AN ABSTRACT OF THE THESIS OF

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Title: THE STRUCTURE AND THERMODYNAMIC PROPERTIES OF 2-BROMOETHANOL
       _____

       AS DETERMINED BY GAS PHASE ELECTRON DIFFRACTION
       _____

Abstract approved: Redacted for privacy
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The molecular structure of gaseous 2-bromoethanol has been

investigated by electron diffraction with nozzle tip temperatures

of 55 $^{\circ}$C, 103 $^{\circ}$C, 135 $^{\circ}$C, 175 $^{\circ}$C, and 200 $^{\circ}$C. The molecule exists

in both trans and gauche conformers at all of these temperatures.

By least squares refinements the values for the mole fraction of the

gauche conformer, x_g, are as follows (in order of increasing temper-

ature): 0.822 ± 0.097, 0.863 ± 0.129, 0.895 ± 0.139, 0.859 ± 0.096,

and 0.812 ± 0.122. The errors are 2σ. Based upon a comparison of the

areas of the peaks associated with the two conformers, the following

values were obtained: 0.860, 0.848, 0.835, 0.785, 0.791. Calculation

of $\Delta H^{\circ}_{t,g} = H^{\circ}_t - H^{\circ}_g$ and $\Delta S^{\circ}_{t,g} = S^{\circ}_t - S^{\circ}_g$ using the former set of

data yields -0.107 ± 2.680 kcal./mole and -2.38 ± 6.77 e. u., respec-

tively; using the latter set yields 1.15 ± 0.67 kcal./mole and

1.17 ± 1.69 e. u., respectively (using an estimated error in x_g of

± 0.02 in the latter set of results). Both values are lower than

corresponding values for 2-chloroethanol, the difference being

attributed to a weaker intramolecular hydrogen bond and a greater

steric interaction in the 2-bromoethanol molecule than in 2-chloroethanol .

The structure of the molecule yielded results comparable to the other halo-ethanols. The following bond distances and angles were determined (associated amplitudes are in parentheses, errors are 2σ): C-C = 1.517 ± 0.003 (0.045 ± 0.006), C-O = 1.417 ± 0.003 (0.045 ± 0.006), O-H = 0.996 ± 0.008, C-H = 1.096 ± 0.008, C-Br = 1.954 ± 0.003 (0.052 ± 0.005), $\angle$CCBr = 110.5 ± 0.4, $\angle$CCO = 110.7 ± 0.7, dihedral $\angle$BrCCO = 66.1 ± 1.5. In the above values distances and amplitudes are in angstroms, angles in degrees. These values are "average" values resulting from least squares refinements using data from all temperature experiments simultaneously and correspond to an "average" temperature of 134 °C.

The Structure and Thermodynamic Properties
of 2-bromoethanol as Determined by
Gas Phase Electron Diffraction

by

James Roger English

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THE STRUCTURE AND THERMODYNAMIC PROPERTIES OF 2-BROMOETHANOL AS DETERMINED BY GAS PHASE ELECTRON DIFFRACTION

ELECTRON DIFFRACTION METHOD

Only a very brief description of the experimental and theoretical aspects of electron diffraction will be given here. More detailed discussions of scattering theory are available from other sources (8) as well as more complete descriptions of the electron diffraction methods used regularly by our group. Some aspects of the method have been made more efficient and an up-dated description of them is planned for the future.

The apparatus accelerates a beam of electrons through a potential difference of 40-50 kV. The beam is collimated by a series of apertures and focused by a magnetic lens to a point on a photographic plate. The beam passes at right angles through a small jet of the vapor to be studied. The diffracted electrons are circularly symmetric about the undiffracted beam and form a pattern of diffuse rings on the photographic plate. The plates are developed and the density measured by scanning along a diametrical line using a modified (9) Joyce-Loebl microdensitometer while the plates are rotated about the center of the diffraction rings. The data are then reduced (7, 11) to complete the experimental procedure.

The equation relating the total scattered intensity to the components of that intensity may be written in the following form:

$$s^4 I_t = k \sum_{i,j} \frac{|A_i||A_j|}{sr_{ij}} \exp(-<\delta \ell_{ij}^2> s^2/2) \cos|\Delta \eta_{ij}| \sin(r_{ij}s)$$

$$+ k \sum_i A_i^2 + k \sum_i Z_i S_i + I_{ext}$$

$$= I_m + I_a + I_i + I_{ext} \tag{1}$$

where I_m, I_a, I_i, and I_{ext} stand for, respectively, the structure sensitive scattering, atomic scattering, incoherent scattering, and extraneous scattering. The quantities A_i are the electron scattering amplitudes multiplied by s^2 and $\Delta \eta_{ij}$ the phase shifts between atoms of atomic numbers, Z_i and Z_j. The variables r_{ij}, ℓ_{ij}, and s are, respectively, the interatomic distances, the root-mean-square amplitude of vibration, and the diffraction variable ($s = 4\pi \lambda^{-1} \sin\theta$). S_i is the incoherent scattering factor and λ is the wavelength of the electrons. I_a, I_i, and I_{ext} are not dependent upon the structure of the molecule and are subtracted as a smooth background from $s^4 I_t$.

In an electron diffraction investigation of a molecule existing in two different conformations, e. g., gauche and trans, the total structure sensitive scattered intensity can be expressed as the sum of the scattering due to each conformer as follows:

$$I_m = x_{gauche} I_{m_{gauche}} + x_{trans} I_{m_{trans}} \tag{2}$$

where x_{gauche} and x_{trans} are the mole fractions of the gauche and the trans conformers, respectively.

The actual structure determination begins with the determination of a trial structure deduced from the fourier transform

of the intensity data. The fourier transform is related to the probability $P(r)$ of finding an interatomic distance in the molecule between r and $r + dr$, and is often termed the radial distribution curve. The calculation of the radial distribution curve is done as follows:

$$\frac{P(r)}{r} = \frac{2}{\pi} \sum_{s_{min}}^{s_{max}} I'_m(s) \exp(-Bs^2) \sin(rs)\Delta s \qquad (3)$$

where the factor $\exp(-Bs^2)$ reduces the error associated with the finiteness of the intensity data, and $I'_m(s)$ is a "constant coefficient" curve obtained by multiplying I_m by sZ_kZ_1/A_kA_1, which helps produce Gaussian-shaped peaks. $I'_m(s)$ is given by the equation

$$I'_m(s) = k \sum \frac{A_iA_jZ_iZ_j}{A_kA_1r_{ij}} \exp(-<\delta\ell_{ij}^2>s^2/2) \cos|\Delta\eta_{ij}| \sin(r_{ij}s) \qquad (4)$$

The actual refinements are done by adjusting the parameters in the expression given above in equation (1) for I_m so that the difference between the calculated and experimental intensity curves is minimized.

INTRODUCTION

It is generally recognized (14,21,22) that the 1,2-dihalo-ethanes (XCH_2-CH_2Y, where X and Y are F, Cl, Br, or I atoms) exist as two rotational conformers, the trans and the gauche. The trans appears to be the more stable, perhaps because of electrostatic repulsions between the electronegative halogen atoms. When one of the halogen atoms is replaced by a hydroxyl group, the opportunity exists for an attractive interaction between the OH group and the X atom which does not exist between two halogen atoms; this attrac-tive interaction owes to the formation of an intramolecular hydrogen bond. Should the strength of such a bond be sufficiently great, it will dominate the repulsive interactions and one may expect the gauche rotamer to be more stable than the trans.

Several groups of researchers (4, 5, 6, 15, 16, 17, 19, 22) have studied the infrared and/or the Raman spectra of the 2-haloethanols. In almost every case evidence has been found for the coexistance of both the trans and the gauche conformations (although the gauche form is often indistinguishable from a mixture of cis and trans forms). The only exception in solution or vapor phase is that 2-fluoroethanol may exist almost entirely in the gauche form, at least at convenient temperatures. Microwave studies (2, 13) have supported these conclusions. As far as electron diffraction is concerned, a recent investigation of gaseous 2-fluoroethanol in our laboratory (10) found no evidence of the

trans conformation even at a rather high temperature. Likewise,
early electron diffraction studies of 2-chloroethanol (3, 20)
failed to detect any trans conformer, but the experiments were done
at low temperatures where only a small percentage of trans would be
expected. A more recent electron diffraction experiment (1)
utilizing new developments in the technique has detected a sub-
stantial amount of the trans conformer at higher temperatures,
and at least some of the trans form at lower temperatures. No
electron diffraction experiments have been reported for 2-bromoethanol.

The difference in energy between the trans and the gauche
conformations of the 2-haloethanols is of considerable interest.
By determining the ratio of gauche to trans forms at a particular
temperature, one determines an equilibrium constant from which the
free energy difference may be obtained. Moreover, by repeating this
determination at different temperatures, the enthalpy and entropy
differences between the two conformations may be calculated. The
values obtained for the enthalpy differences between the conformations
from different types of experiments have usually been in the range of
about one to two kilocalories per mole for 2-chloroethanol and
slightly less for 2-bromoethanol, with the trans form being the
less stable.

Gas phase electron diffraction may be used in certain cases
to measure the relative amounts of the trans and gauche conformers
at various temperatures. In the case of 2-bromoethanol, figure 1
shows that while many of the interatomic distances are basically the
same in the two conformations, the distance between the largest two

atoms, oxygen and bromine, is quite different. The large atomic
numbers of these atoms causes them to be good scatterers of high
energy electrons. A theoretical radial distribution curve (Figure 2)
for a mixture of the two conformations shows prominent peaks at the
interatomic distances corresponding to the Br$\cdot\cdot$O interaction in each
of the conformations. The area of each peak is proportional to
$x_i Z_O Z_{Br} r_{Br\cdot\cdot O}^{-1}$, where x_i is the mole fraction of that conformer.
Thus, the electron diffraction analysis at a given temperature
yields both the composition of the sample at that temperature and the
overall structure of 2-bromoethanol.

THERMODYNAMIC EXPRESSIONS FOR CONFORMATIONAL ANALYSIS

The interconversion of the gauche conformer and the trans conformer can be expressed by the following equilibrium expression (1):
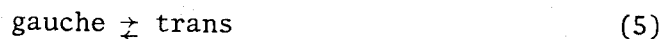
$$\text{gauche} \rightleftharpoons \text{trans} \tag{5}$$

for which the equilibrium constant is

$$K = \frac{x_t}{x_g} \tag{6}$$

where x_t and x_g are the mole fractions of the trans and the gauche conformers, respectively.

The expression for the Gibbs free energy,

$$\Delta G^O = -RT\ln K \ , \tag{7}$$

leads to

$$-R\ln \frac{x_t}{x_g} = \frac{\Delta H^O}{T} - \Delta S^O \ . \tag{8}$$

The entropy difference (ΔS^O) in equation (8) is the entropy change for the reaction of equation (5), i. e., the standard entropy for trans molecules minus that for gauche molecules. Now, because there are two equivalent forms of gauche molecules and only one of trans, the standard entropy of the former includes a statistical factor of $R\ln 2$. If one is interested in the standard entropy difference between the trans and one of the gauche conformers ($\Delta S^O_{t,g}$), one has

$$\Delta S^O = S^O_t - S^O_g - R\ln 2 \tag{9}$$

$$= \Delta S^O_{t,g} - R\ln 2 \ . \tag{10}$$

Equation (8) becomes

$$-R\ln \frac{x_t}{x_g} = \frac{\Delta H^O}{T} - \Delta S^O_{t,g} + R\ln 2 \ . \tag{11}$$

Rearranging and combining terms gives

$$-R\ln \frac{2x_t}{x_g} = \frac{\Delta H^O}{T} - \Delta S^O_{t,g} \ . \tag{12}$$

Equation (12) is the equation of a straight line in the slope-intercept form. A straight line fitted to a plot of $-R\ln \frac{2x_t}{x_g}$ versus $1/T$ will yield a y-intercept equal to $-\Delta S^O_{t,g}$ and a slope equal to ΔH^O.

In the case of conformation analysis studied at extremely low pressures, the partial pressures of the two conformers can be assumed ideal. Since under these circumstances $\Delta(PV) = 0$, we have

$$\Delta H^O = \Delta E^O . \tag{13}$$

EXPERIMENTAL AND DATA REDUCTION

A sample of 2-bromoethanol was obtained from Eastman Kodak Company. The infrared spectrum compared favorably with that given by Wyn-Jones and Orville-Thomas (19). Nuclear magnetic resonance scans were taken on both 100 MHz. and 60 MHz. instruments and appeared to be of pure 2-bromoethanol. There was a possibility of some water being present because its infrared and nmr peaks could have been obscured by those for 2-bromoethanol. However, the areas of the nmr peaks suggested that there could be no more than five percent water in the sample. The sample boiling point was determined to be 149.6°C; the literature value is 150.3°C. The sample was used without further purification.

