BOND LENGTHS AND ANGLES IN GAS-PHASE MOLECULES

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Internuclear distances and bond angles are represented in units of Å (1 Å = 10^{-10} m) and degrees, respectively. The same but inequivalent atoms are discriminated by subscripts a, b, etc. In some molecules ax for axial and eq for equatorial are also used. All measurements were made in the gas phase. The methods used are abbreviated as follows. UV: ultraviolet (including visible) spectroscopy; IR: infrared spectroscopy; R: Raman spectroscopy; MW: microwave spectroscopy; ED: electron diffraction; NMR: nuclear magnetic resonance; LMR: laser magnetic resonance; EPR: electron paramagnetic resonance; MBE: molecular beam electric resonance. If two methods were used jointly for structure determination, they are listed together, as (ED, MW). If the numerical values listed refer to the equilibrium values, they are specified by r_e and θ_e. In other cases the listed values represent various average values in vibrational states; it is frequently the case that they represent the r_s structure derived from several isotopic species for MW or the r_g structure (i.e., the average internuclear distances at thermal equilibrium) for ED. These internuclear distances for the same atom pair with different definitions may sometimes differ as much as 0.01 Å. Appropriate comments are made on the symmetry and conformation in the equilibrium structure.

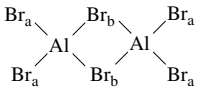
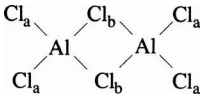
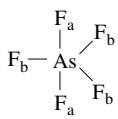
In general, the numerical values listed in the following tables contain uncertainties in the last digits. However, for certain molecules such as diatomic molecules, with experimental uncertainties of the order of 10^{-5} Å or smaller, numerical values are listed to four decimal places.

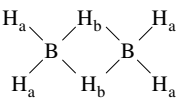
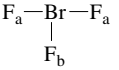
References

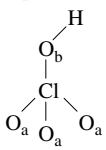
1. L. E. Sutton, Ed., *Tables of Interatomic Distances and Configuration in Molecules and Ions,* The Chemical Society Special Publication, No. 11, 18, The Chemical Society (London) (1958, 1965).
2. K.-H. Hellwege, Ed., *Landolt-Börnstein Numerical Data and Functional Relations in Science and Technology,* New Series, II/7, J. H. Callomon, E. Hirota, K. Kuchitsu, W. J. Lafferty, A. G. Maki, C. S. Pote, with assistance of I. Buck and B. Starck, *Structure Data of Free Polyatomic Molecules*, Springer-Verlag (1976).
3. K. P. Huber and G. Herzberg, *Molecular Spectra and Molecular Structure IV. Constants of Diatomic Molecules,* Van Nostrand Reinhold Co., London (1979).
4. B. Starck, *Microwave Catalogue and Supplements.*
5. B. Starck, *Electron Diffraction Catalogue and Supplements.*

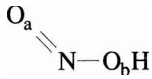
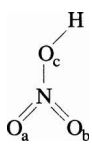
STRUCTURES OF ELEMENTS AND INORGANIC COMPOUNDS

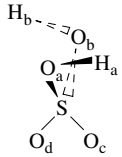
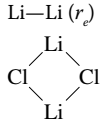
Compounds are arranged in alphabetical order by their chemical formulas (Lengths in Å and Angles in Degrees)

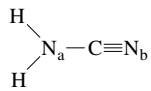
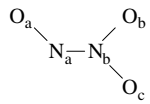
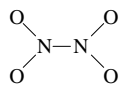
Compound	Structure					Method
AgBr	Ag—Br (r_e)	2.3931				MW
AgCl	Ag—Cl (r_e)	2.2808				MW
AgF	Ag—F (r_e)	1.9832				MW
AgH	Ag—H (r_e)	1.617				UV
AgI	Ag—I (r_e)	2.5446				MW
AgO	Ag—O (r_e)	2.0030				UV
AlBr	Al—Br (r_e)	2.295				UV
AlCl	Al—Cl (r_e)	2.1301				MW
AlF	Al—F (r_e)	1.6544				MW
AlH	Al—H (r_e)	1.6482				UV
AlI	Al—I (r_e)	2.5371				MW
AlO	Al—O (r_e)	1.6176				UV
Al_2Br_6				$Al—Br_a$	2.22	ED
				$Al—Br_b$	2.38	
				$\angle Br_bAlBr_b$	82	
				$\angle Br_aAlBr_a$	118	
				(D_{2h})		
Al_2Cl_6				$Al—Cl_a$	2.04	ED
				$Al—Cl_b$	2.24	
				$\angle Cl_bAlCl_b$	87	
				$\angle Cl_aAlCl_a$	122	
				(D_{2h})		
$AsBr_3$	As—Br	2.324		$\angle BrAsBr$	99.6	ED
$AsCl_3$	As—Cl	2.165		$\angle ClAsCl$	98.6	ED, MW
AsF_3	As—F	1.710		$\angle FAsF$	95.9	ED, MW
AsF_5		$As—F_a$	1.711	$As—F_b$	1.656	
				(D_{3h})		

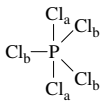
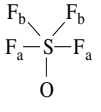
Compound	Structure							Method
AsH_3	As—H (r_e)		1.511			∠HAsH (θ_e)	92.1		MW, IR
AsI_3	As—I		2.557			∠IAsI	100.2		ED
AuH	Au—H (r_e)		1.5237						UV
BBr_3	B—Br		1.893			(D_{3h})			ED
BCl_3	B—Cl		1.742			(D_{3h})			ED
BF	B—F (r_e)		1.2626						UV
BF_2H	B—H	1.189		B—F	1.311		∠FBF	118.3	MW
BF_2OH	B—F	1.32		B—O	1.34		O—H	0.941	MW
	∠FBF	118		∠FBO	123		∠BOH	114.1	
BF_3	B—F		1.313			(D_{3h})			ED, IR
BH	B—H (r_e)		1.2325						UV
BH_3PH_3	B—P	1.937		B—H	1.212		P—H	1.399	MW
	∠PBH	103.6		∠BPH	116.9		∠HBH	114.6	
	∠HPH	101.3		staggered form					
BI_3	B—I		2.118			(D_{3h})			ED
BN	B—N (r_e)		1.281						UV
BO	B—O (r_e)		1.2045						EPR
BO_2	B—O		1.265			linear			UV
BS	B—S		1.6091						UV
B_2H_6						B—H_a	1.19		IR, ED
						B—H_b	1.33		
						B···B	1.77		
						∠H_aBH_a	122		
						∠H_bBH_b	97		
$B_3H_3O_3$	B—O		1.376			∠BOB≅∠OBO	120		ED
$B_3H_6N_3$	B—N	1.435		B—H	1.26		N—H	1.05	ED
	∠NBN	118		∠BNB	121		(C_2)		
BaH	Ba—H (r_e)		2.2318						UV
BaO	Ba—O (r_e)		1.9397						MW
BaS	Ba—S (r_e)		2.5074						MBE
BeF	Be—F (r_e)		1.3609						UV
BeH	Be—H (r_e)		1.3431						UV
BeO	Be—O (r_e)		1.3308						UV
BiBr	Bi—Br (r_e)		2.6095						MW
$BiBr_3$	Bi—Br		2.63			∠BrBiBr	90	(C_{3v})	ED
BiCl	Bi—Cl (r_e)		2.4716						MW
$BiCl_3$	Bi—Cl		2.423			∠ClBiCl	100	(C_{3v})	ED
BiF	Bi—F (r_e)		2.0516						MW
BiH	Bi—H (r_e)		1.805						UV
BiI	Bi—I (r_e)		2.8005						MW
BiO	Bi—O (r_e)		1.934						UV
BrCN	C—N (r_e)		1.157			C—Br (r_e)	1.790		IR
BrCl	Br—Cl (r_e)		2.1361						MW
BrF	Br—F (r_e)		1.7590						MW
BrF_3				Br—F_a	1.810		Br—F_b	1.721	MW
				∠F_aBrF_b	86.2		(C_{2v})		
BrF_5	Br—F (average)		1.753						ED, MW
	(Br—F_{eq}) – (Br—F_{ax}) = 0.069								
	∠$F_{ax}BrF_{eq}$		85.1			(C_{4v})			
BrO	Br—O (r_e)		1.7172						MW
Br_2	Br—Br (r_e)		2.2811						R
CBr_4	C—Br		1.935			(T_d)			ED
CCl	C—Cl		1.6512						UV
$CClF_3$	C—Cl	1.752		C—F	1.325		∠FCF	108.6	ED, MW
CCl_3F	C—Cl	1.754		C—F	1.362		∠ClCCl	111	MW
							(C_{3v})		
CCl_4	C—Cl		1.767			(T_d)			ED
CF	C—F (r_e)		1.2718						EPR
CF_3I	C—I	2.138		C—F	1.330		∠FCF	108.1	ED, MW
CF_4	C—F		1.323			(T_d)			ED

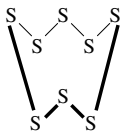
Compound	Structure							Method
CH	C—H (r_e)	1.1199						UV
CI_4	C—I	2.15			(T_d)			ED
CN	C—N (r_e)	1.1718						MW
CO	C—O (r_e)	1.1283						MW
$COBr_2$	C—O	1.178			C—Br	1.923		ED, MW
	∠BrCBr	112.3						
COClF	C—F	1.334	C—O	1.173		C—Cl	1.725	ED, MW
	∠FCCl	108.8	∠ClCO	127.5				
$COCl_2$	C—O	1.179			C—Cl	1.742		ED, MW
	∠ClCCl	111.8						
COF_2	C—F	1.3157			C—O	1.172		ED, MW
	∠FCF	107.71						
CO_2	C—O (r_e)	1.1600						IR
CP	C—P (r_e)	1.562						UV
CS	C—S (r_e)	1.5349						MW
CS_2	C—S (r_e)	1.5526						IR
C_2	C—C (r_e)	1.2425						UV
C_3O_2	C—O	1.163			C—C	1.289		ED
	linear (large-amplitude bending vibration)							
CaH	Ca—H (r_e)	2.002						UV
CaO	Ca—O (r_e)	1.8221						UV
CaS	Ca—S (r_e)	2.3178						UV
CdH	Cd—H (r_e)	1.781						EPR
$CdBr_2$	Cd—Br	2.35			linear			ED
$CdCl_2$	Cd—Cl	2.24			linear			ED
CdI_2	Cd—I	2.56			linear			ED
ClCN	C—Cl (r_e)	1.629			C—N (r_e)	1.160		MW
ClF	Cl—F (r_e)	1.6283						MW
ClF_3	F_a—Cl(F_b)—F_a		Cl—F_a	1.698		Cl—F_b	1.598	MW
			∠F_aClF_b	87.5		(C_{2v})		
ClO	Cl—O (r_e)	1.5696						MW, UV
ClOH	O—Cl	1.690	O—H	0.975		∠HOCl	102.5	MW, IR
ClO_2	Cl—O	1.470			∠OClO	117.38		MW
$ClO_3(OH)$	O_a—Cl	1.407			O_b—Cl	1.639		ED
			∠O_aClO_a		114.3	∠O_aClO_b	104.1	
Cl_2	Cl—Cl (r_e)	1.9878						UV
Cl_2O	Cl—O	1.6959			∠ClOCl	110.89		MW
CoH	Co—H (r_e)	1.542						UV
Cr $(CO)_6$	C—O	1.16			Cr—C	1.92		ED
	∠CrCO	180						
CrO	Cr—O (r_e)	1.615						UV
CsBr	Cs—Br (r_e)	3.0723						MW
CsCl	Cs—Cl (r_e)	2.9063						MW
CsF	Cs—F (r_e)	2.3454						MW
CsH	Cs—H (r_e)	2.4938						UV
CsI	Cs—I (r_e)	3.3152						MW
CsOH	Cs—O (r_e)	2.395			O—H (r_e)		0.97	MW
CuBr	Cu—Br (r_e)	2.1734						MW
CuCl	Cu—Cl (r_e)	2.0512						MW
CuF	Cu—F (r_e)	1.7449						MW
CuH	Cu—H (r_e)	1.4626						UV
CuI	Cu—I (r_e)	2.3383						MW
FCN	C—F	1.262			C—N	1.159		MW
FOH	O—H	0.96	O—F	1.442		∠HOF	97.2	MW
F_2	F—F (r_e)	1.4119						R

