

See discussions, stats, and author profiles for this publication at:  
<https://www.researchgate.net/publication/244284667>

# Molecular structure and conformational composition of 1-iodopropane as determined from gas-phase electron diffraction, microwave spectroscopy data and ab initio calculations

ARTICLE *in* JOURNAL OF MOLECULAR STRUCTURE · FEBRUARY 1995

Impact Factor: 1.6 · DOI: 10.1016/0022-2860(94)09003-8

---

CITATIONS

7

---

READS

37

3 AUTHORS, INCLUDING:



Kolbjørn Hagen

Norwegian University of Science and T...

102 PUBLICATIONS 1,145 CITATIONS

SEE PROFILE

# Molecular structure and conformational composition of 1-iodopropane as determined from gas-phase electron diffraction, microwave spectroscopy data and ab initio calculations<sup>☆</sup>

Kolbjørn Hagen\*, Reidar Stølevik, Per Christian Sæbø

*Department of Chemistry, University of Trondheim, AVH, N-7055 Trondheim, Norway*

Received 21 June 1994

## Abstract

1-Iodopropane has been studied by gas-phase electron diffraction (ED). Earlier published values for rotational constants from microwave spectroscopy, together with results from ab initio molecular orbital calculations (HF/LANL1DZ) have been included in the ED analysis. Two conformers with C–C–C–I torsion angles of 180° (anti) or 66.1(5)° (gauche) have been observed. The results obtained for the bond distances ( $r_g$ ) and valence angles ( $\angle_\alpha$ ) from this combined ED/microwave spectroscopy analysis, with the ab initio calculations used as constraints, are:  $\langle r(\text{C–H}) \rangle = 1.110(4)\text{Å}$ ,  $r(\text{C}_1\text{–C}_2) = 1.521(5)\text{Å}$ ,  $r(\text{C}_2\text{–C}_3) = 1.537(5)\text{Å}$ ,  $r(\text{C}_1\text{–I}) = 2.164(8)\text{Å}$ ,  $\angle(\text{C–C–C})_{\text{anti}} = 110.2(9)^\circ$ ,  $\angle(\text{C–C–C})_{\text{gauche}} = 113.9(9)^\circ$ ,  $\angle(\text{C–C–I})_{\text{anti}} = 111.8(4)^\circ$ ,  $\angle(\text{C–C–I})_{\text{gauche}} = 113.0(4)^\circ$ ,  $\angle\text{C}_2\text{–C}_1\text{–H} = 112.4^\circ$  (ab initio value),  $\angle\text{C}_2\text{–C}_3\text{–H} = 111.0^\circ$  (ab initio value),  $\angle\text{H–C}_2\text{–H} = 109.5^\circ$  (ab initio value). Error limits are given as  $2\sigma$  where  $\sigma$  includes estimates of uncertainties in voltage/height measurements and correlation in the experimental data. The observed amount of gauche conformer is 72(13)%, corresponding to an energy difference of  $\Delta E = E_{\text{anti}} - E_{\text{gauche}} = 0.2(4)\text{ kcal mol}^{-1}$ . The results are compared with those obtained earlier for other halopropanes.

## 1. Introduction

Structures and conformational compositions of several halogen-substituted propanes have been investigated by gas-phase electron diffraction [1]. Our continuing interest in the structures and conformations of these molecules have led us to investigate 1-iodopropane (Fig. 1). Some information about the conformational composition of 1-iodopropane has been published. Niide et al. [2] have shown, by microwave spectroscopy (MW),

that 1-iodopropane in the gas phase consists of two conformers with the I–C–C–C torsion angle either anti or gauche. Fujitake and Hyaashi [3], in another MW investigation, determined rotational constants for both these conformers. Brown and Sheppard [4] have observed both conformers in liquid and solid phase by infrared and Raman spectroscopy. The presence of these two forms has also been shown in two low-resolution MW investigations by Armstrong [5] and Steinmetz et al. [6]. By combining data from some of these earlier investigations with electron diffraction data and ab initio molecular orbital calculations, accurate values for geometrical parameters and conformational composition can be determined.

<sup>☆</sup> Dedicated to Professor Ken Hedberg on the occasion of his 75th birthday.

\* Corresponding author.