For a sample vapor pressure of 10-15 torr, which experience shows is necessary for diffraction photographs of a molecule of this type, a sample bath temperature of about 55°C was required. This temperature is thus the minimum nozzle-tip temperature; lower nozzle temperatures would have led to condensation in the nozzle. Electron diffraction photographs were made at both the long and the middle camera positions using 8 x 10 inch Kodak lantern slide (medium) plates. Because the diffraction data were very weak at about s equal to 25 or 30, no short camera plates were exposed. Experiments were carried out at five different nozzle temperatures: 55°C, 103°C, 135°C, 175°C, and 200°C. At least five plates were exposed at each camera distance for each temperature. Exposure data are listed in Table 1.

All of the usable plates were scanned in the usual manner (18) using a modified (9) Joyce-Loebl microdensitometer. The potentiometer output was sent through a voltage to frequency converter and the digitalized results automatically punched on paper tape. The data was read into the computer and was reduced using a computer program written by Lise Hedberg. Smooth backgrounds were calculated for the curves using another program written by Lise Hedberg. As the structure refinement proceeded, this background program was used to obtain progressively better backgrounds and thus to improve the experimental intensity data. More complete descriptions of the data reduction are available elsewhere (7, 9, 11).

STRUCTURE DETERMINATION AND CONFORMATIONAL ANALYSIS

In order to obtain trial values for the principal geometrical
and vibrational parameters, a radial distribution curve was calculated
according to equation (3) using a composite intensity curve made by
combining data from one middle camera plate and one long camera plate
from the 55°C experiment. The radial distribution curve (like figure
2) has important peaks at 1.02, 1.47, 1.95, 2.40, 2.86, 3.23, and
4.12 (angstroms), which are due, respectively, to following distances
in the molecule: C-H and O-H, C-C and C-O, C-Br, $C \cdot \cdot O$, $C \cdot \cdot Br$, $Br \cdot \cdot O_g$,
and $Br \cdot \cdot O_t$. From these peak positions sufficiently accurate
parameter values were obtained to permit least squares refinements
to be done.

A coordinate and distance subroutine was written to be used
with the standard least squares computer program now used by the
electron diffraction group. Some simplifying assumptions were made
because of the relative complexity of the structure arising from
the lack of symmetry in the molecule: 1) The structures of the trans
and the gauche conformers were assumed to be identical except for
the distances changing with rotation about the carbon-carbon bond.
2) The plane formed by the HCH atoms around each C were assumed to
bisect the angle formed by the C and the other two atoms attached
to it. 3) Both HCH angles were assumed equal. With these assump-
tions the geometry of the molecule may be described by the
following parameters: <C-C,O> (the average of the C-C and the C-O
bond lengths), Δ(C-C,O) (the difference between the C-C and the C-O

bond lengths), r(C-BR) (the C-Br bond length), <C,O-H>, Δ(C,O-H),

∠CCBr (the CCBr bond angle), ∠CCO, ∠COH, ∠HCH, ∠CCOH (the angle

of rotation about the C-O bond with 0° being with the alcoholic H

cis to the β-C), ∠BrCCO (the angle of rotation about the C-C bond,

0° being with the Br and the O eclipsed), and r(Br··O)$_t$ (the trans

Br··O nonbond length). The final parameter was put in as a separate

refinable variable to allow for a possible shortening of the nonbond

length in the case that the trans rotational angle, ∠BrCCO, is not

exactly 180°.

Besides the twelve geometrical parameters listed above, there

were the compositional parameter, x_g (the mole fraction of the

trans conformer in the sample), and 23 vibrational amplitude

parameters associated with distinctly different distances in the

molecule. Not all of these variables could be refined, it was

discovered, so that some had to be given values taken from other

diffraction experiments on less complicated molecules.

Several steps were taken to assure comparable results for the

experiments run at different temperatures: 1) Only the best three

long camera plates and the best three middle camera plates were

selected from the experiments at each temperature. 2) The ranges

of data from corresponding plates from each temperature were chosen

to be identical. 3) The composite curves from the five temperatures

were placed on a common amplitude scale using an average theoretical

curve as basis of comparison.

Although the overall structure of the molecule was readily

determined, even with the precautions taken as mentioned above to obtain comparable results, the determination of the composition (the variable x_g) proved to be very difficult. Three parameters which are sensitive to the conformation, the amplitudes of the gauche and the trans Br··O distances and also the trans Br··O distance, were poorly determined by the least squares refinements judging from their respective standard errors. It was also found that simultaneous refinement of the $r(Br··O)_t$ distance, its amplitude of vibration and the composition was impossible. Thus, one of these variables had to be held constant to obtain values for the others.

Different values for the amplitude were inserted and held constant while the other variables were allowed to refine. It was found that for a wide reange of values for the amplitude, only small differences in the other variables were obtained. Variation of the $r(Br··O)_t$ distance, however, made much larger differences in the values of the refined variables. Hence, an approximate value for the amplitude was inserted and held constant during refinements of the other variables.

The amplitudes of all the distances were expected to increase systematically with temperature, and the results demonstrated such a trend. To compensate for this temperature dependence, the ratio of the refinable amplitudes at one temperature to those at another temperature was calculated and used to adjust those amplitudes which were held constant during the actual refinements.

Even with these corrections, the standard errors associated with the composition parameter, x_g, were large with respect to the values themselves (Table 2). Plotting the radial distribution curves for the five different temperature experiments (Figure 4), a noticeable trend was observed in the relative sizes of the outermost major peak, namely that associated with the $r(Br\cdot\cdot O)_{tr}$ distance. This trend seemed to be lacking in the values obtained from the least squares refinements for x_g, although the error limits associated with these values could easily include such a trend. To get some empirical data for this apparent trend, the peaks associated with the gauche and the trans $Br\cdot\cdot O$ distances were cut out and weighed. The weights of these peaks, just as the areas, are proportional to the mole fractions of the two conformers divided by their respective $Br\cdot\cdot O$ distances. This predicts a linear dependence on the ratio of the peak weights to the composition parameter, x_g. Therefore, three theoretical intensity curves were calculated, which were identically the average of the five final models obtained from least squares with the exception of the compositional parameter. The radial distribution curves were calculated and plotted (Figure 5). The appropriate peaks were cut out and weighed. A plot of x_g versus the ratio of peak weights (trans to gauche), yielded a straight line, as predicted. The ratios obtained from the experimental curves were converted to x_g values on the basis of the plot. For the five experiments in order of increasing temperature, the x_g values obtained in this manner are as follows: 0.860, 0.848, 0.835, 0.785, and 0.791. The values obtained for x_g from the least squares refinements,

arranged in the same order are as follows (errors are 2σ):

0.822 ± 0.097, 0.863 ± 0.129, 0.895 ± 0.139, 0.859 ± 0.096, and

0.812 ± 0.122. Comparing these two sets of results, one may

detect a noticeable trend in the first set which seems to be

lacking in the second.

The geometrical and vibrational parameters proved to be

well determined by the least squares refinements. Moreover, the

values varied only slightly from one experimental temperature to

another (with the exception of the systematic trend of the ampli-

tudes as described above). Because of the slight variance of the

geometrical parameters, all the data was used together in one

large refinement, yielding a set of "average" values for the

refined parameters corresponding to an "average" temperature

of 134 $^{\circ}$C (Table 3).

DISCUSSION

Nothing unusual was found in the final structure of 2-bromo-
ethanol. The r(C-C) and the r(C-O) values are in good agreement
with values reported on 2-chloroethanol and 2-fluoroethanol (Table 5).
There is an apparent trend of increasing $\underline{/}$CCX in the series X =
F, Cl, Br. There may also be a trend of increasing torsional angle,
$\underline{/}$XCCO, in the gauche form for the same series. Both of these
trends can be understood in terms of increasing steric interactions
between the oxygen and the halogen atoms as the halogen atom
increases in size. Another noticeable and expected trend is the
increase in amplitude values as the temperature is increased.

Although the conformational analysis proved to be more
difficult than was originally anticipated, it is felt that some
conclusions may be drawn. The values for the conformational
parameter obtained from the least squares refinements had extremely
large errors associated with them (Table 2). A plot of $-R\ln\frac{2x_t}{x_g}$
versus 1/T yielded a least squares straight line of nearly zero
slope (Figure 6). The thermodynamic quantities ΔH^O and $\Delta S^O_{t,g}$ were
determined to be -0.107 ± 2.680 kcal./mole and -2.38 ± 6.77 e. u.,
respectively. Using the values for the conformational parameter
obtained by weight comparisons of the radial distribution peaks
associated with each particular conformer, other values for ΔH^O and
$\Delta S^O_{t,g}$ were obtained: 1.15 ± 0.67 kcal./mole and 1.17 ± 1.69 e. u.,
respectively. The data used to determine the latter values fit
a straight line much better than the least squares data (Figure 7).

The errors given for the latter values correspond to an estimated error of ± 0.002 in the x_g values.

Values obtained for ΔH^O (or ΔE^O) for 2-chloroethanol (16, 17, 22) have been in the range 0.95 - 2.60 kcal./mole and for $\Delta S^O_{t,g}$ in the range 3.6 - 7.4 e. u. The present study suggests that ΔH^O has a lower value in the case of 2-bromoethanol than in the case of 2-chloroethanol. This corresponds to a gauche form which is not quite as stable relative to the trans form as in the 2-chloroethanol molecule. This can readily be understood as arising from a lower Br$\cdot\cdot$H bond strength relative to the Cl$\cdot\cdot$H and also to a larger steric repulsion between the Br and O atoms than between the Cl and O atoms.

There is also an apparent difference in the entropy values obtained for the two molecules: 2-bromoethanol has a lower value for $\Delta S^O_{t,g}$ than does 2-chloroethanol. This corresponds to a trans form which is more nearly equal in entropy to the gauche form than in the 2-chloroethanol molecule.

Table 1. Data for electron diffraction photographs used for the structure determination of 2-bromoethanol. All plates were 8X10 inches. The usable s-range for the 75 cm. nozzle to plate distance was from 2.00 to 10.75 and for the 30 cm. distance was from 8.00 to 28.00.

Plate I.D.	Voltage (volts)	Wavelength (Å)	Exposure time (min)	Beam current (µamp)	Nozzle temp. (°C)	Bath temp. (°C)	Ambient pressure (torr)	Nozzle to plate distance (cm)
203305	44424	0.056961	1.5	.90	55	50	3.0×10^{-6}	74.9964
203304	44419	0.056965	.75	.60	55	50	3.0×10^{-6}	74.9964
203303	44419	0.056965	1.0	.60	55	51	2.6×10^{-6}	74.9964
202804	44378	0.056992	4.0	.30	55	48	1.6×10^{-6}	29.9869
202802	44375	0.056994	3.5	.46	55	50	2.0×10^{-6}	29.9869
202805	44384	0.056988	3.0	.82	55	46	1.5×10^{-6}	29.9869
211401	44144	0.057149	2.0	.36	103	58	6.0×10^{-6}	74.9617
211402	44148	0.057146	1.5	.36	103	58	6.0×10^{-6}	74.9617
211404	44149	0.057146	2.5	.36	103	58	6.0×10^{-6}	74.9617
211304	44137	0.057154	2.5	.38	105	58	6.0×10^{-6}	29.9566
211303	44131	0.057158	2.25	.38	103	58	6.0×10^{-6}	29.9566
211302	44126	0.057161	2.0	.38	104	58	6.0×10^{-6}	29.9566
207101	44249	0.057078	1.0	.52	135	55	6.0×10^{-6}	74.9844
207102	44252	0.057076	1.5	.52	135	55	6.0×10^{-6}	74.9844
207104	44253	0.057076	2.0	.52	135	55	6.0×10^{-6}	74.9844
202904	44371	0.056997	3.5	.86	135	55	2.1×10^{-6}	29.9728
202901	44363	0.057002	3.0	.80	135	55	2.4×10^{-6}	29.9728
202905	44374	0.056995	4.0	.32	135	53	2.2×10^{-6}	29.9728
210403	44155	0.057142	2.5	.64	175	55	1.0×10^{-5}	74.9651
210404	44155	0.057142	3.0	.64	174	55	1.0×10^{-5}	74.9651
210402	44155	0.057142	3.5	.64	175	55	1.0×10^{-5}	74.9651
210301	44208	0.057106	1.5	.62	176	55	2.0×10^{-6}	29.6327
210603	44163	0.057136	2.0	.40	174	55	8.0×10^{-6}	29.6327
210602	44162	0.057137	2.0	.40	174	55	1.2×10^{-5}	29.6327
207202	44131	0.057158	1.25	.42	199	48	4.6×10^{-6}	74.9844
207203	44137	0.057154	1.5	.42	200	48	4.6×10^{-6}	74.9844
207205	44153	0.057143	1.5	.42	200	48	4.6×10^{-6}	74.9844
207305	44207	0.057107	4.0	.44	200	52	5.1×10^{-6}	29.9927
207304	44205	0.057108	3.5	.44	200	50	5.8×10^{-6}	29.9927
207302	44200	0.057111	3.0	.45	200	52	5.6×10^{-6}	29.9927