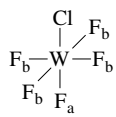
Compound			Structure				Method
$Fe(CO)_5$	Fe—C (average)	1.821					ED
	$(Fe—C)_{eq} - (Fe—C)_{ax}$		0.020				
	C—O (average)	1.153		(D_{3h})			
GaBr	Ga—Br (r_e)	2.3525					MW
GaCl	Ga—Cl (r_e)	2.2017					MW
GaF	Ga—F (r_e)	1.7744					MW
GaF_3	Ga—F	1.88		(D_{3h})			ED
GaI	Ga—I (r_e)	2.5747					MW
GaI_3	Ga—I	2.458		(D_{3h})			ED
GdI_3	Gd—I	2.841		∠IGdI	108	(C_{3v})	ED
$GeBrH_3$	Ge—H	1.526		Ge—Br	2.299		MW, IR
	∠HGeH	106.2					
$GeBr_4$	Ge—Br	2.272		(T_d)			ED
$GeClH_3$	Ge—H	1.537		Ge—Cl	2.150		IR, MW
	∠HGeH	111.0					
$GeCl_2$	Ge—Cl	2.183		∠ClGeCl	100.3		ED
$GeCl_4$	Ge—Cl	2.113		(T_d)			ED
$GeFH_3$	Ge—H	1.522		Ge—F	1.732		MW, IR
	∠HGeH	113.0					
GeF_2	Ge—F (r_e)	1.7321		∠FGeF (θ_e)	97.17		MW
GeH	Ge—H (r_e)	1.5880					UV
GeH_4	Ge—H	1.5251		(T_d)			IR, R
GeO	Ge—O (r_e)	1.6246					MW
GeS	Ge—S (r_e)	2.0121					MW
GeSe	Ge—Se (r_e)	2.1346					MW
GeTe	Ge—Te (r_e)	2.3402					MW
Ge_2H_6	Ge—H	1.541		Ge—Ge	2.403		ED
	∠HGeH	106.4		∠GeGeH	112.5		
HBr	H—Br (r_e)	1.4145					MW
HCN	C—H (r_e)	1.0655		C—N (r_e) linear	1.1532		MW, IR
HCNO	H—C	1.027	C—N	1.161	N—O linear	1.207	MW
HCl	H—Cl (r_e)	1.2746					MW
HF	H—F (r_e)	0.9169					MW
HI	H—I (r_e)	1.6090					MW
HNCO	N—H	0.986	N—C	1.209	C—O	1.166	MW
	∠HNC	128.0					
HNCS	N—H	0.989	N—C	1.216	C—S	1.561	MW
	∠HNC	135.0	∠NCS	180			
HNO	N—H	1.063	N—O	1.212	∠HNO	108.6	UV
HNO_2			*s-trans* conformer		*s-cis* conformer		MW
			O_b—H	0.958	0.98		
			N—O_b	1.432	1.39		
			N—O_a	1.170	1.19		
			∠O_aNO_b	110.7	114		
			∠NO_bH	102.1	104		
HNO_3			O_c—H	0.96	N—O_c	1.41	MW
			N—O_a	1.20	N—O_b	1.21	
			∠HO_cN	102.2	∠O_cNO_a	113.9	
			∠O_cNO_b	115.9	planar		
HNSO	N—H	1.029	N—S	1.512	S—O	1.451	MW
	∠HNS	115.8	∠NSO planar	120.4			
H_2	H—H (r_e)	0.7414					UV
H_2O	O—H (r_e)	0.9575		∠HOH (θ_e)	104.51		MW, IR
H_2O_2	O—O	1.475		∠OOH	94.8		IR
	dihedral angle of internal rotation			119.8	(C_2)		
H_2S	H—S (r_e)	1.3356		∠HSH (θ_e)	92.12		MW, IR

Compound	Structure							Method
H_2SO_4			$O—H$	0.97		$S—O_a$	1.574	MW
			$S—O_c$	1.422		$\angle H_aO_aS$	108.5	
			$\angle O_aSO_b$	101.3		$\angle O_cSO_d$	123.3	
			$\angle O_aSO_c$	108.6		$\angle O_aSO_d$	106.4	
	dihedral angle between the H_aO_aS and O_aSO_c planes						20.8	
	dihedral angle between the H_aO_aS and O_aSO_b planes						90.9	
	dihedral angle between the H_aSO_b and O_cSO_d planes						88.4 (C_2)	
H_2S_2	$S—S$	2.055	$S—H$	1.327		$\angle SSH$	91.3	ED, MW
	dihedral angle of internal rotation		90.6	(C_2)				
$HfCl_4$	$Hf—Cl$	2.33			(T_d)			ED
$HgCl_2$	$Hg—Cl$	2.252			linear			ED
HgH	$Hg—H$ (r_e)	1.7404						UV
HgI_2	$Hg—I$	2.553			linear			ED
IBr	$I—Br$ (r_e)	2.4691						MW
ICN	$C—I$	1.995			$C—N$	1.159		MW
ICl	$I—Cl$ (r_e)	2.3210						MW
IF_5	$I—F$ (average)	1.860			$(I—F)_{eq} - (I—F)_{ax}$	0.03		ED, MW
	$\angle F_{ax}IF_{eq}$	82.1	(C_{4v})					
IO	$I—O$ (r_e)	1.8676						MW
I_2	$I—I$ (r_e)	2.6663						R
InBr	$In—Br$ (r_e)	2.5432						MW
InCl	$In—Cl$ (r_e)	2.4012						MW
InF	$In—F$ (r_e)	1.9854						MW
InH	$In—H$ (r_e)	1.8376						UV
InI	$In—I$ (r_e)	2.7537						MW
IrF_6	$Ir—F$	1.830			(O_h)			ED
KBr	$K—Br$ (r_e)	2.8208						MW
KCl	$K—Cl$ (r_e)	2.6667						MW
KF	$K—F$ (r_e)	2.1716						MW
KH	$K—H$ (r_e)	2.244						UV
KI	$K—I$ (r_e)	3.0478						MW
KOH	$O—H$	0.91			$K—O$	2.212 linear		MW
K_2	$K—K$ (r_e)	3.9051						UV
KrF_2	$Kr—F$	1.89			linear			ED
LiBr	$Li—Br$ (r_e)	2.1704						MW
LiCl	$Li—Cl$ (r_e)	2.0207						MW
LiF	$Li—F$ (r_e)	1.5639						MW
LiH	$Li—H$ (r_e)	1.5949						MW
LiI	$Li—I$ (r_e)	2.3919						MW
Li_2	$Li—Li$ (r_e)	2.6729						UV
Li_2Cl_2					$Li—Cl$	2.23		ED
					$Cl—Cl$	3.61		
					$\angle ClLiCl$	108		
$LuCl_3$	$Lu—Cl$	2.417			$\angle ClLuCl$	112	(C_{3v})	ED
MgF	$Mg—F$ (r_e)	1.7500						UV
MgH	$Mg—H$ (r_e)	1.7297						UV
MgO	$Mg—O$ (r_e)	1.749						UV
MnH	$Mn—H$ (r_e)	1.7308						UV
$Mo(CO)_6$	$Mo—C$	2.063	$C—O$	1.145		(O_h)		ED
$MoCl_4O$	$Mo—Cl$	2.279			$Mo—O$	1.658		ED
	$\angle ClMoCl$	87.2			(C_{4v})			
MoF_6	$Mo—F$	1.820			(O_h)			ED
$NClH_2$	$N—H$	1.017			$N—Cl$	1.748		MW, IR
	$\angle HNCl$	103.7			$\angle HNH$	107		
NCl_3	$N—Cl$	1.759			$\angle ClNCl$	107.1		ED
NF_2	$N—F$	1.3528			$\angle FNF$	103.18		MW
NH_2	$N—H$	1.024			$\angle HNH$	103.3		UV
NH_2CN	$N—H$	1.00			$N_a—C$	1.35		MW

Compound	Structure						Method
		C—N_b	1.160	∠HNH	114		
		angle between the NH_2 plane and the N—C bond			142		
NH_2NO_2	N—N	1.427		N—H	1.005		MW
	∠HNH	115.2		∠ONO	130.1		
	dihedral angle between the NH_2 and NNO_2 planes				128.2		
NH_3	N—H (r_e)	1.012		∠HNH (θ_e)	106.7		IR
NH_4Cl	N—H	1.22	N—Cl	2.54	(C_{3v})		ED
NF_2CN	F_2N_b—C≡N_a		C—N_a	1.158	C—N_b	1.386	MW
	N_b—F	1.399	∠N_aCN_b	174			
	∠CN_bF	105.4	∠FN_bF	102.8			
NH	N—H (r_e)	1.0362					LMR
NH_2OH	N—H	1.02	N—O	1.453	O—H	0.962	MW
	∠HNH	107	∠HNO	103.3	∠NOH	101.4	
	The bisector of H—N—H angle is *trans* to the O—H bond						
NO	N—O (r_e)	1.1506					IR
NOCl	N—Cl	1.975	N—O	1.14	∠ONCl	113	MW
NOF	O—N	1.136	N—F	1.512	∠FNO	110.1	MW
NO_2	N—O	1.193		∠ONO	134.1		MW
NO_2Cl	N—Cl	1.840		N—O	1.202		MW
	∠ONO	130.6		(C_{2v})			
NO_2F	N—O	1.1798		N—F	1.467		MW
	∠ONO	136		(C_{2v})			
NS	N—S (r_e)	1.4940					IR
N_2	N—N (r_e)	1.0977					UV
N_2H_4	N—H	1.021		N—N	1.449		ED, MW
	∠HNH	106.6 (assumed)		∠NNH_a	112		
	∠NNH_b	106	dihedral angle of internal rotation		91		
	H_a: the H atom closer to the C_2 axis, H_b: the H atom farther from the C_2 axis						
N_2O	N—N (r_e)	1.1284		N—O (r_e)	1.1841		MW, IR
N_2O_3		N_a—N_b	1.864	N_a—O_a	1.142		MW
		N_b—O_b	1.202	N_b—O_c	1.217		
		∠$O_aN_aN_b$	105.05				
		∠$N_aN_bO_b$	112.72				
		∠$N_aN_bO_c$	117.47				
N_2O_4		N—N	1.782	N—O	1.190		ED
		∠ONO	135.4	(D_{2h})			
NaBr	Na—Br (r_e)	2.5020					MW
NaCl	Na—Cl (r_e)	2.3609					MW
NaF	Na—F (r_e)	1.9260					MW
NaH	Na—H (r_e)	1.8873					UV
NaI	Na—I (r_e)	2.7115					MW
Na_2	Na—Na (r_e)	3.0789					UV
$NbCl_5$	Nb—Cl_{eq}	2.241	Nb—Cl_{ax}	2.338 (D_{3h})	ED		
NbO	Nb—O (r_e)	1.691					UV
$Ni(CO)_4$	Ni—C	1.838	C—O	1.141	(T_d)		ED
NiH	Ni—H (r_e)	1.476					UV
NpF_6	Np—F	1.981		(O_h)			ED
OCS	C—O (r_e)	1.1578		C—S (r_e)	1.5601		MW
OCSe	C—O	1.159		C—Se	1.709		MW
OF	O—F (r_e)	1.3579					LMR
OF_2	O—F (r_e)	1.4053		∠FOF (θ_e)	103.07	(C_{2v})	MW
$O(SiH_3)_2$	Si—H	1.486		Si—O	1.634		ED
	∠SiOSi	144.1					
O_2	O—O (r_e)	1.2074					MW
O_2F_2	O—O	1.217		F—O	1.575		MW
	∠OOF	109.5	dihedral angle of internal rotation		87.5	(C_2)	

