BOND LENGTHS AND ANGLES IN GAS-PHASE MOLECULES

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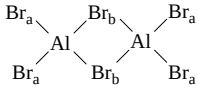
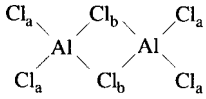
Internuclear distances and bond angles are represented in units of Å (1 Å = 10^{-10} m) and degrees, respectively. The same but inequivalent atoms are discriminated by subscripts a, b, etc. In some molecules ax for axial and eq for equatorial are also used. All measurements were made in the gas phase. 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.

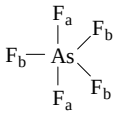
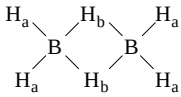
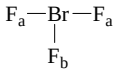
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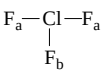
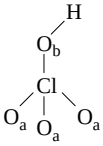
STRUCTURES OF ELEMENTS AND INORGANIC COMPOUNDS
Compounds are Arranged in Alphabetical Order by their Chemical Formulas
(Lengths in Å and Angles in Degrees)

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

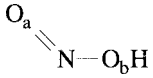
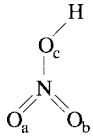
BOND LENGTHS AND ANGLES IN GAS-PHASE MOLECULES (continued)

Compound	Structure									Method
AsF_5		$As—F_a$	1.711			$As—F_b$	1.656			
						(D_{3h})				
AsH_3	$As—H$ (r_e)	1.511				$\angle HAsH$ (θ_e)	92.1			MW, IR
AsI_3	As—I	2.557				$\angle IAsI$	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		$\angle FBF$	118.3		MW
BF_2OH	B—F	1.32		B—O	1.34		O—H	0.941		MW
	$\angle FBF$	118		$\angle FBO$	123		$\angle BOH$	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
	$\angle PBH$	103.6		$\angle BPH$	116.9		$\angle HBH$	114.6		
	$\angle HPH$	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			
						$\angle H_aBH_a$	122			
						$\angle H_bBH_b$	97			
$B_3H_3O_3$	B—O	1.376				$\angle BOB \cong \angle OBO$	120			ED
$B_3H_6N_3$	B—N	1.435		B—H	1.26		N—H	1.05		ED
	$\angle NBN$	118		$\angle BNB$	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				$\angle BrBiBr$	90	(C_{3v})		ED
BiCl	Bi—Cl (r_e)	2.4716								MW
$BiCl_3$	Bi—Cl	2.423				$\angle ClBiCl$	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
				$\angle F_aBrF_b$	86.2		(C_{2v})			
BrF_5	Br—F (average)	1.753								ED, MW
	$(Br—F_{eq}) - (Br—F_{ax}) = 0.069$									
	$\angle F_{ax}BrF_{eq}$	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

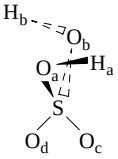
BOND LENGTHS AND ANGLES IN GAS-PHASE MOLECULES (continued)

Compound	Structure								Method
$CClF_3$	C—Cl	1.752		C—F	1.325		∠FCF	108.6	ED, MW
CCl_3F	C—Cl	1.754		C—F	1.362		∠ClCCl (C_{3v})	111	MW
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
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				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

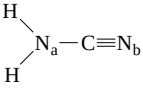
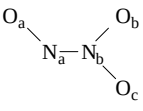
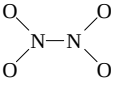
BOND LENGTHS AND ANGLES IN GAS-PHASE MOLECULES (continued)

Compound	Structure								Method
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
$Fe(CO)_5$	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)	1.1532			MW, IR
					linear				
HCNO	H—C	1.027	C—N	1.161	N—O	1.207			MW
					linear				
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				

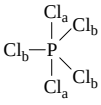
BOND LENGTHS AND ANGLES IN GAS-PHASE MOLECULES (continued)