Table 2. Final structural results for 2-bromoethanol for the five different temperature experiments.[a]

Structural Feature	55°C $r_a, \ell, \angle$	2σ	103°C $r_a, \ell, \angle$	2σ	135°C $r_a, \ell, \angle$	2σ	175°C $r_a, \ell, \angle$	2σ	200°C $r_a, \ell, \angle$	2σ
<C-C,O>	1.469	.006	1.459	.007	1.469	.008	1.468	.005	1.470	.006
Δ(C-C,O)	(.100)		(.100)		(.100)		(.100)		(.100)	
<C,O-H>	1.022	.013	1.082	.017	1.030	.018	1.057	.015	1.051	.016
Δ(C,O-H)	(.100)		(.100)		(.100)		(.100)		(.100)	
r(C-Br)	1.954	.005	1.951	.006	1.956	.007	1.955	.005	1.955	.006
$\angle$CCBr	110.6	0.6	110.5	0.8	110.6	0.9	110.5	0.6	110.4	0.8
$\angle$CCO	109.6	1.3	112.5	1.3	110.4	1.5	110.3	1.1	110.7	1.3
$\angle$HCH	(109.4)		(109.4)		(109.4)		(109.4)		(109.4)	
$\angle$HOC	(105.7)		(105.7)		(105.7)		(105.7)		(105.7)	
ϕ	67.8	2,5	64.4	3.2	66.0	3.7	66.3	2.8	66.2	3.3
% gauche	82.2	9.7	86.3	12.9	89.5	13.9	85.9	9.6	81.2	12.2
r(Br··O)$_{tr}$	4.129	.045	4.085	.075	4.130	.109	4.116	.056	4.123	.056
gauche										
ℓ(C-C)	.044 }	.009	.041 }	.012	.053 }	.013	.040 }	.009	.050 }	.010
ℓ(C-O)	.044		.041		.053		.040		.050	
ℓ(C-Br)	.048	.008	.051	.010	.059	.011	.054	.007	.052	.009
ℓ(C-H)	(.077)		(.078)		(.079)		(.081)		(.082)	
ℓ(O-H)	(.070)		(.071)		(.072)		(.074)		(.075)	
ℓ(C··Br)	.065	.010	.067	.013	.070	.014	.072	.010	.073	.012
ℓ(C··O)	.076	.015	.054	.014	.065	.016	.071	.012	.063	.014
ℓ(O··Br)	.123	.020	.137	.027	.150	.031	.159	.024	.150	.029
trans										
ℓ(O··Br)	(.060)		(.063)		(.066)		(.0685)		(.071)	
R[b]	.140		.179		.199		.130		.162	

Table 2. Continued.

[a]Distances (r_a) and root-mean-amplitudes (ℓ) are in Ångstroms, angles are in degrees. Parenthesized values were assumed. Bracketted values were set equal and refined as a group.

[b]The ratio (R) is given by the expression: $R = [\sum_i w_i \Delta_i^2 / \sum_i w_i I_i(obs)^2]^{1/2}$, where $\Delta_i = I_i(obs) - I_i(calc)$ and w_i are weighting factors.

Table 3. Final "average" parameter values from the least squares refinements using the composites of all five experiments simultaneously.[a]

Independent Geometrical Parameters

Parameter	Value	2σ	Amplitude	2σ
<C-C,O>	1.467	.003		
Δ(C-C,O)	(.100)			
r(C-Br)	1.954	.003	.052	.005
<O,C-H>	1.046	.008		
Δ(O,C-H)	(.100)			
∠CCBr	110.5	0.4		
∠COH	(105.7)			
∠CCO	110.7	0.7		
∠BrCCO	66.1	1.5		
∠CCOH	(60.0)			
∠HCH	(109.4)			
$r(Br \cdot \cdot O_{tr})$	4.118	.033	(.0657)	

Dependent Distances

Distance	Value	2σ	Amplitude	2σ
C-C	1.517	} .003	.045	} .006
C-O	1.417		.045	
O-H	0.996	} .008	(.0724)	
C-H	1.096		(.0794)	
C··Br	2.863	.006	.069	.006
C··O	2.415	.009	.066	.008
$Br \cdot \cdot O_g$	3.232	.017	.144	.014
5-9	1.940	.006	(.110)	
1-2	2.537	.007	(.110)	
1-7	2.960	.016	(.150)	
1-6	3.841	.009	(.130)	
1-9	2.692	.021	(.130)	
4-9	2.553	.011	(.130)	
4-6	2.144	.007	(.110)	
7-8	2.057	.007	(.110)	
2-8	3.349	.009	(.130)	
3-8	2.623	.018	(.150)	
H··H	1.789	.013	(.125)	
6-1'	3.013	.008	(.150)	
9-1'	4.323	.033	(.150)	
8-3'	2.665	.009	(.140)	

[a] This corresponds to an "average" set of results with a temperature of about 134°C. Units are defined as in footnote [a] of Table 2.

Table 4. Correlation matrix for 2-bromoethanol, using the "average" results (Table 3).

<C-C,O>	r(C-Br)	<O,C-H>	/CCBr	/CCO	/BrCCO	$r(Br\cdot\cdot O_{tr})$	ℓ(C-C)	ℓ(C-Br)	ℓ(C$\cdot\cdot$Br)	ℓ(C$\cdot\cdot$O)	ℓ(O$\cdot\cdot$Br)	x_g
σ^a .0011	.0009	.0027	.1304	.2344	.5470	.0115	.0018	.0016	.0020	.0025	.0045	.0206
1.000	-.008	-.048	-.390	-.501	.258	.003	.037	.037	.051	.025	.015	.012
	1.000	-.011	-.327	-.053	.062	.004	-.085	-.111	-.089	-.094	-.021	-.006
		1.000	.064	.016	-.076	.034	.189	.111	.019	-.060	.037	.044
			1.000	.275	-.182	.013	.000	.013	.083	.029	-.292	-.064
				1.000	-.577	-.001	-.132	-.103	-.084	-.104	-.063	-.031
					1.000	-.010	.041	.025	.288	.066	-.071	-.058
						1.000	..015	.008	.000	-.007	-.011	-.005
							1.000	.479	.267	.188	.099	.078
								1.000	.296	.246	.101	.082
									1.000	.167	-.056	-.046
										1.000	.036	.027
											1.000	.438
												1.000

a "σ" is the standard deviation obtained from the least squares program. The values for the distances and root-mean-amplitudes are in angstroms, angles are in degrees.

Table 5. Comparison of 2-bromoethanol with 2-chloroethanol and 2-fluoroethanol.[a]

| Structural feature | 2-bromoethanol | | 2-chloroethanol | | 2-fluoroethanol |
	This Study	Microwave	Electron Diffraction	Microwave	Electron Diffraction
r(C-X)	1.954 ± .003	(1.950)	$1.80_2 \pm .01_3$	1.7886 ± .0038	1.400 ± .005
r(C-C)	1.517 ± .003	(1.518)	$1.51_6 \pm .02$	1.5191 ± .0009	1.513 ± .003
r(C-O)	1.417 ± .003	(1.411)	$1.41_6 \pm .02$	1.4107 ± .0014	1.418 ± .006
∠CCX	110.5 ± 0.4	(110.13)	110.6 ± 2.1	110.08 ± .33	107.7 ± 1.4
∠CCO	110.7 ± 0.7	(112.77)	111.8 ± 3.2	112.77 ± .10	112.2 ± 1.9
∠XCCO	66.1 ± 1.5	64.17 ± .50	60 – 70	63.25 ± .58	64.6 ± 1.1
%trans (200°C)	18.8 ± 12.2		15 – 25		<10 (156°C)
		[ref. (2)]	[ref. (1)]	[ref. (2)]	[ref. (10)]

[a] Distances (r) are in Ångstroms, angles are in degrees. Reported errors from microwave and electron diffraction do not necessarily have the same meaning.

Table 6. Experimental intensity data [$sI_m(s)$] for 2-bromoethanol. Long camera distance (75 cm) plates have an s-range from 2.00 to 10.75, middle camera distance (30 cm) plates have an s-range from 8.00 to 28.00.

EXPERIMENTAL INTENSITY CURVES FOR 55 DEGREE DATA
CURVE NUMBER 1 (203305)

Δs / s	0.00	0.25	0.50	0.75
2.00	-8.32	-9.27	-5.32	-1.11
3.00	-3.12	-9.21	-16.18	-19.03
4.00	-15.79	-4.96	5.77	10.99
5.00	4.10	-13.36	-21.02	-22.51
6.00	-8.38	14.17	33.21	38.96
7.00	34.47	22.60	10.46	-0.30
8.00	-10.29	-21.63	-32.88	-37.14
9.00	-27.41	-2.74	23.35	50.23
10.00	58.40	48.05	33.77	13.20

CURVE NUMBER 4 (202804)

Δs / s	0.00	0.25	0.50	0.75
8.00	-4.96	-12.37	-13.72	-22.36
9.00	-14.71	-4.21	10.29	28.78
10.00	28.16	22.41	20.45	7.96
11.00	-2.03	-15.34	-27.71	-41.34
12.00	-50.03	-49.43	-46.48	-19.78
13.00	8.05	41.47	73.72	83.68
14.00	73.13	38.38	.93	-33.31
15.00	-46.41	-39.88	-36.35	-13.90
16.00	3.14	-9.98	-2.03	-0.68
17.00	-6.68	-8.19	7.28	5.90
18.00	7.95	10.44	13.61	4.86
19.00	2.64	1.54	-0.36	8.31
20.00	14.33	10.32	1.43	-9.33
21.00	-20.35	-26.26	-19.62	-5.68
22.00	-9.05	2.64	-0.47	12.67
23.00	18.60	23.77	20.75	13.71
24.00	-0.77	.25	-7.19	-17.54
25.00	-17.72	-13.39	-30.53	-11.88
26.00	.97	19.87	16.23	13.33
27.00	1.40	19.03	15.66	-1.20
28.00	-12.31			

Table 6. Continued.

CURVE NUMBER 2 (203304)

Δs / s	0.00	0.25	0.50	0.75
2.00	-3.34	-3.69	-2.48	-0.47
3.00	-1.21	-3.86	-6.30	-7.75
4.00	-6.38	-1.83	2.26	4.11
5.00	1.03	-4.52	-9.13	-8.92
6.00	-2.69	6.89	14.89	16.20
7.00	13.81	8.14	3.57	-1.39
8.00	-3.75	-9.52	-12.11	-16.44
9.00	-11.98	.14	11.18	20.50
10.00	23.18	19.78	14.08	4.87

CURVE NUMBER 5 (202802)

Δs / s	0.00	0.25	0.50	0.75
8.00	-5.47	-10.80	-16.44	-19.10
9.00	-15.88	-7.75	10.77	26.96
10.00	29.95	32.40	17.50	11.92
11.00	-2.61	-19.63	-31.44	-46.23
12.00	-53.34	-53.69	-43.38	-18.70
13.00	8.88	48.06	78.09	86.32
14.00	71.28	36.68	1.68	-36.07
15.00	-41.66	-41.82	-29.46	-8.89
16.00	-6.85	-14.60	.21	-7.87
17.00	-9.97	-9.68	3.77	8.85
18.00	16.96	11.70	11.71	7.59
19.00	2.80	-10.15	8.05	8.07
20.00	12.82	7.38	3.41	-8.20
21.00	-19.65	-22.36	-9.67	-7.80
22.00	-6.79	4.53	5.14	13.42
23.00	17.74	11.43	14.39	-9.13
24.00	-13.44	9.59	-8.52	-5.69
25.00	-5.87	-0.51	-20.18	-10.91
26.00	-9.22	5.83	17.69	19.55
27.00	6.66	12.29	7.05	4.15
28.00	-7.49			

Table 6. Continued.

CURVE NUMBER 3 (203303)

s \ Δs	0.00	0.25	0.50	0.75
2.00	-4.67	-5.26	-3.34	-0.79
3.00	-1.90	-5.34	-8.79	-11.23
4.00	-8.50	-2.40	3.35	6.76
5.00	2.15	-6.04	-12.79	-13.16
6.00	-6.14	7.84	19.27	22.50
7.00	20.46	12.53	4.98	2.06
8.00	-4.25	-11.31	-20.19	-21.80
9.00	-15.05	-2.18	14.48	26.53
10.00	32.08	27.90	21.29	7.24

CURVE NUMBER 6 (202805)

s \ Δs	0.00	0.25	0.50	0.75
8.00	-5.53	-15.80	-20.11	-26.19
9.00	-17.26	-1.90	10.83	31.00
10.00	36.72	33.73	21.97	8.00
11.00	-2.61	-10.13	-28.50	-56.03
12.00	-70.99	-71.79	-55.49	-30.61
13.00	11.46	48.31	92.14	112.45
14.00	90.28	62.29	6.84	-33.87
15.00	-54.81	-51.98	-46.81	-27.93
16.00	-20.93	-14.24	5.83	-0.94
17.00	-1.94	-1.92	12.37	10.79
18.00	10.59	11.55	15.73	-7.78
19.00	-15.00	-2.45	2.01	7.57
20.00	22.04	20.54	7.10	-2.67
21.00	-18.42	-36.59	-12.49	-5.21
22.00	6.00	1.91	11.80	4.60
23.00	11.41	28.67	5.22	2.58
24.00	-11.54	-12.55	-19.39	-21.00
25.00	-17.02	1.23	-18.56	22.13
26.00	14.70	13.65	-4.57	16.59
27.00	11.11	.15	11.59	-8.49
28.00	4.04			

Table 6. Continued.

