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Tables of Interatomic Distances and Molecular Configurations obtained by Electron Diffraction in the Gas Phase

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In this compilation are tabulated all available results of investigations of the molecular structures of substances by study of the diffraction of electrons by their vapours. A substantial fraction of these is as yet unpublished. The total number of substances described is 500. Results obtained by other methods of investigation of structure in the gas phase are also given for direct comparison, where available.

The following tables of data on bond lengths and molecular configurations determined by the method of electron diffraction in the vapour phase have been compiled partly in order that such information may be available in a readily accessible form and partly to test the reliability and consistency of the method. With the latter end in view, the tables have been extended to include *strictly comparable* data obtained by other methods, such as spectroscopy (including that of the microwave region), wherever it leads to definite quantitative results for molecular dimensions, and X-ray diffraction by gases. The latter method has been little used; for an account see Pirenne (1946). Results obtained by X-ray crystallographic examinations of solids have not been included, because in many cases (e.g. the alkali halides and phosphorus pentachloride) the results refer to so different an environment that they are not comparable.

No independent attempt has been made to assess the accuracy of the determinations, so the original authors' own estimates of error are given. The expression of error in many cases is not a simple matter; for often it turns out that in, for example, a two-parameter problem, the permitted range of values of the second parameter depends upon the value taken for the first, and vice versa; the ranges of variation are thus not independent though they are commonly written as if they are. Such information must be sought from the original papers. It should be pointed out that results obtained by the rotating-sector technique (Viervoll, 1947) are likely to be somewhat more reliable than those obtained by visual methods.

For a discussion of the overall accuracy of microwave measurements the authors are indebted to Dr D. H. Whiffen. Some workers in this field have attached too fine a limit of error to their results. Very accurate values (in which uncertainty in Planck's constant is the limiting factor) can be obtained for moments of inertia, but errors are introduced in calculating interatomic distances from them. These arise from zero-point vibrations and anharmonicity and are especially serious in polyatomic molecules, where isotopic substitution methods are used. In the absence of a detailed consideration of these factors the error is liable to be as much as $\pm 0{\cdot}01$ A. for polyatomic molecules (Townes, Holden & Merritt, 1948; Gordy, 1948). Similar considerations apply to calculations of interatomic distances from electronic and vibrational spectra. In these tables, spectroscopic results are quoted as values of r_0, the average value of the distance for the molecule in the lowest vibrational state and the ground electronic state. Where references are not given, they will be found in one or other of the works by G. Herzberg (1939, 1945).

In order to save space, and because early electron diffraction measurements vary considerably in reliability, it was decided not to give detailed references to work done prior to 1936, but to quote the weighted values given in a review paper by L. O. Brockway (1936). Hence references to work done before 1936 will be found in his paper, to which users of this table are referred.

The tables are divided into two parts:

Table 1: Compounds containing carbon;
Table 2: Compounds not containing carbon.

Organo-metallic compounds will hence be found in Table 1. Compounds in Table 1 are classified according to the American *Chemical Abstracts* system, while those in Table 2 are arranged in order of the Periodic Table group of the main atom. All references in the tables are to be found at the end, arranged in chronological groups.

In compiling these tables, various sources have been used, in addition to *Chemical Abstracts*. These include a table published by Maxwell (1940), a list of measurements on organic compounds drawn up by T. L. Cottrell (private communication) and a comparison between electron diffraction and spectroscopy compiled by R. W. Livingston (private circulation).

In addition to published results, the tables contain hitherto unpublished results on nearly one hundred compounds, which have been very kindly communicated by the following:

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Note added in proof. No further relevant results have been reported in copies of the following Journals received here to 28 September 1949, since the compilation was made:

Acta Chim. Scand., Canad. J. Res., J. Amer. Chem. Soc., J. Chem. Phys., J. Chim. phys., J. Chem. Soc., Phys. Rev., Proc. Phys. Soc., Proc. Roy. Soc., Trans. Faraday Soc.

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Notes on the Tables

(1) Bond distances are in Ångström units and angles in degrees, followed by the quoted errors in brackets. These errors are, in all cases, understood to be ±.

(2) No attempt is made to indicate bond type. The symbol *A*—*B* corresponds to the *distance* between the atoms *A* and *B*, and does not indicate that the bond is a single bond, or that there is, in fact, an actual chemical bond between the two atoms. Symbols such as C—C, C═C, C≡C are used to avoid confusion in molecules containing several different types of bond between the same atoms (e.g. diacetylene), and where confusion might otherwise arise atoms are numbered.

(3) In general, the configuration of carbon valencies may be taken as tetrahedral unless specific measurements of bond angles are quoted.

(4) It is often necessary in determining structures by the visual comparison method to assume certain distances which are not sufficiently important in the molecule to be evaluated independently but of which some account must be taken: the C—H distance is a case in point. Where such values are quoted, they are distinguished by the symbol *ass.*

(5) Results obtained by different workers on the same compound are arranged in chronological order save that spectroscopic and X-ray results are put last of all.

(6) Symbols:

S.	Rotating sector employed.
Spec.	Spectroscopic results.
X.	Results obtained by X-ray diffraction by the gas.
ass.	Assumed value—see (4) above.

Table 1. *Compounds containing carbon*

C_1

(*1*)	$CBrCl_3$, bromotrichloromethane		
	C—Br	2·01	
	C—Cl	1·76	
	Br—Cl	3·00	
	Cl—Cl	2·95	**19**
(*2*)	$CBrN$, cyanogen bromide		
	C—Br	1·79 (0·02)	**63**
		1·790	*Spec.* **195**
	C—N	1·13 (0·04)	**63**
		1·158	*Spec.* **195**
	Linear		
(*3*)	CBr_2Cl_2, dibromodichloromethane		
	C—Br	1·93	
	C—Cl	1·75	**8**
(*4*)	CBr_2O, carbonyl bromide		
	C—Br	2·05 (0·04)	
	C—O	1·13	**6**
	Planar		
(*5*)	CBr_3F, fluorotribromomethane		
	C—Br	1·91 (0·04)	
	C—F	1·44 (0·06)	
	Br—Br	3·20 (0·03)	
	F—Br	2·70 (0·02)	**60**
(*6*)	CBr_4, carbon tetrabromide		
	C—Br	1·93 (0·03)	**6**
		1·91 (0·02)	**26**
		1·93	**46**
		1·93 (0·02)	*S.* **107**
		1·94 (0·02)	**111**
		1·942 (0·003)	*S.* **135**
(*7*)	$CClN$, cyanogen chloride		
	C—Cl	1·67 (0·02)	**63**
		1·629	*Spec.* **195**
	C—N	1·13 (0·03)	**63**
		1·163	*Spec.* **195**
	Linear		
(*8*)	CCl_2F_2, dichlorodifluoromethane		
	C—Cl	1·74 (0·03)	
	C—F	1·35 (0·03)	**15**
	∠Cl—C—Cl > ∠Cl—C—F > ∠F—C—F		
(*9*)	CCl_2O, carbonyl chloride		
	C—Cl	1·68 (0·02)	**6**
		1·74 (0·02)	**176**
	C—O	1·28 (0·02)	**6**
		1·18 (0·03)	**176**
	Cl—Cl	2·90 (0·04)	**176**
	Cl—O	2·59 (0·03)	**176**
	∠Cl—C—Cl	117° (2°)	**6**
		112·5° (1·5°)	**176**

Table 1 (*cont.*)

C_1 (*cont.*)

(*10*)	CCl_2S, thiophosgene		
	C—Cl	1·70 (0·02)	
	C—S	1·63	**6**
	∠Cl—C—Cl	116°	**6**
(*11*)	CCl_3F, trichlorofluoromethane		
	C—Cl	1·76 (0·02)	**15**
		1·76 (0·02)	**60**
	C—F	1·40 (0·04)	**15**
		1·44 (0·04)	**60**
	Cl—Cl	2·94 (0·03)	**60**
	Cl—F	2·56 (0·04)	**60**
	∠Cl—C—Cl > ∠Cl—C—F		**15**
(*12*)	CCl_4, carbon tetrachloride		
	C—Cl	1·755 (0·005)	**6**
		1·77	**46**
		1·76	**92**
		1·761	*S.* **105**
		1·77 (0·02)	*S.* **107**
		1·765 (0·015)	**196**
		1·75	*X.* **163**
	Tetrahedral model confirmed by *Spec.*		
(*13*)	CCl_4S, perchlorthiophosgene		
	C—Cl	1·76	
	C—S	1·81	**116**
	S—Cl	2·03	
	∠Cl—C—S	109° (4)	
(*14*)	CF_4, carbon tetrafluoride		
	C—F	1·36 (0·02)	**6**
(*15*)	$CHBr_3$, bromoform		
	C—Br	2·03 (0·05)	**6**
		1·91	**26**
	∠Br—C—Br	111°	**26**
(*16*)	$CHClF_2$, chlorodifluoromethane		
	C—Cl	1·73 (0·03)	
	C—F	1·36 (0·03)	**15**
	∠Cl—C—F > ∠F—C—F		**15**
(*17*)	$CHCl_2F$, dichlorofluoromethane		
	C—Cl	1·73 (0·04)	
	C—F	1·41 (0·03)	**15**
	∠Cl—C—Cl > ∠Cl—C—F		
(*18*)	$CHCl_3$, chloroform		
	C—Cl	1·77 (0·02)	**6**
		1·81	*X.* **163**
	∠Cl—C—Cl	112° (2°)	**6**
(*19*)	CHF_3, fluoroform		
	C—F	1·35 (0·03)	**122**
		1·34 (0·02)	**202**
		1·322	*Spec.* **189**
	∠F—C—F	108° (1·5°)	**122**
		109° (2°)	**202**
(*20*)	CHI_3, iodoform		
	C—I	2·12 (0·03)	**6**
		2·12 (0·04)	*S.* **156**
	∠I—C—I	113°	*S.* **156**
(*21*)	CHNO, cyanic acid		
	C—N	1·19 (0·03)	
	C—O	1·19	**84**
	Cyanate group linear. Angle between cyanate group and N—H is 125°		
(*22*)	CH_2Br_2, methylene bromide		
	C—Br	1·91 (0·03)	**6**
		1·91 (0·02)	**26**
	∠Br—C—Br	112° (2°)	**6, 26**
(*23*)	CH_2ClF, chlorofluoromethane		
	C—Cl	1·76 (0·02)	
	C—F	1·40 (0·03)	**15**
(*24*)	CH_2Cl_2, methylene chloride		
	C—Cl	1·77 (0·02)	**6**
	∠Cl—C—Cl	112° (2°)	
(*25*)	CH_2F_2, methylene fluoride		
	C—F	1·36 (0·02)	**15**
		1·32 (0·002)	*Spec.* **179**
(*26*)	CH_2I_2, methylene iodide		
	C—I	2·28 (0·05)	**6**
		2·12 (0·04)	*S.* **156**
	∠I—C—I	114·7°	*S.* **156**
(*27*)	CH_2N_2, diazomethane		
	C—N	1·34 (0·05)	
	N—N	1·13 (0·04)	**6**
	Linear		
(*28*)	CH_2O, formaldehyde		
	C—O	1·15 (0·05)	**6**
		1·21 (0·01)	**74**
		1·225	*Spec.*
	∠H—C—H	120° (1°) *ass. Spec.* moments of inertia	**74**
(*29*)	CH_2O_2, formic acid (see (108) for dimer)		
	C—O	1·42 (0·03)	**144**
		1·368 (0·03)	**177**
		1·41 (0·02)	*Spec.* **180**
	C=O	1·24 (0·03)	**144**
		1·213 (0·03)	**177**
		1·225 (0·02)	*Spec.* **180**
	∠O—C=O	117° (2°)	**144**
		123·5°	**177**
		125° (1°)	*Spec.* **180**
(*30*)	CH_3BF_2, methyl boron fluoride		
	C—B	1·60 (0·02)	
	B—F	1·30 (0·02)	
	C—F	2·53 (0·03)	**121**
	∠C—B—F	121° planar	
(*31*)	CH_3BO, borine carbonyl		
	C—B	1·57 (0·03)	**13**
		1·540	*Spec.* **189**
	C—O	1·13 (0·03)	**13**
		1·13 *ass.*	*Spec.* **189**
	B—H	1·20 (0·03)	**13**
		1·20 *ass.*	*Spec.* **189**
	B—C—O	linear	**13**
	Boron angles tetrahedral		
(*32*)	Withdrawn		
(*33*)	CH_3Br, methyl bromide		
	C—Br	2·06 (0·05)	**6**
		1·91 (0·06)	**26**
		1·936	*Spec.* **194**
(*34*)	CH_3Br_3Sn, methyl stannic bromide		
	C—Sn	2·17 approx.	
	Sn—Br	2·45 (0·02)	**150**
	∠Br—Sn—Br	109·5° (2°)	

Table 1 (*cont.*)

