	0.000000	0	0.000000	0	1	0	0.0142
C	1.406793	1	120.545122	1	0.000000	0	2	1	0.0110
C	1.407750	1	120.333044	1	-0.001633	1	3	2	-0.0817
C	1.419040	1	120.096108	1	0.001343	1	1	2	0.1120
C	1.438231	1	119.154621	1	-0.000705	1	5	1	0.0421
O	1.354267	1	116.224803	1	179.998056	1	5	1	-0.2398
O	1.360328	1	117.326465	1	180.008420	1	6	5	-0.2594
H	1.091297	1	119.490531	1	180.000151	1	4	3	0.0829
Cl	1.747156	1	121.727141	1	179.990383	1	3	2	-0.0783
Cl	1.747132	1	121.491192	1	180.000878	1	2	3	-0.0760
H	1.091564	1	119.916954	1	180.002063	1	1	2	0.0996
H	0.947437	1	114.589743	1	-179.998782	1	7	5	0.2135
H	0.947622	1	113.151759	1	179.998987	1	8	6	0.2065
O	0.000000	0	0.000000	0	0.000000	0	0	0	0

SUMMARY OF MNDO CALCULATION

VERSION 5.01

C6 H4 O2 Cl2

13- 3-1990

3,4-dichlorocatechol

HERBERTS TEST WAS SATISFIED IN BFGS
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION = -83.591412 KCAL
ELECTRONIC ENERGY = -8534.116763 EV
CORE-CORE REPULSION = 6356.712008 EV
GRADIENT NORM = 2.738719
DIPOLE = 2.37360 DEBYE
NO. OF FILLED LEVELS = 27
IONIZATION POTENTIAL = 9.093790 EV
MOLECULAR WEIGHT = 179.002
SCF CALCULATIONS = 209
COMPUTATION TIME = 55.644 SECONDS

FINAL GEOMETRY OBTAINED

CHARGE

3,4-dichlorocatechol

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.1088
C	1.406936	1	0.000000	0	0.000000	0	1	0	0	-0.0327
C	1.402496	1	119.772408	1	0.000000	0	2	1	0	0.0156
C	1.412647	1	120.831467	1	-0.001145	1	3	2	1	-0.0507
C	1.412735	1	120.741077	1	0.050543	1	1	2	3	0.0985
C	1.444791	1	119.704309	1	-0.041708	1	5	1	2	0.1198
O	1.356243	1	123.079887	1	179.960148	1	5	1	2	-0.2228
O	1.352145	1	116.541574	1	-179.974957	1	6	5	1	-0.2201
Cl	1.750110	1	119.846680	1	180.015251	1	4	3	2	-0.0806
Cl	1.747874	1	117.962574	1	179.997886	1	3	2	1	-0.0799
H	1.090398	1	120.919091	1	-179.982810	1	2	3	1	0.0846
H	1.091350	1	118.452725	1	-179.997198	1	1	2	3	0.0729
H	0.948575	1	112.735736	1	0.032200	1	7	5	1	0.1963
H	0.948750	1	113.996981	1	180.029739	1	8	6	5	0.2078
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MNDO CALCULATION

VERSION 5.01

C6 H2 O2 Cl4

7- 3-1990

2,4,5,6-chlororesorcinol

HERBERTS TEST WAS SATISFIED IN BFGS
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION = -90.166525 KCAL
ELECTRONIC ENERGY = -11665.643013 EV
CORE-CORE REPULSION = 8807.534781 EV
GRADIENT NORM = 6.787970
DIPOLE = 3.35570 DEBYE
NO. OF FILLED LEVELS = 33
IONIZATION POTENTIAL = 9.589263 EV
MOLECULAR WEIGHT = 247.893
SCF CALCULATIONS = 94
COMPUTATION TIME = 43.069 SECONDS

FINAL GEOMETRY OBTAINED

CHARGE

2,4,5,6-chlororesorcinol

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.0752
C	1.409094	1	0.000000	0	0.000000	0	1	0	0	0.1047
C	1.408574	1	120.003733	1	0.000000	0	2	1	0	-0.0740
C	1.429503	1	120.544352	1	-0.281597	1	3	2	1	0.2208
C	1.425993	1	120.922786	1	0.517615	1	1	2	3	0.2209
C	1.422915	1	118.660637	1	-0.208818	1	5	1	2	-0.1877
O	1.346503	1	117.145261	1	179.886661	1	5	1	2	-0.2137
O	1.345787	1	116.872094	1	-179.764572	1	4	3	2	-0.2140
Cl	1.753688	1	119.484196	1	-179.937483	1	6	5	1	-0.0920
Cl	1.745552	1	119.851267	1	179.317724	1	3	2	1	-0.0453
Cl	1.742905	1	120.296009	1	-179.720579	1	2	3	1	-0.0355
Cl	1.746507	1	119.650055	1	-179.689261	1	1	2	3	-0.0466
H	0.948822	1	114.736482	1	179.853811	1	7	5	1	0.2186
H	0.949992	1	114.837793	1	179.778416	1	8	4	3	0.2191
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MNDO CALCULATION