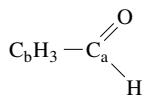
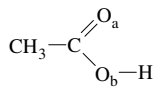
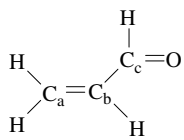
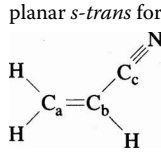
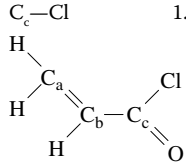
Compound	Structure							Method
O_3	O—O (r_e)		1.2716			∠OOO (θ_e)	117.47 (C_{2v})	MW
OsF_6	Os—F		1.831			(O_h)		ED
OsO_4	Os—O		1.712			(T_d)		ED
PBr_3	P—Br		2.220			∠BrPBr	101.0	ED
PCl_3	P—Cl		2.039			∠ClPCl	100.27	ED
PCl_5				$P—Cl_a$	2.124		$P—Cl_b$ 2.020 (D_{3h})	ED
PF	P—F (r_e)		1.5896					UV
PF_3	P—F		1.570			∠FPF	97.8	ED, MW
PF_5	$P—F_{ax}$	1.577		$P—F_{eq}$	1.534		(D_{3h})	ED
PH	P—H (r_e)		1.4223					LMR
PH_2	P—H		1.418			∠HPH	91.70	UV
PH_3	P—H		1.4200			∠HPH	93.345	MW
PN	N—P (r_e)		1.4909					MW
PO	O—P (r_e)		1.4759					UV
$POCl_3$	P—O		1.449			P—Cl	1.993	ED
	∠ClPCl		103.3					
POF_3	P—O	1.436		P—F	1.524		∠FPF 101.3	ED, MW
P_2	P—P (r_e)		1.8931					UV
P_2F_4	P—F		1.587			P—P	2.281	ED
	∠PPF		95.4			∠FPF	99.1	
	The two PF_2 planes are *trans* to each other (the *gauche* conformer is less than 10%)							
P_4	P—P		2.21			(T_d)		ED
P_4O_6	P—O	1.638		∠POP	126.4		(T_d)	ED
PbH	Pb—H (r_e)		1.839					UV
PbO	Pb—O (r_e)		1.9218					MW
PbS	Pb—S (r_e)		2.2869					MW
PbSe	Pb—Se (r_e)		2.4022					MW
PbTe	Pb—Te (r_e)		2.5950					MW
PrI_3	Pr—I	2.904		∠IPrI	113		(C_{3v})	ED
PtO	Pt—O (r_e)		1.7273					UV
PuF_6	Pu—F		1.971			(O_h)		ED
RbBr	Rb—Br (r_e)		2.9447					MW
RbCl	Rb—Cl (r_e)		2.7869					MW
RbF	Rb—F (r_e)		2.2703					MW
RbH	Rb—H (r_e)		2.367					UV
RbI	Rb—I (r_e)		3.1768					MW
RbOH	Rb—O	2.301		O—H	0.957		linear	MW
$ReClO_3$	Re—O		1.702			Re—Cl	2.229	MW
	∠ClReO		109.4			(C_{3v})		
ReF_6	Re—F		1.832			(O_h)		ED
RuO_4	Ru—O		1.706			(T_d)		ED
SCSe	C—Se		1.693			C—S	1.553	MW
SCTe	C—S		1.557			C—Te	1.904	MW
SCl_2	S—Cl	2.006		∠ClSCl	103.0		(C_{2v})	ED
SF	S—F (r_e)		1.6006					MW
SF_2	S—F		1.5921			∠FSF	98.20	MW
SF_6	S—F		1.561			(O_h)		ED
SO	S—O (r_e)		1.4811					MW
$SOCl_2$	S—O		1.44			S—Cl	2.072	MW
	∠ClSCl		97.2			∠OSCl	108.0	
SOF_2	S—O		1.420			S—F	1.583	ED
	∠OSF		106.2			∠FSF	92.2	
SOF_4				S—O	1.403		$S—F_a$ 1.575	ED
				$S—F_b$	1.552		$∠OSF_a$ 90.7	
				$∠OSF_b$	124.9		$∠F_aSF_b$ 89.6	
				$∠F_bSF_b$	110.2		(C_{2v})	
SO_2	S—O (r_e)		1.4308			∠OSO (θ_e)	119.329	MW

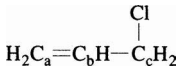
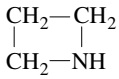
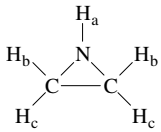
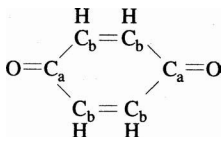
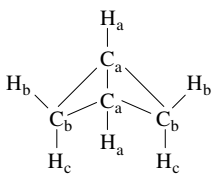
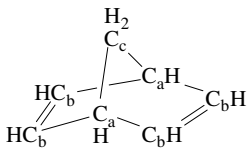
Compound	Structure								Method
SO_2Cl_2	S—O	1.404		S—Cl	2.011		∠OSO	123.5	ED
	∠ClSCl	100.0		(C_{2v})					
SO_2F_2	S—O	1.397		S—F	1.530		∠OSO	123	ED
	∠FSF	97		(C_{2v})					
SO_3	S—O		1.4198			(D_{3h})			IR
$S(SiH_3)_2$	Si—H	1.494		Si—S	2.136		∠SiSSi	97.4	ED
S_2	S—S (r_e)		1.8892						R
S_2Br_2	S—Br		2.24			S—S	1.98		ED
	∠SSBr		105	dihedral angle of internal rotation			83.5		
S_2Cl_2	S—Cl		2.057			S—S	1.931		ED
	∠SSCl		108.2	dihedral angle of internal rotation			84.1	(C_2)	
S_2O_2	S—O	1.458		S—S	2.025		∠OSS	112.8	MW
							planar *cis* form		
S_8				S—S	2.07				ED
				∠SSS	105				
				(D_{4d})					
$SbCl_3$	Sb—Cl		2.333			∠ClSbCl	97.2		ED
SbH_3	Sb—H		1.704			∠HSbH	91.6		MW
SeF	Se—F		1.742						MW
SeF_6	Se—F		1.69			(O_h)			ED
SeO	Se—O (r_e)		1.6393						MW
$SeOF_2$	Se—O		1.576			Se—F	1.730		MW
	∠OSeF		104.82			∠FSeF	92.22		
SeO_2	Se—O (r_e)		1.6076			∠OSeO (θ_e)	113.83		MW
SeO_3	Se—O		1.69			(D_{3h})			ED
Se_2	Se—Se (r_e)		2.1660						UV
Se_6	Se—Se		2.34			∠SeSeSe	102		ED
	six-membered ring with chair conformation								
$SiBrF_3$	Si—F		1.560			Si—Br	2.153		MW
	∠FSiBr		108.5			(C_{3v})			
$SiBrH_3$	Si—H		1.485			Si—Br	2.210		MW
	∠HSiBr		107.8			(C_{3v})			
$SiClH_3$	Si—H		1.482			Si—Cl	2.048		MW
	∠HSiCl		107.9			(C_{3v})			
$SiCl_4$	Si—Cl		2.019			(T_4)			ED
SiF	Si—F		1.6008						UV
$SiFH_3$	Si—H		1.484			Si—F	1.593		MW, IR
	∠HSiH		110.63			(C_{3v})			
SiF_2	Si—F (r_e)		1.590			∠FSiF (θ_e)	100.8		MW
SiF_3H	Si—H (r_e)		1.4468			Si—F (r_e)	1.5624		MW
	∠HSiF (θ_e)		110.64						
SiF_4	Si—F		1.553			(T_d)			ED
SiH	Si—H (r_e)		1.5201						UV
SiH_3I	Si—H		1.485			Si—I	2.437		MW
	∠HSH		107.8						
SiH_4	Si—H		1.4798			(T_d)			IR
SiN	N—Si (r_e)		1.572						UV
SiO	Si—O (r_e)		1.5097						MW
SiS	Si—S (r_e)		1.9293						MW
SiSe	Se—Si (r_e)		2.0583						MW
Si_2	Si—Si (r_e)		2.246						UV
Si_2Cl_6	Si—Si		2.32			Si—Cl	2.009		ED
	∠ClSiCl		109.7						
Si_2F_6	Si—Si		2.317			Si—F	1.564		ED
	∠FSiF		108.6						
Si_2H_6	Si—H		1.492			Si—Si	2.331		ED
	∠SiSiH		110.3			∠HSiH	108.6		
						staggered form (assumed)			

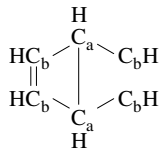
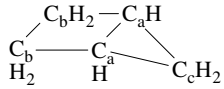
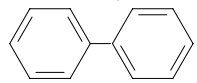
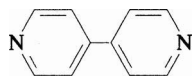
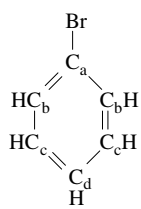
Compound	Structure					Method
$SnCl_4$	Sn—Cl	2.280	(T_d)			ED
SnH	Sn—H (r_e)	1.7815				UV
SnH_4	Sn—H	1.711	(T_d)			R, IR
SnO	Sn—O	1.8325				MW
SnS	S—Sn (r_e)	2.2090				MW
SnSe	Se—Sn (r_e)	2.3256				MW
SnTe	Sn—Te (r_e)	2.5228				MW
SrH	Sr—H (r_e)	2.1455				UV
SrO	Sr—O (r_e)	1.9198				MW
SrS	S—Sr (r_e)	2.4405				UV
$TaCl_5$	Ta—Cl_{eq}	2.227	Ta—Cl_{ax}	2.369	(D_{3h})	ED
TaO	Ta—O (r_e)	1.6875				UV
TeF_6	Te—F	1.815	(O_h)			ED
Te_2	Te—Te (r_e)	2.5574				UV
$ThCl_4$	Th—Cl	2.58	(T_d)			ED
ThF_4	Th—F	2.14	(T_d)			ED
TlBr	Tl—Br (r_e)	2.6182				MW
TlCl	Tl—Cl (r_e)	2.4848				MW
TlF	Tl—F (r_e)	2.0844				MW
TlH	Tl—H (r_e)	1.870				UV
TlI	Tl—I (r_e)	2.8137				MW
$TiBr_4$	Ti—Br	2.339	(T_d)			ED
$TiCl_4$	Ti—Cl	2.170	(T_d)			ED
TiO	Ti—O (r_e)	1.620				UV
TiS	Ti—S (r_e)	2.0825				UV
UF_6	U—F	1.996	(O_h)			ED
$V(CO)_6$	V—C	2.015	C—O	1.138		ED
	(O_h, involving dynamic Jahn-Teller effect)					
VCl_3O	V—O	1.570	V—Cl	2.142		ED, MW
	∠ClVCl	111.3				
VCl_4	V—Cl	2.138	(T_d, involving dynamic Jahn-Teller effect)			ED
VF_5	V—F (average)	1.71				ED
VO	V—O (r_e)	1.5893				UV
$W(CO)_6$	W—C	2.059	C—O	1.149	(O_h)	ED
$WClF_5$				W—Cl	2.251	MW
				W—F (average)	1.836	
				∠F_aWF_b	88.7	
WF_4O	W—O	1.666	W—F	1.847		ED
	∠FWF	86.2	(C_{4v})			
WF_6	W—F	1.832	(O_h)			ED
XeF_2	Xe—F	1.977	linear			IR
XeF_4	Xe—F	1.94	(D_{4h})			ED
XeF_6	Xe—F	1.890	(large-amplitude bending vibration around the O_h structure)			ED
XeO_4	Xe—O	1.736	(T_d)			ED
ZnH	Zn—H (r_e)	1.5949				UV
$ZrCl_4$	Zr—Cl	2.32	(T_d)			ED
ZrF_4	Zr—F	1.902	(T_d)			ED
ZrO	Zr—O (r_e)	1.7116				UV

STRUCTURES OF ORGANIC MOLECULES

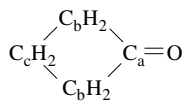
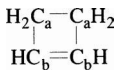
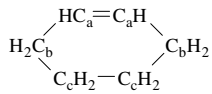
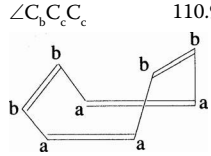
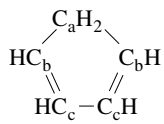
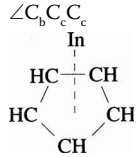
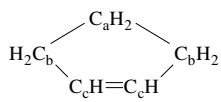
Compounds are arranged in alphabetical order by chemical name; cross references are given for common synonyms (lengths in Å and angles in degrees)