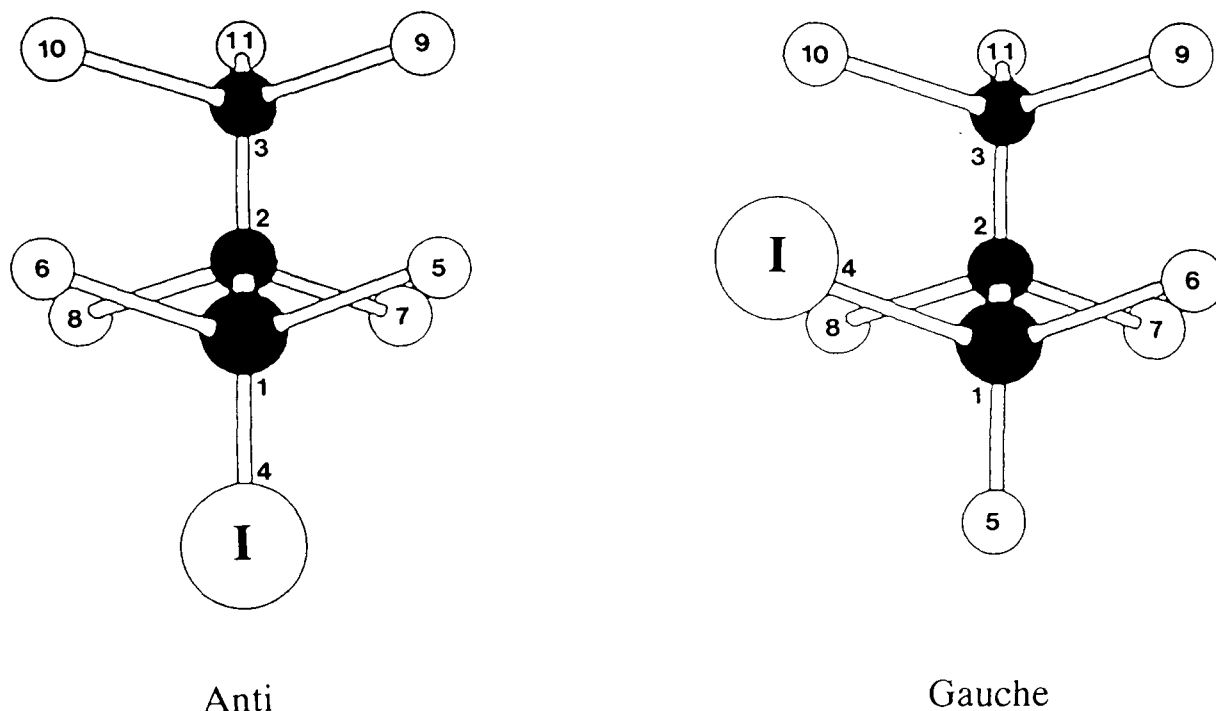


Fig. 1. Diagram, with atom numbering, of the anti and gauche conformers of 1-iodopropane.

These results may then be compared with results for related molecules.

## 2. Experimental section and data reduction

The sample of 1-iodopropane (99%) was obtained from Aldrich. Sample purity was checked by GC before use. Electron diffraction patterns were recorded with Balzers Eldigraph KDG-2 at University of Oslo [7,8] with a nozzle-tip temperature of 25°C. Voltage/distance calibration was made with benzene as reference. Data were obtained at two different nozzle-to-plate distances (497.76 and 247.92 mm). Six diffraction photographs from each of two nozzle-to-plate distances were used. Optical densities were measured using a Joyce Loeble double beam microdensitometer and the data were reduced in the usual way [9–11]. The ranges of data were  $2.00 \leq s(\text{\AA}^{-1}) \leq 14.75$  and  $5.00 \leq s(\text{\AA}^{-1}) \leq 25.000$ . A calculated background [12] was subtracted from the data for each plate to yield

experimental molecular intensity curves in the form  $sI_m(s)$ . The average experimental intensity curves are shown in Fig. 2. Fig. 3 shows the final experimental radial distribution (RD) curve calculated in the usual way from the modified molecular intensity curve  $I'(s) = sI_m(s)Z_C Z_I (A_C A_I)^{-1} \exp(-0.002s^2)$ , where  $A = s^2 F$  and  $F$  is the absolute value of the complex electron scattering amplitudes. The scattering amplitudes and phases were taken from Tables [13].

## 3. Structure analysis

The geometrical parameters chosen to define each of the conformers are as follows:  $r(\text{C-H})$ ,  $\langle r(\text{C-C}) \rangle = 0.5[r(\text{C}_1\text{-C}_2) + r(\text{C}_2\text{-C}_3)]$ ,  $\Delta r(\text{C-C}) = r(\text{C}_2\text{-C}_3) - r(\text{C}_1\text{-C}_2)$ ,  $r(\text{C-I})$ ,  $\angle \text{C-C-C}$ ,  $\angle \text{C-C-I}$ ,  $\angle \text{C}_2\text{-C}_1\text{-H}$ ,  $\angle \text{H-C}_1\text{-H}$ ,  $\angle \text{C}_1\text{-C}_2\text{-H}$ ,  $\angle \text{H-C}_2\text{-H}$ ,  $\angle \text{C}_2\text{-C}_3\text{-H}$ ,  $\phi(\text{I-C}_1\text{-C}_2\text{-C}_3)$ , and  $\phi(\text{C}_1\text{-C}_2\text{-C}_3\text{-H})$ . Local  $C_{3v}$  symmetry was assumed for the methyl group.