Compound	Structure									Method
HNSO	N—H	1.029		N—S	1.512		S—O	1.451		MW
	∠HNS	115.8		∠NSO	120.4					
				planar						
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
H_2SO_4				O—H	0.97		$S—O_a$	1.574		MW
				$S—O_c$	1.422		$∠H_aO_aS$	108.5		
				$∠O_aSO_b$	101.3		$∠O_cSO_d$	123.3		
				$∠O_aSO_c$	108.6		$∠O_aSO_d$	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		∠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
	$∠F_{ax}IF_{eq}$	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			
						∠ClLiCl	108			
$LuCl_3$	Lu—Cl	2.417				∠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
	∠ClMoCl	87.2				(C_{4v})				

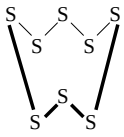
BOND LENGTHS AND ANGLES IN GAS-PHASE MOLECULES (continued)

Compound	Structure								Method
MoF_6	Mo—F	1.820			(O_h)				ED
$NClH_2$	N—H	1.017			N—Cl	1.748			MW, IR
	∠HNCl	103.7			∠HNH	107			
NCl_3	N—Cl	1.759			∠ClNCl	107.1			ED
NF_2	N—F	1.3528			∠FNF	103.18			MW
NH_2	N—H	1.024			∠HNH	103.3			UV
NH_2CN	N—H	1.00			N_a—C	1.35			MW
			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

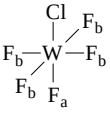
BOND LENGTHS AND ANGLES IN GAS-PHASE MOLECULES (continued)

Compound	Structure								Method
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)	
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 (D_{3h})	2.020		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

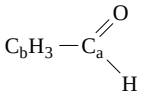
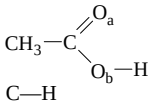
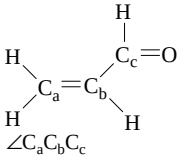
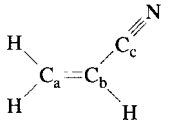
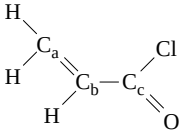
BOND LENGTHS AND ANGLES IN GAS-PHASE MOLECULES (continued)

Compound	Structure								Method
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
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

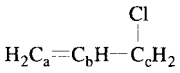
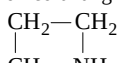
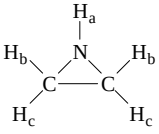
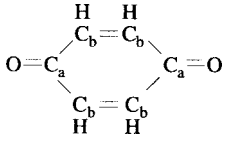
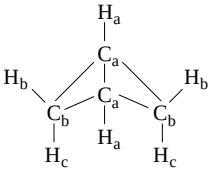
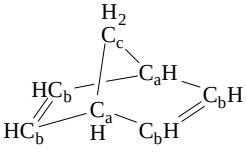
BOND LENGTHS AND ANGLES IN GAS-PHASE MOLECULES (continued)

Compound	Structure					Method
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)			
$SnCl_4$	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

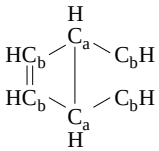
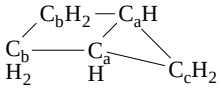
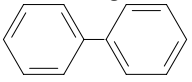
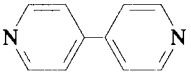
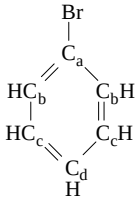
STRUCTURES OF ORGANIC MOLECULES
Compounds are Arranged in Alphabetical Order by Chemical Name; Cross References are Given for Common Synonyms (Lengths in Å and Angles in Degrees)

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	

BOND LENGTHS AND ANGLES IN GAS-PHASE MOLECULES (continued)

