

## Errata: Molecular Composition of Alkali Halide Vapors

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# Errata: Dissociation Energies of Carbon Monoxide and Nitrogen from Reflected Shock Wave Studies

[J. Chem. Phys. 26, 655 (1957)]

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THE theoretical curves in Figs. 2 and 3, page 656, are slightly in error. The results of new calculations for both N<sub>2</sub> and CO using the NBS Series III and Fickett and Cowan's values for the energy content of CO are given in Table I.

TABLE I. Corrected values for the reflected shock velocity,  $U_R$ , as a function of incident shock Mach number,  $M_1$ .

N <sub>2</sub>				CO					
<i>D</i> (ev)	<i>P</i> <sub>1</sub> (mm)	<i>M</i> <sub>1</sub>	<i>U<sub>R</sub></i> mm/μ sec ±0.002	<i>D</i> (ev)	<i>P</i> <sub>1</sub> (mm)	<i>M</i> <sub>1</sub>	<i>U<sub>R</sub></i> mm/μ sec ±0.002		
7.38	0.1	6.01	0.526	9.14	0.5	6.24	0.568		
		7.51	0.504			7.34	0.557		
	1.0	9.64	0.495		5.0	8.96	0.541		
		5.68	0.545			9.04	0.581		
		6.61	0.546			6.03	0.585		
		8.00	0.537			6.70	0.598		
		9.54	0.544			7.70	0.593		
9.76	0.1	7.35	0.584		0.5	9.04	0.581		
		8.08	0.576			6.41	0.616		
	1.0	8.93	0.571		5.0	7.15	0.619		
		10.26	0.570			8.22	0.609		
		7.35	0.620			9.66	0.593		
		8.08	0.621			6.37	0.619		
		8.79	0.611			6.84	0.639		
		9.64	0.614			7.48	0.648		
						8.36	0.646		
						9.55	0.637		
						5.96	0.591		
						7.40	0.707		
				8.67	0.801				
				<hr/>					
				α=0					

Iodine heptafluoride is cubic from 0°C to -120°C, and orthorhombic below -120°C. Complete three-dimensional x-ray data for the cubic phase were recorded at -110°C. The unit cell constant is  $a=6.28$  Å, with two molecules in the cell. The most probable space groups are  $I43m$ ,  $I432$ , or  $Im3m$ . The electron density projection suggests that the structure is so disordered that the statistical symmetry  $Im3m$  is attained by a free rotation or random orientation of the molecules around a molecular axis which is distributed with equal probability along each of the three cube axes. Electron density sections based on  $Im3m$  are consistent with this interpretation.

Complete three-dimensional data for the orthorhombic phase were recorded at -145°C. The unit cell constants are  $a=8.74$  Å,  $b=8.87$  Å,  $c=6.14$  Å, with four molecules in the cell. The most probable space groups are  $C^{17}_{2v}=Aba2$  or  $D^{18}_{2h}=Abam$ . The fourfold positions in  $Abam$  have the symmetry  $2/m$  which is impossible for a sevenfold coordination in an ordered structure. No evidence was found for the type of disorder which would give rise to  $Abam$  and  $Aba2$  was accepted as the correct space group. The iodine atom and one fluorine atom are in special position ( $a$ ), the remaining fluorine atoms are in general position ( $b$ ). A suitable trial structure was obtained and refined as far as a series of six three-dimensional difference syntheses giving the following positional and temperature parameters:

	$x$	$y$	$z$	$u$	$v$	$w$
I	0	0	0	0.47 <sub>6</sub>	0.70	0.97 <sub>5</sub>
F <sub>1</sub>	0	0	0.2777	3.4	3.4	0
F <sub>2</sub>	0.0862	0.0974	-0.2361	1.4	1.4	1.4
F <sub>3</sub>	0.1235	0.1566	0.0585	1.0	1.0	1.0
F <sub>4</sub>	0.1695	-0.1189	0.0310	1.0	1.0	1.0