From the experimental RD curve and from

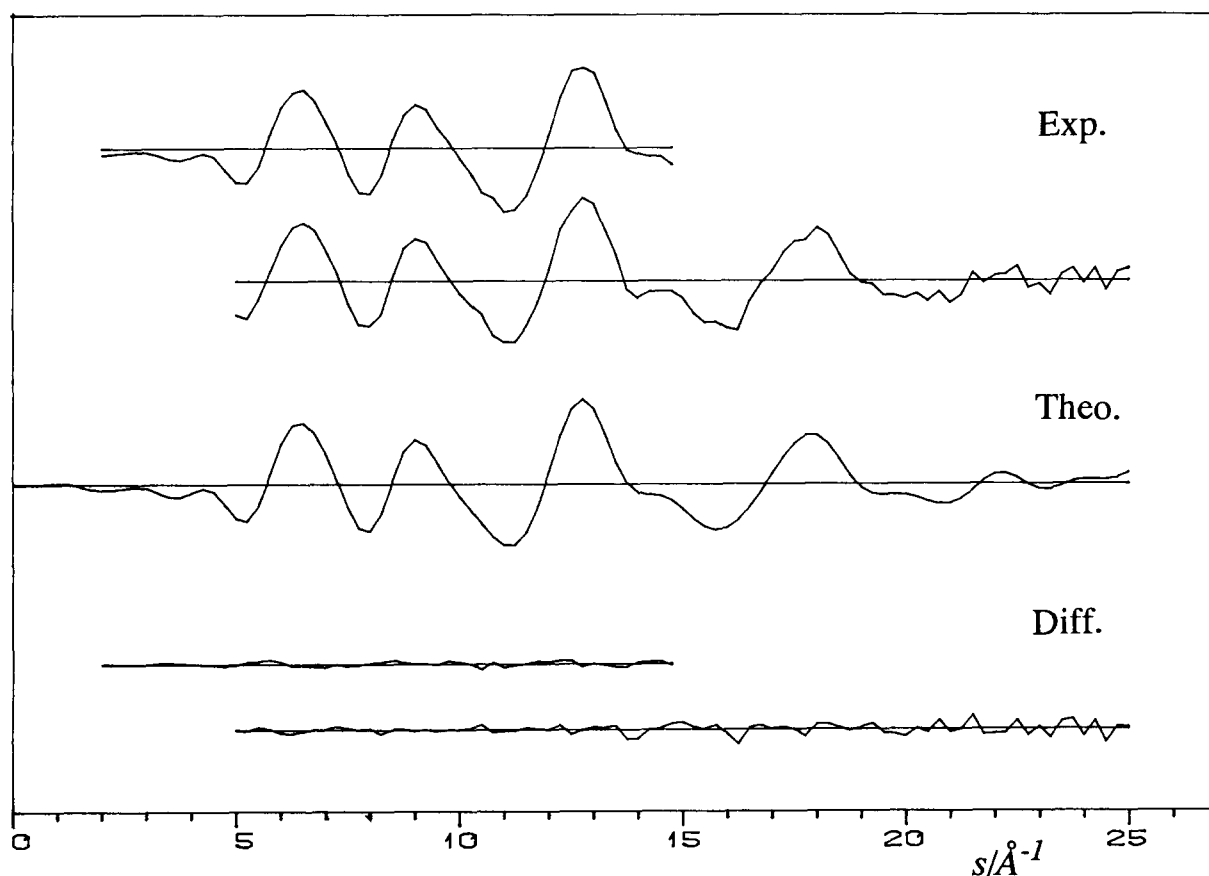


Fig. 2. Intensity curves,  $sI_m(s)$ , for 1-diodopropane. The experimental curves are averages of all plates for the two camera distances. The theoretical curve was calculated from the structural parameters shown in Tables 2 and 3. The difference curves result from subtracting the relevant part of the theoretical curve from the experimental curves.

results obtained for related molecules, trial values for bond distances and valence angles could be obtained. Calculations of theoretical RD curves for the gauche and anti conformers clearly showed that a model with only one conformer could not fit the experimental data. However, by using a model with a mixture of both anti and gauche conformers a good fit to the experimental data could be obtained.