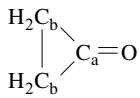
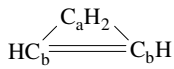
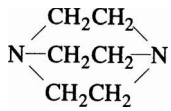
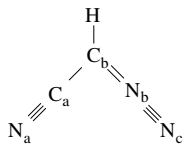
Compound	Structure				Method
Acetaldehyde			C_a—O	1.210	ED, MW
			C_b—H	1.107	
			C_a—H	1.128	
	C_a—C_b	1.515	∠C_bC_aO	124.1	
	∠HC_bH	109.8	∠C_bC_aH	115.3	
Acetamide	C—O	1.220	C—N	1.380	ED
CH_3CONH_2	C—C	1.519	N—H	1.022	
	C—H	1.124	∠NCO	122.0	
	∠CCN	115.1			
Acetic acid			C—C	1.520	ED
			C—O_a	1.214	
			C—O_b	1.364	
	C—H	1.10	∠CCO_a	126.6	
	∠CCO_b	110.6			
Acetone	C—C	1.520	C—O	1.213	ED, MW
$(CH_3)_2CO$	C—H	1.103	∠CCC	116.0	
	∠HCH	108.5	symmetry axis of each methyl group is tilted 2° from the C—C bond		
Acetonitrile	C—H	1.107	C—C	1.468	ED, MW
CH_3CN	C—N	1.159	∠CCH	109.7	
Acetonitrile oxide	C—C	1.442	C—N	1.169	MW
CH_3CNO	N—O	1.217	(C_{3v})		
Acetyl chloride	C—H	1.105	C—O	1.187	ED, MW
CH_3COCl	C—C	1.506	C—Cl	1.798	
	∠HCH	108.6	∠OCCl	121.2	
	∠CCCl	111.6			
Acetyl cyanide → Pyruvonitrile					
Acetylene	C—H (r_e)	1.060	C—C (r_e)	1.203	IR
HC≡CH					
Acrolein → Acrylaldehyde					
Acrylaldehyde			C_b—C_c	1.484	ED, MW
			C_a—C_b	1.345	
			C_c—O	1.217	
			C_a—H	1.10	
			C_c—H	1.13	
	∠$C_aC_bC_c$	120.3	∠C_bC_cO	123.3	
	∠HC_cC_b	114	other CCH angles (average)	122	
	planar *s-trans* form				
Acrylonitrile			C_a—C_b	1.343	ED, MW
			C_b—C_c	1.438	
			C_c—N	1.167	
			C_a—H	1.114	
			∠$C_aC_bC_c$	121.7	
	∠C_bC_cN	178	∠HCC	120	
Acryloyl chloride	C—H	1.086 (assumed)	C_b—C_c	1.48	MW
	C_c—Cl	1.82	C_a—C_b	1.35	
			C_c—O	1.19	
			∠C_aC_bH	120 (assumed)	
			∠C_bC_aH	121.5 (assumed)	
			∠$C_aC_bC_c$	123	
			∠C_bC_cCl	116	
			∠C_bC_cO	127	

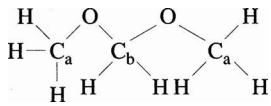
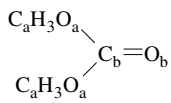
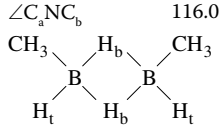
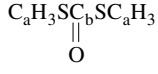
Compound	Structure					Method
Allene	C—C	1.3084	C—H		1.087	IR
$CH_2=C=CH_2$	∠HCH	118.2				
Allyl chloride			*cis* conformer	C—Cl	1.811	MW
				∠CCCl	115.2	
			skew conformer	C—Cl	1.809	
	∠CCCl	109.6	CCCCl	dihedral angle of internal rotation	122.4	
Aniline	C—C	1.392	C—N		1.431	MW
$C_6H_5NH_2$	N—H	0.998	∠HNH		113.9	
	dihedral angle between the NH_2 plane and the N—C bond				140.6	
Azetidine			C—N		1.482	ED
			C—C		1.553	
			C—H		1.107	
	N—H	1.03	∠CNC		92.2	
	∠CCC	86.9	∠CCN		85.8	
	dihedral angle between the CCC and CNC planes				147	
Aziridine			N—H		1.016	MW
			N—C		1.475	
			C—C		1.481	
			C—H		1.084	
			∠CNC		60.3	
			$\angle H_aNC$		109.3	
	$\angle H_bCH_c$	115.7	$\angle H_bCC$		117.8	
	$\angle H_bCN$	118.3	$\angle H_cCC$		119.3	
	$\angle H_cCN$	114.3				
Azomethane	C—N	1.482	N—N		1.247	ED
$CH_3N=NCH_3$	∠CNN	112.3	*trans* conformer			
Benzene	C—C	1.399	C—H		1.101	ED, IR
C_6H_6						
p-Benzoquinone			C_a—O		1.225	ED
			C_b—C_b		1.344	
			C_a—C_b		1.481	
			$\angle C_bC_aC_b$		118.1	
Biacetyl	C—O	1.215	C—C (average)		1.524	ED
$CH_3COCOCH_3$	C—H	1.108	∠CCO		119.5	
	∠CCC	116.2	*trans* conformer			
Bicyclo[1.1.0]butane			C_a—C_a		1.497	MW
			C_a—C_b		1.498	
			C_a—H_a		1.071	
			C_b—H_b, C_b—H_c		1.093	
			$\angle H_bC_bH_c$		115.6	
	$\angle C_bC_aH_a$	130.4	$\angle C_aC_bC_a$		60.0	
	$\angle C_aC_aH_a$	128.4	dihedral angle between the two $C_aC_aC_b$ planes		121.7	
Bicyclo[2.2.1]hepta-2,5-diene			C_a—C_b		1.535	ED
			C_b—C_b		1.343	
			C_a—C_c		1.573	
			C—H		1.12	
			$\angle C_aC_cC_a$		94	
	dihedral angle between the two $C_aC_bC_bC_a$ planes				115.6 (C_{2v})	
Bicyclo[2.2.1]heptane	See the preceding molecule for the labels of the C atoms					ED
C_7H_{12}	C_a—C_b	1.54	C_b—C_b		1.56	
	C_a—C_c	1.56	C—C (average)		1.549	
	$-C_aC_cC_a$	93.1	dihedral angle between the two $C_aC_bC_bC_a$ planes		113.1	

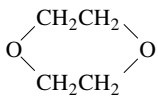
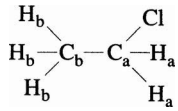
Compound	Structure				Method
Bicyclo[2.2.0]hexa-2,5-diene			$C_b—C_b$	1.345	ED
			$C_a—C_a$	1.574	
			$C_a—C_b$	1.524	
		dihedral angle between the two $C_aC_bC_bC_a$ planes		117.3	
Bicyclo[2.2.2]octane	$HC_a(C_bH_2C_bH_2)_3C_aH$		$C_a—C_b$	1.54	ED
	$C_b—C_b$	1.55	$\angle C_aC_bC_b$	109.7	
	C—C (average)	1.542			
	large-amplitude torsional motion about the D_{3h} symmetry axis				
Bicyclo[1.1.1]pentane	C—C	1.557	∠CCC	74.2	ED
C_5H_8					
Bicyclo[2.1.0]pentane			$C_a—C_a$	1.536	MW
			$C_b—C_b$	1.565	
			$C_a—C_b$	1.528	
			$C_a—C_c$	1.507	
	Dihedral angle between the $C_aC_aC_bC_b$ and $C_aC_aC_c$ planes			112.7	
Biphenyl			C—C (intra-ring)	1.396	ED
			(inter-ring)	1.49	
			torsional dihedral angle between the two rings	~40	
4,4′-Bipyridyl	C—C, C—N (intra-ring)		1.375		ED
			C—C (inter-ring)	1.465	
			torsional dihedral angle between the two rings	~37	
Bis (cyclopentadienyl) beryllium	Be—(cyclopentadienyl plane)		1.470, 1.92		ED
$(C_5H_5)_2Be$	C—C 1.423 (C_{5v}) (The Be atom has two equilibrium positions)				
Bis (cyclopentadienyl) iron → Ferrocene					
Bis (cyclopentadienyl) lead	C—C	1.430	Pb—C	2.79	ED
$(C_5H_5)_2Pb$	dihedral angle between the two C_5H_5 planes 40~50 (The two rings are not parallel.)				
Bis (cyclopentadienyl) manganese	Mn—C 2.383	C—C 1.429	(D_{5h})		ED
$(C_5H_5)_2Mn$					
Bis (cyclopentadienyl) nickel	Ni—C	2.196	C—C	1.430 (D_{5h})	ED
$(C_5H_5)_2Ni$					
Bis (cyclopentadienyl) ruthenium	C—C	1.439	Ru—C	2.196	ED
$(C_5H_5)_2Ru$					
Bis (cyclopentadienyl) tin	C—C	1.431	Sn—C	2.71	ED
$(C_5H_5)_2Sn$	C—H	1.14	(D_{5h})		
Bis (trifluoromethyl) peroxide	O—O	1.42	C—O	1.399	ED
CF_3OOCF_3	C—F	1.320	∠COO	107	
	∠FCF	109.0	COOC dihedral angle of internal rotation	123	
Borine carbonyl	B—H	1.194	B—C	1.540	MW
BH_3CO	C—O	1.131	∠HBH	113.9	
	∠BCO	180	(C_{3v})		
Bromobenzene			C—H	1.072	MW
			$C_c—C_d$	1.401	
			$C_b—C_c$	1.375	
			C—Br	1.85	
			$C_a—C_b$	1.42	
			$\angle C_bC_aC_b$	117.4	
Bromoform	C—Br	1.924	C—H	1.11	ED, MW
$CHBr_3$	∠BrCBr	111.7	(C_{3v})		
Bromoiodoacetylene	C—I	1.972	C—C	1.206	ED
IC≡CBr	C—Br	1.795			

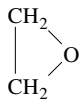
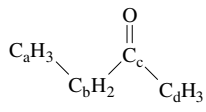
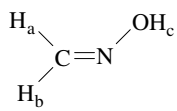
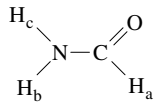
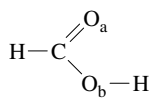
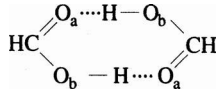
Compound	Structure				Method
1,3-Butadiene	C_aH_2		$C_b—C_b$	1.467	ED
	$C_bH—C_bH$		$C_a—C_b$	1.349	
	C_aH_2		C—H (average)	1.108	
			∠CCC	124.4	
	$\angle C_bC_aH$	120.9	*anti* conformer	(C_{2h})	
1,3-Butadiyne	$HC_a≡C_b—C_b≡C_aH$		C—H	1.09	ED
	$C_a—C_b$	1.218	$C_b—C_b$	1.384	
			linear		
Butane	C—C	1.531	C—H	1.117	ED
$CH_3CH_2CH_2CH_3$	∠CCC	113.8	∠CCH	111.0	
	trans conformer	54%	dihedral angle for the *gauche* conformer		65
2-Butanone → Ethyl methyl ketone					
Butatriene	$H_2C_a=C_b=C_b=C_aH_2$		C—H	1.08	ED
	$C_a—C_b$	1.32	$C_b—C_b$	1.28 (D_{2h})	
2-Butene	$C_aH_3—C_bH=C_bH—C_aH_3$				ED
	$C_a—C_b$	*cis* conformer	1.506	*trans* conformer 1.508	
	$C_b—C_b$	1.346	1.347		
	$\angle C_aC_bC_b$	125.4	123.8		
3-Buten-1-yne → Vinylacetylene					
tert-Butyl chloride	C—H	1.102	C—C	1.528	ED, MW
$(CH_3)_3CCl$	C—Cl	1.828	∠CCCl	107.3	
	∠CCH	110.8	∠CCC	111.6	
tert-Butyl cyanide → Pivalonitrile					
2-Butyne	$C_aH_3—C_b≡C_b—C_aH_3$	C—H	1.116	ED	
	$C_b—C_b$	1.214	$C_a—C_b$	1.468	
	$\angle C_bC_aH$	110.7			
Carbon C_2	C—C (r_e)	1.3119			UV
Carbon C_3	C—C	1.277	linear		UV
Carbon suboxide → Tricarbon dioxide					
Carbon tetrabromide	C—Br	1.935	(T_d)		ED
CBr_4					
Carbon tetrachloride	C—Cl	1.767	(T_d)		ED
CCl_4					
Carbon tetrafluoride	C—F	1.323	(T_d)		ED
CF_4					
Carbon tetraiodide	C—I	2.15	(T_d)		ED
CI_4					
Carbonyl cyanide	C—O	1.209	C—C	1.466	ED, MW
$CO(CN)_2$	C—N	1.153	∠CCC	115	
	∠CCN	180			
Chloroacetylene	C—H	1.0550	C—C	1.2033	MW
HC≡CCl	C—Cl	1.6368			
Chlorobenzene	C—C	1.400	C—Cl	1.737	ED
C_6H_5Cl	C—H	1.083	∠CC(Cl)C	121.7	
	∠CC(H)C	120			
Chlorobromoacetylene	Cl—C	1.636	C—C	1.206	ED
ClC≡CBr	C—Br	1.784			
Chlorocyanoacetylene	C—Cl	1.624	C—C	1.205	ED
ClC≡CCN	C—CN	1.362	C—N	1.160	
Chloroethane → Ethyl chloride					
2-Chloroethanol	C—O	1.413	C—C	1.519	ED
$ClCH_2CH_2OH$	C—Cl	1.801	C—H	1.093	
	O—H	1.033	∠CCCl	110.7	∠CCO 113.8
	fraction of the *gauche* conformer at 37°C is 92 ∼ 94%,				
	dihedral angle of internal rotation		62.4		
Chloroethylene → Vinyl chloride					
Chloroform	C—H	1.100	C—Cl	1.758	MW
$CHCl_3$	∠ClCCl	111.3	(C_{3v})		
Chloroiodoacetylene	C—Cl	1.63	C—I	1.99	MW
ClC≡CI	C—C	1.209 (assumed)			