COMPOSITE CURVE FCR 55 DEGREE DATA

s \ Δs	0.00	0.25	0.50	0.75
2.00	-94.89	-105.84	-66.27	-13.97
3.00	-36.21	-167.72	-180.73	-221.77
4.00	-173.06	-52.48	66.00	126.47
5.00	39.92	-123.03	-252.85	-259.21
6.00	-97.99	172.09	397.71	453.93
7.00	400.33	247.91	107.44	-0.45
8.00	-96.85	-234.92	-328.70	-411.79
9.00	-294.61	-52.85	236.51	527.05
10.00	595.16	527.80	371.58	158.87
11.00	-41.16	-261.36	-497.63	-804.17
12.00	-972.47	-975.27	-815.51	-382.60
13.00	158.51	778.40	1369.80	1579.13
14.00	1315.91	758.93	49.14	-585.86
15.00	-801.37	-743.80	-627.37	-274.42
16.00	-124.39	-218.41	17.38	-56.32
17.00	-110.39	-117.75	127.34	142.02
18.00	202.47	190.61	230.28	37.56
19.00	-40.10	-64.01	56.30	136.30
20.00	272.44	207.52	63.94	-119.39
21.00	-332.48	-473.23	-238.49	-107.09
22.00	-66.86	52.80	85.77	180.60
23.00	276.06	353.48	238.69	42.69
24.00	-142.20	-1.62	-189.75	-243.44
25.00	-226.20	-78.55	-398.19	-30.39
26.00	21.72	222.64	183.49	280.18
27.00	102.98	190.58	170.17	-23.56
28.00	-100.51			

Table 6. Continued.

EXPERIMENTAL INTENSITY DATA FOR 103 DEGREE DATA
CURVE NUMBER 1 (211401)

s \ Δs	0.00	0.25	0.50	0.75
2.00	-12.54	-15.24	-11.47	-4.93
3.00	-7.19	-15.40	-25.86	-29.73
4.00	-24.16	-8.02	8.80	19.04
5.00	9.03	-12.76	-27.27	-29.54
6.00	-3.11	31.19	60.73	71.65
7.00	61.75	38.37	15.75	-5.46
8.00	-21.23	-49.91	-63.69	-71.72
9.00	-52.55	-14.17	33.45	70.74
10.00	75.50	63.48	50.81	17.03

CURVE NUMBER 4 (211304)

s \ Δs	0.00	0.25	0.50	0.75
8.00	-23.31	-31.04	-36.22	-41.02
9.00	-32.43	-9.78	13.94	41.25
10.00	49.08	42.16	26.45	11.10
11.00	1.98	-23.68	-44.20	-64.12
12.00	-75.09	-74.48	-52.17	-17.96
13.00	26.95	75.00	112.62	128.15
14.00	101.92	47.83	-9.64	-54.47
15.00	-71.54	-74.71	-46.22	-31.06
16.00	-12.03	-13.80	-6.29	-18.23
17.00	-18.95	-12.72	5.67	30.89
18.00	23.64	37.03	38.06	24.13
19.00	19.64	7.14	-9.30	1.27
20.00	4.35	-7.43	-6.68	-21.82
21.00	-32.63	-34.66	-29.05	-15.43
22.00	-4.96	6.34	8.48	23.73
23.00	22.36	29.74	24.21	8.88
24.00	5.95	-1.96	-6.03	-6.81
25.00	-6.97	-30.09	-23.84	-14.04
26.00	-5.99	3.81	7.95	19.07
27.00	17.05	18.95	11.10	-7.59
28.00	-9.26			

Table 6. Continued.

CURVE NUMBER 2 (211402)

s \ Δs	0.00	0.25	0.50	0.75
2.00	-5.27	-6.54	-4.85	-1.77
3.00	-3.03	-6.16	-10.97	-13.46
4.00	-10.59	-3.13	3.92	8.84
5.00	4.46	-4.38	-12.23	-12.46
6.00	-3.71	11.07	27.81	31.91
7.00	26.01	16.50	5.38	-2.16
8.00	-10.44	-20.44	-27.28	-28.12
9.00	-21.82	-3.43	13.25	27.24
10.00	31.17	27.59	19.26	9.13

CURVE NUMBER 5 (211303)

s \ Δs	0.00	0.25	0.50	0.75
9.00	-21.27	-28.26	-33.32	-34.88
9.00	-27.94	-15.11	17.68	32.11
10.00	44.03	37.13	26.22	11.18
11.00	-2.01	-17.31	-43.40	-55.75
12.00	-67.30	-67.38	-50.96	-19.82
13.00	14.07	67.04	102.83	115.84
14.00	92.56	58.68	8.76	-28.49
15.00	-75.02	-74.32	-48.88	-32.99
16.00	-24.37	-18.47	-14.03	-13.17
17.00	-7.84	2.93	8.34	14.41
18.00	23.11	29.72	20.05	14.38
19.00	7.84	2.66	5.06	20.16
20.00	20.81	4.72	-7.61	-13.45
21.00	-23.38	-27.82	-27.06	-16.57
22.00	-12.45	1.49	2.45	9.81
23.00	19.39	21.00	7.86	7.18
24.00	-1.35	1.03	-4.02	-5.39
25.00	-1.06	-9.19	-15.14	-8.83
26.00	13.43	3.08	.90	7.06
27.00	15.43	-9.54	5.64	3.66
28.00	-0.31			

Table 6. Continued.

CURVE NUMBER 3 (211434)

s \ Δs	0.00	0.25	0.50	0.75
2.00	-12.37	-15.38	-10.95	-4.24
3.00	-7.12	-15.14	-26.35	-30.80
4.00	-24.56	-8.77	6.57	19.56
5.00	9.83	-13.59	-27.42	-27.74
6.00	-6.05	33.46	60.05	70.46
7.00	61.84	36.17	15.94	-7.05
8.00	-19.14	-46.18	-66.21	-64.67
9.00	-55.96	-16.15	29.18	73.07
10.00	78.34	64.37	46.98	16.48

CURVE NUMBER 6 (211332)

s \ Δs	0.00	0.25	0.50	0.75
8.00	-21.67	-38.44	-49.04	-53.36
9.00	-39.39	-12.39	15.29	48.90
10.00	59.01	58.78	40.38	16.38
11.00	-1.25	-22.53	-50.91	-78.61
12.00	-91.84	-96.48	-68.52	-28.19
13.00	27.73	87.67	134.13	145.56
14.00	122.82	63.93	-2.78	-60.49
15.00	-86.27	-75.47	-70.64	-46.88
16.00	-17.67	-11.01	-5.11	-5.32
17.00	1.69	6.28	8.60	26.57
18.00	27.93	50.03	44.42	-11.45
19.00	-12.05	-12.56	-5.49	2.66
20.00	11.25	1.38	8.20	-19.44
21.00	-38.15	-26.46	-32.95	-6.08
22.00	-3.12	12.65	8.60	19.92
23.00	38.31	33.02	23.40	-0.77
24.00	4.04	.41	-14.58	-28.77
25.00	-35.11	-23.42	-15.37	-0.97
26.00	-5.33	15.73	16.13	36.24
27.00	10.74	11.34	-0.94	-13.49
28.00	1.22			

Table 6. Continued.

CCMPOSITE CURVE FCR 1J3 DEGREE DATA

s \ Δs	0.00	0.25	0.50	0.75
2.00	-91.09	-109.52	-81.22	-29.76
3.00	-47.84	-110.09	-183.94	-221.34
4.00	-187.34	-68.02	63.10	148.33
5.00	77.94	-76.32	-195.58	-199.77
6.00	-36.52	210.40	441.52	510.27
7.00	435.27	276.22	112.07	-37.28
8.00	-167.39	-582.61	-529.90	-611.76
9.00	-471.57	-154.66	236.50	624.75
10.00	712.61	594.71	468.56	222.08
11.00	35.31	-140.63	-380.06	-643.54
12.00	-890.97	-885.81	-684.80	-345.64
13.00	141.13	709.12	1134.29	1388.25
14.00	1193.99	724.46	66.52	-487.01
15.00	-804.52	-826.90	-572.32	-356.14
16.00	-161.02	-83.76	-9.16	-70.22
17.00	-134.30	-26.77	25.33	231.35
18.00	261.25	422.38	279.49	128.52
19.00	14.96	41.99	-99.52	7.66
20.00	-19.31	67.70	16.15	-99.38
21.00	-247.33	-293.13	-394.40	-261.92
22.00	-60.00	97.26	97.26	77.37
23.00	257.98	516.80	325.75	137.08
24.00	167.41	73.36	14.35	-358.27
25.00	-643.05	-233.37	-196.35	-19.17
26.00	-177.91	157.15	220.17	331.98
27.00	183.86	127.68	59.06	-36.29
28.00	-87.28			

Table 6. Continued.

EXPERIMENTAL INTENSITY CURVES FOR 135 DEGREE DATA
CURVE NUMBER 1 (207101)

s \ Δs	0.00	0.25	0.50	0.75
2.00	-3.33	-3.85	-2.23	.03
3.00	-1.06	-4.07	-8.48	-9.03
4.00	-7.02	-2.63	3.10	6.36
5.00	3.03	-3.91	-9.15	-8.93
6.00	-1.74	7.30	15.09	17.96
7.00	16.99	11.87	4.60	1.10
8.00	-3.72	-11.54	-18.35	-23.69
9.00	-15.19	-5.87	13.55	21.14
10.00	22.84	16.95	13.47	3.69

CURVE NUMBER 4 (202904)

s \ Δs	0.00	0.25	0.50	0.75
8.00	-9.41	-14.33	-15.30	-20.75
9.00	-12.62	-1.29	10.30	22.24
10.00	28.77	13.11	11.00	1.77
11.00	-6.34	-23.77	-34.50	-51.93
12.00	-54.05	-59.35	-42.13	-21.58
13.00	15.45	59.87	85.99	94.12
14.00	73.45	45.23	6.40	-37.86
15.00	-37.94	-35.24	-17.58	-19.69
16.00	-11.42	-1.05	8.29	-9.18
17.00	-11.15	-0.14	9.51	15.66
18.00	16.13	9.22	8.77	1.68
19.00	-13.59	-2.90	-1.64	1.36
20.00	21.61	-6.64	4.19	-2.44
21.00	-26.64	-22.03	-21.81	-24.40
22.00	-1.13	20.44	-1.94	-0.45
23.00	10.02	4.13	12.93	-14.10
24.00	20.94	4.20	2.01	-7.28
25.00	-5.99	-10.50	15.44	-23.52
26.00	22.74	-4.74	-6.57	30.82
27.00	17.77	11.41	-0.13	-11.36
28.00	-11.67			

Table 6. Continued.

CURVE NUMBER 2 (207102)

s \ Δs	0.00	0.25	0.50	0.75
2.00	-6.42	-7.65	-4.89	-0.03
3.00	-2.97	-7.39	-19.04	-18.33
4.00	-15.07	-5.37	7.14	11.92
5.00	6.03	-6.83	-19.69	-19.83
6.00	-5.35	16.27	33.77	39.10
7.00	35.35	22.62	8.62	-4.16
8.00	-10.52	-25.10	-35.66	-38.59
9.00	-34.36	-1.12	21.71	33.33
10.00	44.31	44.07	25.70	4.62

CURVE NUMBER 5 (202901)

s \ Δs	0.00	0.25	0.50	0.75
8.00	-4.03	-12.83	-13.59	-15.23
9.00	-10.84	-0.65	7.78	17.89
10.00	17.61	10.35	12.30	3.30
11.00	-9.87	-16.20	-30.19	-41.66
12.00	-51.61	-50.62	-35.42	-11.76
13.00	14.14	48.05	68.51	76.70
14.00	62.12	29.69	1.29	-17.63
15.00	-29.29	-27.88	-27.47	-10.37
16.00	-3.75	2.39	7.23	-13.88
17.00	8.04	5.33	4.99	8.85
18.00	6.52	21.45	21.80	11.26
19.00	5.09	-9.29	-5.92	-6.52
20.00	14.03	1.84	-10.97	-3.31
21.00	-14.59	-36.35	-26.47	-26.45
22.00	-18.90	-14.92	2.26	1.28
23.00	9.35	6.72	36.85	4.54
24.00	9.57	6.94	8.01	-1.03
25.00	-17.11	-6.33	-2.00	-5.16
26.00	11.14	21.77	21.80	.21
27.00	32.69	12.83	-12.29	-22.47
28.00	-13.02			

Table 6. Continued.