VERSION 5.01

C6 H3 O2 Cl3

13- 3-1990

2,4,5-TRICHLORORESORCINOL

HERBERTS TEST WAS SATISFIED IN BFGS
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION = -88.952967 KCAL
ELECTRONIC ENERGY = -10022.062016 EV
CORE-CORE REPULSION = 7504.215587 EV
GRADIENT NORM = 4.770350
DIPOLE = 2.97346 DEBYE
NO. OF FILLED LEVELS = 30
IONIZATION POTENTIAL = 9.457775 EV
MOLECULAR WEIGHT = 213.447
SCF CALCULATIONS = 220
COMPUTATION TIME = 1 MINUTES AND 7.420 SECONDS

FINAL GEOMETRY OBTAINED

CHARGE

2,4,5-TRICHLORORESORCINOL

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.1152
C	1.401937	1	0.000000	0	0.000000	0	1	0	0	0.0893
C	1.410546	1	121.471223	1	0.000000	0	2	1	0	-0.0710
C	1.427894	1	119.477301	1	0.354355	1	3	2	1	0.2091
C	1.423747	1	119.793367	1	-0.364670	1	1	2	3	0.1975
C	1.422038	1	119.432622	1	0.031699	1	5	1	2	-0.1819
O	1.349625	1	115.775453	1	-179.833855	1	5	1	2	-0.2294
O	1.348237	1	116.841093	1	-179.941851	1	4	3	2	-0.2188
Cl	1.753625	1	119.721628	1	-179.788511	1	6	5	1	-0.0986
Cl	1.744300	1	120.263057	1	-179.665501	1	3	2	1	-0.0501
Cl	1.746874	1	120.999828	1	179.743547	1	2	3	1	-0.0654
H	1.091628	1	120.336985	1	179.743181	1	1	2	3	0.1043
H	0.948332	1	114.615966	1	-179.923265	1	7	5	1	0.2143
H	0.950169	1	114.581929	1	-178.812022	1	8	4	3	0.2159
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MNDO CALCULATION

VERSION 5.01

C6 H4 O2 Cl2

21- 3-1990

2,4-dichlororesorcinol

HERBERTS TEST WAS SATISFIED IN BFGS
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION = -85.444396 KCAL
ELECTRONIC ENERGY = -8533.186055 EV
CORE-CORE REPULSION = 6355.700949 EV
DIPOLE = 1.86745 DEBYE
NO. OF FILLED LEVELS = 27
IONIZATION POTENTIAL = 9.216961 EV
MOLECULAR WEIGHT = 179.002
SCF CALCULATIONS = 202
COMPUTATION TIME = 52.702 SECONDS

FINAL GEOMETRY OBTAINED CHARGE
PRECISE GRAD
2,4-dichlororesorcinol

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.1282
C	1.399052	1	0.000000	0	0.000000	0	1	0	0	0.0382
C	1.407439	1	120.796502	1	0.000000	0	2	1	0	-0.0800
C	1.423517	1	120.614247	1	-0.039108	1	3	2	1	0.2047
C	1.424859	1	120.007303	1	0.011477	1	1	2	3	0.1929
C	1.421994	1	119.379242	1	0.014329	1	5	1	2	-0.1832
O	1.350358	1	115.950838	1	-179.988552	1	5	1	2	-0.2337
O	1.348669	1	117.359063	1	-179.962790	1	4	3	2	-0.2219
Cl	1.755261	1	119.719552	1	179.986875	1	6	5	1	-0.1072
Cl	1.748212	1	117.992884	1	179.975855	1	3	2	1	-0.0792
H	1.091980	1	120.097108	1	-179.989006	1	2	3	1	0.0830
H	1.090378	1	119.603935	1	180.011540	1	1	2	3	0.0897
H	0.948464	1	114.521265	1	-179.977416	1	7	5	1	0.2117
H	0.948731	1	114.468956	1	180.027744	1	8	4	3	0.2131
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MNDO CALCULATION