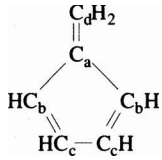
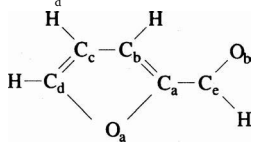
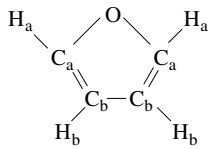
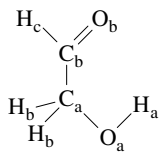
Compound	Structure				Method
Chloromethane → Methyl chloride					
3-Chloropropene → Allyl chloride					
Cyanamide	N_a—C	1.346	C—N_b	1.160	MW
$H_2N_aCN_b$	N—H	1.00	∠HNH	114	
	dihedral angle between the NH_2 plane and the N—C bond			142	
Cyanoacetylene	C_b—H	1.058	C_a—C_b	1.205	MW
H—C_b≡C_a—C_c≡N	C_a—C_c	1.378	C_c—N	1.159	
Cyanocyclopropane	C—C (ring)	1.513	C—C_a	1.472	MW
$C_3H_5C_aN$	C—H	1.107	C_a—N	1.157	
	∠HCH	114.6	∠C_aCH	119.6	
Cyanogen	C—N	1.163	C—C	1.393	ED
$(CN)_2$				linear	
Cyclobutane	C—H	1.113	C—C	1.555	ED
$(CH_2)_4$	dihedral angle between the two CCC planes 145				
Cyclobutanone			C_a—C_b	1.527	MW
			C_b—C_c	1.556	
			∠$C_bC_aC_b$	93.1	
			∠$C_aC_bC_c$	88.0	
Cyclobutene		C_b—C_b	1.342	C_a—C_a 1.566	MW
		C_a—C_b	1.517	C_a—H 1.094	
		C_b—H	1.083		
	∠$C_aC_bC_b$	94.2	∠C_bC_bH	133.5	
	∠C_aC_aH	114.5	∠$C_aC_aC_b$	85.8	
	∠HC_aH	109.2	dihedral angle between the CH_2 plane and the C_a—C_a bond	135.8	
Cyclohexane	C—C	1.536	C—H	1.119	ED
C_6H_{12}	∠CCC	111.3	chair form		
Cyclohexene			C_a—C_a	1.334	ED
			C_a—C_b	1.50	
			C_b—C_c	1.52	
			C_c—C_c	1.54	
	∠$C_aC_aC_b$	123.4	∠$C_aC_bC_c$	112.0	
	∠$C_bC_cC_c$	110.9	(C_2)	half-chair form	
Cyclooctatetraene			C_a—C_b	1.476	ED
			C—H	1.100	
			C_a—C_a,C_b—C_b	1.340	
			∠$C_bC_aC_a$, ∠$C_aC_bC_b$	126.1	
	dihedral angle between the $C_aC_aC_aC_a$ and $C_aC_bC_bC_a$ planes			136.9	
	tub form (D_{2d})				
1,3-Cyclopentadiene			C_a—C_b	1.509	MW
			C_b—C_c	1.342	
			C_c—C_c	1.469	
			∠$C_aC_bC_c$	109.3	
	∠$C_bC_cC_c$	109.4	∠$C_bC_aC_b$	102.8	
Cyclopentadienylindium			In—C	2.621	ED
			C—C	1.426	
			(C_{5v})		
Cyclopentane	C—H	1.114	C—C	1.546	ED
$(CH_2)_5$	∠CCH	111.7			
	(The out-of-plane vibration of the C atoms is essentially free pseudorotation; average value of the displacements of the C atoms from the molecular plane 0.43)				
Cyclopentene			C_a—C_b	1.546	ED
			C_b—C_c	1.519	
			C_c—C_c	1.342	
			∠$C_bC_aC_b$	104.0	
	∠$C_bC_cC_c$	110.0	∠$C_aC_bC_c$	103.0	
	dihedral angle between the $C_bC_aC_b$ and $C_bC_cC_cC_b$ planes			151.2	

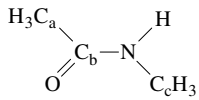
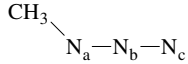
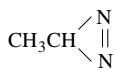
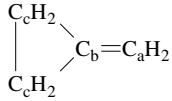
Compound	Structure						Method
Cyclopropane	C—C	1.512	C—H	1.083			R
$(CH_2)_3$	∠HCH	114.0					
Cyclopropanone		C—H	1.086	C_a—C_b	1.475		MW
		C_b—C_b	1.575	C_a—O	1.191		
		$\angle C_aC_bC_b$	57.7				
	$\angle HC_bH$	114	dihedral angle between the CH_2 plane and the C_b—C_b bond		151		
Cyclopropene			C_b—C_b	1.304			ED
			C_a—C_b	1.519			
			C_b—H	1.077			
	C_a—H	1.112	$\angle C_bC_bH$	133			
	$\angle HC_aH$	118					
Decalin	C—C (average)	1.530	C—H (average)	1.113			ED
$C_{10}H_{18}$	∠CCC (average)	111.4					
Dewer benzene → Bicyclo[2.2.0] hexa-2,5-diene							
Diacetylene → 1,3-Butadiyne							
1,4-Diazabicyclo[2.2.2]octane			C—N	1.472			ED
			C—C	1.562			
			∠NCC	110.2			
			∠CNC	108.7			
	large-amplitude torsional motion about the D_{3h} symmetry axis						
2,3-Diaza-1,3-butadiene → Formaldehyde azine							
Diazirine			C—H	1.09			MW
			C—N	1.482			
			N—N	1.228			
			∠HCH	117			
Diazoacetonitrile			C_b—N_b	1.280			MW
			N_b—N_c	1.132			
			C_a—N_a	1.165			
			C—H	1.082			
			C_a—C_b	1.424			
	$\angle C_aC_bH$	117	$\angle C_aC_bN_b$	119.5			
Diazomethane	C—H	1.075	C—N	1.32			MW, IR
CH_2N_2	N—N	1.12	∠HCH	126.0 linear			
1,2-Dibromoethane	C—C	1.506	C—Br	1.950			ED
CH_2BrCH_2Br	C—H	1.108	∠CCBr	109.5			
	∠CCH 110		fraction of the *trans* conformer at 25°C	95%			
Dibromomethane	C—H	1.08	C—Br	1.924			ED
CH_2Br_2	∠HCBr	109	∠BrCBr	113.2			
2,2′-Dichlorobiphenyl	C—C	1.398	C—C inter-ring	1.495			ED
C_6H_4Cl—C_6H_4Cl	C—Cl	1.732	C—H	1.10			
	∠CCCl	121.4	∠CCH	126			
	dihedral angle between the two aromatic rings 74 (defined to be 0 for that of the *cis* conformer)						
trans-1,4-Dichlorocyclohexane	C—H	1.102	C—Cl	1.810			ED
$C_6H_{10}Cl_2$	C—C	1.530	∠CCC	111.5			
	∠CCCl (*ee*)	108.6	∠CCCl (*aa*)	110.6			
	∠HCCl (*ee*)	111.5	∠HCCl (*aa*)	107.6			
	ee 49%		aa 51%	e: equatorial, a: axial			
1,1-Dichloroethane	C—Cl	1.766	C—C	1.540			MW
$CHCl_2CH_3$	∠ClCCl	112.0	∠CCCl	111.0			
1,2-Dichloroethane	C—C	1.531	C—Cl	1.790			ED
CH_2ClCH_2Cl	C—H	1.11	∠CCCl	109.0			
	∠CCH	113					
	fraction of the *trans* conformer at room temperature 73%, that of the *gauche* conformer 27%						

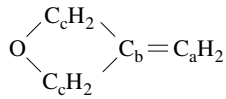
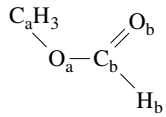
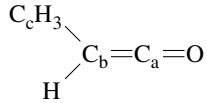
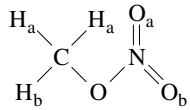
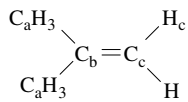
Compound	Structure				Method
1,1-Dichloroethylene	C—C	1.32 (assumed)	C—Cl	1.73	MW
$CH_2{=}CCl_2$	∠ClCC	123	(C_{2v})		
cis-1,2-Dichloroethylene	C—Cl	1.718	C—C	1.354	ED
CHCl=CHCl	∠ClCC	123.8			
Dichloromethane	C—H (r_e)	1.087	C—Cl (r_e)	1.765	MW, IR
CH_2Cl_2	∠HCH (θ_e)	111.5	∠ClCCl (θ_e)	112.0	
1,1-Difluoroethane	C—C	1.498	C—H (average)	1.081	ED
CH_3CHF_2	C—F	1.364	∠CCH (average)	111.0	
	∠CCF 110.7	dihedral angle between the two CCF planes		118.9	
1,2-Difluoroethane	C—F	1.389	C—C	1.503	ED
CH_2FCH_2F	C—H	1.103	∠CCF	110.3	
	∠CCH 111	dihedral angle of internal rotation		109	
	fraction of the *gauche* conformer at 22°C 94%				
1,1-Difluoroethane	C—C	1.340	C—F	1.315	ED, MW
$CH_2{=}CF_2$	C—H	1.091	∠CCF	124.7	
	∠CCH	119.0			
cis-1,2-Difluoroethylene	C—C	1.33	C—F	1.342	ED, MW
CHF=CHF	C—H	1.099	∠CCF	122.0	
	∠CCH	124.1			
Difluoromethane	C—H	1.093	C—F	1.357	MW
CH_2F_2	∠HCH	113.7	∠FCF	108.3	
Dimethoxymethane			C_a—O	1.432	ED
			C_b—O	1.382	
			C—H (average)	1.108	
	∠COC	114.6	∠OCO	114.3	
	∠OCH	110.3			
Dimethylacetylene → 2-Butyne					
Dimethylamine	C—H	1.106	N—H	1.00	ED
$(CH)_2NH$	C—N	1.455	∠CNC	111.8	
	∠CNH	107	∠NCH	112	
	∠HCH	107			
Dimethylberyllium	Be—C	1.698	C—H	1.127	ED
$(CH_3)_2Be$	∠BeCH	113.9	CBeC linear		
Dimethylcadmium	C—Cd	2.112	∠HCH	108.4	R
$(CH_3)_2Cd$					
Dimethyl carbonate			C_b—O_b	1.209	ED
			C_b—O_a	1.34	
			C_a—O_a	1.42	
	∠$O_aC_bO_a$	107	∠$C_bO_aC_a$	114.5	
Dimethylcyanamide	C_b—N_b	1.161	C_b—N_a	1.338	ED
$(C_aH_3)_2N_a—C_b{\equiv}N_b$	C_a—N_a	1.463	∠C_aNC_a	115.5	
	∠C_aNC_b	116.0			
1,2-Dimethyldiborane			B—B	1.799	ED
			B—C	1.580	
			B—H_b	1.358 (*cis*), 1.365 (*trans*)	
	B—H_t	1.24			
	∠BBC	122.6 (*cis*), 121.8 (*trans*)			
Dimethyl diselenide	C—H	1.13	C—Se	1.95	ED
$(CH_3)_2Se_2$	Se—Se	2.326	∠CSeSe	98.9	
	∠HCSe 108	dihedral angle between the CSeSe and SeSeC planes		88	
Dimethyl disulfide	C—S	1.816	S—S	2.029	ED
$(CH_3)_2S_2$	C—H	1.105	∠SSC	103.2	
	∠SCH 111.3	CSSC dihedral angle of internal rotation		85	
S,S′-Dimethyl dithiocarbonate			C_b—O	1.206	ED
			C_b—S	1.777	
			C_a—S	1.802	
	∠OCS	124.9	∠CSC	99.3	
			syn-syn conformer		