CURVE NUMBER 3 (207104)

s \ Δs	0.00	0.25	0.50	0.75
2.00	-7.30	-8.82	-6.08	-1.11
3.00	-3.74	-9.00	-16.76	-19.58
4.00	-16.34	-7.05	6.23	12.45
5.00	4.07	-9.25	-20.04	-23.48
6.00	-8.94	18.68	41.59	46.42
7.00	43.72	28.81	18.39	3.93
8.00	-11.34	-31.15	-47.31	-45.76
9.00	-37.95	-16.56	22.67	36.26
10.00	45.55	45.02	31.28	25.67

CURVE NUMBER 6 (202905)

s \ Δs	0.00	0.25	0.50	0.75
8.00	-10.73	-10.89	-10.72	-10.68
9.00	-7.32	.12	7.77	18.67
10.00	15.00	13.40	10.71	2.62
11.00	.74	-6.97	-20.00	-29.09
12.00	-29.14	-26.55	-25.02	-8.62
13.00	7.07	27.56	46.91	40.69
14.00	39.28	23.04	3.61	-13.21
15.00	-21.30	-22.12	-17.20	-11.21
16.00	-5.12	-2.35	-7.77	-6.26
17.00	-8.12	-7.79	-1.74	.85
18.00	1.62	2.27	8.03	4.73
19.00	2.48	9.93	8.32	5.93
20.00	-1.56	3.67	-2.77	-5.53
21.00	-2.91	-10.79	2.56	-1.59
22.00	3.57	8.10	-1.83	6.99
23.00	9.49	-2.24	13.70	2.80
24.00	-4.3?	-0.15	.23	-9.81
25.00	-5.5?	-9.43	-13.22	5.82
26.00	3.7?	-3.25	5.86	3.85
27.00	7.5?	-1.96	4.35	-1.79
28.00	3.5?			

Table 6. Continued.

COMPOSITE CURVE FOR 135 DEGREE DATA

s	Δs 0.00	0.25	0.50	0.75
2.00	-80.56	-95.33	-60.68	-3.82
3.00	-34.16	-96.85	-193.24	-221.71
4.00	-179.70	-69.46	77.87	147.21
5.00	65.25	-94.12	-229.95	-240.98
6.00	-68.65	195.41	415.06	478.48
7.00	445.09	296.12	139.74	5.67
8.00	-160.23	-304.83	-388.63	-435.83
9.00	-319.32	-61.61	243.87	455.50
10.00	500.34	393.70	301.70	63.25
11.00	-89.48	-332.53	-641.40	-916.02
12.00	-1010.23	-1005.21	-779.87	-307.12
13.00	270.24	987.63	1518.01	1553.07
14.00	1313.00	735.38	87.57	-496.17
15.00	-670.01	-653.53	-490.96	-315.55
16.00	-151.47	-15.98	11.72	-222.35
17.00	-101.05	-51.56	71.31	163.98
18.00	159.08	230.60	295.59	142.54
19.00	-16.17	30.11	42.90	29.37
20.00	208.12	13.98	-83.70	-100.23
21.00	-292.10	-507.01	-285.36	-347.34
22.00	-99.01	107.25	-16.22	85.40
23.00	225.01	46.15	489.82	-19.44
24.00	141.02	71.77	70.71	-161.05
25.00	-190.08	-212.97	-72.72	-198.92
26.00	254.30	88.16	180.66	226.45
27.00	413.32	135.14	-37.82	-244.95
28.00	-119.53			

Table 6. Continued.

CURVE NUMBER 2 (210404)

Δs \ s	0.00	0.25	0.50	0.75
2.00	-9.13	-12.15	-9.27	-2.95
3.00	-4.98	-11.06	-19.64	-24.35
4.00	-19.61	-5.86	9.64	22.02
5.00	10.74	-16.85	-28.73	-32.23
6.00	-10.38	21.69	53.38	63.62
7.00	57.45	38.63	9.99	-7.28
8.00	-29.00	-46.74	-65.22	-65.82
9.00	-41.06	-4.34	35.56	74.43
10.00	71.40	55.56	40.10	2.72

CURVE NUMBER 5 (210603)

Δs \ s	0.00	0.25	0.50	0.75
8.00	-42.27	-54.12	-60.97	-65.58
9.00	-49.13	-27.32	18.56	68.46
10.00	71.73	65.73	53.53	21.43
11.00	.42	-20.36	-46.02	-91.87
12.00	-142.37	-135.09	-97.00	-41.36
13.00	36.92	134.46	192.98	214.16
14.00	166.11	105.53	-14.09	-68.28
15.00	-97.78	-112.47	-94.42	-58.43
16.00	-47.47	-19.85	-18.70	-8.90
17.00	-21.22	-20.99	-0.80	-0.84
18.00	17.84	33.31	17.83	7.96
19.00	18.13	6.17	9.09	21.15
20.00	43.89	17.53	18.62	7.58
21.00	-26.76	-26.55	-37.38	-4.32
22.00	3.05	30.55	7.69	15.31
23.00	35.27	49.60	44.12	2.97
24.00	-11.59	-3.07	-36.59	-30.05
25.00	-33.28	-73.74	-23.51	-41.28
26.00	-11.87	16.97	20.18	25.97
27.00	16.49	34.21	26.58	-0.65
28.00	16.32			

Table 6. Continued.

CURVE NUMBER 5 (215402)

s \ Δs	0.00	0.25	0.50	0.75
2.00	-13.42	-17.44	-13.87	-4.80
3.00	-8.24	-14.78	-27.50	-33.43
4.00	-29.71	-9.40	10.94	29.13
5.00	17.87	-11.51	-37.56	-42.70
6.00	-16.72	32.82	72.64	89.59
7.00	79.55	49.38	11.60	-14.46
8.00	-35.39	-66.19	-87.54	-98.91
9.00	-65.56	-9.22	61.81	97.46
10.00	115.02	100.97	90.51	-45.63

CURVE NUMBER 6 (215602)

s \ Δs	0.00	0.25	0.50	0.75
8.00	-49.75	-71.54	-74.73	-86.10
9.00	-50.67	-6.34	42.54	87.99
10.00	76.98	85.65	60.14	26.69
11.00	14.14	-23.81	-72.82	-122.51
12.00	-153.40	-149.02	-101.58	-43.79
13.00	40.79	124.81	191.64	206.09
14.00	171.04	92.53	-10.77	-67.97
15.00	-107.03	-106.27	-88.27	-48.11
16.00	-30.44	-23.71	2.81	-21.40
17.00	2.13	-3.61	18.50	39.82
18.00	37.41	52.61	35.56	-4.45
19.00	-5.50	12.55	-18.13	19.23
20.00	-7.40	-20.44	-18.34	-32.47
21.00	-51.58	-38.49	-64.71	-32.04
22.00	18.09	19.62	58.56	47.59
23.00	69.19	103.43	39.57	-6.25
24.00	26.05	7.43	-33.28	-51.97
25.00	-64.32	-46.61	-19.02	-27.90
26.00	.87	9.07	38.41	43.96
27.00	16.47	7.74	-39.66	-19.81
28.00	53.87			

Table 6. Continued.

COMPOSITE CURVE FOR 175 DEGREE DATA

s \ Δs	0.00	0.25	0.50	0.75
2.00	-69.95	-94.36	-74.32	-23.50
3.00	-40.51	-79.64	-150.33	-185.46
4.00	-156.37	-48.01	70.66	159.09
5.00	94.21	-68.21	-220.95	-243.93
6.00	-88.86	174.94	398.50	494.86
7.00	434.65	274.79	83.66	-55.20
8.00	-260.42	-403.87	-489.06	-520.92
9.00	-351.13	-66.75	257.06	537.21
10.00	565.67	484.39	381.48	171.05
11.00	41.65	-177.76	-436.97	-745.23
12.00	-1000.62	-974.96	-673.70	-262.91
13.00	272.70	894.05	1335.32	1471.32
14.00	1186.86	713.00	-76.74	-502.36
15.00	-779.19	-803.78	-644.37	-425.91
16.00	-277.12	-155.63	-92.51	-52.56
17.00	-79.08	-30.59	91.96	151.83
18.00	239.49	319.41	205.75	89.40
19.00	69.86	42.77	21.94	85.18
20.00	139.17	-6.52	-32.32	-106.53
21.00	-231.62	-306.22	-329.74	-120.20
22.00	11.46	149.44	251.00	227.16
23.00	303.63	422.69	266.22	66.24
24.00	-6.24	43.54	-183.23	-253.90
25.00	-323.14	-405.16	-162.95	-198.44
26.00	20.20	69.34	281.53	211.55
27.00	124.11	106.30	25.52	-33.93
28.00	119.15			

Table 6. Continued.

EXPERIMENTAL INTENSITY CURVES FOR 200 DEGREE DATA
CURVE NUMBER 1 (207202)

s \ Δs	0.00	0.25	0.50	0.75
2.00	-7.20	-9.51	-6.80	-2.24
3.00	-3.28	-8.98	-17.70	-18.66
4.00	-15.19	-2.68	10.25	18.26
5.00	10.45	-9.64	-28.07	-32.96
6.00	-14.39	18.36	41.68	48.70
7.00	50.12	28.54	12.70	4.50
8.00	-10.52	-28.22	-51.15	-52.32
9.00	-38.23	-10.33	22.30	42.43
10.00	47.66	40.23	25.58	24.90

CURVE NUMBER 4 (207309)

s \ Δs	0.00	0.25	0.50	0.75
8.00	-23.82	-33.72	-36.41	-36.45
9.00	-26.98	.49	22.62	42.65
10.00	40.51	37.58	28.56	16.15
11.00	.27	-14.13	-44.14	-70.99
12.00	-81.02	-83.60	-47.63	-16.72
13.00	18.37	77.22	105.08	123.42
14.00	106.85	33.16	-12.61	-39.47
15.00	-72.23	-48.15	-50.96	-22.06
16.00	-14.38	-1.62	-0.46	-10.83
17.00	7.41	-2.69	3.62	15.14
18.00	13.55	11.82	10.42	-5.19
19.00	-10.37	10.42	-9.29	21.88
20.00	1.95	3.63	-2.82	-13.79
21.00	-21.34	-8.70	-37.72	-29.15
22.00	-3.12	14.30	44.40	33.04
23.00	9.29	43.40	45.64	-0.93
24.00	.95	2.65	-9.09	-25.74
25.00	-37.08	-15.23	-18.59	-29.11
26.00	-3.00	18.56	6.35	.34
27.00	16.07	13.54	17.35	5.55
28.00	-10.14			

Table 6. Continued.

CURVE NUMBER 2 (207203)

s \ Δs	0.00	0.25	0.50	0.75
2.00	-10.48	-13.13	-10.14	-2.81
3.00	-6.06	-12.65	-21.88	-27.04
4.00	-24.51	-7.33	13.13	22.65
5.00	14.80	-11.06	-35.77	-40.28
6.00	-13.05	26.74	58.13	69.46
7.00	61.09	42.74	18.01	.06
8.00	-7.89	-48.99	-74.84	-76.43
9.00	-53.52	-13.43	24.27	65.59
10.00	82.26	63.78	35.78	25.87

CURVE NUMBER 5 (207304)

s \ Δs	0.00	0.25	0.50	0.75
8.00	-26.11	-33.90	-36.77	-41.68
9.00	-18.76	.14	24.77	46.61
10.00	43.04	31.74	27.86	9.70
11.00	-4.54	-20.98	-45.56	-61.15
12.00	-80.74	-69.13	-56.98	-18.35
13.00	31.15	71.53	114.83	123.57
14.00	99.22	56.61	-9.82	-49.79
15.00	-77.15	-65.45	-49.89	-34.46
16.00	-19.07	-8.18	-7.39	2.87
17.00	-3.92	4.69	14.17	5.68
18.00	12.43	22.66	21.68	10.36
19.00	.76	8.14	13.72	2.48
20.00	7.49	-3.50	-3.48	5.73
21.00	-22.75	-32.07	-25.28	-23.98
22.00	-17.76	4.41	11.60	-5.03
23.00	25.95	42.32	40.52	13.24
24.00	27.50	9.88	-0.33	-15.13
25.00	-17.76	-23.22	-16.20	-18.86
26.00	-12.94	15.73	1.97	29.68
27.00	14.16	-13.27	-6.05	5.80
28.00	12.97			

Table 6. Continued.