VERSION 5.01

C6 H4 O2 Cl2

22- 3-1990

4,5-dichlororesorcinol

HERBERTS TEST WAS SATISFIED IN BFGS
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION = -86.025141 KCAL
ELECTRONIC ENERGY = -8473.503235 EV
CORE-CORE REPULSION = 6295.992945 EV
DIPOLE = 2.44820 DEBYE
NO. OF FILLED LEVELS = 27
IONIZATION POTENTIAL = 9.336703 EV
MOLECULAR WEIGHT = 179.002
SCF CALCULATIONS = 45
COMPUTATION TIME = 13.506 SECONDS

FINAL GEOMETRY OBTAINED									CHARGE
PRECISE									
4,5-dichlororesorcinol									
C	0.000000	0	0.000000	0	0.000000	0	0	0	-0.1076
C	1.401016	1	0.000000	0	0.000000	0	1	0	0.0877
C	1.411418	1	121.609515	1	0.000000	0	2	1	-0.1202
C	1.424146	1	119.375637	1	-0.012986	1	3	2	0.1867
C	1.425752	1	118.975244	1	0.020964	1	1	2	0.1612
C	1.415417	1	120.534983	1	-0.016562	1	5	1	-0.1763
O	1.354047	1	116.579660	1	179.987107	1	5	1	-0.2370
O	1.351780	1	124.565480	1	180.000506	1	4	3	-0.2372
H	1.090820	1	120.807784	1	-179.996538	1	6	5	0.0874
Cl	1.748775	1	120.392872	1	179.989821	1	3	2	-0.0833
Cl	1.749197	1	120.843085	1	180.007588	1	2	3	-0.0769
H	1.090311	1	120.653644	1	180.012665	1	1	2	0.1000
H	0.948465	1	113.369226	1	179.995546	1	7	5	0.2025
H	0.948556	1	114.331335	1	-0.001347	1	8	4	0.2129
O	0.000000	0	0.000000	0	0.000000	0	0	0	0

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faded.

SUMMARY OF RMC0 CALCULATION

VERSION 5.01

06 FEB 08 2014

EL- 3-1981

2,3,5-Enterocyanonylhydroxycarbene

RESTART TEST WAS SATISFIED IN FREE
SCF FIELD WAS PROVIDED

HEAT OF FORMATION = -69.800748 KCAL
ELECTRONIC ENERGY = -1.0660112897 EV
CORE-CORE REACTION = 2871.026424 EV
DIPOLE = 1.374817 DEBYE
NO. OF FILLED LEVELS = 22
IONIZATION POTENTIAL = 8.437459 EV
MOLECULAR WEIGHT = 240.059
SCF ITERATIONS = 189
CONVERGENCE TIME = 57.455 SECONDS

FINAL GEOMETRY OBTAINED

D-9422

PRECISE 9422

2,3,5-Enterocyanonylhydroxycarbene

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.0390
C	1.401887	1	0.000000	0	0.000000	0	1	0	0	-0.0390
C	1.428823	1	120.565555	1	0.000000	0	2	1	0	0.1204
C	1.421338	1	118.771845	1	0.000221	1	3	2	1	0.0148
O	1.351358	1	124.440357	1	179.998070	1	2	2	1	-0.2800
C	1.493308	1	120.885540	1	-0.002211	1	1	2	2	0.1204
C	1.431458	1	118.755422	1	0.004859	1	5	1	2	0.0148
O	1.751357	1	124.429754	1	180.000250	1	6	1	2	-0.2800
O1	1.744454	1	119.503450	1	179.998075	1	7	6	1	-0.0375
O1	1.744454	1	119.599321	1	179.997641	1	4	2	2	-0.0375
O1	1.745791	1	119.551052	1	179.994054	1	2	2	1	-0.0359
O1	1.745791	1	119.674572	1	-179.999662	1	1	2	3	-0.0552
H	0.948812	1	114.324849	1	-0.051553	1	8	5	1	0.2147
H	0.948810	1	114.327216	1	0.026553	1	5	3	2	0.2147
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MNDO CALCULATION

VERSION 5.01

C6 H3 O2 Cl3

21- 3-1990

2,3,6-trichlorohydroquinone

PETERS TEST WAS SATISFIED IN BFGS OPTIMIZATION
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION = -87.565455 KCAL
ELECTRONIC ENERGY = -10019.515308 EV
CORE-CORE REPULSION = 7501.729046 EV
DIPOLE = 1.39051 DEBYE
NO. OF FILLED LEVELS = 30
IONIZATION POTENTIAL = 9.254362 EV
MOLECULAR WEIGHT = 213.447
SCF CALCULATIONS = 161
COMPUTATION TIME = 50.084 SECONDS