Refinements of the structure were made by the least-squares method [14] by simultaneously fitting a single theoretical intensity curve to the two average experimental curves, and theoretical rotational constants to the six experimental values, three for each of the two conformers. In the combined electron diffraction (ED)/MW analysis the  $r_a$  distances

used to calculate the theoretical intensity curves were converted to the geometrically consistent  $r_\alpha^0 = r_z$  distances according to procedures described by Kuchitsu and Cyvin [15]. These distances were used to obtain  $B_z$  values which were then compared with the experimental  $B_z$  values obtained from the reported  $B_0$  values as follows:

$$B_z = B_0 + 0.5 \sum \sigma_s^{\text{harm}}$$

The necessary corrections for converting  $r_a$  to  $r_\alpha^0$  as well as from  $B_0$  to  $B_z$  were calculated from an assumed valence force field. The force constants were taken from force fields developed for related molecules. This force field was also used to calculate values for the vibrational amplitudes for the 27

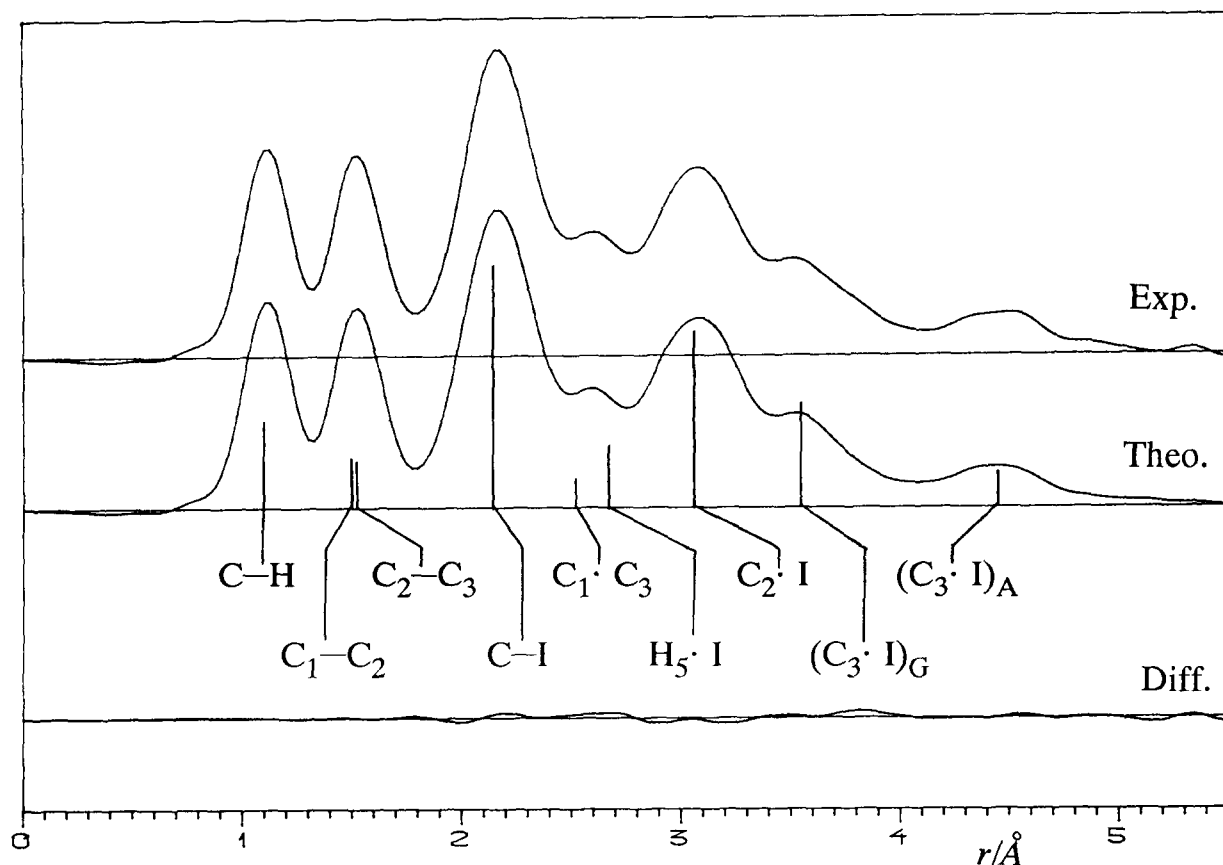


Fig. 3. Radial distribution curves for 1-iodopropane. The experimental curve was calculated from the composite of the two average intensity curves shown in Fig. 2 with the use of theoretical data for the region  $0 \leq s(\text{\AA}^{-1}) \leq 1.75$  and  $B(\text{\AA}^2) = 0.0020$ . Difference curve is experimental minus theoretical. The vertical lines indicate the interatomic distances and have lengths proportional to the distance weights.

different interatomic distances of each conformer. In the early refinements it was assumed that only  $\phi$ , the  $C_1-C_2$  torsion angle differed in the two conformers. This is clearly not a very good assumption, and to get more information about the structure of 1-iodopropane, some theoretical calculations were made. The structure of 1-iodopropane was optimized at the ab initio HF/LANL1DZ [16–18] level with the use of the program GAUSSIAN 92 [19] for the gauche and anti conformers. These ab initio results were used to modify our electron diffraction model of the molecule in such a way that the calculated differences in the corresponding valence angles between the two conformers could be introduced as constraints in our model. In order to get some more information about the

potential for torsion about the  $C_1-C_2$  bond, ab initio calculations were also made for several additional values of the I-C-C-C torsion angle  $\phi$ . These results are shown in Table 1 and Fig. 4, together with the results obtained from molecular mechanics calculations [20].