CURVE NUMBER 3 (207205)

s \ Δs	0.00	0.25	0.50	0.75
2.00	-7.16	-9.31	-7.00	-2.67
3.00	-4.01	-9.06	-15.17	-16.13
4.00	-17.24	-6.34	10.53	16.84
5.00	7.70	-10.23	-23.33	-24.61
6.00	-10.96	16.29	38.60	50.42
7.00	41.63	31.74	10.86	4.28
8.00	-14.36	-32.68	-48.38	-56.35
9.00	-36.16	-6.21	18.09	48.53
10.00	54.76	49.43	24.34	11.92

CURVE NUMBER 6 (207302)

s \ Δs	0.00	0.25	0.50	0.75
8.00	-20.87	-30.21	-43.15	-34.09
9.00	-35.17	-2.31	21.78	41.43
10.00	45.07	38.02	27.26	24.62
11.00	.23	-22.33	-41.18	-58.25
12.00	-76.03	-80.12	-53.31	-22.91
13.00	17.92	71.23	114.25	121.91
14.00	113.42	44.78	-12.22	-45.27
15.00	-71.54	-65.81	-49.22	-29.77
16.00	-9.68	-21.84	-17.17	-17.30
17.00	3.20	-7.10	11.60	15.53
18.00	20.51	15.21	14.08	24.17
19.00	24.72	4.01	-6.41	-4.71
20.00	-4.86	30.08	-4.60	15.98
21.00	-7.54	-8.92	-25.88	-3.69
22.00	-18.38	-11.28	20.39	-3.32
23.00	15.92	5.96	37.47	-10.16
24.00	6.94	-23.16	-3.91	-8.09
25.00	-31.58	-10.53	-11.73	-13.69
26.00	11.05	14.09	24.46	34.30
27.00	34.14	16.48	.89	-16.13
28.00	-25.56			

Table 6. Continued.

COMPOSITE CURVE FOR 2JU DEGREE DATA

s \ Δs	0.00	0.25	0.50	0.75
2.10	-73.36	-94.70	-71.66	-23.24
3.00	-38.96	-90.93	-162.94	-181.57
4.00	-167.61	-47.85	101.35	172.31
5.00	96.37	-93.39	-258.43	-289.99
6.00	-116.64	180.40	438.97	499.46
7.00	454.83	304.93	122.26	29.87
8.00	-196.82	-361.83	-495.68	-504.52
9.00	-355.40	-47.28	239.04	499.71
10.00	534.51	447.61	298.62	207.54
11.00	-16.40	-235.62	-537.61	-782.65
12.00	-976.85	-957.18	-648.28	-238.09
13.00	276.49	903.91	1372.27	1515.41
14.00	1312.76	551.69	-142.43	-552.16
15.00	-907.30	-736.15	-616.57	-353.91
16.00	-177.01	-129.29	-102.40	-104.26
17.00	23.02	-21.27	120.26	149.70
18.00	191.00	203.61	189.21	119.69
19.00	61.35	92.87	-9.09	81.71
20.00	18.57	124.14	-44.74	31.54
21.00	-212.10	-203.12	-365.73	-233.85
22.00	-160.57	31.08	315.30	103.24
23.00	209.41	376.89	508.14	8.27
24.00	144.21	-43.82	-55.14	-201.66
25.00	-355.86	-221.27	-191.24	-253.80
26.00	-19.72	198.85	134.73	262.81
27.00	264.42	69.91	51.17	-19.52
28.00	-94.27			

Table 7. Theoretical intensity data for 2-bromoethanol.

THEORETICAL INTENSITY CURVE FOR 55 DEGREE EXPERIMENT

s \ Δs	0.00	0.25	0.50	0.75
0	0	.11	2.80	13.48
1.00	28.16	27.52	-4.66	-57.87
2.00	-96.80	-96.47	-66.74	-42.22
3.00	-53.22	-105.25	-172.79	-206.84
4.00	-163.17	-42.16	93.30	147.56
5.00	62.20	-127.36	-298.72	-321.65
6.00	-153.46	126.23	372.37	476.33
7.00	430.42	307.22	181.00	67.47
8.00	-65.73	-235.46	-394.28	-448.19
9.00	-329.25	-57.81	260.19	498.99
10.00	586.26	527.72	374.64	172.83
11.00	-61.05	-324.78	-601.66	-848.21
12.00	-1004.67	-1011.72	-822.36	-415.21
13.00	179.69	851.08	1408.20	1642.28
14.00	1432.93	833.99	70.27	-570.11
15.00	-884.39	-849.17	-601.60	-331.21
16.00	-164.65	-118.09	-130.34	-131.32
17.00	-88.19	-7.57	86.79	170.57
18.00	220.75	216.61	153.04	57.14
19.00	-14.33	-8.45	81.83	200.93
20.00	260.81	199.89	26.08	-186.92
21.00	-347.40	-398.77	-341.07	-214.43
22.00	-65.32	74.89	168.80	262.43
23.00	283.00	247.59	171.61	82.48
24.00	2.94	-63.26	-128.98	-195.16
25.00	-254.29	-274.22	-227.94	-115.04
26.00	33.05	168.58	251.79	267.32
27.00	223.59	142.22	46.89	-41.09
28.00	-163.46	-127.86	-112.69	-70.95
29.00	-25.04	4.13	8.10	-6.56
30.00	-25.39			

Table 7. Continued.

THEORETICAL INTENSITY CURVE FOR 103 DEGREE EXPERIMENT

s	Δs 0.00	0.25	0.50	0.75
0	0	.11	2.80	13.45
1.00	27.89	26.31	-7.85	-63.06
2.00	-101.75	-97.98	-64.52	-41.42
3.00	-62.34	-130.66	-214.40	-258.30
4.00	-214.78	-81.98	81.11	181.71
5.00	154.60	15.14	-138.42	-185.69
6.00	-68.49	165.69	398.84	515.14
7.00	487.68	359.13	194.33	20.94
8.00	-174.72	-399.01	-602.33	-684.89
9.00	-562.73	-240.56	171.07	514.29
10.00	675.00	638.27	472.08	261.06
11.00	49.16	-173.24	-420.30	-675.67
12.00	-873.50	-925.01	-761.82	-371.96
13.00	184.59	780.80	1248.74	1429.05
14.00	1236.47	712.92	30.76	-573.09
15.00	-905.28	-906.12	-665.68	-357.04
16.00	-132.67	-50.91	-71.79	-110.02
17.00	-98.13	-18.43	104.57	230.33
18.00	322.61	356.70	322.25	228.98
19.00	110.79	15.00	-22.46	-2.69
20.00	32.84	28.48	-47.20	-177.59
21.00	-307.98	-380.00	-364.56	-271.87
22.00	-135.87	9.84	144.80	258.27
23.00	339.73	375.01	353.09	274.14
24.00	152.30	8.69	-135.69	-261.82
25.00	-349.33	-375.72	-323.96	-196.32
26.00	-22.53	146.51	258.94	235.08
27.00	228.86	122.92	10.98	-70.58
28.00	-103.14	-87.54	-38.96	18.79
29.00	61.02	69.34	36.83	-19.06
30.00	-80.92			

Table 7. Continued.

THEORETICAL INTENSITY CURVE FOR 135 DEGREE EXPERIMENT

s	Δs	J.00	0.25	C.50	0.75
0		0	.11	2.81	13.53
1.00		28.22	27.10	-6.60	-61.36
2.00		-99.00	-93.08	-57.09	-32.49
3.00		-52.69	-117.82	-191.66	-219.6
4.00		-163.87	-37.40	92.32	139.92
5.00		61.34	-106.37	-257.46	-282.24
6.00		-141.28	106.38	343.21	469.31
7.00		457.08	347.22	199.11	44.85
8.00		-114.23	-273.77	-396.10	-418.84
9.00		-300.01	-59.49	221.37	438.81
10.00		531.08	492.96	362.55	180.96
11.00		-33.49	-280.51	-551.91	-809.74
12.00		-984.23	-993.93	-777.57	-327.75
13.00		285.50	914.35	1369.31	1489.44
14.00		1219.62	650.34	-12.42	-540.17
15.00		-787.21	-747.44	-532.58	-292.99
16.00		-135.03	-84.44	-101.86	-127.74
17.00		-119.33	-63.79	27.18	127.33
18.00		204.60	231.76	200.58	131.35
19.00		66.38	44.59	74.24	123.58
20.00		140.36	87.95	-28.86	-165.51
21.00		-265.68	-293.18	-246.63	-151.94
22.00		-42.72	55.35	128.33	170.64
23.00		182.09	167.44	136.01	96.69
24.00		52.28	-1.99	-71.14	-149.37
25.00		-215.29	-239.47	-201.19	-103.24
26.00		26.15	145.56	218.82	228.96
27.00		181.13	96.79	3.84	-71.80
28.00		-112.20	-111.50	-77.05	-27.24
29.00		16.01	36.21	28.98	2.45
30.00		-28.57			

Table 7. Continued.

THEORETICAL INTENSITY CURVE FOR 175 DEGREE EXPERIMENT

s \ Δs	0.00	0.25	0.50	0.75
0	0	.11	2.86	13.46
1.00	27.97	26.65	-7.02	-61.92
2.00	-101.16	-98.81	-66.23	-41.18
3.00	-56.03	-115.26	-190.27	-229.77
4.00	-189.08	-67.18	77.98	156.77
5.00	109.57	-41.77	-195.01	-231.62
6.00	-100.33	144.36	380.31	500.43
7.00	474.66	346.63	178.67	1.97
8.00	-184.09	-371.02	-508.57	-520.80
9.00	-363.66	-72.12	247.24	477.53
10.00	558.06	504.77	374.92	211.89
11.00	18.73	-222.43	-507.75	-786.19
12.00	-969.94	-971.47	-741.19	-290.44
13.00	302.25	899.33	1332.43	1455.23
14.00	1208.92	664.96	9.42	-536.8
15.00	-820.37	-820.05	-634.27	-405.82
16.00	-238.07	-155.64	-122.46	-89.36
17.00	-30.23	52.34	141.49	219.37
18.00	269.84	277.99	237.17	160.34
19.00	82.31	41.38	51.84	97.97
20.00	97.53	38.14	-90.93	-244.17
21.00	-357.33	-384.61	-319.81	-191.29
22.00	-39.74	101.67	213.14	283.81
23.00	307.51	283.74	221.14	135.29
24.00	41.60	-51.55	-141.78	-223.93
25.00	-282.61	-294.97	-243.63	-132.60
26.00	10.82	144.53	231.03	252.53
27.00	214.10	137.13	48.20	-29.30
28.00	-79.34	-95.25	-80.31	-47.35
29.00	-13.96	4.46	1.58	-17.79
30.00	-41.61			

Table 7. Continued.