(*35*)	CH_3Cl, methyl chloride		
	C—Cl	1·77 (0·02)	**6**
		1·77 (0·01)	**213**
		1·779	*Spec.* **194**
(*36*)	CH_3Cl_2N, methyl dichloramine		
	N—Cl	1·74 (0·02)	**101**
		1·74 (0·02)	**150**
	∠Cl—N—Cl	108° (2°)	**101**
	∠C—N—Cl	109° (2°)	**150**
(*37*)	CH_3Cl_3Si, methyl silicon trichloride		
	Si—Cl	2·01 (0·02)	
	Cl—Cl	3·27 (0·03)	**146**
	∠Cl—Sn—Cl	109° (3°)	
(*38*)	CH_3Cl_3Sn, methyl stannic chloride		
	C—Sn	2·19 (0·05)	
	Sn—Cl	2·32 (0·03)	**150**
	∠Cl—Sn—Cl	108° (4°)	
(*39*)	CH_3F, methyl fluoride		
	C—F	1·42 (0·02)	**6**
		1·42 (0·02)	**15**
		1·39	**115**
		1·384	*Spec.* **190**
(*40*)	CH_3I, methyl iodide		
	C—I	2·28 (0·05)	**6**
		2·132	*Spec.* **194**
(*41*)	CH_3I_3Sn, methyl stannic iodide		
	Sn—I	2·68 (0·02)	**150**
	∠I—Sn—I	109·5° (2°)	
(*42*)	CH_3NO_2, methyl nitrite		
	CH_3—O—N—O′		
	C—O	1·44 (0·02)	
	N—O	1·37 (0·02)	
	N—O′	1·22 (0·02)	**128**
	O—N—O′ group linear		
(*43*)	CH_3NO_2, nitromethane		
	C—N	1·46 (0·02)	**6**
		1·47 (0·02)	**128**
	N—O	1·21 (0·02)	**6**
		1·22 (0·02)	**128**
	∠O—N—O	127° (3°)	**6**
		130°–140°	**128**
(*44*)	CH_3NO_3, methyl nitrate		
	CH_3—O′—NO_2		
	C—O′	1·43 (0·05)	**30**
		1·44 (0·03)	**128**
	N—O	1·26	**30**
		1·22 (0·04)	**128**
	N—O′	1·36	**30**
		1·37 (0·03)	**128**
	∠O—N—O	125·2°	
	∠O—N—O′	105° (5°)	**30**
(*45*)	CH_3N_3, methyl azide		
	CH_3—N=N′=N″		
	C—N	1·47 (0·02)	**6**
		1·47 (0·02)	**30**
	N—N′	1·26 (0·02)	**6**
		1·24 (0·02)	**30**
	N′—N″	1·10 (0·02)	**6**
		1·10 (0·02)	**30**
	∠C—N=N′	120° (5°)	**30**
	Azide group linear		
(*46*)	CH_4O, methyl alcohol		
	C—O	1·44 (0·01)	**213**
(*47*)	CH_4S, methyl mercaptan		
	C—S	1·82 (0·01)	**213**
(*48*)	CH_5N, methylamine		
	C—N	1·47 (0·01)	**213**
		1·48	*Spec.*
(*49*)	CH_5NO, *O*-methyl hydroxylamine		
	C—O	1·44 (0·02)	
	N—O	1·37 (0·02)	**6**
	∠C—O—N	111° (3°)	
(*50*)	CI_4, carbon tetraiodide		
	C—I	2·12 (0·02)	*S.* **86**
		2·15 (0·02)	**111**
(*51*)	CN_4O_8, tetranitromethane		
	C—N	1·47 (0·02)	**77**
	N—O	1·22 (0·02)	
	∠O—N—O	127°	
(*52*)	COS, carbon oxysulphide		
	C—O	1·16 (0·03)	**6**
		1·161	*Spec.* **195**
	C—S	1·56 (0·04)	**6**
		1·561	*Spec.* **195**
	Linear		
(*53*)	CO_2, carbon dioxide		
	C—O	1·13 (0·02)	**6**
		1·15 (0·02)	*S.* **105**
		1·1632	*Spec.*
	Linear		
(*54*)	CS_2, carbon disulphide		
	C—S	1·54 (0·03)	**6**
		1·56 (0·02)	*S.* **105**
		1·554	*Spec.*
	Linear		

C_2

(*55*)	C_2Br_2, dibromoacetylene		
	C—C	1·20 (0·03)	
	C—Br	1·80 (0·03)	**6**
(*56*)	C_2Br_4, tetrabromoethylene		
	C—Br	1·91 (0·05)	**6**
(*57*)	C_2Cl_2, dichloroacetylene		
	C—C	1·195	*S.* **105, 109**
	C—Cl	1·640	*S.* **105, 109**
(*58*)	$C_2Cl_2I_2$, dichloro-diiodoethylene		
	C—C	1·34	**86**
	C—I	2·05	
	∠C—C—Cl	123·5°	
	Trans		
(*59*)	$C_2Cl_2O_2$, oxalyl chloride		
	C—C	1·50 (0·03)	
	C—Cl	1·72 (0·03)	**210**
	C=O	1·20 *ass.*	
	∠C—C—O	123° (2°)	
	∠Cl—C—O	123° (2°)	

Table 1 (*cont.*)

C_2 (*cont.*)

(*60*)	C_2Cl_4, tetrachloroethylene		
	C—C	1·38	**6**
		1·34 (0·05)	**208**
	C—Cl	1·73 (0·02)	**6**
		1·71 (0·02)	**208**
	∠Cl—C—C	123·7° (1°)	**6**
		122·2° (1°)	**208**
(*61*)	C_2Cl_6, hexachloroethane		
	C—Cl	1·770	
	Cl—Cl	4·275	*S.* **143**
	Normal form is *trans*		
(*62*)	C_2F_6, hexafluoroethane		
	C—C	1·45 (0·06)	**122**
		1·62–1·52	**202**
	C—F	1·35	**122**
		1·37–1·34	**202**
	∠F—C—F	107·5°	**122**
		107·5°–109·5°	**202**
(*63*)	$C_2FeN_2O_4$, iron nitrosocarbonyl		
	C—O	1·15 (0·03)	
	C—Fe	1·84 (0·02)	
	N—O	1·12 (0·03)	**16**
	N—Fe	1·77 (0·02)	
	Tetrahedral; Fe—C—O and Fe—N—O groups linear		
(*64*)	C_2HBr, bromoacetylene		
	C—Br	1·80 (0·03)	**40**
(*65*)	C_2HBr_3, tribromoethylene		
	C—C	1·32 (0·08)	
	C—Br	2·05 (0·08)	**6**
(*66*)	C_2HCl, chloroacetylene		
	C—C	1·21 (0·04)	
	C—Cl	1·68 (0·04)	**40**
(*67*)	C_2HCl_3, trichloroethylene		
	C—C	1·38	**6**
		1·36 (0·04)	**208**
	C—Cl	1·71 (0·03)	**6**
		1·72 (0·02)	**208**
	Cl′ClC=CHCl″		
	∠Cl′—C—C	123° (2°)	**6**
		121·5° (1°)	**208**
	∠Cl″—C—C	123° (2°)	**6**
		124° (2°)	**208**
(*68*)	C_2HCl_3O, chloral		
	C—C	1·52 (0·02)	
	C—Cl	1·76 (0·02)	**42**
	C—O	1·15 (0·02)	
	CCl_3 pyramidal; CHO planar and lies in symmetry plane of pyramid		
(*69*)	$C_2HF_3O_2$, trifluoroacetic acid (see (185) for dimer)		
	C—F	1·36 (0·05)	**144**
	∠F—C—F	110° (4°)	
(*70*)	C_2H_2, acetylene		
	C—C	1·22 (0·10)	**6**
		1·205 (0·008)	*S.* **181**
		1·204	*Spec.*
		1·15	*X.* **49**
	C—H	1·06 (0·05)	*S.* **181**
		1·057	*Spec.*
	Linear		

(*71*)	$C_2H_2AsCl_3$, lewisite (isomers)		
	C—As	1·90	
	As—Cl	2·17	**170**
(*72*)	$C_2H_2Br_2$, 1:2-dibromoethylene		
	Cis		
	C—C	1·32 (0·08)	**6**
	C—Br	2·05 (0·08)	
	Trans		
	C—Br	1·91 (0·05)	**6**
		1·86 (0·04)	**50**
	∠C—C—Br	121° (3°)	**50**
(*73*)	$C_2H_2Br_4$, *sym.*-tetrabromoethane		
	C—Br	1·941	*S.* **143**
	Br—Br	4·594	
	Stable form is *trans*		
(*74*)	$C_2H_2Cl_2$, 1:1-dichloroethylene		
	C—Cl	1·69 (0·02)	**6**
	∠Cl—C—C	122° (1°)	
(*75*)	$C_2H_2Cl_2$, 1:2-dichloroethylene		
	Cis		
	C—Cl	1·67 (0·02)	**6**
	Cl—Cl	3·7	*X.* **1**
	∠Cl—C—C	123·5° (1°)	**6**
	Trans		
	C—Cl	1·69 (0·03)	**6**
	Cl—Cl	4·7	*X.* **1**
	∠Cl—C—C	122·5° (1°)	**6**
(*76*)	$C_2H_2Cl_4$, *sym.*-tetrachloroethane		
	Cl—Cl	4·32	**95**
		4·275	*S.* **143**
	C—Cl	1·770	*S.* **143**
	Stable form is *trans*		**143**
(*77*)	$C_2H_2I_2$, *sym.*-diiodoethylene		
	Cis		
	C—I	2·03 (0·04)	**50**
		2·05	**86**
	∠C—C—I	125° (2°)	**50**
		125·5°	**86**
	Trans		
	C—I	2·03 (0·04)	**50**
		2·05	**86**
	∠C—C—I	122° (2°)	**50**
		121·1°	**86**
(*78*)	C_2H_2O, ketene (see (*190*) for dimer)		
	C—C	1·35 (0·02)	**59**
		1·353	*Spec.* **172**
	C—O	1·17 (0·02)	**59**
		1·102	*Spec.* **172**
	C—C—O linear		**59**
(*79*)	$C_2H_2O_2$, glyoxal		
	C—C	1·47 (0·02)	
	C—O	1·20 (0·01)	**68**
	∠C—C—O	123° (2°)	**68**
	Trans configuration		
(*80*)	C_2H_3Br, vinyl bromide		
	C—Br	1·86 (0·04)	**50**
	∠C—C—Br	121° (3°)	**50**
(*81*)	$C_2H_3Br_3$, 1:1:2-tribromoethane		
	C—Br	1·941	*S.* **143**
	Br—Br	4·594	

Table 1 (*cont.*)

(82)	C_2H_3BrO, acetyl bromide		
	C—C	1·54	
	C—Br	2·06 (0·10)	**6**
	C—O	1·13 (0·05)	
(83)	C_2H_3Cl, vinyl chloride		
	C—C	1·38	
	C—Cl	1·69 (0·02)	**6**
	∠C—C—Cl	122° (3°)	
(84)	$C_2H_3ClF_2$, methyl-difluorochloromethane		
	C—F	1·37 (0·03)	
	C—Cl	1·77 (0·03)	**217**
	∠C—C—F = ∠C—C—Cl	111° (5°)	
	∠F—C—F = ∠F—C—Cl	108° (5°)	
(85)	C_2H_3ClO, acetyl chloride		
	C—C	1·54	
	C—Cl	1·82 (0·10)	
	C—O	1·14 (0·05)	**6**
(86)	$C_2H_3ClO_2$, methyl chloroformate		
	C=O	1·19 (0·03)	
	C—O	1·35 (0·04) (carboxyl)	**211**
		1·46 (0·04) (methoxyl)	
	C—Cl	1·74 (0·02)	
	∠O=C—O	126° (4°)	
	∠C—O—C	111° (4°)	
	∠O—C—Cl	112° (2°)	
	Angle between C—O—C plane and plane of carboxyl group is 20° (10°)		
(87)	$C_2H_3Cl_2F$, methyl fluorodichloromethane		
	C—F	1·40 (0·03)	
	C—Cl	1·78 (0·03)	**217**
	∠C—C—F	109·5° (3°)	
	∠C—C—Cl	111° (3°)	
	∠Cl—C—Cl	109·5° (3°)	
(88)	$C_2H_3Cl_3$, methyl chloroform		
	C—Cl	1·76 (0·02)	**62**
	∠Cl—C—Cl	109° (2°)	
(89)	$C_2H_3Cl_3$, 1:1:2-trichloroethane		
	C—Cl	1·75 (0·03)	**79**
		1·770	*S.* **143**
	Cl—Cl	4·275	*S.* **143**
	∠Cl—C—Cl	111·5° (2°)	**79**
	Stable configuration is rotated about 50° from *trans*		**79**
	Stable configuration is *trans*		*S.* **143**
(90)	C_2H_3FO, acetyl fluoride		
	C—F	1·41 (0·05)	
	C—O	1·14 (0·05)	**116**
	∠O—C—F	125° (5°)	
	∠O—C—C	125° (5°)	
	∠C—C—F	105° (5°)	
(91)	$C_2H_3F_3$, methyl fluoroform		
	C—C	1·45 (0·04)	**122**
		1·53 (0·04)	**217**
		1·54	*Spec.* **188**
	C—F	1·33 (0·03)	**122**
		1·36 (0·02)	**217**
		1·33	*Spec.* **188**
	∠C—C—F	112° (2°)	**217**
	∠F—C—F	108·5°	**122**
		107° (3°)	**217**
(92)	C_2H_3I, vinyl iodide		
	C—I	2·03 (0·04)	**50**
	∠I—C—C	122° (2°)	
(93)	C_2H_3N, methyl cyanide		
	C—C	1·54 (0·02)	**5**
		1·49 (0·03)	**70**
	C—N	1·16 (0·02)	**5**
		1·16 (0·03)	**70**
	Linear		*Spec.* **174**
(94)	C_2H_3N, methyl *iso*cyanide		
	C—N	1·48 (0·03)	**5**
		1·44 (0·02)	**123**
		1·426	*Spec.* **189**
	N—C	1·17 (0·02)	**5**
		1·18 (0·02)	**123**
		1·167	*Spec.* **189**
(95)	C_2H_3NO, methyl *iso*cyanate		
	C—O	1·18 (0·03)	
	C—N	1·19 (0·03)	**84**
	N—O	2·37 (0·03)	
	∠C—N=C	125° (5°)	
(96)	C_2H_4, ethylene		
	C—C	1·30 (0·10)	**6**
		1·34 (0·02)	**31**
		1·33	**176**
		1·353 (0·01)	*Spec.*
	C—H	1·06 (0·03)	**31**
		1·071	*Spec.*
(97)	C_2H_4BrCl, 1-bromo-2-chloroethane		
	C—Cl	1·75 (0·02)	
	C—Br	1·90 (0·02)	**64**
	Oscillates about *trans*		
(98)	$C_2H_4Br_2$, 1:1-dibromoethane		
	Br—Br	3·56 (0·15)	**6**
(99)	$C_2H_4Br_2$, 1:2-dibromoethane		
	C—Br	1·92 (0·02)	**64**
		1·941	*S.* **143**
	Br—Br	4·75 (0·15)	**6**
		4·594	*S.* **143**
	Stable form is *trans*		
(100)	$C_2H_4Cl_2$, 1:1-dichloroethane		
	Cl—Cl	2·9 (0·3)	**6**
(101)	$C_2H_4Cl_2$, 1:2-dichloroethane		
	C—Cl	1·76 (0·02)	**35**
		1·770	*S.* **143**
	Cl—Cl	4·275	*S.* **143**
	Stable form is *trans*		
(102)	C_2H_4O, acetaldehyde		
	C—C	1·51 (0·05)	**6**
		1·50 (0·02)	**73**
	C—O	1·20 (0·05)	**6**
		1·22 (0·02)	**73**
	∠C—C—O	121° (2°)	**73**
(103)	C_2H_4O, ethylene oxide		
	C—C	1·49 (0·1)	**6**
		1·4728	*Spec.* **192, 204**
	C—O	1·49 (0·1)	**6**
		1·4363	*Spec.* **192, 204**