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	

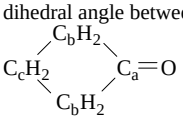
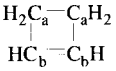
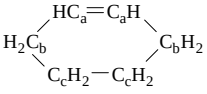
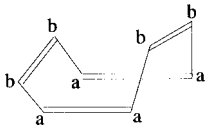
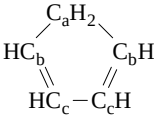
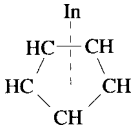
BOND LENGTHS AND ANGLES IN GAS-PHASE MOLECULES (continued)

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	ED
$(C_5H_5)_2Ni$				(D_{5h})	
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			

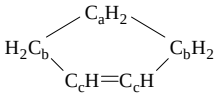
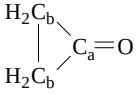
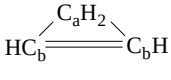
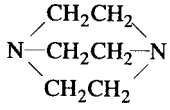
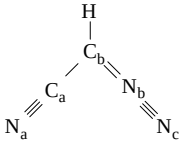
BOND LENGTHS AND ANGLES IN GAS-PHASE MOLECULES (continued)

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—H (average)	1.108		
	C_aH_2			∠CCC	124.4		
	∠C_bC_aH	120.9		*anti* conformer	(C_{2h})		
1,3-Butadiyne	$HC_a{\equiv}C_b$—$C_b{\equiv}C_aH$			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			
	∠$C_aC_bC_b$	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—$C_b{\equiv}C_b$—C_aH_3	C—H		1.116	ED		
	C_b—C_b	1.214		C_a—C_b	1.468		
	∠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
$HC{\equiv}CCl$	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
$ClC{\equiv}CBr$	C—Br	1.784					
Chlorocyanoacetylene	C—Cl	1.624		C—C	1.205		ED
$ClC{\equiv}CCN$	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})			

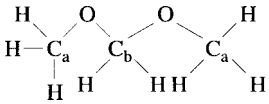
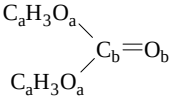
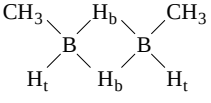
BOND LENGTHS AND ANGLES IN GAS-PHASE MOLECULES (continued)

Compound	Structure				Method
Chloroiodoacetylene	C—Cl	1.63	C—I	1.99	MW
ClC≡CI	C—C	1.209 (assumed)			
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)				

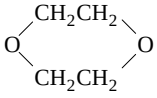
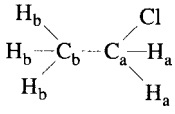
BOND LENGTHS AND ANGLES IN GAS-PHASE MOLECULES (continued)

Compound	Structure						Method
Cyclopentene				C_a—C_b	1.546		ED
				C_b—C_c	1.519		
				C_c—C_c	1.342		
				$\angle C_bC_aC_b$	104.0		
	$\angle C_bC_cC_c$	110.0		$\angle C_aC_bC_c$	103.0		
	dihedral angle between the $C_bC_aC_b$ and $C_bC_cC_cC_b$ planes				151.2		
Cyclopropane	C—C	1.512		C—H	1.083		R
$(CH_2)_3$	$\angle$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
$C_{10}H_{18}$	$\angle$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		
				$\angle$NCC	110.2		
				$\angle$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		
				$\angle$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		$\angle$HCH	126.0 linear		
1,2-Dibromoethane	C—C	1.506		C—Br	1.950		ED
CH_2BrCH_2Br	C—H	1.108		$\angle$CCBr	109.5		
	$\angle$CCH 110		fraction of the *trans* conformer at 25°C		95%		
Dibromomethane	C—H	1.08		C—Br	1.924		ED
CH_2Br_2	$\angle$HCBr	109		$\angle$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		
	$\angle$CCCl	121.4		$\angle$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		$\angle$CCC	111.5		
	$\angle$CCCl (*ee*)	108.6		$\angle$CCCl (*aa*)	110.6		
	$\angle$HCCl (*ee*)	111.5		$\angle$HCCl (*aa*)	107.6		
	ee 49%		*aa* 51%		e: equatorial, a: axial		