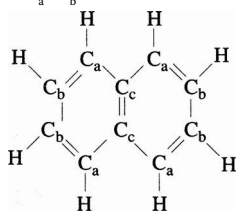
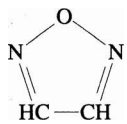
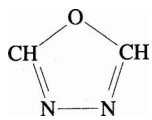
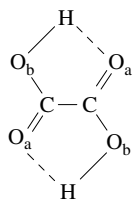
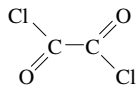
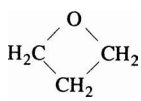
Compound	Structure				Method
Dimethyl ether	C—O	1.416	C—H	1.121	ED
$(CH_3)_2O$	∠COC	112	∠HCH	108	
Dimethylglyoxal → Biacetyl					
N,N′-Dimethylhydrazine	N—N	1.42	C—N	1.46	ED
$CH_3NH—NHCH_3$	N—H	1.03	C—H	1.12	
	∠NNC 112	CNNC dihedral angle of internal rotation		90	
Dimethylmercury	C—Hg	2.083	C—H	1.160 (assumed)	ED
$(CH_3)_2Hg$	Hg···H	2.71			
Dimethylphosphine	C—P	1.848	P—H	1.419	MW
$(CH_3)_2PH$	∠CPC	99.7	∠CPH	97.0	
Dimethyl selenide	C—H	1.093	Se—C	1.943	MW
$(CH_3)_2Se$	∠CSeC	96.2	∠SeCH	108.7	
	∠HCH	110.3			
Dimethyl sulfide	C—S	1.807	C—H	1.116	ED, MW
$(CH_3)_2S$	∠CSC	99.05	∠HCH	109.3	
Dimethyl sulfone	C—H	1.114	S—O	1.435	ED
$(CH_3)_2SO_2$	S—C	1.771	∠CSC	102	
	∠OSO	121			
Dimethyl sulfoxide	C—H	1.081	C—S	1.799	MW
$(CH_3)_2SO$	S—O	1.485	∠CSC	96.6	
	∠CSO	106.7	∠HCH	110.3	
	dihedral angle between the SCC plane and the S—O bond			115.5	
Dimethylzinc	Zn—C	1.929	∠HCH	107.7	R
$(CH_3)_2Zn$					
1,4-Dioxane	C—C	1.523	C—O	1.423	ED
	C—H	1.112	∠COC	112.45	
	∠CCO	109.2	chair form		
Ethanal → Acetaldehyde					
Ethane	C—C	1.5351	C—H	1.0940	MW
C_2H_6	∠CCH	111.17	staggered conformation		
Ethanethiol	$C_bH_3—C_aH_2—SH$		$C_a—H$	1.090	MW
	$C_b—H$	1.093	$C_a—C_b$	1.530	
	$C_a—S$	1.829	S—H	1.350	
	$∠C_bC_aH$	109.6	$∠C_aC_bH$	109.7	
	$∠C_bC_aS$	108.3	$∠C_aSH$	96.4	
Ethanol	$C_bH_3C_aH_2OH$		C—C	1.512	MW
	C—O	1.431	O—H	0.971	
	$C_a—H$	1.10	$C_b—H$	1.09	
	∠CCO	107.8	∠COH	105	
	$∠C_bC_aH$	111	$∠C_aC_bH$	110	
	staggered conformation				
Ethyl chloride			C—C	1.528	ED, MW
			C—Cl	1.802	
			C—H	1.103	
			$C_a—H_a=C_b—H_b$ (assumed)		
			∠CCCl	110.7	
	$∠H_bC_bH_b$	109.8	$∠H_aC_aH_a$	109.2	
	$∠C_bC_aH_a$	110.6			
Ethylene	C—H	1.087	C—C	1.339	MW
$CH_2=CH_2$	∠CCH	121.3			
Ethylenediamine	C—N	1.469	C—C	1.545	ED
$H_2NCH_2CH_2NH_2$	C—H	1.11	∠CCN	110.2	
	gauche conformer	dihedral angle between the NCC and CCN planes		64	
Ethylene dibromide → 1,2-Dibromoethane					
Ethylene dichloride → 1,2-Dichloroethane					
Ethyleneimine → Aziridine					

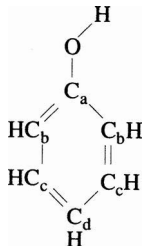
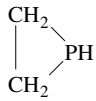
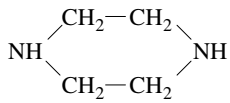
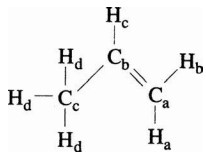
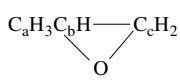
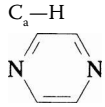
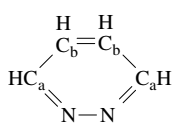
Compound	Structure						Method
Ethylene oxide	C—C	1.466	C—H		1.085		MW
	C—O	1.431	∠HCH		116.6		
	dihedral angle between the NH_2 plane and the N—C bond				158.0		
Ethylene sulfide → Thiirane							
Ethyl methyl ether	C—O (average)	1.418	C—C		1.520		ED
$C_2H_5OCH_3$	C—H (average)	1.118	∠COC		111.9		
	∠OCC	109.4	∠HCH		109.0		
	fraction of the *trans* conformer at 20°C		80%				
Ethyl methyl ketone			C—C (average)		1.518		ED
			C_c—O		1.219		
			C—H (average)		1.102		
			$\angle C_aC_bC_c$		113.5		
	$\angle C_bC_cO$, $\angle C_dC_cO$	121.9	trans conformer		95%		
Ethyl methyl sulfide	C—S (average)	1.813	C—C		1.536		ED
$C_2H_5SCH_3$	C—H	1.111	∠CSC		97		
	∠SCC	114.0	∠HCH		110		
	fraction of the *gauche* conformer at 20°C		75%				
Ferrocene	C—C	1.440	C—H		1.104		ED
$(C_5H_5)_2Fe$	Fe—C	2.064	(D_{5h})				
Fluoroform	C—H	1.098	C—F		1.332		MW
CHF_3	∠FCF	108.8	(C_{3v})				
Formaldehyde	C—H	1.116	C—O		1.208		MW
H_2CO	∠HCH	116.5					
Formaldehyde azine	$H_2C{=}N{-}N{=}CH_2$	N—N	1.418				ED
	C—N	1.277	C—H		1.094		
	∠CNN	111.4	∠HCN		120.7		
	fraction of the *trans* conformer at –30°C		91%				
Formaldehyde dimethylacetal → Dimethoxymethane							
Formaldoxime			$C{-}H_a$		1.085		MW
			$C{-}H_b$		1.086		
			C—N		1.276		
	N—O	1.408	$O{-}H_c$		0.956		
	$\angle H_bCN$	115.6	∠CNO		110.2		
	$\angle H_aCN$	121.8	$\angle NOH_c$		102.7		
Formamide			$C{-}H_a$		1.125		ED, MW
			N—H		1.027		
			C—N		1.368		
	C—O	1.212	∠NCO		125.0		
	∠CNH (average)	119.2					
Formic acid			$C{-}O_a$		1.202		MW
			$C{-}O_b$		1.343		
	O_b—H	0.972	C—H		1.097		
	$\angle HCO_a$	124.1	$\angle O_aCO_b$		124.9		
	$\angle CO_bH$	106.3	planar				
Formic acid dimer			$O_a{\cdots}O_b$		2.703		ED
			$C{-}O_a$		1.220		
			$C{-}O_b$		1.323		
			$\angle O_aCO_b$		126.2		
			$\angle CO_aO_b$		108.5		
Formyl radical		C—H	1.110	C—O		1.1712	MW
		∠HCO	127.43				

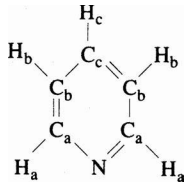
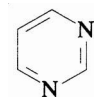
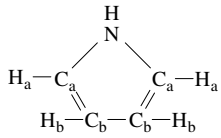
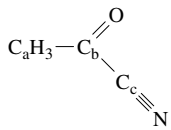
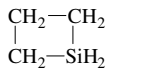
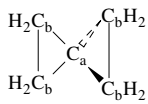
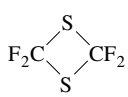
Compound	Structure				Method
Fulvene			$C_a—C_d$	1.349	MW
			$C_a—C_b$	1.470	
			$C_b—C_c$	1.355	
			$C_c—C_c$	1.476	
			$C_b—H$	1.078	
			$C_c—H$	1.080	
	$C_d—H$	1.13	$\angle C_bC_aC_b$	106.6	
	$\angle C_aC_bC_c$	107.7	$\angle C_bC_cC_c$	109	
	$\angle C_aC_bH$	124.7	$\angle C_bC_cH$	126.4	
	$\angle HC_dH$	117			
2-Furaldehyde			$C_a—C_e$	1.458	MW
			$C_e—O_b$	1.250	
			$C_e—H$	1.088	
			$\angle C_eC_aC_b$	133.9	
	$\angle C_aC_eH$	116.9	$\angle C_aC_eO$	121.6	
	trans conformer (with respect to the O_a and O_b atoms)				
Furan			$C_b—C_b$	1.431	MW
			$C_a—C_b$	1.361	
			$C_a—O$	1.362	
			$C_a—H_a$	1.075	
			$C_b—H_b$	1.077	
	$\angle C_aC_bC_b$	106.1	$\angle C_aOC_a$	106.6	
	$\angle C_bC_aO$	110.7	$\angle OC_aH_a$	115.9	
	$\angle C_bC_bH_b$	128.0			
Furfural → 2-Furaldehyde					
Glycolaldehyde			$C_b—O_b$	1.209	MW
			$C_a—O_a$	1.437	
			$C_a—C_b$	1.499	
			$O_a—H_a$	1.051	
			$C_b—H_c$	1.102	
			$C_a—H_b$	1.093	
	$\angle C_aC_bO_b$	122.7	$\angle C_aC_bH_c$	115.3	
	$\angle C_bC_aO_a$	111.5	$\angle C_aO_aH_a$	101.6	
	$\angle C_bC_aH_b$	109.2	$\angle H_bC_aH_b$	107.6	
	$\angle H_bC_aO_a$	109.7			
Glyoxal	C—C	1.526	C—O	1.212	ED, UV
CHOCHO	C—H	1.132	∠CCO	121.2	
	∠HCO	112	*trans* conformer	(C_{2h} (assumed))	
Hexachloroethane	C—C	1.56	C—Cl	1.769	ED
Cl_3CCCl_3	∠CCCl	110.0			
2,4-Hexadiyne	$C_aH_3—C_b≡C_c—C_c≡C_b—C_aH_3$				ED
	$C_a—C_b$	1.450	$C_b—C_c$	1.208	
	$C_c—C_c$	1.377	$C_a—H$	1.09	
Hexafluoroethane	C—C	1.545	C—F	1.326	ED
F_3CCF_3	∠CCF	109.8	staggered conformation		
Hexafluoropropene	average value of the C=C and C—F distances			1.329	ED
$CF_2=CFCF_3$	C—C	1.513	∠CCC	127.8	
	∠FCC (CF_2)	124	∠FCC (CF)	120	
	∠FCC (CF_3)	110			
1,3,5-Hexatriene	$H_2C_a=C_bH—C_cH=C_cH—C_bH=C_aH_2$				ED
	$C_a—C_b$	1.337	$C_b—C_c$	1.458	
	$C_c—C_c$	1.368	$\angle C_aC_bC_c$	121.7	
	$\angle C_bC_cC_c$	124.4			
Iminocyanide radical	N—H	1.034	N···N	2.470	UV
HNCN	∠HNC	116.5	∠NCN	∼180	
Iodocyanoacetylene	$I—C_a$	1.985	$C_a—C_b$	1.207	MW
$I—C_a≡C_b—C_c≡N$	$C_b—C_c$	1.370	$C_c—N$	1.160	