Some of the parameters used to define the model in the least-squares refinements could not be determined well from the ED/MW data, and they were therefore kept constant at the values obtained in the ab initio calculations. These parameters were  $\Delta r(C-C)$ ,  $\angle C_2-C_1-H$ ,  $\angle H-C_1-H$ ,  $\angle C_1-C_2-H$ ,  $\angle H-C_2-H$ ,  $\angle C_2-C_3-H$ , and  $\phi(C_1-C_2-C_3-H)$ . This procedure of using ab initio results as constraints in the ED analysis has been shown to be very useful [21–23]. Some of the vibrational

Table 1

Relative energies ( $\text{kcal mol}^{-1}$ ) for 1-iodopropane as a function of the I–C–C–C torsion angle  $\phi$  calculated from ab initio (HF/LANL1DZ) and molecular mechanics (mm) [20]

$\phi$ (deg)	$E$ (ab initio) ( $\text{kcal mol}^{-1}$ )	$E$ (MM) ( $\text{kcal mol}^{-1}$ )
0	6.45	5.5
30	4.12	4.1
67.7	–	0.0
69.1	0.65	–
90	1.80	1.8
120	3.83	3.1
150	1.90	1.3
180	0.00	0.0

amplitudes were refined together in groups. The vibrational amplitudes which could not be refined were kept constant at values calculated in the normal coordinate analysis. In the final refinement six geometrical parameters, six amplitude parameters and a composition parameter were refined simultaneously. The results of this refinement are given in Table 2 where also the values from the ab initio calculations are given. In Table 3 the final values for some selected distances are shown together with refined and/or calculated values from the normal coordinate analysis for the vibrational amplitudes. Table 4 shows the experimental values for the rotational constants together with those calculated from the final model. The intensity curve calculated for the final model is shown in Fig. 2 together with experimental and difference curves. Fig. 3 shows the corresponding RD curves, and the correlation matrix for the refined parameters is given in Table 5.

#### 4. Discussion

The agreement between the experimental values for the rotational constants and those calculated for the final model is quite good. Some of the differences probably arise from the calculations of the  $B_0$  to  $B_c$  corrections, and from the ab initio calculated differences in bond distances and valence angle not being accurate enough. Including the rotational constants in the analysis is,

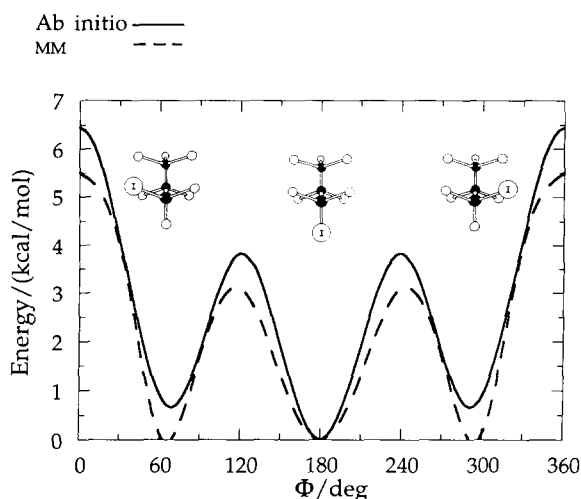


Fig. 4. Potential energy for 1-iodopropane, from ab initio calculations [19] using the HF/LANL1DZ basis set [16–18], and from molecular mechanics (MM) calculations [20], as a function of the H–C–C–I torsion angle,  $\phi$ .

however, important in order to get as good a structure determination as possible.

If we use the entropy difference between conformers ( $\Delta S = S_{\text{anti}} - S_{\text{gauche}} = R \cdot \ln 2 + 0.33 \text{ cal mol}^{-1} \text{ K}^{-1}$ ) and the difference in zero-point vibrational energy ( $-0.04 \text{ kcal mol}^{-1}$ ), both obtained from the ab initio calculations, then the conformational composition of 72(13)% gauche, 28(13)% anti conformer corresponds to an energy difference of  $\Delta E = E_{\text{anti}} - E_{\text{gauche}} = 0.2(4) \text{ kcal mol}^{-1}$ . This is significantly different from the ab initio value of  $\Delta E = -0.65 \text{ kcal mol}^{-1}$ , but within error limits of the value determined from molecular mechanics calculations [20] where the two conformers are found to have approximately equal energy. Ab initio calculations at the HF/LANL1DZ level therefore have not reproduced the relative energy of the two conformers in 1-iodopropane very well, but this is not very surprising with these relatively low level calculations.