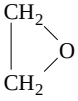
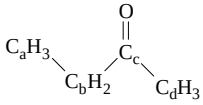
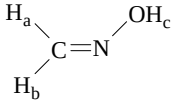
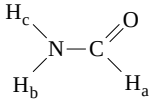
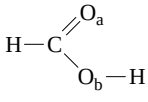
BOND LENGTHS AND ANGLES IN GAS-PHASE MOLECULES (continued)

Compound	Structure				Method
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%				
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	
	$\angle O_aC_bO_a$	107	$\angle C_bO_aC_a$	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	$\angle C_aNC_a$	115.5	
	$\angle C_aNC_b$	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	

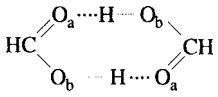
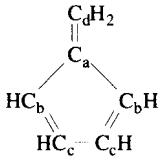
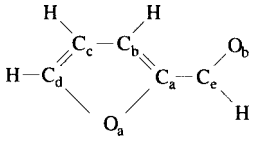
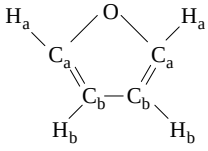
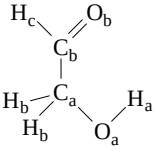
BOND LENGTHS AND ANGLES IN GAS-PHASE MOLECULES (continued)

Compound	Structure				Method
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	$C_aH_3SC_bSC_aH_3$ (O)		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		
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			

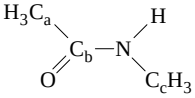
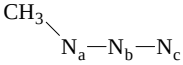
BOND LENGTHS AND ANGLES IN GAS-PHASE MOLECULES (continued)

Compound	Structure					Method
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						
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			

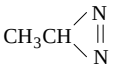
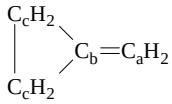
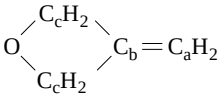
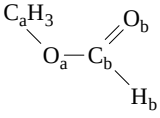
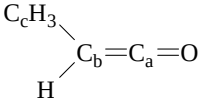
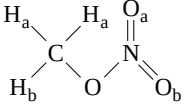
BOND LENGTHS AND ANGLES IN GAS-PHASE MOLECULES (continued)

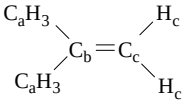
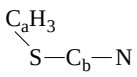
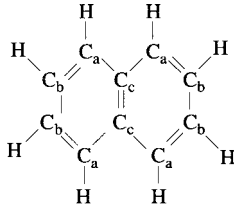
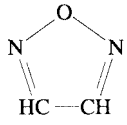
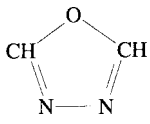
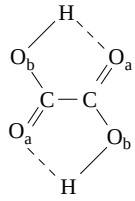
Compound	Structure					Method
Formic acid dimer			$O_a\cdots O_b$	2.703		ED
			C—O_a	1.220		
			C—O_b	1.323		
			$\angle O_aCO_b$	126.2		
			$\angle CO_aO_b$	108.5		
Formyl radical		C—H	1.110	C—O	1.1712	MW
		$\angle$HCO	127.43			
Fulvene			C_a—C_d	1.349		MW
			C_a—C_b	1.470		
			C_b—C_c	1.355		
			C_c—C_c	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	$\angle$CCO	121.2		
	$\angle$HCO	112	*trans* conformer	(C_{2h} (assumed))		
Hexachloroethane	C—C	1.56	C—Cl	1.769		ED
Cl_3CCCl_3	$\angle$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	$\angle$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	$\angle$CCC	127.8		
	$\angle$FCC (CF_2)	124	$\angle$FCC (CF)	120		
	$\angle$FCC (CF_3)	110				

BOND LENGTHS AND ANGLES IN GAS-PHASE MOLECULES (continued)