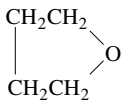
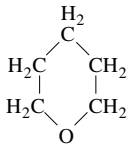
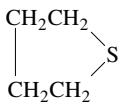
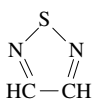
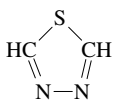
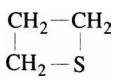
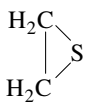
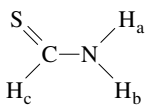
Compound	Structure					Method
Isobutane	C_a—H	1.122	C_b—H		1.113	ED, MW
$(C_bH_3)_3C_aH$	C_a—C_b	1.535	∠$C_bC_aC_b$		110.8	
	∠C_aC_bH	111.4				
Isobutylene → 2-Methylpropene						
Ketene	C—C	1.317	C—O		1.161	MW
CH_2=C=O	C—H	1.080	∠HCH		123.0	
Malononitrile	C—H	1.091	C—C		1.480	MW
$C_aH_2(C_bN)_2$	C—N	1.147	∠CCC		110.4	
	∠HCH	108.4	∠CCN		176.6	
	(The two N atoms are bent away from each other in the plane of C_b—C_a—C_b)					
Methane	C—H (r_e)	1.0870	(T_d)			MW
CH_4						
Methanethiol	C—H	1.09	C—S		1.819	MW
CH_3SH	S—H	1.34	∠HSC		96.5	
	∠HCH	109.8				
	angle between the CH_3 symmetry axis and the C—S bond 2.2. (The axis of the CH_3 group is tilted away from the H atom with respect to the C—S bond.)					
Methanol	C—H	1.0936	C—O		1.4246	MW
CH_3OH	O—H	0.9451	∠HCH		108.63	
	∠COH	108.53				
	angle between the CH_3 symmetry axis and the C—O bond (The axis of the CH_3 group is tilted away from the H atom with respect to the C—O bond.)				3.27	
Methyl radical	C—H	1.08	planar			UV
$\cdot CH_3$						
N-Methylacetamide			C_a—C_b		1.520	ED
			N—C_c		1.469	
			C—H		1.107	
	C_b—N	1.386	C_b—O		1.225	
	∠C_bNC_c	119.7				
	∠NC_bO	121.8				
	∠C_aC_bN	114.1				
Methylacetylene → Propyne						
Methylal → Dimethoxymethane						
Methylamine	N—H	1.010	C—N		1.471	MW
CH_3NH_2	C—H	1.099	∠HNH		107.1	
	∠HNC	110.3	∠HCH		108.0	
	dihedral angle between the CH_3 symmetry axis and the C—N bond (The axis of the CH_3 group is tilted away from the NH_2 group with respect to the C—N bond.)				2.9	
Methyl azide			C—H		1.09	ED
			C—N_a		1.468	
			N_a—N_b		1.216	
	N_b—N_c	1.113	∠CN_aN_b		116.8	
	NNN linear					
Methyl bromide	C—H (r_e)	1.086	C—Br (r_e)		1.933	MW, IR
CH_3Br	∠HCH (θ_e)	111.2	(C_{3v})			
Methyl chloride	C—H	1.090	C—Cl		1.785	MW, IR
CH_3Cl	∠HCH	110.8				
Methyldiazirine		C—N	1.481	C—C	1.501	MW
		N—N	1.235	∠NCN	49.3	
		dihedral angle between the CNN plane and the C—C bond		122.3		
Methylene	C—H	1.078	∠HCH	130		LMR
:CH_2						
Methylenecyclopropane			C_a—C_b	1.332		MW
			C_b—C_c	1.457		
			C_c—C_c	1.542		
	C_c—H	1.09	∠$C_cC_bC_c$	63.9		

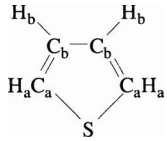
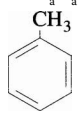
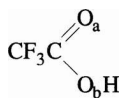
Compound	Structure					Method
	$\angle HC_aH$	114.3	$\angle HC_cH$	113.5		
	dihedral angle between the C_cH_2 plane and the $C_c—C_c$ bond			150.8		
3-Methyleneoxetane			$C_b—C_c$	1.52		MW
			$C_c—O$	1.45		
			$C_a—C_b$	1.33		
	C—H	1.09 (assumed)	$\angle C_cC_bC_c$	87		
	$\angle HC_cH$	114 (assumed)	$\angle HC_aH$	120 (assumed		
Methyl fluoride	C—H (r_e)	1.095				MW, IR
CH_3F	C—F (r_e)	1.382	$\angle$HCH (θ_e)	110.45	(C_{3v})	
Methyl formate			$C_a—H$	1.08		ED
			$C_b—O_b$	1.206		
			C—O (average)	1.393		
			$C_b—H$	1.101 (assumed)		
	$\angle O_aC_bO_b$	127	$\angle$COC	114		
	$\angle O_aC_aH$	110				
Methylgermane	C—H	1.083	Ge—H	1.529		MW
CH_3GeH_3	C—Ge	1.945	$\angle$HCH	108.4		
	$\angle$HGeH	109.3				
Methyl hypochlorite	C—H	1.103	O—Cl	1.674		MW
CH_3OCl	O—C	1.389	$\angle$HCH	109.6		
	$\angle$COCl	112.8				
Methylidyne radical	C—H (r_e)	1.1198				UV
:CH						
Methylidyne phosphide	H—C (r_e)	1.0692	C—P (r_e)	1.5398		MW
HCP						
Methyl iodide	C—H (r_e)	1.084	C—I (r_e)	2.132		MW, IR
CH_3I	$\angle$HCH (θ_e)	111.2	(C_{3v})			
Methyl isocyanide	$C_aH_3—N≡C_b$	$C_a—H$	1.102	$C_a—N$	1.424	MW
	$N—C_b$	1.166	$\angle NC_aH$	109.12		
Methylketene			O—C_a	1.171		MW
			$C_b—C_c$	1.518		
			$C_c—H$	1.10		
	$C_a—C_b$	1.306	$C_b—H$	1.083		
	$\angle OC_aC_b$	180.5	$\angle C_aC_bC_c$	122.6		
	$\angle C_aC_bH$	113.7	$\angle C_cC_bH$	123.7		
	$\angle$HCH	109.2				
Methylmercury chloride	Hg—Cl	2.282	C—H	1.15		MW,
CH_3HgCl	Hg—C	1.99	(C_{3v})			NMR
Methyl nitrate			$C—H_a$	1.10		MW
			$C—H_b$	1.09		
			C—O	1.437		
			O—N	1.402		
	$N—O_a$	1.205	$N—O_b$			
	$\angle OCH_a$	110	$\angle OCH_b$	103		
	$\angle$CON	112.7	$\angle ONO_a$	118.1		
	$\angle ONO_b$	112.4				
Methylphosphine	C—P	1.858	C—H	1.094		ED
CH_3PH_2						
2-Methylpropane → Isobutane						
2-Methylpropene			$C_a—H$		1.119	ED, MW
			$C_c—H_c$		1.10	
			$C_a—C_b$		1.508	
			$C_b—C_c$		1.342	
	$\angle HC_aC_b$ (average)	111.4	$\angle H_cC_cH_c$		118.5	
	$\angle C_aC_bC_a$	115.6	$\angle C_aC_bC_c$		122.2	
	$\angle HC_aH$	107.9	$\angle C_bC_cH$		121	

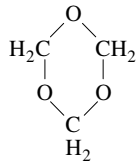
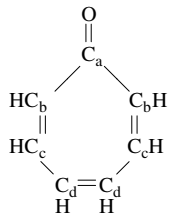
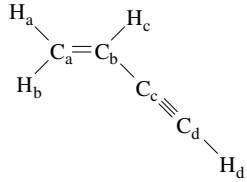
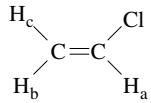
Compound	Structure						Method
Methylsilane	C—H	1.093	C—Si		1.867		MW
CH_3SiH_3	Si—H	1.485	∠HCH		107.7		
	∠HSiH	108.3	(C_{3v})				
Methylstannane	C—Sn	2.143	Sn—H		1.700		MW
CH_3SnH_3			(C_{3v})				
Methyl thiocyanate	C_aH_3	S—C_b	1.684	S—C_a		1.824	MW
	S—C_b—N	C_b—N	1.170	C—H		1.081	
	∠C_aSC_b	99.0	∠HCH	110.6	∠HCS	108.3	
Naphthalene			C_a—C_b		1.37		ED
			C_b—C_b		1.41		
			C_a—C_c		1.42		
			C_c—C_c		1.42		
			C—C (average)		1.40		
			∠$C_aC_cC_c$		119.4		
Neopentane	C—C	1.537	C—H		1.114		ED
$C(CH_3)_4$	∠CCH	112					
Nickelocene → Bis (cyclopentadienyl) nickel							
Nitromethane	C—H	1.088 (assumed)	C—N		1.489		MW
CH_3NO_2	N—O	1.224	∠NCH		107		
	∠ONO	125.3					
N-Nitrosodimethylamine	N—O	1.235	N—N		1.344		ED
$(CH_3)_2NNO$	C—N	1.461	∠ONN		113.6		
	∠CNC	123.2	∠CNN		116.4		
Nitrosomethane	C—N	1.49	N—O		1.22		MW
CH_3NO	C—H	1.084	∠CNO		112.6		
	∠NCH	109.0					
Norbornane → Bicyclo[2.2.1]heptane							
Norbornadiene → Bicyclo[2.2.1]hepta-2,5-diene							
1,2,5-Oxadiazole		O—N	1.380	∠NON	110.4		MW
		C—N	1.300	∠ONC	105.8		
		C—C	1.421	∠CCN	109.0		
		C—H	1.076	∠CCH	130.2		
		∠NCH	120.9	planar			
1,3,4-Oxadiazole		O—C	1.348	∠COC	102.0		MW
		C—N	1.297	∠OCN	113.4		
		N—N	1.399	∠CNN	105.6		
		C—H	1.075	∠OCH	118.1		
		∠NCH	128.5	planar			
Oxalic acid			C—C		1.544		ED
			C—O_a		1.205		
			C—O_b		1.336		
			O_b—H		1.05		
			∠CCO_a		123.1		
			∠O_aCO_b		125.0		
			∠CO_bH		104		
Oxalyl dichloride			C—O		1.182		ED
			C—C		1.534		
			C—Cl		1.744		
	∠CCO	124.2	∠CCCl		111.7		
	fraction of the *trans* conformer at 0°C 68%, that of the *gauche* conformer 32%						
Oxetane			C—O		1.448		MW
			C—C		1.546		
			C—H (average)		1.090		
			∠COC		92		

Compound	Structure						Method
	∠CCC	85	∠OCC	92			
	∠HCH (average)	109.9					
Oxirane → Ethylene oxide							
Phenol			C—C (average)	1.397			MW
			C_b—H	1.084			
			C_c—H	1.076			
			C_d—H	1.082			
			C_a—O	1.364			
			O—H	0.956			
			∠COH	109.0			
Phosphirane		C—P	1.867	P—H		1.43	MW
		C—C	1.502	C—H		1.09	
		∠CPC	47.4	∠HCH		114.4	
	∠HPC 95.2	∠CCH	118				
	dihedral angle between the PCC plane and the PH bond		95.7				
Piperazine			C—C	1.540			ED
			C—N	1.467			
			C—H	1.110			
	∠CNC	109.0	∠CCN (C_{2h})	110.4			
Pivalonitrile	C_a—C_b	1.495	C_a—N	1.159			MW
$(C_cH_3)_3C_b$—C_a≡N	C_b—C_c	1.536	∠$C_cC_bC_c$	110.5			
Propadiene → Allene							
Propane	C—C	1.532	C—H	1.107			ED
C_3H_8	∠CCC	112	∠HCH	107			
Propenal → Acrylaldehyde							
Propene			C_a—H_a	1.104			ED, MW
			C_a—C_b	1.341			
			C_c—H_d	1.117			
			C_b—C_c	1.506			
			∠$C_bC_aH_{a,b,c}$	121.3			
	∠$C_bC_cH_d$	110.7	∠$C_aC_bC_c$	124.3			
l-Propenyl chloride	CH_3—C_bH=C_aH—Cl	C_a—Cl	1.728	MW			
	∠C_bC_aCl	121.9	*trans* conformer				
Propiolaldehyde	H_aC_a≡C_b—C_cH_cO		C_a—H_a	1.085			ED, MW
	C_a—C_b	1.211	C_b—C_c	1.453			
	C_c—H_c	1.130	C_c—O	1.214			
	∠C_bC_cO	124.2	∠$C_bC_cH_c$	113.7			
	∠$C_aC_bC_c$	178.6	planar				
Propylene → Propene							
Propylene oxide			C_a—C_b	1.51			MW
			∠$C_aC_bC_c$	121.0			
			dihedral angle between the C_bC_cO plane and the C_aC_b bond	123.8			
Propynal → Propiolaldehyde							
Propyne	H_3C_c—C_b≡C_aH		C_c—H	1.105			MW
	C_c—C_b	1.459	C_b—C_a	1.206			
	C_a—H	1.056	∠HC_cC_b	110.2			
Pyrazine			C—C	1.339	C—N	1.403	ED
			C—H	1.115	∠CCN	115.6	
			∠CCH	123.9			
Pyridazine			N—C_a	1.341			ED, MW
			C_a—C_b	1.393			
			N—N	1.330			
			C_b—C_b	1.375			
	∠NCC	123.7	∠NNC	119.3			