FINAL GEOMETRY OBTAINED

										CHARGE
PRECISE GRAD										
2,3,6-trichlorohydroquinone										
C	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.0503
C	1.399582	1	0.000000	0	0.000000	0	1	0	0	-0.0195
C	1.424039	1	119.875467	1	0.000000	0	2	1	0	0.1075
C	1.421972	1	119.185852	1	0.010516	1	3	2	1	-0.0370
O	1.354247	1	115.667819	1	180.014758	1	3	2	1	-0.2348
C	1.425416	1	121.674204	1	-0.029814	1	1	2	3	0.1268
C	1.425217	1	118.184501	1	0.032944	1	6	1	2	0.0128
O	1.351903	1	124.431476	1	180.023969	1	6	1	2	-0.2222
Cl	1.745435	1	119.737586	1	179.983153	1	7	6	1	-0.0470
Cl	1.749511	1	119.574329	1	180.003617	1	4	3	2	-0.0726
H	1.091838	1	119.918433	1	179.989873	1	2	3	1	0.1029
Cl	1.751973	1	117.568788	1	179.983596	1	1	2	3	-0.0898
H	0.949683	1	114.025625	1	0.006916	1	8	6	1	0.2123
H	0.948295	1	114.184816	1	180.059254	1	5	3	2	0.2110
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MNDO CALCULATION

VERSION 4.01

C6 H3 N CL4
2,3,4,5-tetrachloroaniline

HERBERTS TEST WAS SATISFIED IN BFGS
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	2.971105 KCAL/MOL
HEAT OF FORMATION	=	12.448929 KJ/MOL
ELECTRONIC ENERGY	=	-9748.686265 EV
CORE-CORE REPULSION	=	7313.872303 EV
GRADIENT NORM	=	2.866118
DIPOLE	=	3.43251 DEBYE
NO. OF FILLED LEVELS	=	30
IONIZATION POTENTIAL	=	9.593450 EV
MOLECULAR WEIGHT	=	230.908
SCF CALCULATIONS	=	122

FINAL GEOMETRY OBTAINED

CHARGE

2,3,4,5-tetrachloroaniline

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.0826
C	1.401531	1	0.000000	0	0.000000	0	1	0	0	0.0518
C	1.413008	1	120.836448	1	0.000000	0	2	1	0	-0.0147
C	1.411655	1	119.170446	1	-0.270670	1	3	2	1	0.0595
C	1.423469	1	120.641778	1	-0.106437	1	1	2	3	0.1003
C	1.422477	1	118.374792	1	0.578911	1	5	1	2	-0.0366
N	1.410768	1	119.075614	1	-173.740495	1	5	1	2	-0.2341
CL	1.748357	1	119.872889	1	179.113138	1	6	5	1	-0.0661
CL	1.744339	1	119.747093	1	-179.757197	1	4	3	2	-0.0441
CL	1.742424	1	120.239528	1	179.835737	1	3	2	1	-0.0455
CL	1.746194	1	121.297382	1	179.921677	1	2	3	1	-0.0635
H	1.091980	1	119.281932	1	-179.738671	1	1	2	3	0.0917
H	1.005528	1	114.148987	1	-154.917615	1	7	5	1	0.1465
H	1.006029	1	113.002854	1	-31.277973	1	7	5	1	0.1372
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MNDO CALCULATION

VERSION 5.01

C6 H4 N C13

21- 3-1990

2,3,4-trichloroaniline

HERBERTS TEST WAS SATISFIED IN BFGS
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION = 6.194323 KCAL
ELECTRONIC ENERGY = -8267.168889 EV
CORE-CORE REPULSION = 6172.718875 EV
GRADIENT NORM = 3.780358
DIPOLE = 3.71641 DEBYE
NO. OF FILLED LEVELS = 27
IONIZATION POTENTIAL = 9.388959 EV
MOLECULAR WEIGHT = 196.463
SCF CALCULATIONS = 28
COMPUTATION TIME = 7.860 SECONDS