Table 1 (*cont.*)

C_2 (*cont.*)

(*104*) C_2H_4OS, thioacetic acid

C—C	1·54 (0·06)	
C—O	1·24 (0·04)	**158**
C—S	1·78 (0·02)	
∠C—C—S	110° (5°)	
∠C—C—O	125° (5°)	

(*105*) $C_2H_4O_2$, acetic acid (see (*210*) for dimer)

C—C	1·54 (0·04)	
C—O	1·43 (0·03)	**144**
C=O	1·24 (0·03)	
∠O=C—O	122–138°	
∠C—C—O	113–128°	

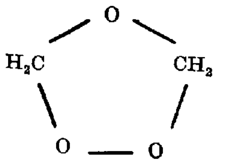
(*106*) $C_2H_4O_2$, methyl formate

C—O	1·36 (0·04) (carboxyl)	
	1·46 (0·04) (methoxyl)	**211**
C=O	1·21 (0·03)	
∠O=C—O	124° (4°)	
∠C—O—C	112° (3°)	

∠C—O—C plane is 30° (10°) out of *cis* planar configuration

(*107*) $C_2H_4O_3$, ethylene ozonide

Non-planar 5-membered ring with average ring-bond distance of 1·44 and average angle of 103°. Two possible structures which cannot be distinguished by electron diffraction **214**



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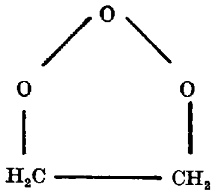


II

(*108*) $C_2H_4O_4$, formic acid dimer

C—O	1·36 (0·04)	**144**
C=O	1·29 (0·02)	**6**
	1·25 (0·03)	**144**
O—H—O	2·67 (0·04)	**6**
	2·73 (0·05)	**144**
∠O—C=O	125° (5°)	**6**
	121° (2°)	**144**

(*109*) C_2H_5Br, ethyl bromide

C—Br	2·02 (0·07)	**6**
	1·91 (0·02)	**62**
	2·81 (0·02)	**62**
∠C—C—Br	109° (2°)	**62**

(*110*) C_2H_5Cl, ethyl chloride

C—C	1·54 (0·02)	**213**
C—Cl	1·81 (0·1)	**6**
	1·76 (0·02)	**62**
	2·74 (0·02)	**62**
	1·77 (0·01)	**213**
∠C—C—Cl	111·5° (2°)	**62**
	110° (2°)	**213**

(*111*) C_2H_5ClO, ethylene chlorhydrin

C—C	1·54	
C—Cl	1·76	
C—O	1·43	*S.* **198**

Angle between CCO and CCCl planes is 74°. One H bond assumed

(*112*) C_2H_5I

C—I	2·32 (0·05)	**6**

(*113*) C_2H_6, ethane

C—C	1·52 (0·10)	**6**
	1·55 (0·03)	**31**
	1·573	*Spec.*
C—H	1·09 (0·03)	**31**

(*114*) C_2H_6AsBr, dimethyl arsenic bromide

As—Br	2·34 (0·04)	**150**
∠C—As—Br	96° (3°)	

(*115*) C_2H_6AsCl, dimethyl arsenic chloride

As—Cl	2·18 (0·04)	**150**
∠C—As—Cl	98° (3°)	

(*116*) C_2H_6AsI, dimethyl arsenic iodide

As—I	2·52 (0·03)	**150**
C—As	1·98 *ass.*	
∠C—As—I	98° (4°)	

(*117*) C_2H_6BF, dimethyl boron fluoride

C—B	1·55 (0·02)	
B—F	1·29 (0·02)	**121**
C—F	2·48 (0·03)	
∠C—B—F	121·5°	

Planar

(*118*) $C_2H_6BF_3O$, dimethyl ether–boron trifluoride

C—O	1·45 (0·03)	
B—F	1·43 (0·03)	**133, 151**
B—O	1·50 (0·06)	

Boron angles tetrahedral
Oxygen angles tetrahedral

(*119*) $C_2H_6Br_2Sn$, dimethyl stannic bromide

C—Sn	2·17 approx.	
Sn—Br	2·48 (0·02)	**150**
∠Br—Sn—Br	109° (3°)	

(*120*) C_2H_6ClN, *N*-chlorodimethylamine

C—N	1·47 (0·02)	**101**
	1·47 *ass.*	
Cl—N	1·77 (0·02)	**101**
	1·77 (0·02)	**150**

(*121*) $C_2H_6Cl_2Si$, dimethyl silicon chloride

C—Si	1·83 (0·06)	
Si—Cl	1·99 (0·03)	**146**
C—Cl	3·12 (0·06)	
Cl—Cl	3·25 (0·04)	

(*122*) $C_2H_6Cl_2Sn$, dimethyl stannic chloride

Sn—Cl	2·34 (0·03)	**150**

(*123*) C_2H_6Hg, dimethyl mercury

C—Hg	2·23 (0·04)	**20**

(*124*) $C_2H_6I_2Sn$, dimethyl stannic iodide

Sn—I	2·69 (0·03)	**150**
∠I—Sn—I	109·5° (3°)	

Table 1 (*cont.*)

(*125*)	$C_2H_6N_2$, azomethane			
		C—N	1·47 (0·06)	
		N—N	1·24 (0·05)	6
		∠C—N=N	110° (10°)	
(*126*)	$C_2H_6N_2O_2$, dimethylnitramine			
		C—N	1·48	
		N—N	1·30	*S.* 198
		N—O	1·30	
		∠N—N—O	120°	
		∠C—N—N	123°	
		Planar		
(*127*)	C_2H_6O, dimethyl ether			
		C—O	1·42 (0·03)	6
			1·43 (0·03)	213
		∠C—O—C	111° (3°)	213
(*128*)	C_2H_6O, ethyl alcohol			
		C—C	1·55 (0·02)	
		C—O	1·43 (0·02)	213
		∠C—C—O	110° (3°)	
(*129*)	C_2H_6OS, dimethyl sulphoxide			
		C—S	1·82	*S.* 182
			1·84 (0·02)	212
		S—O	1·47	*S.* 182
			1·47 (0·04)	212
		C—O	2·65 (0·03)	212
		C—H	1·08	*S.* 182
		∠C—S—C	100°	*S.* 182
		∠C—S—O	107°	*S.* 182
			106° (6°)	212
		Pyramidal		182
(*130*)	$C_2H_6O_2$, ethylene glycol			
		C—C	1·54	*S.* 198
			1·52 (0·02)	205
		C—O	1·43	*S.* 198
			1·43 (0·02)	
		C—H	1·08	*S.* 198
		O—H	0·97 *ass.*	205
		Angle between CCO planes is 74°. One H bond assumed		*S.* 198
(*131*)	$C_2H_6O_2$, dimethyl peroxide			
		No determination of separate bond distances possible		214
		∠C—O—O	105° (3°)	
(*132*)	$C_2H_6O_2S$, dimethyl sulphone			
		C—S	1·90 (0·03)	67
			1·80 (0·02)	212
		S—O	1·44 (0·03)	67
			1·43 (0·02)	212
		C—O	2·58 (0·02)	212
		∠C—S—O	105° (3°)	
		∠C—S—C	115° (15°)	212
		∠O—S—O	125° (15°)	
(*133*)	C_2H_6S, dimethyl thio-ether			
		C—S	1·82 (0·03)	6
			1·82 (0·01)	213
(*134*)	C_2H_6S, ethyl mercaptan			
		C—C	1·54 (0·02)	
		C—S	1·81 (0·01)	213
		∠C—C—S	113° (2°)	
(*135*)	$C_2H_6S_2$, dimethyl disulphide			
		C—S	1·78 (0·03)	
		S—S	2·04 (0·03)	58
		∠C—S—S	107° (3°)	
(*136*)	$C_2H_6S_3$, dimethyl trisulphide			
		C—S	1·78 (0·04)	
		S—S	2·04 (0·02)	187
		∠C—C—C	104° (5°)	
		∠S—S—S	104° (5°)	
		Chain configuration		
(*137*)	C_2H_7N, dimethylamine			
		C—N	1·46 (0·03)	33
			1·47 (0·02)	213
		C—H	1·08 (0·03)	33
		∠C—N—C	108° (4°)	33
			111° (3°)	213
(*138*)	C_2H_7N, ethylamine			
		C—C	1·54 (0·02)	213
		C—N	1·47 (0·02)	
		∠C—C—N	110° (3°)	
(*139*)	$C_2H_8N_2$, dimethylhydrazine			
		C—N	1·47 (0·03)	
		N—N	1·45 (0·03)	183
		∠C—N—N	110° (4°)	
		∠C—N—C	110° (4°)	
(*140*)	C_2I_2, diiodoacetylene			
		C—C	1·18	
		C—I	2·03 (0·05)	6
(*141*)	C_2I_4, tetraiodoethylene			
		C—I	2·10 (0·05)	6
(*142*)	C_2N_2, cyanogen			
		C—C	1·43 (0·02)	6
			1·37 (0·02)	70
		C—N	1·16 (0·02)	6
			1·16 (0·02)	70

C_3

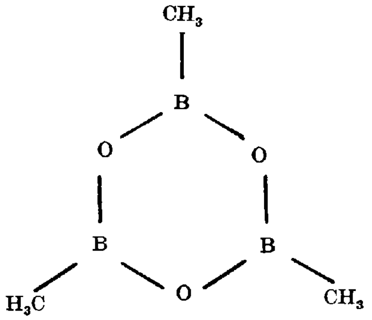
(*143*)	C_3CoNO_4, cobalt nitrosocarbonyl			
		C—O	1·14 (0·04)	
		C—Co	1·83 (0·02)	
		N—O	1·10 (0·04)	16
		N—Co	1·76 (0·02)	
		Tetrahedral, with linear Co—C—O and Co—N—O groups		
(*144*)	C_3F_6, hexafluoropropene			
		C—C	1·52	
		C=C	1·31	185
(*145*)	C_3H_3Br, 3-bromo-1-propyne			
		C_2—C_3	1·47 (0·02)	
		C_3—Br	1·95 (0·02)	127
		∠C_2—C_3—Br	112° (2°)	
(*146*)	C_3H_3Cl, 3-chloro-1-propyne			
		C_2—C_3	1·47 (0·02)	
		C_3—Cl	1·82 (0·02)	127
		∠C_2—C_3—Cl	111° (2°)	

Table 1 (*cont.*)

C_3 (*cont.*)

(*147*)	C_3H_3I, 3-iodo-1-propyne			
		C_2—C_3	1·47 (0·02)	
		C_3—I	2·13 (0·03)	**127**
		∠C_2—C_3—I	111° (3°)	
(*148*)	C_3H_4, allene			
		C—C	1·31 (0·05)	**6**
			1·34 (0·02)	**31**
			1·330	*Spec.*
		Linear		
(*149*)	C_3H_4, methyl acetylene			
		C—C	1·46 (0·02)	**70**
			1·469	*Spec.*
		C≡C	1·20 (0·03)	**70**
(*150*)	$C_3H_4Cl_2$, 1:1-dichlorocyclopropane			
		C—C	1·52 (0·02)	**162**
		C—Cl	1·76 (0·02)	
		Angle between C—Cl and ring is 56° (2°)		
(*151*)	$C_3H_4O_2$, *β*-propiolactone			
		C—C	1·54	
		C—O	1·44	*S.* **203**
		C=O	1·21–1·24	
		∠C—C—C	89°	
		∠O—C=O	133°	
		Best model is a planar ring		
(*152*)	C_3H_5Cl, chlorcyclopropane			
		C—C	1·52 (0·02)	
		C—Cl	1·76 (0·02)	**162**
		Angle between C—Cl and ring is 56° (2°)		
(*153*)	C_3H_6, cyclopropane			
		C—C	1·53 (0·02)	**6**
			1·53 (0·03)	**31**
			1·54	*S.* **157**
		C—H	1·08	*S.* **157**
		∠C—C—H	116·4° (2°)	
		∠H—C—H	118·2° (2°)	*S.* **157**
(*154*)	$C_3H_6Br_2$, propylene bromide			
		C—Br	1·92 (0·02)	**94**
		∠C—C—Br	110° (1°)	
		Normal structure is *trans*		
(*155*)	$C_3H_6Cl_2$, 2:2-dichloropropane			
		C—C	1·54 (0·02)	
		C—Cl	1·78 (0·02)	**211**
		∠C—C—C	114 (4°)	
		∠C—C—Cl	108·5° (3°)	
		∠Cl—C—Cl	110° (2°)	
(*156*)	C_3H_6O, acetone			
		C—C	1·57 (0·04)	**6**
			1·56	*S.* **182**
		C—O	1·14	*S.* **182**
		C—H	1·09	*S.* **182**
		∠C—C—O	123°	*S.* **182**
		Planar		
(*157*)	C_3H_6O, trimethylene oxide			
		C—C	1·54 (0·03)	
		C—O	1·46 (0·03)	**214**
		∠C—C—O	88·5° (3°)	
		∠C—O—C	94·5° (3°)	
(*158*)	$C_3H_6O_2$, methyl acetate			
		C—C	1·51 (0·03)	
		C—O	1·36 (0·04) (carboxyl)	**211**
			1·46 (0·04) (methoxyl)	
		C=O	1·22 (0·03)	
		∠C—O—C	113° (3°)	
		∠O—C=O	124° (4°)	
		∠C—O—C is 25° (8°) out of *cis* planar configuration		
(*159*)	$C_3H_6O_2$, ethylene methylene dioxide			
		C—C	1·54 (0·05)	
		C—O	1·42 (0·03)	**214**
		Angles close to tetrahedral. Better model has puckered, non-planar ring		
(*160*)	$C_3H_6O_3$, trioxane			
		C—O	1·40 (0·02)	**214**
		∠C—O—C=∠O—C—O	112° (3°)	
(*161*)	$C_3H_6S_3$, *sym.*-trithioformaldehyde			
		C—S	1·81	
		S—S	3·05	*S.* **171**
		∠S—C—S	106·5°	
		'Chair' form		
(*162*)	C_3H_7Br, *i*-propyl bromide			
		C—Br	1·91 (0·03)	
			2·81 (0·03)	**62**
		∠C—C—C	tetrahedral	
		∠C—C—Br	109·5° (3°)	
(*163*)	C_3H_7Cl, *i*-propyl chloride			
		C—Cl	1·75 (0·02)	
			2·66 (0·03)	**62**
		∠C—C—C	109° (3°)	
		∠C—C—Cl	110° (3°)	
(*164*)	C_3H_8, *n*-propane			
		C—C	1·52 (0·05)	**6**
			1·54 (0·02)	**31**
		∠C—C—C	111·5° (3°)	**31**
(*165*)	$C_3H_8N_2$, pyrazolidine			
		C—C	1·51	
		C—N	1·47 *ass.*	**214**
		N—N	1·47 *ass.*	
		∠C—C—C	107°	
		∠C—C—N	107·5°	
		∠C—N—N	109°	
		Ring assumed coplanar		
(*166*)	$C_3H_8O_2$, methylal			
		C—O	1·42 (0·02)	
		C—H	1·09 (0·04)	**205**
		∠C—O—C ∠O—C—O	Average of these angles is 112° (2°)	
(*167*)	$C_3H_8O_3$, glycerol			
		C—C	1·54	
		C—O	1·43	*S.* **198**
		C—H	1·08	
		Angle between CCO planes is 71°. Two H bonds assumed		
(*168*)	C_3H_9As, trimethyl arsine			
		C—As	1·98 (0·02)	**57**
		∠C—As—C	96° (5°)	