Compound	Structure						Method
Pyridine			$N—C_a$			1.340	MW
			$C_b—C_c$			1.394	
			$C_b—H_b$			1.081	
			$C_a—C_b$			1.395	
			$C_a—H_a$			1.084	
			$C_c—H_c$			1.077	
	$\angle C_aNC_a$	116.8	$\angle NC_aC_b$			123.9	
	$\angle C_aC_bC_c$	118.5	$\angle C_bC_cC_b$			118.3	
	$\angle NC_aH_a$	115.9	$\angle C_cC_bH_b$			121.3	
Pyrimidine			N—C	1.340	C—C	1.393	ED
			∠NCN	127.6	∠CNC	115.5	
	(C_{2v} assumed)						
Pyrrole			N—Ca			1.370	MW
			$C_b—C_b$			1.417	
			$C_a—C_b$			1.382	
			N—H			0.996	
			$C_a—H_a$			1.076	
	$C_b—H_b$	1.077	$\angle C_aNC_a$			109.8	
	$\angle NC_aC_b$	107.7	$\angle C_aC_bC_b$			107.4	
	$\angle NC_aH_a$	121.5	$\angle C_bC_bH$			127.1	
Pyruvonitrile			C—H			1.12	ED, MW
			C—N			1.17	
			C—O			1.208	
			$C_b—C_c$			1.477	
	$C_a—C_b$	1.518	∠HCH			109.2	
	$\angle C_aC_bO$	124.5	$\angle C_aC_bC_c$			114.2	
	∠CCN	179					
Ruthenocene → Bis (cyclopentadienyl) ruthenium							
Silacyclobutane			Si—C			1.892	ED
			C—C			1.600	
			Si—H			1.47	
	C—H	1.14	∠CSiC			80.7	
	∠SiCC	84.8	∠CCC			99.8	
	dihedral angle between the CCC and CSiC planes					146	
Spiropentane			$C_b—C_b$			1.52	ED
			$C_a—C_b$			1.47	
			C—H			1.09	
			$\angle C_bC_aC_b$			62	
	∠HCH	118	(D_{2d})				
Succinonitrile	CH_2CN	C—C	1.561	C—C(N)		1.465	ED
	CH_2CN	C—N	1.161	C—H		1.09	
		∠CCC	110.4				
	fraction of the *anti* conformer at 170°C 74%,						
	dihedral angle of CCCC for the *gauche* conformer					75	
Tetrachloroethylene	C—Cl	1.718	C—C			1.354	ED
$CCl_2=CCl_2$	∠ClCCl	115.7					
Tetracyanoethylene	C—N	1.162	C—C			1.435	ED
$(CN)_2C=C(CN)_2$	C=C	1.357	∠CC=C			121.1	
Tetrafluoro-1,3-dithietane			C—S			1.785	ED
			C—F			1.314	
			∠CSC			83.2	
	∠FCS	113.7	(D_{2h} assumed)				
Tetrafluoroethylene	C—C	1.31	C—F			1.319	ED
$CF_2=CF_2$	∠CCF	123.8	(D_{2h} assumed)				

Compound	Structure						Method
Tetrahydrofuran	C—H	1.115	C—O		1.428		ED
	C—C	1.536					
	The skeletal bending vibration of the molecular plane is essentially free pseudorotation						
Tetrahydropyran			C—O		1.420		ED
			C—C		1.531		
			C—H		1.116		
			∠COC		111.5		
			∠OCC		111.8		
	∠CCC (C)	108	∠CCC (O)		111		
	chair form						
Tetrahydrothiophene	C—S	1.839	C—H		1.120		
	C—C	1.536	∠CSC		93.4		
	∠SCC	106.1	∠CCC		105.0		
Tetramethylgermane	Ge—C	1.945	C—H		1.12		ED
$(CH_3)_4Ge$	∠GeCH	108	(T_d excluding the H atoms)				
Tetramethyllead	Pb—C	2.238	(T_d excluding the H atoms)				ED
$(CH_3)_4Pb$							
Tetramethylsilane	C—H	1.115	C—Si		1.875		ED
$(CH_3)_4Si$	∠HCH	109.8	(T_d excluding the H atoms)				
Tetramethylstannane	C—Sn	2.144					ED
$(CH_3)_4Sn$	C—H	1.12	(T_d excluding the H atoms)				
1,2,5-Thiadiazole		S—N	1.631	∠NSN		99.6	MW
		C—N	1.328	∠CCN		113.8	
		C—C	1.420	∠CCH		126.2	
		C—H	1.079	planar			
1,3,4-Thiadiazole		S—C	1.721	∠CSC		86.4	MW
		N—N	1.371	∠SCN		114.6	
		C—N	1.302	∠CCN		112.2	
		C—H	1.08	∠SCH		121.9	
		∠NCH	123.5			planar	
Thietane			C—S		1.847		ED, MW
			C—C		1.549		
			C—H (average)		1.100		
	∠CSC	76.8	∠HCH (average)		112		
	dihedral angle between the CCC and CSC planes				154		
Thiirane		C—C	1.484	∠HCH		116	MW
		C—H	1.083	∠CSC		48.3	
		C—S	1.815	∠CCS		65.9	
		dihedral angle between the CH_2 plane and the C—C bond		152			
Thioformaldehyde	C—S	1.611	C—H		1.093		MW
CH_2S	∠HCH	116.9					
Thioformamide			N—H_a		1.002		MW
			N—H_b		1.007		
			C—N		1.358		
	C—S	1.626	C—H_c		1.10		
	∠H_aNH_b	121.7	∠H_aNC		117.9		
	∠H_bNC	120.4	∠NCS		125.3		
	∠NCH_c	108	∠SCH_c		127		
Thiolane → Tetrahydrothiophene							

Compound	Structure					Method
Thiophene			$C_a—H_a$	1.078		MW
			$C_b—H_b$	1.081		
			$C_a—S$	1.714		
			$C_a—C_b$	1.370		
			$C_b—C_b$	1.423		
			$\angle C_aSC_a$	92.2		
	$\angle SC_aC_b$	115.5	$\angle C_aC_bC_b$	112.5		
	$\angle SC_aH_a$	119.9	$\angle C_bC_bH_b$	124.3		
Toluene		C—C (ring)	1.399	$C—CH_3$	1.524	ED
		C—H (average)	1.11			
		the difference between the C—H(CH_3) and C—H(ring): about 0.01				
1,1,1-Tribromoethane	C—Br	1.93	C—H	1.095 (assumed)		MW
CH_3CBr_3	C—C	1.51 (assumed)	∠CCBr	108		
	∠BrCBr	111	∠CCH	109.0 (assumed)		
Tribromomethane → Bromoform						
Tri-*tert*-butyl methane	$C_a—C_b$	1.611	C—H	1.111		ED
$HC_a[C_b(C_cH_3)_3]_3$	$C_b—C_c$	1.548	$\angle C_aC_bC_c$	113.0		
Tricarbon dioxide	C—O	1.163	C—C	1.289		ED
OCCCO	linear (with a large-amplitude bending vibration)					
Trichloroacetonitrile	C—N	1.165	C—C	1.460		ED
CCl_3CN	C—Cl	1.763	∠ClCCl	110.0		
1,1,1-Trichloroethane	C—H	1.090	C—C	1.541		MW
CH_3CCl_3	C—Cl	1.771	∠HCH	110.0		
	∠CCH	108.9	∠ClCCl	109.4		
	∠CCCl	109.6				
Trichloro(methyl)germane	Ge—Cl	2.132	Ge—C	1.89		ED, MW
CH_3GeCl_3	C—H	1.103 (assumed)	∠ClGeCl	106.4		
	∠GeCH	110.5 (assumed)				
Trichloro(methyl)silane	C—Si	1.876	Si—Cl	2.021		MW
CH_3SiCl_3			(C_{3v})			
Trichloro(methyl)stannane	Sn—Cl	2.304	Sn—C	2.10		ED
CH_3SnCl_3	C—H	1.100	∠CSnCl	113.9		
	∠ClSnCl	104.7	∠SnCH	108		
Triethylenediamine → 1,4-Diazabicyclo [2.2.2]octane						
Trifluoroacetic acid			C—F	1.325		ED
			C—C	1.546		
			$C—O_a$	1.192		
	$C—O_b$	1.35	O—H	0.96 (assumed)		
	$\angle CCO_a$	126.8	$\angle CCO_b$	111.1		
	∠CCF	109.5				
1,1,1-Trifluoroethane	C—C	1.494	C—F	1.340		ED
CH_3CF_3	C—H	1.081	∠CCF	119.2		
	∠CCH	112				
Trifluoromethane → Fluoroform						
1,1,1-Trifluoro-2,2,2-trichloroethane	C—C	1.54	C—F	1.33		MW
CF_3CCl_3	C—Cl	1.77	∠CCF	110		
	∠CCCl	109.6	staggered conformation			
Trimethylaluminium	C—H	1.113	Al—C	1.957		ED
$(CH_3)_3Al$	∠AlCH	111.7	∠CAlC	120		
Trimethylamine	C—N	1.458	C—H	1.100		ED
$(CH_3)_3N$	∠CNC	110.9	∠HCH	110		
Trimethylarsine	C—As	1.979	∠CAsC	98.8		ED
$(CH_3)_3As$	∠AsCH	111.4				
Trimethylbismuth	Bi—C	2.263	C—H	1.07		ED
$(CH_3)_3Bi$	∠CBiC	97.1				
Trimethylborane	C—B	1.578	C—H	1.114		ED
$(CH_3)_3B$	∠CBC	120.0	∠BCH	112.5		

Compound	Structure				Method
Trimethyleneimine → Azetidine					
Trimethylphosphine	C—P	1.847	C—H	1.091	ED
$(CH_3)_3P$	∠CPC	98.6	∠PCH	110.7	
1,3,5-Trioxane			C—O	1.422	MW
			∠OCO	112.2	
			∠COC	110.3	
Triphenylamine	C—C	1.392	C—N	1.42	ED
$(C_6H_5)_3N$	∠CNC	116	(C_3)		
	torsional dihedral angle of the two phenyl rings 47° (defined to be 0 when the symmetry axis is contained in the phenyl planes)				
Tropone			C_a—O	1.23	ED
			C_a—C_b	1.45	
			C_b—C_c	1.36	
			C_c—C_d	1.46	
			C_d—C_d	1.34	
			$\angle C_bC_aC_b$	122	
			$\angle C_aC_bC_c$	133	
	$\angle C_bC_cC_d$	126	$\angle C_cC_dC_d$	130	
				(C_{2v})	
Vinylacetylene			C_b—C_c	1.434	ED, MW
			C_a—C_b	1.344	
			C_c—C_d	1.215	
			C_a—H_a	1.11	
			C_d—H_d	1.09	
			$\angle C_aC_bC_c$	123.1	
	$\angle C_bC_cC_d$	178	$\angle H_aC_aC_b$	119	
	$\angle H_bC_aC_b$	122	$\angle H_cC_bC_a$	122	
	$\angle C_cC_dH_d$	182			
Vinyl chloride			C—C	1.342	ED, MW
			C—Cl	1.730	
			C—H	1.09	
	∠CCCl	122.5	$\angle CCH_a$	124	
	$\angle CCH_b$	120	$\angle CCH_c$	121.1	