THEORETICAL INTENSITY CURVE FOR 200 DEGREE EXPERIMENT

| s \ Δs	0.00	0.25	0.50	0.75
0	0	.11	2.80	13.40
1.00	27.79	26.61	-6.16	-59.71
2.00	-98.87	-98.96	-69.85	-44.84
3.00	-54.92	-107.41	-179.87	-224.07
4.00	-191.07	-71.93	78.31	164.01
5.00	116.09	-46.46	-214.36	-258.65
6.00	-125.67	125.32	362.11	478.69
7.00	455.38	345.65	208.91	59.57
8.00	-121.12	-328.76	-459.17	-535.84
9.00	-383.93	-84.19	242.68	471.62
10.00	546.23	492.44	371.09	218.14
11.00	25.69	-226.80	-526.17	-808.45
12.00	-981.59	-966.44	-728.09	-276.72
13.00	310.02	916.69	1346.43	1472.71
14.00	1214.53	642.57	-42.27	-598.77
15.00	-863.74	-824.22	-598.50	-346.11
16.00	-174.08	-99.59	-78.13	-58.48
17.00	-17.34	41.85	107.86	171.52
18.00	220.84	236.59	203.13	127.73
19.00	47.55	8.58	31.05	88.56
20.00	122.82	85.26	-27.68	-171.05
21.00	-282.33	-319.89	-281.76	-190.68
22.00	-80.39	30.19	130.67	211.00
23.00	258.08	261.63	222.67	153.00
24.00	67.32	-25.73	-122.04	-212.79
25.00	-277.42	-268.79	-229.27	-106.61
26.00	44.38	176.19	250.05	251.37
27.00	190.90	95.63	-3.74	-81.52
28.00	-121.24	-118.08	-79.68	-24.97
29.00	22.69	44.80	35.81	4.53
30.00	-31.89			
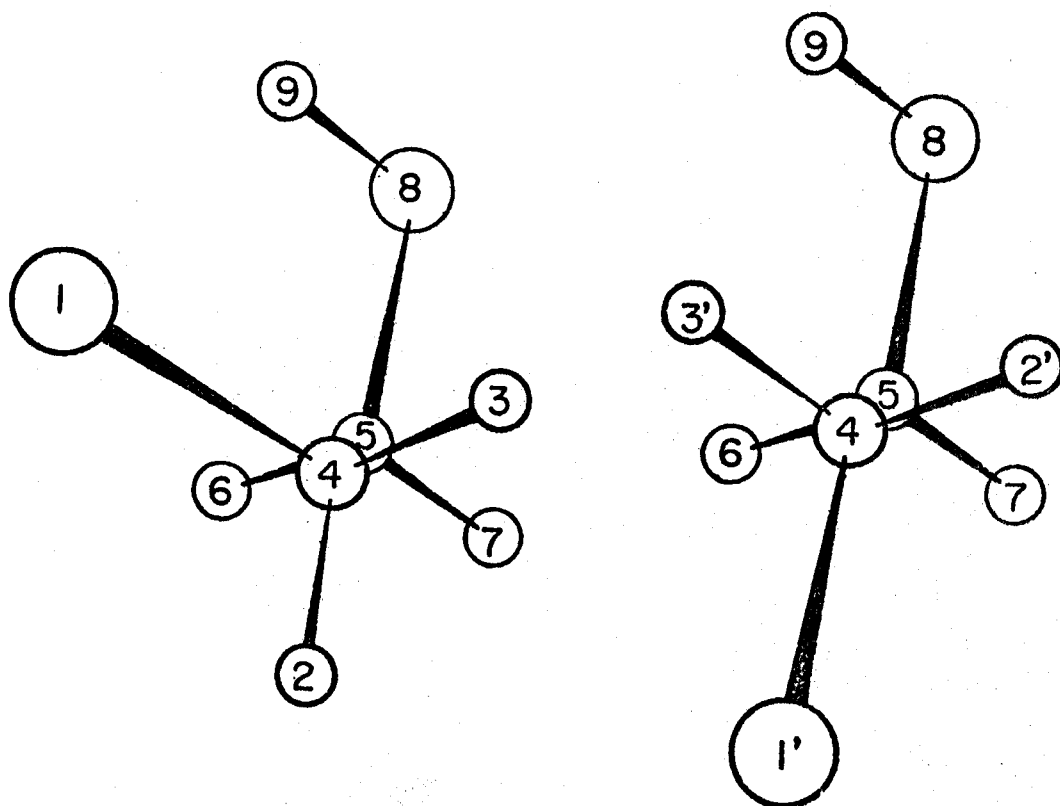
Figure 1. Gauche (left) and trans (right) conformations and atom
numbering of 2-bromoethanol.
Br: 1, 1'
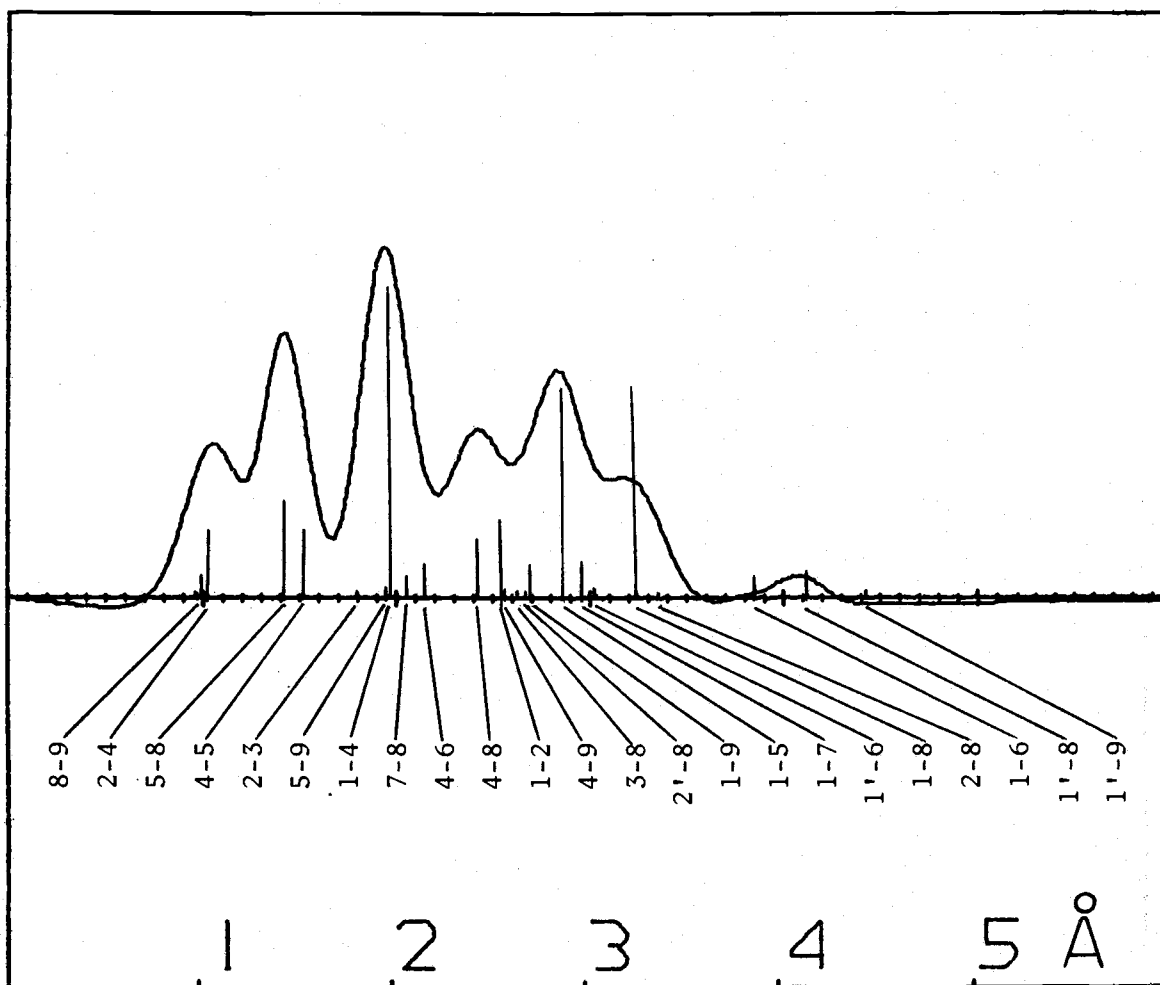C: 4, 5
H: 2, 2', 3, 3', 6, 7, 9
O: 8

Figure 2. Average final theoretical radial distribution curve for
2-bromoethanol showing the relative contributions for the
different interatomic distances with the atoms numbered as
in Figure 1.

Figure 3. Composite experimental intensity curves for 2-bromoethanol for the five different temperature experiments. The lower five curves are the difference curves (i. e., experimental minus theoretical) using theoretical curves determined independently for each experiment.