FINAL GEOMETRY OBTAINED

CHARGE

2,3,4-trichloroaniline

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.0938
C	1.399100	1	0.000000	0	0.000000	0	1	0	0	0.0010
C	1.411152	1	120.322447	1	0.000000	0	2	1	0	-0.0244
C	1.408159	1	120.235617	1	-0.090244	1	3	2	1	0.0589
C	1.424790	1	120.387900	1	-0.176018	1	1	2	3	0.0935
C	1.421191	1	118.928249	1	0.465266	1	5	1	2	-0.0397
N	1.413396	1	118.774620	1	-173.894829	1	5	1	2	-0.2348
Cl	1.749203	1	120.113175	1	179.328801	1	6	5	1	-0.0730
Cl	1.744759	1	120.015074	1	-179.837335	1	4	3	2	-0.0526
Cl	1.746302	1	118.035958	1	179.989311	1	3	2	1	-0.0733
H	1.091400	1	120.263359	1	180.043771	1	2	3	1	0.0849
H	1.090953	1	118.850799	1	-179.811416	1	1	2	3	0.0789
H	1.005614	1	114.008279	1	-155.291900	1	7	5	1	0.1423
H	1.006209	1	112.697965	1	-32.424446	1	7	5	1	0.1321
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MNDO CALCULATION

VERSION 4.01

C6 H4 N CL3
2,3,5-trichloroaniline

HERBERTS TEST WAS SATISFIED IN BFGS
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	4.577403	KCAL/MOL
HEAT OF FORMATION	=	19.179319	KJ/MOL
ELECTRONIC ENERGY	=	-8208.774209	EV
CORE-CORE REPULSION	=	6114.239080	EV
GRADIENT NORM	=	3.567332	
DIPOLE	=	2.41051	DEBYE
NO. OF FILLED LEVELS	=	27	
IONIZATION POTENTIAL	=	9.494249	EV
MOLECULAR WEIGHT	=	196.463	
SCF CALCULATIONS	=	129	

FINAL GEOMETRY OBTAINED

CHARGE

2,3,5-trichloroaniline

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.0788
C	1.401890	1	0.000000	0	0.000000	0	1	0	0	0.0373
C	1.407664	1	121.344298	1	0.000000	0	2	1	0	-0.0555
C	1.406476	1	118.584613	1	-0.139065	1	3	2	1	0.0448
C	1.423622	1	120.313469	1	-0.053531	1	1	2	3	0.0873
C	1.424352	1	118.501343	1	0.401227	1	5	1	2	-0.0325
N	1.413517	1	118.904265	1	-173.829210	1	5	1	2	-0.2317
CL	1.748213	1	120.287129	1	179.112987	1	6	5	1	-0.0727
CL	1.747822	1	117.462677	1	180.052186	1	4	3	2	-0.0709
H	1.090289	1	120.713943	1	179.849624	1	3	2	1	0.0991
CL	1.748583	1	119.299547	1	179.913737	1	2	3	1	-0.0879
H	1.091693	1	119.657417	1	-179.690636	1	1	2	3	0.0880
H	1.005713	1	113.836219	1	-156.775548	1	7	5	1	0.1414
H	1.006579	1	112.497645	1	-34.321210	1	7	5	1	0.1322
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MNDO CALCULATION

VERSION 4.01

C6 H4 N CL3
2,4,5-trichloroaniline

HERBERTS TEST WAS SATISFIED IN BFGS
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	3.997804	KCAL/MOL
HEAT OF FORMATION	=	16.750798	KJ/MOL
ELECTRONIC ENERGY	=	-8193.471371	EV
CORE-CORE REPULSION	=	6098.911109	EV
GRADIENT NORM	=	4.060578	
DIPOLE	=	2.64917	DEBYE
NO. OF FILLED LEVELS	=	27	
IONIZATION POTENTIAL	=	9.427281	EV
MOLECULAR WEIGHT	=	196.463	
SCF CALCULATIONS	=	120	

FINAL GEOMETRY OBTAINED

CHARGE

2,4,5-trichloroaniline

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	0.0516
C	1.410073	1	0.000000	0	0.000000	0	1	0	0	-0.0247
C	1.407704	1	119.833622	1	0.000000	0	2	1	0	0.0136
C	1.405854	1	119.859223	1	0.040629	1	3	2	1	-0.0436
C	1.405399	1	120.340480	1	-0.105025	1	1	2	3	-0.0868
C	1.423266	1	120.654472	1	-0.211161	1	5	1	2	0.0944
N	1.412286	1	119.341473	1	-173.778461	1	6	5	1	-0.2333
CL	1.751437	1	117.364081	1	-179.443254	1	4	3	2	-0.0911
H	1.091715	1	120.066500	1	-179.924375	1	3	2	1	0.0970
CL	1.745296	1	118.394956	1	179.909063	1	2	3	1	-0.0709
CL	1.746339	1	121.508653	1	179.754542	1	1	2	3	-0.0709
H	1.091661	1	119.204685	1	-179.828133	1	5	1	2	0.0887
H	1.005737	1	113.719142	1	-154.634803	1	7	6	5	0.1423
H	1.006160	1	112.845141	1	-31.666811	1	7	6	5	0.1337
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	