Table 1 (*cont.*)

(*169*)	$C_3H_9As_3$, arsenomethane polymer		
	C—As	1·98 (0·04)	
	As—As	2·42 (0·02)	154
	∠As—As—As	90° (average)	
(*170*)	C_3H_9B, trimethyl boron		
	C—B	1·56 (0·02)	
	C—C	2·70 (0·03)	27
	∠C—B—C	120° (3°)	
	Planar		
(*171*)	$C_3H_9BO_3$, methyl borate		
	C—O	1·43 (0·03)	
	B—O	1·38 (0·02)	102
	∠B—O—C	113° (3°)	
	BO_3 group planar		
(*172*)	$C_3H_9B_3O_3$, trimethyl triborine trioxane		
	C—B	1·57 (0·03)	102
	B—O	1·39 (0·02)	
	∠B—O—B	112° (4°)	
	Planar ring, with CH_3 groups in plane of ring: 		
(*173*)	C_3H_9BrSn, trimethyl stannic bromide		
	C—Sn	2·17 (0·05)	
	Sn—Br	2·49 (0·03)	150
	Tetrahedral		
(*174*)	C_3H_9ClSi, trimethyl silicon chloride		
	C—Si	1·89 (0·03)	
	Si—Cl	2·09 (0·03)	161
(*175*)	C_3H_9ClSn, trimethyl stannic chloride		
	C—Sn	2·19 (0·03)	
	Sn—Cl	2·37 (0·03)	150
	∠C—Sn—Cl	108° (4°)	
(*176*)	C_3H_9ISn, trimethyl stannic iodide		
	Sn—I	2·72 (0·03)	150
	Tetrahedral		
(*177*)	C_3H_9In, trimethyl indium		
	C—In	2·16 (0·04)	113
(*178*)	C_3H_9N, trimethylamine		
	C—N	1·47 (0·02)	6
		1·47 (0·01)	213
(*179*)	C_3H_9NO, trimethylamine oxide		
	C—N	1·54 (0·02)	67
		1·49 (0·02)	212
	N—O	1·36 (0·03)	67
		1·44 (0·04)	212
	C—O	2·34 (0·03)	212
	C—C	2·49 (0·03)	212
	∠C—N—O	104° (5°)	212
	∠C—N—C	114° (5°)	212
(*180*)	C_3H_9P, trimethyl phosphine		
	C—P	1·87 (0·02)	57
	∠C—P—C	100° (4°)	
(*181*)	$C_3H_{12}BN$, borine trimethylamine		
	C—N	1·53 (0·06)	
	B—N	1·62 (0·15)	13
(*182*)	C_3O_2, carbon suboxide		
	C—C	1·29 (0·03)	
	C—O	1·20 (0·02)	6
	Linear		

C_4

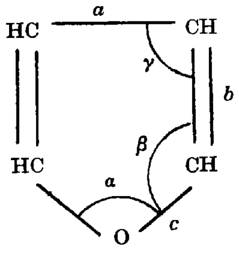
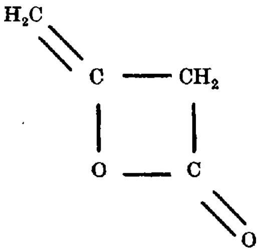
(*183*)	C_4HCoO_4, cobalt carbonyl hydride		
	C—Co	1·75 (0·08) (in COH)	
		1·83 (0·02)	65
	C—O	1·16 (0·05)	
	Tetrahedral. H attached to one CO group		
(*184*)	C_4H_2, diacetylene		
	C—C	1·43 (0·03)	6
		1·36 (0·03)	70
	C≡C	1·21 (0·02)	6
		1·19 (0·03)	70
	Linear		
	Discrepancy between force constant and length of central C—C bond		*Spec.* 173
(*185*)	$C_4H_2F_6O_4$, trifluoroacetic acid dimer		
	C—C	1·47 (0·03)	
	C—F	1·36 (0·03)	144
	O—OH	2·76 (0·06)	
	∠O—C=O	130° (3°)	
	∠F—C—F	109° (2°)	
(*186*)	$C_4H_2FeO_4$, iron carbonyl hydride		
	C—Fe	1·79 (0·04) (in COH)	
		1·84 (0·03)	65
	C—O	1·15 (0·05)	
	Tetrahedral. H attached to one CO group		
(*187*)	$C_4H_4N_2$, pyrazine		
	C—C	1·39 (0·02)	
	C—N	1·35 (0·02)	72
	C—H	1·09 (0·04)	
(*188*)	C_4H_4O, furan 		
	a	1·46 (0·03)	103
	a	1·46 *ass.*	72
	b	1·35 *ass.*	72
	c	1·41 (0·02)	72
		1·40 (0·03)	103
	α	107° (4°)	72
		107° (3°)	103
	β	109° (3°)	72
	γ	107° (2°)	72

Table 1 (*cont.*)

C_4 (*cont.*)

(*189*) $C_4H_4O_2$, dioxadiene
C—C 1·35 (0·03)
C—O 1·41 (0·03) **103**
∠C—O—C 116° (4°)

(*190*) $C_4H_4O_2$, ketene dimer
Electron diffraction cannot distinguish between two models: *S*. **203**



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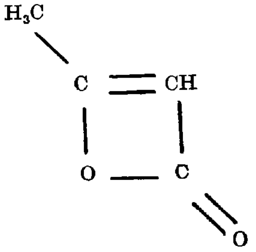


II

(*191*) C_4H_4S, thiophene
Notation as for C_4H_4O (*188*)
a 1·44 *ass.*
b 1·35 *ass.*
c 1·74 (0·03) **72**
α 91° (4°)
β 112° (3°)
γ 113° (3°)

(*192*) C_4H_5N, pyrrol
Notation as for C_4H_4O (*188*)
a 1·44 *ass.*
b 1·35 *ass.*
c 1·42 (0·02) **72**
α 105° (4°)
β 110° (3°)
γ 108° (2°)

(*193*) C_4H_6, dimethyl acetylene
C—C 1·47 (0·02) **70**

(*194*) C_4H_6, 1:3-butadiene
1·52 (0·08) **6**
C—C 1·46 (0·03) **72**
1·47 *S*. **198**
C═C 1·35 (0·02) **72**
1·37 *S*. **198**
C—H 1·06 *S*. **198**
∠C═C—C 122°
∠C═C—H 125° *S*. **198**

(*195*) $C_4H_6Br_4$, 1:2:3:4-tetrabromobutane
C—C 1·54
C—Br 1·94 *S*. **198**
No free rotation. Angle between C—C—Br planes between 60 and 180°

(*196*) $C_4H_6D_2O_4$, deuterium acetate dimer
Identical with acetic acid dimer (*210*) within limits of experimental error **144**

(*197*) C_4H_6O, dihydrofuran
C—C 1·54 (0·03)
C═C 1·35 *ass.*
C—O 1·45 (0·03) **103**
∠C—O—C 110° (3°)

(*198*) C_4H_6O, vinyl ether
C═C 1·34 (0·03)
C—O 1·40 (0·03) **210**
∠C═C—O 121·5° (2°)
∠C—O—C 112° (2°)

(*199*) $C_4H_6O_2$, diacetyl
C_1—C_2 1·54 (0·02)
C_2—C_3 1·47 (0·02)
C—O 1·20 (0·02) **68**
∠CO—C═O 123° (2°)
∠CH_3—C═O 122·5° (1°)
Coplanar. *Trans*

(*200*) C_4H_7Cl, *i*-crotyl chloride
C—Cl 1·72 (0·02) **62**
∠C—C—Cl 123° (2°)
∠C—C—C 111° (3°)

(*201*) C_4H_8, 2-butene
Cis
C—C 1·54 (0·03)
C═C 1·38 (0·02) **7, 17**
Trans
C—C 1·56 (0·04)
C═C 1·40 (0·04) **7, 17**

(*202*) C_4H_8, *i*-butene
C—C 1·54 (0·02) **31**

(*203*) $C_4H_8Br_2$, 2:3-dibromobutane
C—Br 2·83 (0·02)
Br—Br 4·60 (0·03)
C—Br 1·91 *ass.* **76**
C—C 1·54 *ass.*
∠C—C—Br 109·5° (2°)
Trans configuration (meso and racemic forms)

(*204*) $C_4H_8Cl_2$, 2:3-dichlorobutane
Cl—Cl 4·33 (0·03)
C—C 1·55 *ass.* **214**
C—Cl 1·77 *ass.*
Trans configuration

(*205*) $C_4H_8I_2$, 1:4-diiodobutane
Large variety of configurations **24**

(*206*) C_4H_8O, tetrahydrofuran
C—C 1·54 (0·02)
C—O 1·43 (0·03) **103**
∠C—O—C 111° (2°)

(*207*) C_4H_8O, 2-butene oxide
Cis
C—C 1·54 (0·03)
C—O 1·43 (0·03) **7, 17**
Trans
C—C 1·54 (0·03)
C—O 1·43 (0·03)

Table 1 (*cont.*)

(*208*) $C_4H_8O_2$, 1:4-dioxane

C—C	1·54	*S.* **171**
	1·51 (0·04)	**214**
C—O	1·46 (0·04)	**6**
	1·42	*S.* **171**
	1·44 (0·03)	**214**
∠C—O—C	110° (5°)	**6**
	108° (5°)	*S.* **171**
	112° (5°)	**214**
∠C—C—O	106°	*S.* **171**
	109·5° (5°)	**214**
'Chair' form		**6, 171, 214**

(*209*) $C_4H_8O_3$, 2-butene ozonide

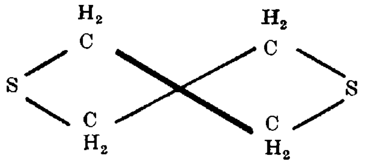
Good agreement with Staudinger ring model **214**

(*210*) $C_4H_8O_4$, acetic acid dimer

C—C	1·54 (0·04)	
C—O	1·36 (0·04)	
C=O	1·25 (0·03)	
OH—O	2·76 (0·06)	**144**
∠O—C=O	130°	

(*211*) $C_4H_8S_2$, 1:4-dithian

Two models cannot be distinguished: I, the normal 'chair' form; II, as below:



S. **171**

(*212*) C_4H_9Br, *tert.*-butyl bromide

C—C	1·54 (0·02)	
C—Br	1·92 (0·03)	**36**
∠C—C—C	111·5° (2°)	

(*213*) C_4H_9Cl, *tert.*-butyl chloride

C—C	1·54 (0·02)	
C—Cl	1·78 (0·03)	**36**
∠C—C—C	111·5° (2°)	

(*214*) C_4H_{10}, *n*-butane

C—C	1·51 (0·05)	**6**

(*215*) C_4H_{10}, *i*-butane

C—C	1·54 (0·02)	**31, 36**
∠C—C—C	111·5° (2°)	**81**

(*216*) $C_4H_{10}N_2$, 1:2-diaminocyclobutane

Cis and *trans*. Angle between C—N and ring plane is 56·5° (1·5°) **216**

(*217*) $C_4H_{10}O$, diethyl ether

C—C	1·50 (0·02)	**213**
C—O	1·33 (0·08)	**6**
	1·43 (0·02)	**213**
∠C—C—O	110° (3°)	
∠C—O—C	108° (3°)	**213**

(*218*) $C_4H_{10}S$, diethyl thio-ether

C—C	1·55 (0·02)	
C—S	1·81 (0·01)	**213**
∠C—C—S	112° (2°)	