55°C

103°C

135°C

175°C

200°C

55°C

103°C

135°C

175°C

200°C

5 10 15 20 25 30 35 S
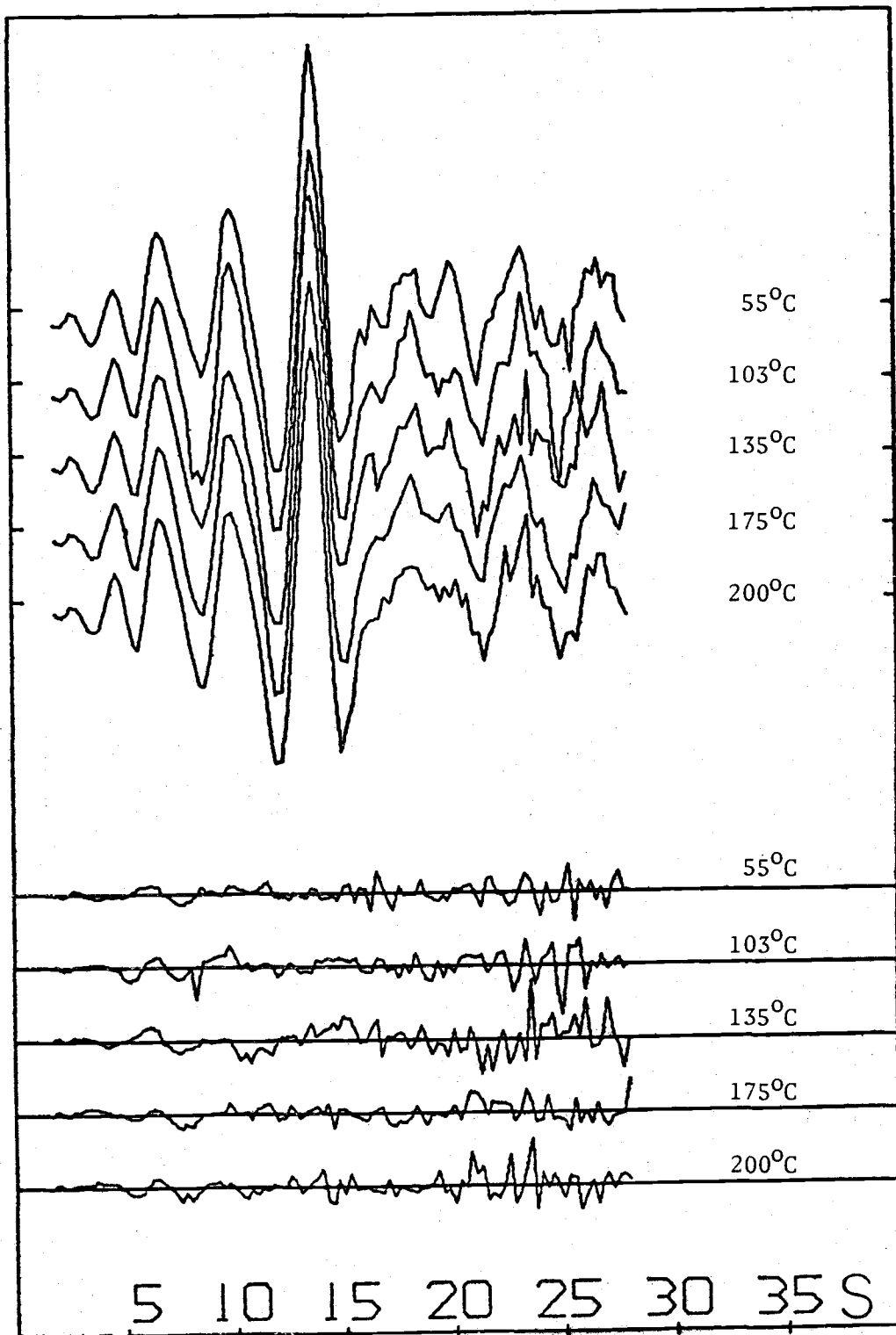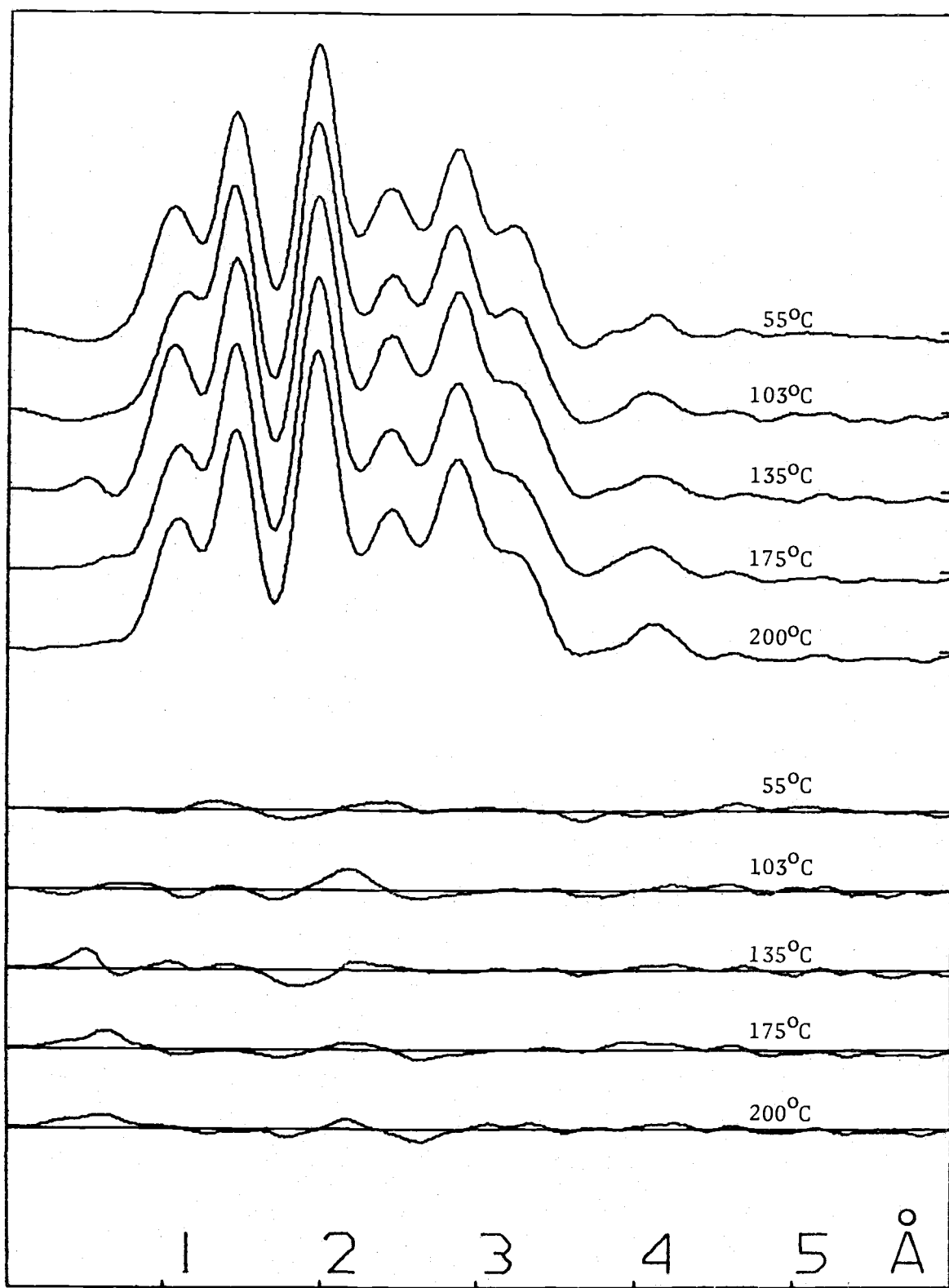
Figure 4. Radial distribution curves for 2-bromoethanol calculated from the experimental curves given in Figure 3.
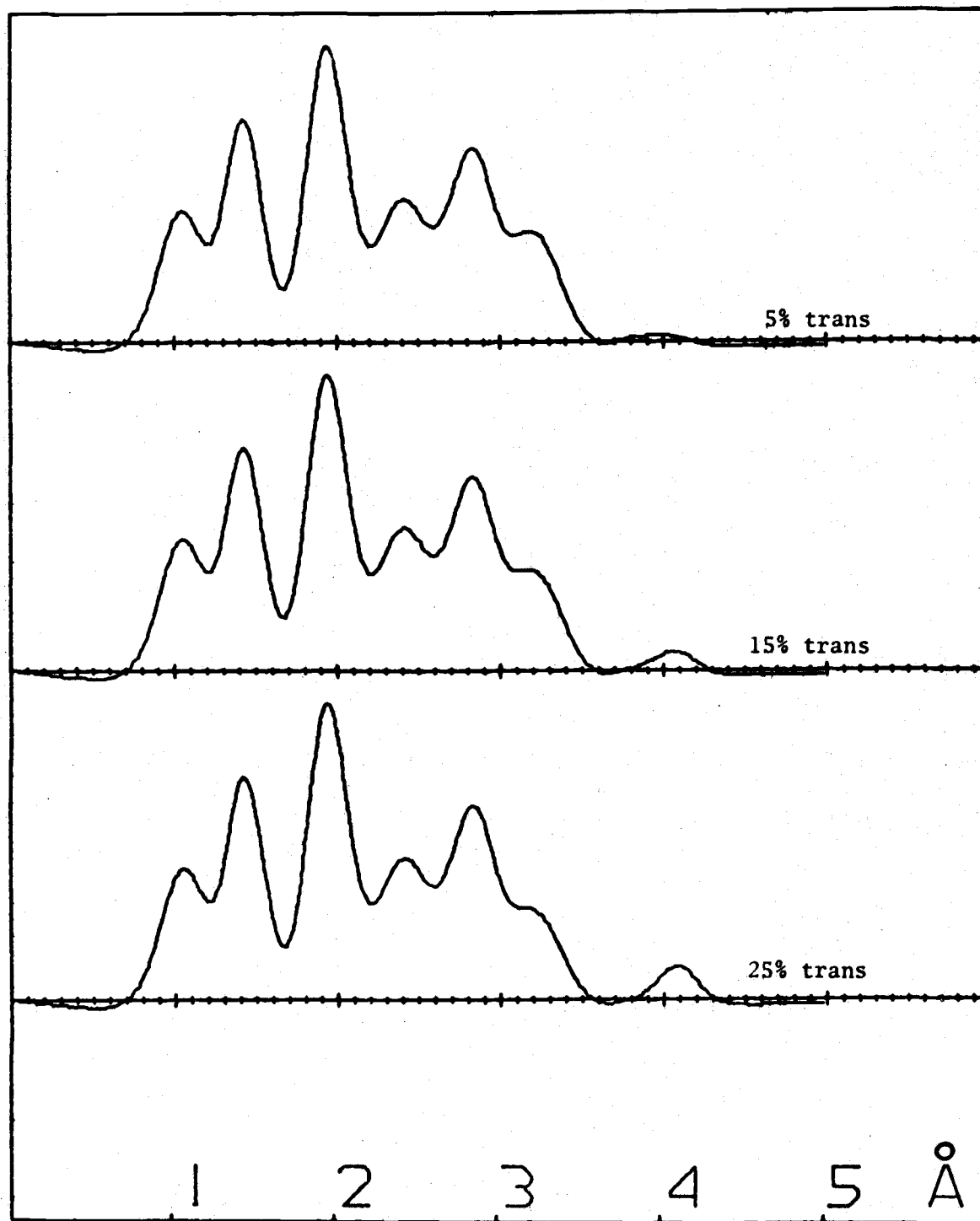
Figure 5. Theoretical radial distribution curves identically equal to the average final theoretical curve in Figure 2 except for the percentage of the trans conformer as given on the figure.
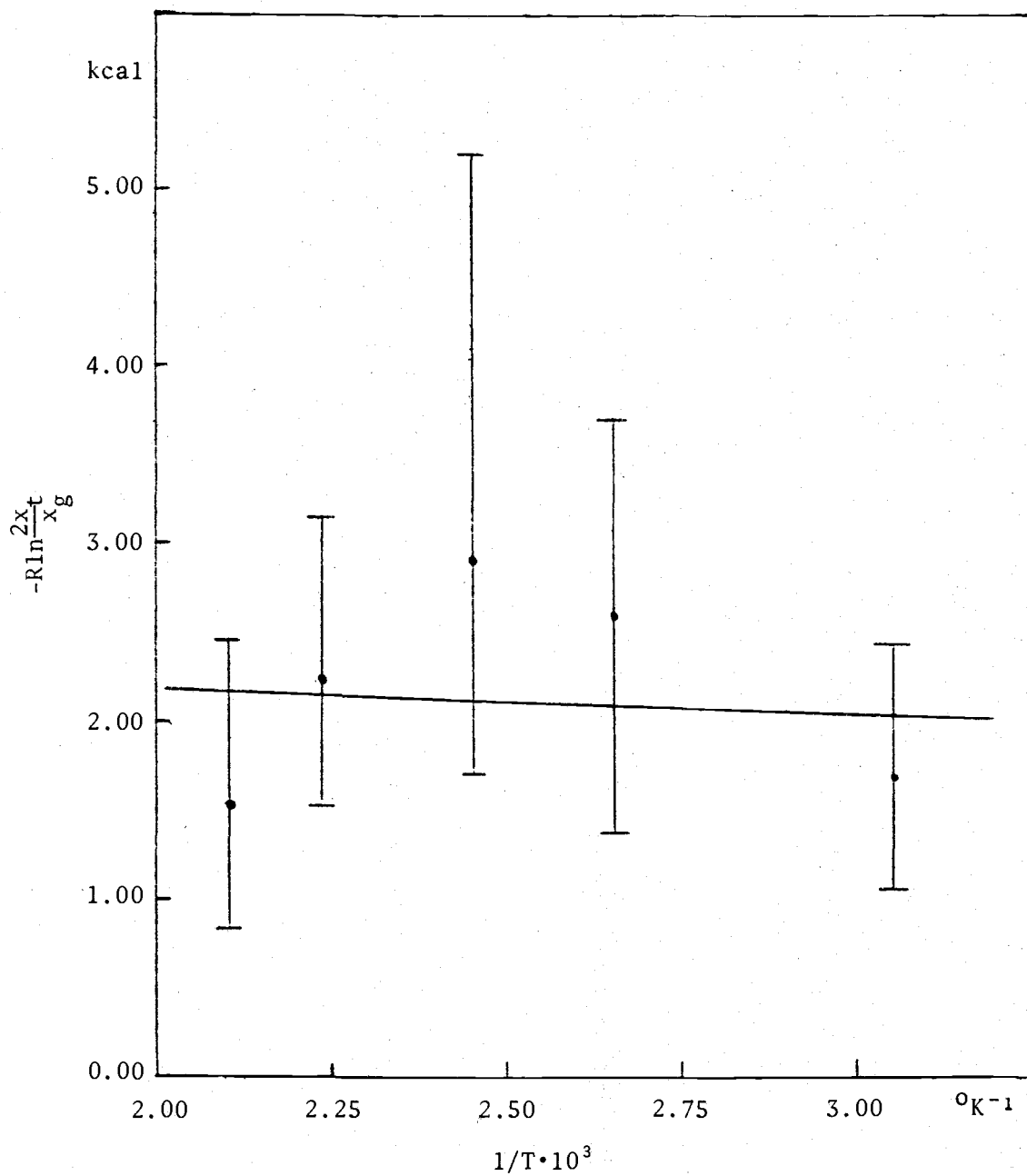
Figure 6. Thermodynamic plot using the least squares values for x_g at each temperature. The best straight line has a slope of -0.107 and a y-intercept of 2.38.
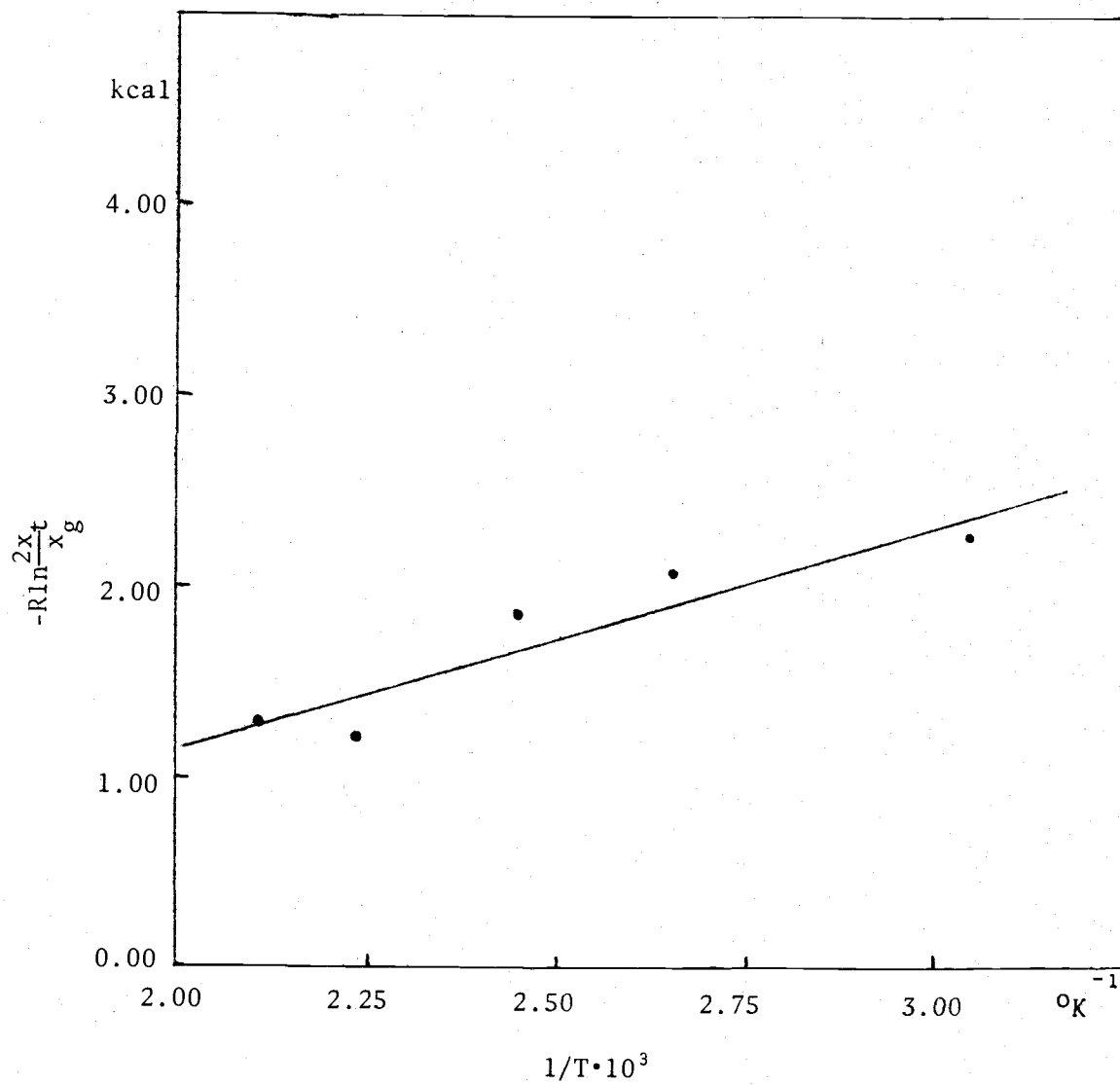
Figure 7. Thermodynamic plot using values for x_g obtained from a weight comparison of peaks.

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