In Table 6 the results obtained for propane and all the 1-halopropanes are shown. For all these halogen-substituted propanes, the energy difference between conformers are quite small. Some of the reported error limits for  $\Delta E$  are probably too small, the two reported values for 1-chloropropane [26,28] for example being significantly different. No

Table 2  
1-Iodopropane: structural parameter values<sup>a</sup>

Parameter	ED/MW <sup>b</sup>		Ab initio <sup>b</sup>
	$r_g$	$r_\alpha; \angle_\alpha$	
$r(\text{C-H})$	1.110(4)	1.092(4)	1.082
$\langle r(\text{C-C}) \rangle$	1.529(5)	1.525(5)	1.535
$\Delta r(\text{C-C})$	[0.016]	[0.012]	0.012
$r(\text{C-I})$	2.164(8)	2.161(8)	2.206
$\angle(\text{C-C-I})_A$		111.8(4)	112.4
$\angle(\text{C-C-I})_G$		113.0(4)	113.6
$\angle(\text{C-C-C})_A$		110.2(9)	110.8
$\angle(\text{C-C-C})_G$		113.9(9)	114.5
$\angle \text{C}_2\text{-C}_1\text{-H}$		[112.5]	112.5
$\angle \text{C}_2\text{-C}_3\text{-H}$		[111.0]	111.0
$\angle \text{H-C}_2\text{-H}$		[109.5]	109.5
$\phi(\text{I-C}_1\text{-C}_2\text{-C}_3)_G$		66.1(5)	69.1
$\phi(\text{C}_1\text{-C}_2\text{-C}_3\text{-H})_G$		[3.5]	3.5
$\alpha_G^c$		0.72(13)	

<sup>a</sup> Distances ( $r$ ) are in Å, angles ( $\angle$ ) are in degrees. Parenthesized values are estimated  $2\sigma$  values and include estimates of uncertainty in voltage/nozzle-height and of correlation in the experimental data. Values in square brackets were kept constant in the final least-squares refinement.

<sup>b</sup> Results from ab initio (HF/LANL1DZ).

<sup>c</sup> Mole fraction of the gauche conformer.

clear trend is obvious from the reported energy values.

If we exclude the value reported for 1-bromopropane, a small, but significant increase in the value for  $\phi(\text{X-C-C-C})$  can be observed as we go from  $\text{X} = \text{F}$  to  $\text{X} = \text{I}$ . Such an increase is probably due to increasing steric repulsion between the  $\text{CH}_3$  group and the halogen atom  $\text{X}$  as the size of  $\text{X}$  is increasing. The torsion angle value for 1-bromopropane is only based on fitting a model

Table 3  
1-Iodopropane: selected distances and root-mean-square amplitudes<sup>a</sup>

Distance	$r_g$	$l_{\text{exp.}}$	$l_{\text{calcd.}}$
$r(\text{C-H})$	1.110(4)	0.057(8)	0.078
$r(\text{C}_1\text{-C}_2)$	1.521(5)	0.066(8) <sup>b</sup>	0.048
$r(\text{C}_2\text{-C}_3)$	1.537(5)	0.066(8) <sup>b</sup>	0.048
$r(\text{C-I})$	2.164(8)	0.079(15)	0.053
$r(\text{C}_1 \cdots \text{C}_3)$	2.506(12)	0.086(23)	0.076
$r(\text{C}_2 \cdots \text{I})$	3.072(7)	0.066(14)	0.081
$r(\text{I} \cdots \text{H}_5)$	2.693(9)		0.115
$r(\text{I} \cdots \text{C}_3)_A$	4.443(56)		0.080
$r(\text{I} \cdots \text{H}_9)_A$	4.763(25)		0.175
$r(\text{I} \cdots \text{H}_{11})_A$	5.232(49)		0.132
$r(\text{I} \cdots \text{H}_7)_A$	3.224(122)		0.188
$r(\text{I} \cdots \text{C}_3)_G$	3.546(9)	0.156(36)	0.182
$r(\text{I} \cdots \text{H}_9)_G$	3.107(15)		0.285
$r(\text{I} \cdots \text{H}_{10})_G$	3.939(13)		0.302
$r(\text{I} \cdots \text{H}_{11})_G$	4.532(11)		0.208
$r(\text{I} \cdots \text{H}_7)_G$	4.064(9)		0.109
$r(\text{I} \cdots \text{H}_8)_G$	3.165(13)		0.183

<sup>a</sup> Distances ( $r_g$ ) and vibrational amplitudes ( $l$ ) are in Angstroms. Parenthesized values are  $2\sigma$  and include uncertainties in voltage/nozzle heights and correlation in the experimental data.