(*219*) $C_4H_{11}ClSi$, siliconeopentyl chloride

$(CH_3)_3SiCH_2Cl$

C—Cl	1·73 (0·03)	
C—Si	1·88 (0·04)	*S.* **207**

Tetrahedral. Staggered configuration preferred

(*220*) $C_4H_{11}N$, ethylamine

C—C	1·54 (0·02)	
C—N	1·47 (0·02)	**213**
∠C—C—N	110° (3°)	
∠C—N—C	112° (3°)	

(*221*) $C_4H_{12}Al_2Br_2$, dimethyl aluminium bromide dimer

C—Al	1·90–2·05	
C—Br	3·59 (0·05)	
Al—Br	2·42 (0·03)	**104**
∠C—Al—C	115–130°	
∠Br—Al—Br	90° (3°)	

Bridge structure

(*222*) $C_4H_{12}Al_2Cl_2$, dimethyl aluminium chloride dimer

C—Al	1·85–2·00	
C—Cl	3·43 (0·05)	
Al—Cl	2·31 (0·03)	**104**
∠C—Al—C	120–135°	
∠Cl—Al—Cl	89° (4°)	

(*223*) $C_4H_{12}Ge$, tetramethyl germanium

C—Ge	1·98 (0·03)	**6**

(*224*) $C_4H_{12}Pb$, tetramethyl lead

C—Pb	2·30 (0·05)	**6**

(*225*) $C_4H_{12}Si$, tetramethyl silicon

C—Si	1·93 (0·03)	**6**

(*226*) $C_4H_{12}Sn$, tetramethyl tin

C—Sn	2·18 (0·03)	**6**

(*227*) C_4NiO_4, nickel carbonyl

C—O	1·15 (0·02)	
C—Ni	1·82 (0·03)	**6**

Tetrahedral. Ni—C—O linear

C_5

(*228*) C_5F_{10}, decafluorocyclopentane

C—C	1·54	
C—F	1·38	*S.* **200**

Deviation from 5-fold symmetry

(*229*) C_5FeO_5, iron pentacarbonyl

C—O	1·15 (0·04)	
C—Fe	1·84 (0·03)	**65**

Trigonal bipyramid

Fe—C—O linear

(*230*) C_5H_5N, pyridine

C—C	1·39 (0·02)	
C—N	1·37 (0·03)	
C—H	1·09 (0·04)	**72**

(*231*) C_5H_6, cyclopentadiene

Notation as for C_4H_4O (*188*)

a	1·46 (0·04)	
b	1·34 *ass.*	
c	1·54 *ass.*	**72**
α	101° (4°)	
β	109° (3°)	
γ	110° (2°)	

Table 1 (*cont.*)

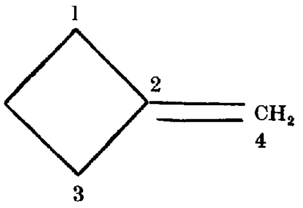
C_5 (*cont.*)

(*232*) C_5H_6, pirylene

CH_3—C≡C—CH=CH_2
1 2 3 4 5

C_1—C_2	1·47	
C_2—C_3	1·20	
C_3—C_4	1·42	
C_4—C_5	1·35	**131**
∠C_3—C_4—C_5	125°	

(*233*) C_5H_8, methylene cyclobutane



C_1—C_2	1·56 (0·03)	**120**
	1·55 (0·02)	**149**
C_2—C_4	1·34 (0·02)	**120**
	1·34 (0·03)	**149**
∠C_1—C_2—C_3	90°	**120**
	92·5° (4°)	**149**

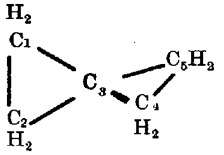
(*234*) C_5H_8, 1-methyl cyclobutene

C—C	1·54 (0·03)	
C=C	1·34 (0·03)	**149**
∠CH_3—C—C	125° (4°)	
∠C=C—C	93·5° (3°)	

(*235*) C_5H_8, spiropentane

C—C	1·54	
C—H	1·08	
Apical angles 60°		**71**

It seems doubtful whether this compound really was spiropentane, vide **120**



C_1—C_2	1·51 (0·04)	
C_1—C_3	1·48 (0·03)	**152**
∠C_2—C_3—C_1	61·5° (2°)	
∠H—C—H	120° (8°)	

(*236*) $C_5H_8Br_4$, tetrabromopentaerythritol

C—C	1·54	
C—Br	1·93	**2**
Halogens in plane with central C		
Disagree with this structure		**47**

(*237*) $C_5H_8Cl_4$, tetrachloropentaerythritol

C—C	1·54	
C—Cl	1·76	**2**
See (*236*)		**47**

(*238*) $C_5H_8I_4$, tetraiodopentaerythritol

C—C	1·54	
C—I	2·10	**2**
See (*236*)		**47**

(*239*) C_5H_{10}, cyclopentane

C—C	1·52 (0·03)	**6**
	1·52 (0·03)	**31**
	1·54	*S.* **159**
C—H	1·09	*S.* **159**
∠H—C—H tetrahedral		*S.* **159**

(*240*) $C_5H_{10}Br_2$, 1:5-dibromopentane

Large variety of configurations		**24**

(*241*) $C_5H_{11}Cl$, neopentyl chloride

$(CH_3)_3C'$—$C''H_2Cl$

C′—C″	1·58 (0·05)	
C—C	1·54 (0·03)	
C—Cl	1·74 (0·03)	*S.* **207**

(*242*) C_5H_{12}, *n*-pentane

C—C	1·53 (0·05)	**6**

(*243*) C_5H_{12}, *neo*-pentane

C—C	1·54 (0·02)	**31**

C_6

(*244*) $C_6Br_4O_2$, bromanil

C—C	1·54	*S.* **197**
C=C	1·36	*S.* **197**
C—Br	1·93	**106**
	1·89	*S.* **197**
C—O	1·14	*S.* **197**
∠C—C—C	114°	*S.* **197**
∠C=C—Br	123·25°	**106**
	124°	*S.* **197**

(*245*) C_6Br_6, hexabromobenzene

C_1—Br_2	2·81	
C_1—Br_3	4·12	
C_1—Br_4	4·64	
Br_1—Br_2	3·30	
Br_1—Br_3	5·62	
Br_1—Br_4	6·50	*S.* **165**

Br bent out of plane of ring by 12°

(*246*) $C_6Cl_4O_2$, chloranil

C—C	1·54	*S.* **197**
C=C	1·36	*S.* **197**
C—Cl	1·71	**106**
	1·72	*S.* **197**
C—O	1·14	*S.* **197**
∠C—C—C	110°	*S.* **197**
∠C=C—Cl	123°	*S.* **197**

(*247*) C_6Cl_6, hexachlorobenzene

C_1—Cl_2	2·68	
C_1—Cl_3	3·99	
C_1—Cl_4	4·51	
Cl_1—Cl_2	3·51	
Cl_1—Cl_3	5·35	
Cl_1—Cl_4	6·19	*S.* **165**

Cl bent out of plane of ring by 12°

(*248*) C_6CrO_6, chromium hexacarbonyl

C—O	1·16 (0·05)	
C—Cr	1·92 (0·04)	**41**

Octahedral. Cr—C—O linear

Table 1 (*cont.*)

(249)	C_6F_{12}, dodecafluorocyclohexane		
	C—C	1·54	
	C—F	1·38	*S.* **200**
	Angles approximately tetrahedral		
(250)	$C_6H_2Br_4$, 1:2:3:5-tetrabromobenzene		
	C_1—Br_2	2·83	
	C_1—Br_3	4·11	
	C_1—Br_4	4·66	
	Br_1—Br_2	3·34	
	Br_1—Br_3	5·62	*S.* **165**
	Br bent out of plane of ring by 15°		
(251)	$C_6H_2Br_4O_2$, tetrabromohydroquinone		
	C—Br	1·87	**106**
	∠C=C—Br	122·5°	
(252)	$C_6H_2Cl_4$, 1:2:4:5-tetrachlorobenzene		
	C_1—Cl_1	1·72 (0·04)	
	C_1—Cl_2	3·20	
	C_2—Cl_4	5·37	
	C_2—Cl_5	6·25	**18**
(253)	$C_6H_2Cl_4O_2$, tetrachlorohydroquinone		
	C—Cl	1·70	**106**
	∠C=C—Cl	122°	
(254)	$C_6H_3Br_3$, *sym.*-tribromobenzene		
	C—C	1·39 (0·02)	
	C—Br	1·84 (0·02)	
	∠C—C—Br	119° (2°)	**110**
(255)	$C_6H_3Cl_3$, *sym.*-trichlorobenzene		
	C—Cl	1·69 (0·03)	**18**
	Cl_1—Cl_3	5·38	
(256)	$C_6H_3I_3$, *sym.*-triiodobenzene		
	C—I	2·05	**6**
(257)	$C_6H_4Br_2$, *o*-dibromobenzene		
	C—C	1·405	*S.* **165**
	C_1—Br_1	1·89	
	C_1—Br_2	2·85	*S.* **165**
	C_1—Br_3	4·13	
	Br_1—Br_2	3·43	*S.* **165**
		3·80 (0·05)	*X.* **11**
	Br bent out of plane of ring by 18°		*S.* **165**
(258)	$C_6H_4Br_2$, *p*-dibromobenzene		
	C—Br	1·88 (0·02)	**6**
	C_1—Br_2	2·85	
	C_1—Br_3	4·15	*S.* **165**
	Br_1—Br_4	6·56	*S.* **165**
		6·55 (0·09)	*X.* **11**
(259)	$C_6H_4Cl_2$, *o*-dichlorobenzene		
	C_1—Cl_1	1·71 (0·03)	**18**
	C_1—Cl_2	2·70	
	C_1—Cl_3	3·97	*S.* **165**
	Cl_2—Cl_3	3·28	*S.* **165**
		3·15	**18**
		3·30 (0·05)	*X.* **11**
	Cl bent out of plane of ring by 18°		*S.* **165**
(260)	$C_6H_4Cl_2$, *m*-dichlorobenzene		
	C—Cl	1·69 (0·03)	**18**
	Cl—Cl	5·35	**18**
		5·35 (0·05)	*X.* **11**
(261)	$C_6H_4Cl_2$, *p*-dichlorobenzene		
	C—Cl	1·69 (0·03)	**18**
	Cl—Cl	6·18	**18**
		6·10 (0·09)	*X.* **11**
(262)	$C_6H_4F_2$, *o*-difluorobenzene		
	C—F	1·35 (0·03)	**91**
(263)	$C_6H_4I_2$, *o*-diiodobenzene		
	C—I	2·00 (0·10)	**6**
(264)	$C_6H_4I_2$, *m*-diiodobenzene		
	C—I	2·00 (0·10)	**6**
(265)	$C_6H_4I_2$, *p*-diiodobenzene		
	C—I	2·00 (0·10)	**6**
(266)	C_6H_5Cl, chlorobenzene		
	C—C	1·39 (0·02)	**18**
		1·42 (0·03)	*X.* **11**
	C—Cl	1·69 (0·03)	**18**
		1·65 (0·03)	*X.* **11**
(267)	C_6H_5F, fluorobenzene		
	C—F	1·34 (0·04)	**91**
		1·31 (0·03)	*S.* **105**
(268)	C_6H_6, benzene		
	C—C	1·39 (0·02)	**72**
		1·40	*S.* **105**
		1·40 (0·01)	*S.* **118**
		1·42 (0·03)	*X.* **3**
	C—H	1·08 (0·04)	**72**
		1·04	*S.* **105**
		1·04 (0·05)	*S.* **118**
	Planar		
(269)	C_6H_6, dimethyldiacetylene		
	C_1—C_2	1·47 (0·02)	
	C_2—C_3	1·20 (0·02)	
	C_3—C_4	1·38 (0·03)	**70**
	Discrepancy between force constant and length of central C—C		*Spec.* **173**
(270)	$C_6H_6Cl_6$, *β*-hexachlorocyclohexane		
	C—C	1·54	
	C—Cl	1·76	*S.* **125**
(271)	$C_6H_6O_3$, phloroglucinol		
	C—C	1·40	
	C—O	1·36	*S.* **171**
	Enol form. C and O coplanar		
(272)	$C_6H_8Br_4$, 1:2:4:5-tetrabromocyclohexane		
	C—C	1·54	
	C—Br	1·93	**66**
	Rigid symmetrical ring		
(273)	$C_6H_{10}Br_2$, 1:3-dibromocyclohexane		
	C—Br	1·93	**44**
(274)	$C_6H_{10}Br_2$, 1:4-dibromocyclohexane		
	C—Br	1·93	**44**
(275)	$C_6H_{10}Cl_2$, 1:4-dichlorocyclohexane		
	C—Cl	1·76	**44**
(276)	$C_6H_{10}I_2$, 1:3-diiodocyclohexane		
	C—I	2·12	**44**
(277)	$C_6H_{10}I_2$, 1:4-diiodocyclohexane		
	C—I	2·12	**44**

Table 1 (*cont.*)

C_6 (*cont.*)