The atomic scattering factors were chosen of the form

$$f=f_0 \exp[-s^2(un_1^2+vn_2^2+wn_3^2)],$$

where  $s=(2 \sin \theta)/\lambda$ ;  $u$ ,  $v$ ,  $w$  are the temperature parameters;  $n_1$ ,  $n_2$ ,  $n_3$  are the direction cosines of the diffraction vector with the axes of the ellipsoid of thermal vibration. The observed electron density indicates that the thermal motion of the fluorine atoms is not entirely accounted for. Limited computing facilities prevented treating the temperature parameters in more general form.

An  $R$  factor of 11% was obtained for the  $hkl$  reflections of observable intensity.† There are only 21 reflections with mixed indices of observable intensity, determined by contributions from fluorine atoms alone, which give an  $R$  factor of 26%. Since the iodine atoms occur in a face-centered arrangement, the reflections with unmixed indices are all strong and may be subject to extinction. Such an effect might account for the peculiar shape (and temperature parameters) of the  $F_1$  peak.

The following bond distances and bond angles were obtained:

I-F <sub>1</sub>	1.71 Å	F <sub>1</sub> -I-F <sub>3</sub>	78°28'
I-F <sub>2</sub>	1.85 Å	F <sub>1</sub> -I-F <sub>4</sub>	84°2'
I-F <sub>3</sub>	1.80 Å	F <sub>2</sub> -I-F <sub>2'</sub>	76°40'
I-F <sub>4</sub>	1.83 Å	F <sub>2</sub> -I-F <sub>3</sub>	63°15'
		F <sub>2</sub> -I-F <sub>4</sub>	91°11'
		F <sub>2</sub> -I-F <sub>4'</sub>	98°11'
		F <sub>3</sub> -I-F <sub>4</sub>	86°29'
		F <sub>3</sub> -I-F <sub>4'</sub>	91°10'

The heavy iodine atom, lack of a center of symmetry, and large thermal motions combine to produce standard errors in the bond distances which average 0.04 Å. The effect of any systemic errors on the bond distances is unknown.

The molecule has one short bond and six longer bonds and possesses only the point group symmetry 2 required by the space group. The idealized description of the molecule, based on the point group symmetry  $mm$ , would be five F atoms forming a tetragonal pyramid with the I atom situated below the base of the pyramid to which are added two more F atoms lying below the I atom. This is in sharp contrast to the pentagonal bipyramid arrangement proposed by Lord *et al.*<sup>1</sup> from a study of infrared and Raman spectra.

\* This document is based on work performed for the U. S. Atomic Energy Commission by Union Carbide and Carbon Corporation at Oak Ridge, Tennessee.

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‡ Tables of observed and calculated structure factors of iodine heptafluoride at -145°C have been deposited as Document number 5340 with the ADI Auxiliary Publications Project, Photoduplication Service, Library of Congress, Washington 25, D. C. A copy may be secured by citing the Document number and by remitting \$ 1.25 for photoprints, or \$1.25 for 35-mm microfilm. Advance payment is required. Make checks or money order payable to: Chief, Photoduplication Service, Library of Congress,

<sup>1</sup> Lord, Lynch, Schumb, and Slowinski, J. Am. Chem. Soc. **72**, 522 (1950).

### Structure of the Interhalogen Compounds. III. Concluding Note on Bromide Tri- fluoride, Bromine Pentafluoride, and Iodine Pentafluoride\*

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UNDER the foregoing general title the crystal structures of chlorine trifluoride and iodine heptafluoride have been reported in this Journal.<sup>1,2</sup> Various circumstances have made it impossible to complete the structure analyses of the remaining compounds in the interhalogen series. However, the partial results we have obtained may be of some interest.

**Bromine trifluoride.**—Complete three-dimensional x-ray data were recorded at -125°C. The crystal system is orthorhombic with  $a=5.34$  Å,  $b=7.35$  Å,  $c=6.61$  Å,