<sup>b</sup> Refined as a group.

to the six rotational constants determined from MW. Most of the geometrical parameter values reported for this molecule have therefore been assumed, and errors in these assumptions will affect the value for  $\phi(\text{Br-C-C-C})$  which is a fitted value. It is therefore reasonable to believe that the value for  $\phi$  is smaller than  $70^\circ$ , probably closer to  $65^\circ$ . In order to get a complete study of all the 1-halopropanes we have started an electron diffraction investigation of 1-bromopropane. The

Table 4  
Rotational constants (in MHz) for the two conformers of 1-iodopropane

	Anti			Gauche		
	Exp. <sup>a</sup>	Exp. <sup>b</sup>	Theor.	Exp. <sup>a</sup>	Exp. <sup>a</sup>	Theor.
A	24710.744(82)	24796.5	24796.5	10595.348(17)	10589.5	10589.7
B	1304.204(3)	1304.8	1302.7	1781.651(2)	1779.5	1780.7
C	1269.366(3)	1268.9	1267.0	1614.186(1)	1613.3	1612.8

<sup>a</sup>  $B_0$  values from Ref. 3. Values in parentheses are reported uncertainties calculated from 2.5 times the standard deviations.

<sup>b</sup>  $B_z$  values as obtained from the  $B_0$  values.

Table 5

Correlation matrix ( $\times 100$ ) for parameters refined in the least squares refinement

Parameter	$\sigma_{LS}^a$	$r_1$	$r_2$	$r_3$	$\angle_4$	$\angle_5$	$\angle_6$	$l_7$	$l_8$	$l_9$	$l_{10}$	$l_{11}$	$l_{12}$	$\alpha_{13}$
1. $r(C-H)$	0.0015	100	-18	-39	63	19	97	9	12	16	15	15	-4	9
2. $\langle r(C-C) \rangle$	0.0016		100	-67	57	-55	-30	-20	-26	-28	22	-18	-18	22
3. $r(C-I)$	0.0027			100	-60	-3	-33	4	8	1	-37	-4	5	-17
4. $\angle C-C-I$	0.1385				100	-53	50	-13	-13	-17	20	-9	-23	25
5. $\angle C-C-C$	0.3150					100	31	24	25	39	5	30	26	-18
6. $\phi(C-C-C-I)_G$	0.1662						100	12	16	20	14	18	1	5
7. $l(C-H)$	0.0028							100	65	64	2	48	14	-21
8. $l(C-C)$	0.0026								100	60	-1	50	14	-21
9. $l(C-I)$	0.0051									100	3	58	19	-29
10. $l(C_1 \cdots C_3)$	0.0080										100	7	1	2
11. $l(C_2 \cdots I)$	0.0047											100	19	-17
12. $l(C_3 \cdots I)_G$	0.0125												100	-38
13. $\alpha_A^b$	0.0477													100

<sup>a</sup> Standard deviations from least squares. Distances ( $r$ ) and amplitudes ( $l$ ) are in Å, angles ( $\angle$ ) are in degrees.<sup>b</sup> Mole fraction of the anti conformer.

Table 6

Results obtained for propane and 1-halopropanes<sup>a</sup>

	Propane	1-Fluoropropane	1-Chloropropane	1-Bromopropane	1-Iodopropane
$r(C-H)$	1.107(5)	1.094(3)	1.113(3)	1.094	1.110(4)
$r(C_1-C_2)$	} 1.532(3)	1.501(2)	} 1.525(2)	} 1.534	1.521(5)
$r(C_2-C_3)$		1.534(1)			1.537(5)
$r(C_1-X)$	1.107(5)	1.401(3)	1.796(2)	1.970	2.164(8)
$\angle(C-C-C)_A$	} 112(1)	110.6(3)	111.3(13)		110.2(9)
$\angle(C-C-C)_G$		112.9(3)	113.9(5)	110.5	113.9(9)
$\angle(C-C-X)_A$		109.9(4)	111.3(7)		111.8(4)
$\angle(C-C-X)_G$		110.0(5)	112.2(6)	111.0	113.0(4)
$\Phi_G$		62.6(5)	63.9(12)	70.0	66.1(5)
$\Delta E = E_A - E_G$		0.35(3) <sup>b</sup>	0.05(7)/0.36(3) <sup>b</sup>	0.11(3) <sup>b</sup>	0.2(4)
Method	ED + MW	MW	ED + MW	MW	ED + MW + ab initio
Ref.	24	25	26	27	This work

<sup>a</sup> Distances ( $r$ ) are in Å, angles ( $\angle$ ) are in degrees. Error limits from different investigations may have different meanings.<sup>b</sup> From Ref. [28].

published results for the rotational constants from MW will be used to supplement the ED data.