(*278*)	$C_6H_{11}Cl$, chlorocyclohexane		
	C—C	1·54	*S.* **171**
	C_1—Cl_1	1·79	*S.* **139**
		1·76	*S.* **171**
	C_2—Cl_1	2·70	
	C_3—Cl_1	4·00	*S.* **139**
	C_4—Cl_1	4·64	
	Cl on bond orthogonal to main axis		*S.* **171**
(*279*)	C_6H_{12}, tetramethylethylene		
	C—C	1·54 (0·02)	**31**
	∠C—C—C	111·5° (2°)	
(*280*)	C_6H_{12}, cyclohexane		
	C—C	1·51 (0·05)	**6**
		1·53 (0·03)	**31**
		1·540 (0·015)	*S.* **124**
	'Chair' form		**31, 87, 124**
	Less symmetric forms may also be present		**124**
(*281*)	$C_6H_{12}N_4$, hexamethylenetetramine		
	C—N	1·47 (0·02)	**45**
		1·48 (0·01)	**178**
	∠C—N—C=∠N—C—N	109·5° (1°)	
(*282*)	$C_6H_{12}O_3$, paraldehyde		
	C—C	1·54 (0·02)	
	C—O	1·43 (0·02)	**6**
	Staggered hexagon		
(*283*)	$C_6H_{12}S$, cyclohexylmercaptan		
	C—S	1·87	*S.* **171**
	SH group on bond orthogonal to main axis of 'chair' form ring		
(*284*)	$C_6H_{12}S_3$, trithioacetaldehyde		
	C—S	1·81	*S.* **171**
	∠C—S—C	106·5°	
	∠S—C—S	114·5°	
	'Chair' form ring. Two isomers (α and β) differing in types of bond to which substituent groups are attached: α: κκε β: κκκ κ bonds are orthogonal to principal axis of ring ε bonds are parallel to trigonal axis of ring		
(*285*)	$C_6H_{13}NO$, 3-dimethylaminocyclobutanol		
	Cyclobutanol structure verified. Two isomers: *cis* is probably the form which is liquid at room temperature. Bond distances normal		**216**
(*286*)	C_6H_{14}, *n*-hexane		
	C—C	1·54 (0·05)	**6**
(*287*)	$C_6H_{15}N$, triethylamine		
	C—C	1·54 (0·02)	
	C—N	1·47 (0·02)	**213**
	∠C—C—N	113° (3°)	
	∠C—N—C	113° (3°)	
(*288*)	$C_6H_{18}Al_2$, hexamethyl dialuminium		
	C—Al	2·05 (0·05)	**83**
		2·01 (0·04)	**104**
	Al—Al	2·02 (0·06)	**83**
		2·20 (0·15)	**104**
	∠C—Al—Al	100° (5°)	**104**
	Ethane-like		**83, 104**
	Ethylenic		*Spec.* **126**

(*289*)	$C_6H_{18}O_3Si_3$, dimethyl cyclosiloxane trimer		
	C—Si	1·88 (0·04)	
	Si—O	1·66 (0·04)	*S.* **220**
	∠O—Si—O	115° (5°)	
	∠Si—O—Si	125° (5°)	
	∠C—Si—C	112° (6°)	
	Planar six-membered Si—O ring. CH_3 groups above and below plane of ring		
(*290*)	$C_6H_{18}Pb_2$, hexamethyl di-lead		
	C—Pb	2·25 (0·06)	
	Pb—Pb	2·88 (0·03)	**98**
	Ethane-like		
(*291*)	$C_6H_{18}Si_2$, hexamethyl disilane		
	C—Si	1·90 (0·02)	
	Si—Si	2·34 (0·10)	**104**
	∠C—Si—C	109° (4°)	
	Ethane-like		
(*292*)	$C_6I_4O_2$, iodo-anil		
	C—C	1·54	*S.* **197**
	C=C	1·36	
	C—I	2·09	**106**
		2·06	*S.* **197**
	C—O	1·14	*S.* **197**
	∠C=C—I	123·5°	**106**
		125°	*S.* **197**
	∠C—C—C	122°	*S.* **197**
(*293*)	C_6MoO_6, molybdenum hexacarbonyl		
	C—O	1·15 (0·05)	
	C—Mo	2·08 (0·04)	**41**
	Octahedral. Mo—C—O linear		
(*294*)	C_6O_6W, tungsten hexacarbonyl		
	C—O	1·13 (0·05)	
	C—W	2·06 (0·04)	**41**
	Octahedral. W—C—O linear		

C_8

(*295*)	C_8H_8, cyclo-octatetraene		
	C—C	$1{\cdot}42_5$ (average)	*S.* **199**
	∠C—C—C	120° (2°)	*S.* **166**, *S.* **199**
	Puckered ring, 'crown' model		
(*296*)	$C_8H_8Br_2$, 4:5-dibrom-*o*-xylene		
	C—C	1·40 (0·02)	
	C—Br	1·88 (0·02)	
	Br—Br	1·39	**110**
	∠C—C—Br	122° (2°)	
(*297*)	C_8H_{10}, *p*-xylene		
	C—C	1·40 (0·02)	
	C—CH_3	1·50 (0·01)	**6**
(*298*)	$C_8H_{12}O_2$, dimethyl ketene dimer		
	C—C	1·56	
	C—CH_3	1·54	
	C—C	1·22	**160**
	∠C—CO—C	93°	
	∠CH_3—C—CH_3	111°	
	Agree with above		*S.* **203**
(*299*)	C_8H_{18}, hexamethylethane		
	C—C	1·58 (0·03)	
	C—CH_3	1·54 (0·02)	**120**
	∠C—C—C	111° (2°)	

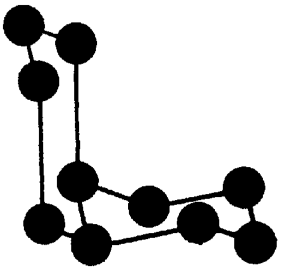
Table 1 (*cont.*)

C_9

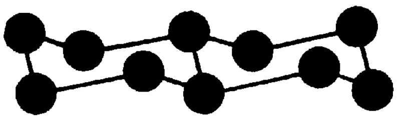
(*300*)	$C_9H_8Br_2$, 5:6-dibromohydrindene		
	C—C	1·42 (0·02)	
	C—Br	1·84 (0·02)	
	Br—Br	3·37	**110**
	∠C—C—Br	122° (2°)	
(*301*)	C_9H_{12}, mesitylene		
	C—C	1·40 (0·01)	**6**
	C—CH_3	1·50 (0·01)	**6**
		1·54 (0·01)	**31**

C_{10}

(*302*)	$C_{10}H_8$, naphthalene		
	C—C	1·397 average	**117**
	Planar		
(*303*)	$C_{10}H_{10}Br_2$, 6:7-dibromotetralin		
	C—C	1·42 (0·02)	
	C—Br	1·86 (0·02)	
	Br—Br	3·41 (0·02)	**110**
	∠C—C—Br	122° (2°)	
(*304*)	$C_{10}H_{16}$, adamantane		
	C—C	1·54 (0·04)	**191**
	Tetrahedral		
(*305*)	$C_{10}H_{18}$, decalin		
	Structures of isomers are:		



Cis



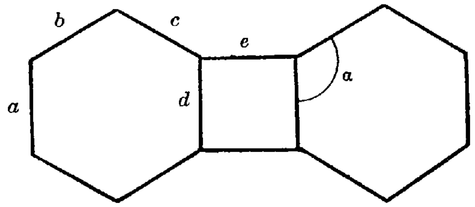
Trans

S. **171**

(*306*)	$C_{10}H_{20}Br_2$, 1:10-dibromodecane		
	Large variety of configurations		**24**

C_{12}

(*307*) $C_{12}H_8$, biphenylene



	a, b, c, d	1·41 (0·02) (average)	
	e	1·46 (0·05)	**142**
	α	121° (3°)	
(*308*)	$C_{12}H_8Br_2$, 3:3′-dibromodiphenyl		
	C—C	1·40	
	C—C′	1·49	
	C—Br	1·88	*S.* **198**
	Angle between ring planes is 54°		
(*309*)	$C_{12}H_8I_2O$, *p-p′*-diiododiphenyl ether		
	∠I—O—I	118° (3°)	**6**
(*310*)	$C_{12}H_{10}$, diphenyl		
	C—C	1·39 (0·02)	**145**
		1·40	*S.* **198**
	C—C′	1·52 (0·04)	**145**
		1·48	*S.* **198**
	C—H	1·06	
	Probably non-coplanar		**145**
	Angle between ring planes is 45°		*S.* **198**
(*311*)	$C_{12}H_{10}Cl_2N_2$, 3:3′-dichlorobenzidine		
	C—C	1·40	
	C—C′	1·50	
	C—Cl	1·73	*S.* **198**
	Rings probably non-coplanar		
(*312*)	$C_{12}H_{18}$, hexamethylbenzene		
	C—CH_3	1·54 (0·01)	**31**

C_{18}

(*313*)	$C_{18}H_{14}$, *o*-terphenyl		
	C—C	1·39 (0·02)	
	C—C′	1·52 (0·04)	**145**
	Non-coplanar. Attached rings roughly orthogonal to central ring		

C_{24}

(*314*)	$C_{24}H_{16}$, tetraphenylene		
	C—C	1·39 (0·02)	
	C—C′	1·52 (0·04)	**145**
	Cyclooctatetraene ring non-planar. Ring angles about 120°		

Table 2. *Compounds not containing carbon*

Group I

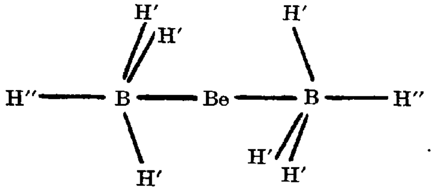
(315)	H_2O_2			
	O—O	1·48 (0·02)		**136**
		1·47 (0·02)		**137**
		1·48		*Spec.*
	O—H	1·01 (0·03)		**136**

Group I halides

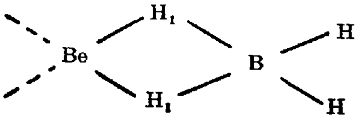
(316)	NaCl		
	Na—Cl	2·51 (0·03)	**29**
(317)	NaBr		
	Na—Br	2·64 (0·01)	**29**
(318)	NaI		
	Na—I	2·90 (0·02)	**29**
(319)	KCl		
	K—Cl	2·79 (0·02)	**29**
(320)	KBr		
	K—Br	2·94 (0·03)	**29**
(321)	KI		
	K—I	3·23 (0·04)	**29**
(322)	Cu_2Cl_2		
	Cu—Cl	2·13	**69**
(323)	Cu_2Br_2		
	Cu—Br	2·25	**69**
(324)	Cu_2I_2		
	Cu—I	2·40	**69**
(325)	RbCl		
	Rb—Cl	2·89 (0·01)	**29**
(326)	RbBr		
	Rb—Br	3·06 (0·02)	**29**
(327)	RbI		
	Rb—I	3·26 (0·02)	**29**
(328)	CsCl		
	Cs—Cl	3·06 (0·03)	**29**
(329)	CsBr		
	Cs—Br	3·14 (0·03)	**29**
(330)	CsI		
	Cs—I	3·41 (0·03)	**29**

Group II

(331)	BeB_2H_8		
	Be—B	1·66 (0·04)	
	B—H′	1·15 (0·05)	
	B—H″	1·19 (0·05)	**164**



A bridge model:



with B—H 1·22
Be—H_1 1·59
B—H 1·17
cannot be distinguished from the earlier model by electron diffraction **215**
See also, for *Spec.*, **184**

Group II halides
(All linear)

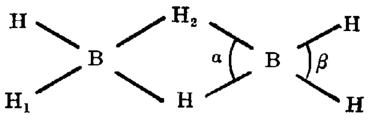
(332)	ZnI_2		
	Zn—I	2·42 (0·02)	**48**
(333)	$CdCl_2$		
	Cd—Cl	2·23 (0·03)	**112**
(334)	$CdBr_2$		
	Cd—Br	2·39 (0·03)	**112**
(335)	CdI_2		
	Cd—I	2·60 (0·02)	**48**
		2·56 (0·03)	**112**
(336)	$HgCl_2$		
	Hg—Cl	2·28 (0·05)	**6**
		2·34 (0·01)	**20**
		2·27 (0·03)	**88**
(337)	$HgBr_2$		
	Hg—Br	2·38 (0·05)	**6**
		2·44 (0·01)	**20**
(338)	HgI_2		
	Hg—I	2·55 (0·05)	**6**
		2·61 (0·01)	**20**
(339)	Hg_2Cl_2		
	Hg—Cl	2·23 (0·03)	**88**

Group III

(340)	BF_3		
	B—F	1·31	**14**
		1·30 (0·02)	**27**
		1·291	*Spec.*
	∠F—B—F	120° (3°)	**27**

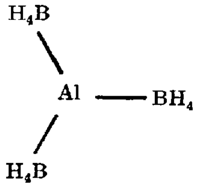
Table 2 (*cont.*)

(341)	BCl_3		
	B—Cl	1·73 (0·02)	**6**
		1·76 (0·02)	**20**
		1·73 (0·02)	**27**
	∠Cl—B—Cl	120° (3°)	**27**
(342)	BBr_3		
	B—Br	1·87 (0·02)	**27**
	∠Br—B—Br	120° (6°)	
(343)	B_2H_6		
	B—B	1·86 (0·04)	
	B—H	1·27 (0·03)	**12**
	Tetrahedral—ethane-like		
	Re-interpreted in terms of bridge model:		



with

	$B—H_1$	1·18	
	$B—H_2$	1·41	
	α	100°	
	β	120°	**119**
	Ethylene-like		*Spec.*
	For reviews of boron hydrides see **119** and **184**		
(344)	B_2H_7N		
	B—N	1·56 (0·03)	**33**
	B—H	1·20 approx.	
	∠B—N—B tetrahedral		
	Most likely structure is: $H_3B—NH—BH_3$ but another possibility is: $H_3B—NH_2—BH_2$		
(345)	$B_3H_6N_3$		
	B—N	1·47 (0·07)	**6**
		1·44 (0·02)	**33**
	Regular hexagon		**6, 33**
(346)	B_4H_{10}		
	B—B	1·84 (0·04)	
	B—H	1·28 (0·03)	**34, 119**
	Butane-like		
	For *Spec.* see **184**		
(347)	B_5H_9		
	B—B	1·76 (0·02)	
	B—H	1·17 (0·04)	**4, 119**
	Planar, 4 boron atoms in square; fifth atom coplanar with ring		
	∠H—B—H tetrahedral		
(348)	B_5H_{11}		
	B—B	1·81 (0·03)	
	B—H	1·26 (0·03)	**34, 119**
	Structure similar to that of pentane or *iso*-pentane. Cannot fix position of trivalent boron atom		
(349)	$B_{10}H_{24}$		
	B—B	1·80 (0·03)	
	B—H	1·29 (0·04)	**193**
	∠B—B—B	109° (3°)	
(350)	AlB_3H_{12}		
	Al—B	2·14 (0·02)	
	B—H	1·27 (0·04)	**80**
	∠B—Al—B	120° (5°)	
	∠Al—B—H	85° (3°)	
	Structure is:		



	Re-interpreted: a bridge model is equally consistent with electron diffraction data		**215**
	For *Spec.* see **184**		
(351)	Al_2Cl_6		
	Al—Al	3·41 (0·2)	**53**
	Al—Cl	2·06 (0·04)	
	Bridge structure		
(352)	Al_2Br_6		
	Al—Al	3·34 (0·1)	
	Al—Br	2·21 (0·04)	**53**
	Bridge structure		
(353)	Al_2I_6		
	Al—Al	3·24 (0·15)	
	Al—I	2·53 (0·04)	**53**
	Bridge structure		

Gallium and indium halides

(Results of Brode (**82**) corrected by Stevenson & Schomaker (**132**))

(354)	$GaCl_3$		
	Ga—Cl	2·22	
(355)	$GaBr_3$		
	Ga—Br	2·34	
(356)	GaI_3		
	Ga—I	2·50	
(357)	$InCl_3$		
	In—Cl	2·46	
(358)	$InBr_3$		
	In—Br	2·58	
(359)	InI_3		
	In—I	2·76	
(360)	TlCl		
	Tl—Cl	2·55 (0·03)	**6**
(361)	TlBr		
	Tl—Br	2·68 (0·03)	**6**
(362)	TlI		
	Tl—I	2·87 (0·03)	**6**
(363)	Withdrawn		

Table 2 (*cont.*)

Group IV

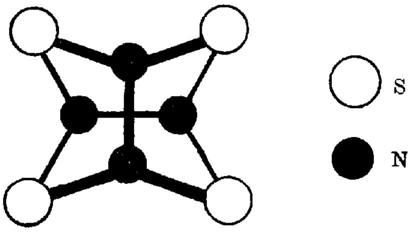
(All compounds in this group are tetrahedral unless otherwise stated.)

