

tering factors.

As I indicated in my Paper the inner regions of the scattering curves are uncertain, and I would not be surprised if there are errors in the bromine curve. However, I agree with Dr. Bonham that the cause of the trouble is more likely to be in the incoherent scattering curve. The theory of incoherent scattering is far more primitive than is the theory of coherent scattering, and the numerical values, based as they are on the Thomas-Fermi atom, are not reliable.

JOURNAL OF THE PHYSICAL SOCIETY OF JAPAN

VOL. 17, SUPPLEMENT B-II, 1962

PROCEEDINGS OF INTERNATIONAL CONFERENCE ON MAGNETISM AND CRYSTALLOGRAPHY, 1961, VOL. II

Electron Diffraction Investigation of the Molecular Structure  
of Some Gaseous Oxides\*

P. A. AKISHIN, L. V. VILKOV, E. Z. ZASORIN, N. G. RAMBIDI  
AND V. P. SPIRIDONOV  
*Moscow State University, Moscow, U.S.S.R.*

Table I.

Molecule	Configuration (symmetry)	Parameters
Li <sub>2</sub> O	Angular	$r(\text{Li-O})=1.82\pm0.02\text{\AA}$
	C <sub>2v</sub>	Li-O-Li=110°
B <sub>2</sub> O <sub>3</sub>	Angular	$r(\text{B-O})=1.36\pm0.02\text{\AA}$
	Planar	$r(\text{B-O})=1.20\pm0.03\text{\AA}$
	C <sub>2v</sub>	B-O-B=95° O-B-O=180°
N <sub>2</sub> O <sub>5</sub>	Angular	$r(\text{N-O})=1.21\pm0.01\text{\AA}$
	Nonplanar	$r(\text{N-O})=1.46\pm0.02\text{\AA}$
	C <sub>2v</sub>	O=N-O=134°±9° N-O-N=95°±3°
P <sub>4</sub> O <sub>10</sub>	Cyclic	$r(\text{P-O})=1.60\pm0.01\text{\AA}$
	T <sub>d</sub>	$r(\text{P-O})=1.40\pm0.03\text{\AA}$
		P-O-P=124°30'±1°
Sb <sub>4</sub> O <sub>6</sub>	Cyclic	$r(\text{Sb-O})=2.00\pm0.02\text{\AA}$
	T <sub>d</sub>	Sb-O-Sb=129°±2.5°
Cl <sub>2</sub> O <sub>7</sub>	Angular	$r(\text{Cl-O})=1.72\pm0.03\text{\AA}$
	Nonplanar	$r(\text{Cl-O})=1.42\pm0.01\text{\AA}$
	C <sub>s</sub>	Cl-O-Cl=115°±5° O-Cl-O=97°±3°

\* Presented at the Conference only by title.

1. Data about the structure and geometrical parameters of gaseous oxides of various elements are of great interest for theory and the explanation of applied problems. The data in the literature are few. In the Electron-Diffraction Laboratory of the Chemical Faculty of Moscow University systematic electron-diffraction investigations of the geometry of various oxides in the vapour state are being carried out.

2. In this paper are communicated the results of electron-diffraction study of the following gaseous oxides:  $\text{Li}_2\text{O}$ ,  $\text{B}_2\text{O}_3$ ,  $\text{N}_2\text{O}_5$ ,  $\text{P}_4\text{O}_{10}$ ,  $\text{Sb}_4\text{O}_6$  and  $\text{Cl}_2\text{O}_7$  (see the table).

3. The analysis of the results and the comparison of them with data in the literature allows us to reach the conclusion that monomeric molecules of the higher oxides are constructed in a similar fashion; atoms or groups of atoms are joined to the central oxygen atom in such a manner that their bonds give the symmetry  $C_{2v}$  or  $C_s$  to these molecules; configurations of still higher symmetry (such as bipyramid  $D_{3h}$ ) are not realized apparently due to steric hindrance. A bicycle structure of high symmetry is characteristic of the dimeric oxides.

JOURNAL OF THE PHYSICAL SOCIETY OF JAPAN

VOL. 17, SUPPLEMENT B-II, 1962

PROCEEDINGS OF INTERNATIONAL CONFERENCE ON MAGNETISM AND CRYSTALLOGRAPHY, 1961, VOL. II

## On the Possibility of Nonplanar Structures of Some Molecules with Conjugated Bonds\*

P. A. AKISHIN AND L. V. VILKOV

Moscow State University, Moscow, U.S.S.R.

1. A problem of fundamental importance for theoretical organic chemistry is the question of the configuration of molecules with conjugated bonds. There is some information concerning the nonplanarity of such aromatic molecules as biphenyl and nitrobenzene. Unfortunately, no structural data are available at present for the nonplanarity of alicyclic molecules with conjugated bonds.

2. The molecular structures of chloroprene  $\text{CH}_2=\text{CH}-\text{CCl}=\text{CH}_2$ ,  $\alpha$ -chloroacrolein  $\text{O}=\text{CH}-\text{ClC}=\text{CH}_2$ , methylglyoxal  $\text{O}=\text{CH}-(\text{CH}_3)\text{C}=\text{OH}_2$  and isoprene  $\text{CH}_2=\text{CH}-(\text{CH}_3)\text{C}=\text{CH}_2$  have been determined from electron diffraction in the vapour. In the case of chloroprene we could not make an unequivocal choice between a planar (with unequal  $\text{C}-\text{C}=\text{C}$

angles) and a nonplanar (with the interplanar angle of vinyl groups approximately  $30^\circ$ ) model. It has been found that  $\alpha$ -chloroacrolein exists in two nonplanar forms: in one the  $\text{C}=\text{O}$  group is twisted  $40^\circ$  relative to the *cis* form; and in the other this angle is about  $55^\circ$  relative to the *trans* form. A planar configuration has been found for the molecule of methylglyoxal.

The molecule of isoprene is nonplanar with interplanar angle about  $50^\circ$  relative to the *trans* form.

3. There have been obtained reliable structural data on the possibility of nonplanar configurations for molecules with conjugated double bonds, in the case of  $\alpha$ -chloroacrolein and isoprene.

\* Presented at the Conference only by title.