### Acknowledgements

The authors are very grateful to the Norwegian National Supercomputer Committee (TRU) for a grant of computing time on the Cray YMP 464, and to Hans Vidar Volden and Snefrid Gundersen at the University of Oslo for help with the data collection.

### References

- [1] K. Kuchitsu (Ed.), Structure Data of Free Polyatomic Molecules, Landolt-Börnstein, New Series, Volume II/7, Springer, Berlin, 1992.
- [2] Y. Niide, I. Ohkoshi and M. Takano, J. Mol. Spectrosc., 122 (1987) 113.
- [3] M. Fujitake and M. Hayashi, J. Mol. Spectrosc., 127 (1988) 112.
- [4] J.K. Brown and N. Sheppard, Trans. Faraday Soc., 50 (1954) 1164.
- [5] S. Armstrong, Appl. Spectrosc., 23 (1969) 575.
- [6] W.E. Steinmetz, F. Hickernell, I.K. Mun and L.H. Scharpen, J. Mol. Spectrosc., 68 (1977) 173.



- [7] W. Zeil, J. Haase and L. Wegmann, *Z. Instrumentenkol.*, 74 (1960) 84.
- [8] O. Bastiansen, R. Graber and L. Wegmann, *Balzers High Vac. Rep.*, 25 (1969) 1.
- [9] K. Hagen and K. Hedberg, *H. Am. Chem. Soc.*, 95 (1973) 1003.
- [10] G. Gundersen and K. Hedberg, *J. Chem. Phys.*, 51 (1969) 2500.
- [11] B. Andersen, H.M. Seip, T.G. Strand and R. Stølevik, *Acta Chem. Scand.*, 23 (1969) 3224.
- [12] L. Hedberg, *Abstracts of Papers, 5th Austin Symp. on Gas-Phase Molecular Structures*, Austin, TX, March 1974, p. 37.
- [13] A.W. Ross, M. Fink and R. Hilderbrandt, *International Tables of Crystallography*, Vol. 4, Kluwer Academic, Dordrecht, 1992, p. 245.
- [14] K. Hedberg and M. Iwasaki, *Acta Crystallogr.*, 17 (1964) 529.
- [15] K. Kuchitsu and S.J. Cyvin, in S.J. Cyvin (Ed.), *Molecular Structure and Vibration*, 5, Elsevier, Amsterdam, 1972; Chapter 12.
- [16] P.J. Hay and W.R. Wadt, *J. Chem. Phys.*, 82 (1985) 270.
- [17] W.R. Wadt and P.J. Hey, *J. Chem. Phys.*, 82 (1985) 284.
- [18] P.J. Hey and W.R. Wadt, *J. Chem. Phys.*, 82 (1985) 299.
- [19] M.J. Frisch, G.W. Trucks, M. Head-Gordon, P.M.W. Gill, M.W. Wong, J.B. Foresman, B.G. Johnson, H.B. Schlegel, M.A. Robb, E.S. Replogle, R. Comperts, J.L. Anders, K. Raghavachari, S.J. Binkley, C. Gonzalez, R.L. Martin, D.J. Fox, D.J. DeFrees, J. Baker, J.J.P. Stewart and J.A. Pople, *GAUSSIAN 92*, Revision C; Gaussian, Inc., Pittsburgh, PA, 1992.
- [20] P.C. Sæbø, Ph.D. Thesis, University of Trondheim, 1993.
- [21] L. Schäfer, J.D. Ewbank, K. Siam, N. Chiu and H.L. Sellers, in I. Hargittai and M. Hargittai (Eds.), *Stereochemical Applications of Gas-Phase Electron Diffraction*, VCH, New York, 1988, p. 301.
- [22] V.J. Klimkowski, J.D. Ewbank, C. Van Alsenoy, J.N. Cardale and L. Schäfer, *J. Am. Chem. Soc.*, 104 (1982) 1476.
- [23] D. Van Hemelrijk, L. Van den Enden, H.J. Geise, H.L. Sellers and L. Schäfer, *J. Am. Chem. Soc.*, 102 (1980) 2189.
- [24] T. Iijima, *Bull. Chem. Soc. Jpn.*, 45 (1972) 1291.
- [25] M. Hayashi and M. Fujitake, *J. Mol. Struct.*, 146 (1986) 9.
- [26] K. Yamanouchi, M. Sugie, H. Takeo, C. Matsumura and K. Kuchitsu, *J. Phys. Chem.*, 88 (1984) 2315.
- [27] Y. Niide, I. Ohkoshi and M. Takano, *J. Mol. Spectrosc.*, 89 (1981) 387.
- [28] J.R. Durig, S.E. Godbey and J.F. Sullivan, *J. Chem. Phys.*, 80 (1984) 5983.