(364)	$SiBr_2F_2$		
	Si—Br	2·16 (0·02)	
	F—Br	3·08 (0·04)	
	Br—Br	3·56 (0·05)	
	F—F	2·35 (0·15)	**130**
	∠Br—Si—Br	111° (3°)	
	∠Br—Si—F	111·3° (3°)	
	∠F—Si—F	99° (10°)	
(365)	$SiClF_3$		
	Si—F	1·55 (0·02)	
	Cl—F	2·94 (0·03)	
	Si—Cl	2·03 (0·03)	
	F—F	2·50 (0·05)	**146**
(366)	SiF_4		
	Si—F	1·54 (0·02)	**6**
		1·54 (0·02)	**14**
(367)	SiH_3Cl		
	Si—Cl	2·06 (0·05)	**40**
(368)	SiH_2Cl_2		
	Si—Cl	2·02 (0·03)	**40**
	∠Cl—Si—Cl	110° (1°)	
(369)	$SiHCl_3$		
	Si—Cl	2·00 (0·03)	**6**
		2·05 (0·03)	**9**
		2·01 (0·03)	**39**
		1·98 (0·02)	*X*, **163**
	∠Cl—Si—Cl	110° (3°)	**6**
		110° (1°)	**39**
(370)	$SiBrCl_3$		
	Si—Cl	2·05 (0·05)	
	Si—Br	2·19 (0·05)	
	Br—Cl	3·41 (0·03)	**21**
(371)	$SiCl_4$		
	Si—Cl	2·02 (0·02)	**6**
(372)	$SiHBr_3$		
	Si—Br	2·19 (0·05)	**32**
		2·16 (0·03)	**130**
	Br—Br	3·63	**32**
		3·55 (0·02)	**130**
(373)	$SiBr_4$		
	Si—Br	2·14 (0·02)	**111**
		2·15 (0·02)	**130**
	Br—Br	3·51 (0·03)	**130**
(374)	SiI_4		
	Si—I	2·43 (0·02)	**111**
(375)	Si_2H_6		
	Si—Si	2·32 (0·03)	**39**
	Si—H	1·47 (0·03)	
(376)	Si_2Cl_6		
	Si—Si	2·32 (0·06)	
	Si—Cl	2·00 (0·05)	**39**
	Trans		
(377)	$TiCl_4$		
	Ti—Cl	2·21 (0·05)	**6**
		2·18 (0·04)	**111**
(378)	$TiBr_4$		
	Ti—Br	2·31 (0·02)	**111**
(379)	$GeCl_4$		
	Ge—Cl	2·08 (0·03)	**6**
(380)	$GeBr_4$		
	Ge—Br	2·32	**55**
		2·34	**92**
		2·29 (0·02)	**111**
(381)	GeI_4		
	Ge—I	2·47	**23**
		2·48	**46**
		2·50 (0·03)	**111**
(382)	Ge_2H_6		
	Ge—Ge	2·41 (0·02)	**54**
(383)	Ge_3H_8		
	Ge—Ge	2·41 (0·02)	**54**
(384)	$ZrCl_4$		
	Zr—Cl	2·33 (0·05)	**111**
(385)	$SnCl_2$		
	Sn—Cl	2·42 (0·02)	**112**
	∠Cl—Sn—Cl	95° *ass.*	
(386)	$SnBr_2$		
	Sn—Br	2·55 (0·02)	**112**
	∠Br—Sn—Br	95° *ass.*	
(387)	SnI_2		
	Sn—I	2·73 (0·02)	**112**
	∠I—Sn—I	95° *ass.*	
(388)	$SnCl_4$		
	Sn—Cl	2·30 (0·03)	**6**
(389)	$SnBr_4$		
	Sn—Br	2·44 (0·02)	**111**
(390)	SnI_4		
	Sn—I	2·64	**46**
		2·64 (0·04)	**111**
(391)	$PbCl_2$		
	Pb—Cl	2·46 (0·02)	**112**
	∠Cl—Pb—Cl	95° *ass.*	
(392)	$PbBr_2$		
	Pb—Br	2·60 (0·03)	**112**
	∠Br—Pb—Br	95° *ass.*	
(393)	PbI_2		
	Pb—I	2·79 (0·02)	**112**
	∠I—Pb—I	95° *ass.*	
(394)	$PbCl_4$		
	Pb—Cl	2·43 (0·04)	**111**
(395)	$ThCl_4$		
	Th—Cl	2·61 (0·03)	**111**

Table 2 (*cont.*)

Group V

(*396*)	NO_2		
	N—O	1·21 (0·02)	**89, 90**
		1·28 (0·03)	*Spec.* **85**
	∠O—N—O	130° (2°)	**89, 90**
		154° (4°)	*Spec.* **85**
(*397*)	NOCl		
	N—O	1·14 (0·02)	
	N—Cl	1·95 (0·01)	
	O—Cl	2·65 (0·01)	**25**
	∠Cl—N—O	116° (2°)	
(*398*)	NOBr		
	N—O	1·15 (0·04)	
	N—Br	2·14 (0·02)	
	O—Br	2·85 (0·02)	**25**
	∠Br—N—O	117° (3°)	
(*399*)	HNO_3		
	N—O	1·22 (0·02)	
	N—O′	1·41 (0·02)	**89, 90**
	∠O—N—O	130° (5°)	
	∠O—N—O′	115° (2·5°)	
	Planar		
(*400*)	NF_3		
	N—F	1·37 (0·02)	**209**
	∠F—N—F	102·5° (1·5°)	
(*401*)	N_2		
	N—N	1·095 (0·008)	*S.* **181**
		1·098	*Spec.*
(*402*)	N_2O		
	N—N—O r_1 r_2		
	r_1+r_2	2·38 (0·05)	**6**
		2·32 (0·02)	**129**
	$0{\cdot}925 < r_1/r_2 < 1{\cdot}08$		**129**
	r_1	1·126	
	r_2	1·191	*Spec.* **168**
	Linear		
(*403*)	N_2O_4		
	N—N	1·6–1·7	**6**
(*404*)	N_2O_5		
	N—O	1·18	
	N—O′	1·3–1·4	**6**
(*405*)	N_2F_2		
	N—N	1·25 (0·04)	
	N—F	1·44 (0·04)	**167**
	Cis and *trans* isomers		
	∠N—N—F	115° (5°)	
(*406*)	N_2H_4		
	N—N	1·47 (0·02)	
	N—H	1·04 (0·06)	**137**
	∠H—N—N	108° (10°)	
(*407*)	N_3H		
	N_1—N_2	1·136 (0·01)	**129**
		1·128	*Spec.*
	N_2—N_3	1·247 (0·01)	**129**
		1·241	*Spec.*
	N_3 group linear, *ass.*		**129**
(*408*)	N_4S_4		
	N—S	1·74	**138**
		1·62 (0·02)	**147**
	S—S	2·63	**138**
		2·69	**147**
	N—N	1·47	**138**
	∠S—N—S	112°	**147**
	∠N—S—N	106°	**147**
		75·9°	**138**
	Various models tried: 'cradle' model preferred		**147**
	Best model is:		**138**



(*409*)	PF_3		
	P—F	1·52 (0·04)	**6**
		1·546 (0·008)	*Spec.* **189**
	∠F—P—F	104° (4°)	**6**
		104° (3°) *ass.*	*Spec.* **189**
(*410*)	$PFCl_2$		
	P—F	1·55 (0·05)	
	P—Cl	2·02 (0·03)	**39**
	∠F—P—Cl = ∠Cl—P—Cl	102° (3°)	
(*411*)	PCl_3		
	P—Cl	2·00 (0·02)	**6**
		2·03 (0·02)	**218**
	∠Cl—P—Cl	101° (2°)	**6**
		100·5° (1·5°)	
(*412*)	PBr_3		
	P—Br	2·23 (0·01)	**20**
		2·18 (0·03)	**218**
	∠Br—P—Br	100° (2°)	**20**
		101·5° (1·5°)	**218**
(*413*)	PI_3		
	P—I	2·52 (0·01)	**20**
		2·46	**46**
		2·43 (0·04)	**218**
	∠I—P—I	98° (4°)	**20**
		100°	**46**
		102° (2°)	**218**
(*414*)	PF_5		
	P—F	1·54	**14**
		1·57 (0·02)	**39**
	Trigonal bipyramid		
(*415*)	PF_3Cl_2		
	P—F	1·59 (0·03)	
	P—Cl	2·05 (0·03)	
	F—Cl	2·59 (0·03)	**39**
	Trigonal bipyramid		
(*416*)	PCl_5		
	P—Cl	2·10, 2·25	**56**
		2·07, 2·01	**92**

Table 2 (*cont.*)

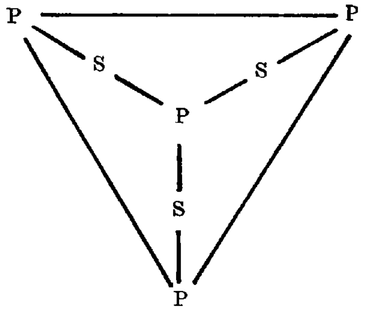
Group V (*cont.*)

(417)	POF$_3$		
	P—F	1·52 (0·02)	
	P—O	1·56 (0·03)	
	F—F	2·44 (0·02)	39
	∠F—P—F	107° (2°)	
(418)	POF$_2$Cl		
	P—F	1·51 (0·03)	
	P—O	1·55 (0·03)	
	P—Cl	2·01 (0·04)	39
	∠F—P—F	106° (3°)	
	∠F—P—Cl	106° (3°)	
(419)	POFCl$_2$		
	P—F	1·50 (0·03)	
	P—Cl	1·99 (0·04)	
	P—O	1·54 (0·03)	39
	∠F—P—Cl	106° (3°)	
	∠Cl—P—Cl	106° (3°)	
(420)	POCl$_3$		
	P—Cl	2·02 (0·03)	
	P—O	1·58	
	Cl—Cl	3·22 (0·03)	39
	∠Cl—P—Cl	106° (1°)	
(421)	POBr$_3$		
	P—Br	2·06 (0·03)	
	P—O	1·41 (0·07)	148
	∠Br—P—Br	108° (3°)	
(422)	PSF$_3$		
	P—F	1·51 (0·02)	
	P—S	1·85 (0·02)	75
	∠F—P—F	99·5° (2°)	
	∠F—P—S	118° (2°)	
(423)	PSCl$_3$		
	P—Cl	2·01 (0·02)	
	P—S	1·94 (0·03)	59
(424)	PSF$_2$Br		
	P—F	1·45 (0·08)	
	P—Br	2·14 (0·04)	
	P—S	1·87 (0·05)	148
	∠F—P—Br	106° (3°)	
(425)	PSFBr$_2$		
	P—F	1·50 (0·10)	
	P—Br	2·18 (0·03)	
	P—S	1·87 (0·05)	148
	∠Br—P—Br	100° (3°)	
(426)	PSBr$_3$		
	P—Br	2·13 (0·03)	
	P—S	1·89 (0·06)	148
	∠Br—P—Br	106° (3°)	
(427)	P$_3$N$_3$Cl$_6$		
	P—Cl	1·97 (0·03)	
	P—N	1·65 (0·03)	134
	Benzene-like ring		
(428)	P$_4$		
	P—P	2·21 (0·02)	6
	Tetrahedral		

(429) P$_4$S$_3$

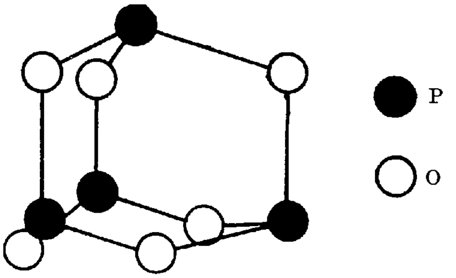
Two important distances at 2·15 and 3·38 *S.* **108**

Structure is:



(430)	P$_4$O$_6$		
	P—O	1·67 (0·03)	28
		1·65 (0·02)	45
	P—P	3·00 (0·05)	28
		2·95 (0·03)	45

Structure is:



(431)	P$_4$O$_6$S$_4$		
	P—O	1·61 (0·02)	
	P—S	1·85 (0·02)	
	P—P	2·85 (0·03)	78
	∠P—O—P	123·5° (1°)	
	∠O—P—O	101·5° (1°)	
	∠O—P—S	116·5° (1°)	

(432) P$_4$O$_8$

Gives electron diffraction pattern similar to that of P$_4$O$_{10}$ **28**

(433)	P$_4$O$_{10}$		
	P—O	1·62 (0·02)	
	P—O′	1·39 (0·02)	
	P—P	2·84 (0·03)	45
	∠O—P—O	101·5° (1°)	
	∠O—P—O′	116·5° (1°)	
	∠P—O—P	123·5° (1°)	

Structure is:

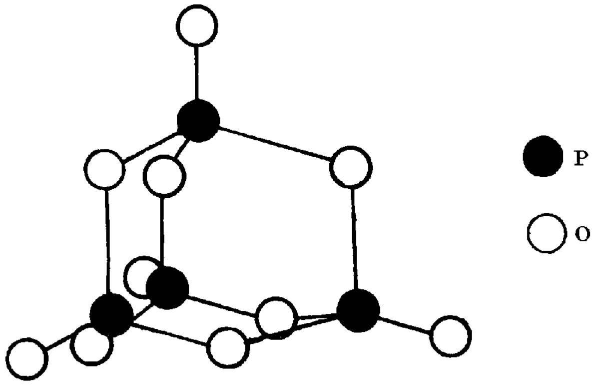


Table 2 (*cont.*)

(*434*)	$VOCl_3$		
	V—O	1·56 (0·04)	
	V—Cl	2·12 (0·03)	
	Cl—O	3·00 (0·04)	
	Cl—Cl	3·50 (0·03)	**51**
	∠Cl—V—Cl	111·2° (2°)	
	∠Cl—V—O	108·1° (2°)	
(*435*)	VCl_4		
	V—Cl	2·03 (0·02)	**153**
	Tetrahedral		
(*436*)	AsF_3		
	As—F	1·72 (0·02)	**6**
		1·712	*Spec.* **186**
	Regular pyramid		
(*437*)	$AsCl_3$		
	As—Cl	2·16 (0·03)	**6**
		2·17 (0·02)	**218**
	∠Cl—As—Cl	103° (3°)	**6**
		99° (2°)	
(*438*)	$AsBr_3$		
	As—Br	2·36 (0·02)	**20**
		2·31	**46**
		2·33 (0·02)	**218**
	∠Br—As—Br	100° (2°)	**20**
		101·5°	**46**
		100·5° (1·5°)	**218**
(*439*)	AsI_3		
	As—I	2·58 (0·01)	**20**
		2·51	**46**
		2·541	*S.* **105**
		2·55 (0·03)	**218**
	∠I—As—I	100° (2°)	**20**
		102·5°	**46**
		98·5°	*S.* **105**
		101° (1·5°)	**218**
(*440*)	As_4		
	As—As	2·44 (0·03)	**6**
	Tetrahedral		
(*441*)	As_4S_4		
	As—S	2·23 (0·02)	
	As—As	2·49 (0·04)	**147**
	∠As—S—As	101° (4°)	
	'Cradle' model preferred		
(*442*)	As_4O_6		
	As—O	1·80 (0·02)	**45**
		1·78 (0·02)	**147**
	As—As	3·20 (0·05)	**28**
		3·20 (0·03)	**45**
		3·20 (0·02)	**147**
	∠As—O—As	126° (3°)	**45**
		128° (2°)	**147**
	∠O—As—O	100° (1·5°)	**45**
		99° (2°)	**147**
(*443*)	As_4S_6		
	As—S	2·25 (0·02)	**147**
	∠As—S—As	100° (2°)	
	∠S—As—S	114° (2°)	
	Same structure as As_4O_6		
(*444*)	$NbCl_5$		
	Nb—Cl	2·29 (0·03)	**96**
	Trigonal bipyramid		
(*445*)	$NbBr_5$		
	Nb—Br	2·46 (0·03)	**96**
(*446*)	$SbCl_3$		
	Sb—Cl	2·37 (0·02)	**20**
		2·37 (0·02)	**218**
	∠Cl—Sb—Cl	104° (2°)	**20**
		96° (4°)	**218**
(*447*)	$SbBr_3$		
	Sb—Br	2·52 (0·02)	**20**
		2·47	**46**
		2·51 (0·02)	**218**
	∠Br—Sb—Br	96° (2°)	**20**
		98°	**46**
		97° (2°)	**218**
(*448*)	SbI_3		
	Sb—I	2·75 (0·02)	**20**
		2·74	**46**
		2·67 (0·03)	**218**
	∠I—Sb—I	98° (2°)	**20**
		99° (1°)	**218**
(*449*)	$SbCl_5$		
	Sb—Cl	2·43, 2·31	**92**
	Trigonal bipyramid		
(*450*)	$TaCl_5$		
	Ta—Cl	2·30 (0·02)	**96**
	Trigonal bipyramid		
(*451*)	$TaBr_5$		
	Ta—Br	2·45 (0·03)	**96**
	Trigonal bipyramid		
(*452*)	$BiCl_3$		
	Bi—Cl	2·48 (0·02)	**97**
	∠Cl—Bi—Cl	100° (6°)	
(*453*)	$BiBr_3$		
	Bi—Br	2·63 (0·02)	**97**
	∠Br—Bi—Br	100° (4°)	

Group VI

(*454*)	O_3		
	O—O	1·26 (0·02)	**141**
		1·0 approx.	*Spec.* **155**
	∠O—O—O	127° (3°)	**141**
		34°	*Spec.* **155**
	Isosceles triangle For earlier *Spec.* see **141**		
(*455*)	SCl_2		
	S—Cl	1·99 (0·03)	**51**
		2·00 (0·02)	**58**
	∠Cl—S—Cl	101° (4°)	**51**
		103° (3°)	**58**

Table 2 (*cont.*)

Group VI (*cont.*)

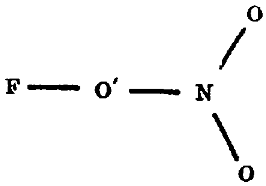
(456)	SOCl$_2$		
	S—O	1·45 (0·02)	
	S—Cl	2·07 (0·03)	
	Cl—O	2·84 (0·03)	**51**
	∠O—S—Cl	106° (1°)	
	∠Cl—S—Cl	114° (2°)	
	Pyramidal		
(457)	SOBr$_2$		
	S—Br	2·27 (0·02)	
	Br—O	3·05 (0·03)	**99**
	∠Br—S—Br	96° (2°)	
	Pyramidal		
(458)	SO$_2$		
	S—O	1·45 (0·02)	**6**
		1·43 (0·01)	**93**
		1·43$_3$	*Spec.* **169**
	∠O—S—O	124° (15°)	**6**
		120° (5°)	**93**
		119°	*Spec.* **169**
(459)	SO$_3$		
	S—O	1·43 (0·02)	
	O—O	2·48 (0·03)	**51**
	∠O—S—O	120° (2°)	
(460)	SO$_2$F$_2$		
	S—O	1·43 (0·02)	
	S—F	1·56 (0·02)	
	F—O	2·37 (0·02)	**75**
	∠F—S—O	105° (2°)	
	∠F—S—F	100° (8°)	
	∠O—S—O	130° (10°)	
(461)	SO$_2$Cl$_2$		
	S—O	1·43 (0·02)	
	S—Cl	1·99 (0·02)	
	O—O	2·48 (0·10)	
	Cl—O	2·76 (0·03)	
	Cl—Cl	3·28 (0·10)	**51**
	∠Cl—S—O	106° (2°)	
	∠Cl—S—Cl	111° (2°)	
	∠O—S—O	119·5° (5°)	
(462)	SF$_6$		
	S—F	1·58 (0·03)	**6**
	Octahedral		
(463)	S$_2$		
	S—S	1·92 (0·03)	**10**
		1·89	*Spec.*
(464)	S$_2$H$_2$		
	S—S	2·05 (0·02)	**58**
(465)	S$_2$Cl$_2$		
	S—Cl	1·98 (0·05)	**6**
		1·99 (0·03)	**51**
		2·01 (0·07)	**206**
	S—S	2·04 (0·05)	**6**
		2·05 (0·03)	**51**
		2·07 (0·10)	**206**
	∠Cl—S—S	103° (2°)	**51**
		104·5° (2·5°)	**206**
	Cis configuration. Angle between S—S—Cl planes is 92° (12°)		**206**

(466)	S$_8$		
	S—S	2·08 (0·02)	**22**
		2·07 (0·02)	**147**
	Puckered ring		
(467)	CrO$_2$Cl$_2$		
	Cr—O	1·57 (0·03)	
	Cr—Cl	2·12 (0·02)	
	O—O	2·49 (0·10)	
	Cl—O	3·03 (0·03)	
	Cl—Cl	3·54 (0·05)	**51**
	∠O—Cr—O	105° (4°)	
	∠Cl—Cr—Cl	113° (3°)	
	∠Cl—Cr—O	109·5° (3°)	
(468)	SeO$_2$		
	Se—O	1·61 (0·03)	**52**
(469)	SeCl$_4$		
	Se—Cl	2·13 (0·04)	**111**
	Tetrahedral		
(470)	SeF$_6$		
	Se—F	1·68 (0·03)	**6**
	Octahedral		
(471)	Se$_2$		
	Se—Se	2·19 (0·03)	**88**
		2·16	*Spec.*
(472)	Se$_6$		
	Se—Se	2·32	**22**
	Puckered ring		
(473)	MoO$_2$Cl$_2$		
	Mo—Cl	2·28	
	Mo—O	1·75	**116**
	∠Cl—Mo—Cl	113° (7°)	
	∠O—Mo—Cl	108° (7°)	
	∠O—Mo—O	109·5° *ass.*	
(474)	MoCl$_5$		
	Mo—Cl	2·27 (0·02)	**43**
	Trigonal bipyramid		
(475)	MoF$_6$		
	Mo—F	1·6 approx.	**14**
(476)	TeCl$_2$		
	Te—Cl	2·36 (0·03)	**6**
	Linear ?		
(477)	TeBr$_2$		
	Te—Br	2·49 (0·03)	**6**
		2·51 (0·02)	**175**
	∠Br—Te—Br	98° (3°)	**175**
(478)	TeCl$_4$		
	Te—Cl	2·33 (0·02)	
	Cl—Cl	3·37 (0·06)	**100**
	∠Cl—Te—Cl	93° (3°)	
	Distorted trigonal bipyramid		
(479)	TeF$_6$		
	Te—F	1·82 (0·03)	**6**
	Octahedral		
(480)	Te$_2$		
	Te—Te	2·59 (0·02)	**88**

Table 2 (*cont.*)

(*481*)	WF_6		
	W—F	1·64, 1·84	
		2·00	**14**
(*482*)	WCl_6		
	W—Cl	2·26 (0·02)	**43**
		2·28 (0·02)	**216**
	Octahedral		**43, 216**
(*483*)	UF_6		
	U—F	1·78, 1·99, 2·17	**14**
		1·86, 2·16	*S.* **201**
	Distorted octahedron, with base edges about 2·88		*S.* **201**

Group VII

(*484*)	$(HF)_n$		
	F—H	1·00 (0·06)	
	F—H′	1·55 (0·06)	
	F—F	2·55 (0·03)	**61**
	Zig-zag chain. Angle 140° (5°)		
(*485*)	FNO_3		
	 		
	N—O	1·29 (0·05)	
	N—O′	1·39 (0·05)	
	F—O′	1·42 (0·05)	**30**
	∠O—N—O	125° (5°)	
	∠N—O′—F	105° (5°)	
(*486*)	F_2		
	F—F	1·45 (0·05)	**38**
		1·435 (0·01)	**114**
(*487*)	F_2O		
	F—O	1·41 (0·05)	**6**
	∠O—F—O	100° (3°)	
(*488*)	ClF		
	Cl—F	1·63 (0·01)	**219**
(*489*)	ClF_3		
	Cl—F	1·69	**219**
	∠F—Cl—F	86·5° (1·5°)	
(*490*)	ClO_2		
	Cl—O	1·53 (0·02)	**6**
	∠O—Cl—O	137° (15°)	
(*491*)	Cl_2		
	Cl—Cl	2·01 (0·03)	**6**
		2·00 (0·02)	**10**
		1·993	*Spec.*
(*492*)	Cl_2O		
	Cl—O	1·68 (0·03)	**6**
	∠Cl—O—Cl	115° (4°)	
(*493*)	Br_2		
	Br—Br	2·28 (0·02)	**6**
		2·279	*S.* **105**
(*494*)	I_2		
	I—I	2·65 (0·10)	**6**
		2·66 (0·01)	**29**
		2·674	*S.* **105**
(*495*)	ICl		
	I—Cl	2·30 (0·03)	**6**
		2·324	*Spec.*
(*496*)	IF_5		
	I—F	2·57	**14**

Group VIII

(*497*)	Fe_2Cl_6		
	Fe—Cl	2·17	*S.* **140**
	Bridge structure		
(*498*)	OsO_4		
	Os—O	1·66 (0·05)	**6**
(*499*)	OsF_8		
	Os—F	2·52 (0·10)	**6**
	Archimedes antiprism ?		
(*500*)	RuO_4		
	Ru—O	1·66, 1·74	**37**
	Rhomboid		

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The numbers in parentheses at the end of each entry refer to the compounds studied in each paper.

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B. California Institute of Technology (received from Prof. L. Pauling and Prof. V. Schomaker).

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Short Communications

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 500 words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible; and proofs will not generally be submitted to authors. Publication will be quicker if the contributions are without illustrations.

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Corrigenda: The accuracy of electron-density maps in X-ray analysis with special reference to dibenzyl.

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(*Received* 19 *July* 1949)

The estimated standard deviation of atomic co-ordinates in non-centrosymmetric structures was originally stated (Cox & Cruickshank 1948) to be $\sqrt{2}$ times the corresponding deviation in centrosymmetric structures; a revised calculation (Cruickshank, 1949*a*) gave this factor as unity; we shall revise the discussion again, now reaching by two methods a factor of 2.

The authors's papers (Cruickshank, 1949*a*, *b*, 1950) will be referred to as A, B and C; the notation of these papers will be used.