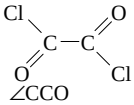
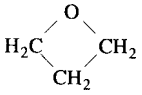
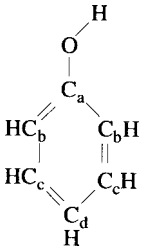
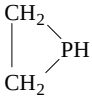
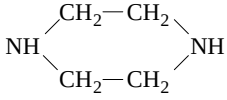
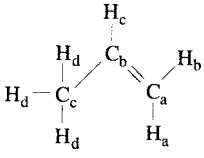
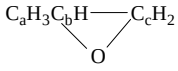
Compound	Structure				Method
1,3,5-Hexatriene	$H_2C_a{=}C_bH{-}C_cH{=}C_cH{-}C_bH{=}C_aH_2$				ED
	$C_a{-}C_b$	1.337	$C_b{-}C_c$	1.458	
	$C_c{-}C_c$	1.368	$\angle C_aC_bC_c$	121.7	
	$\angle C_bC_cC_c$	124.4			
Iminocyanide radical	N—H	1.034	N···N	2.470	UV
$H\dot{N}CN$	∠HNC	116.5	∠NCN	~180	
Iodocyanoacetylene	$I{-}C_a$	1.985	$C_a{-}C_b$	1.207	MW
$I{-}C_a{\equiv}C_b{-}C_c{\equiv}N$	$C_b{-}C_c$	1.370	$C_c{-}N$	1.160	
Isobutane	$C_a{-}H$	1.122	$C_b{-}H$	1.113	ED, MW
$(C_bH_3)_3C_aH$	$C_a{-}C_b$	1.535	$\angle C_bC_aC_b$	110.8	
	$\angle C_aC_bH$	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	
	$\angle C_bNC_c$	119.7			
	$\angle NC_bO$	121.8			
	$\angle C_aC_bN$	114.1			
Methylacetylene → Propyne					
Methylal → Dimethoxymethane					
Methylamine	N—H	1.010	C—N	1.471	MW
CH_3NH_2	C—H	1.099	∠NHN	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	$\angle CN_aN_b$	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			

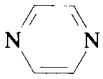
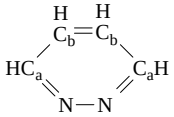
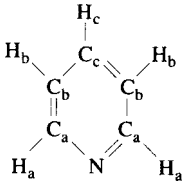
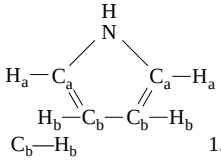
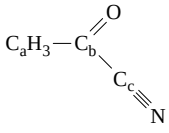
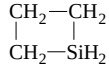
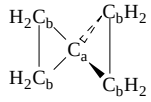
BOND LENGTHS AND ANGLES IN GAS-PHASE MOLECULES (continued)

Compound	Structure				Method
Methyldiazirine		C—N 1.481 N—N 1.235 dihedral angle between the CNN plane and the C—C bond	C—C 1.501 ∠NCN 49.3 122.3		MW
Methylene :CH_2	C—H 1.078	∠HCH 130			LMR
Methylenecyclopropane		C_a—C_b 1.332 C_b—C_c 1.457 C_c—C_c 1.542			MW
	C_c—H 1.09 ∠HC_aH 114.3	∠$C_cC_bC_c$ 63.9 ∠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 C_c—O 1.45 C_a—C_b 1.33			MW
	C—H 1.09 (assumed) ∠HC_cH 114 (assumed)	∠$C_cC_bC_c$ 87 ∠HC_aH 120 (assumed)			
Methyl fluoride CH_3F	C—H (r_e) 1.095 C—F (r_e) 1.382	∠HCH (θ_e) 110.45 (C_{3v})			MW, IR
Methyl formate		C_a—H 1.08 C_b—O_b 1.206 C—O (average) 1.393 C_b—H 1.101 (assumed)			ED
	∠$O_aC_bO_b$ 127 ∠O_aC_aH 110	∠COC 114			
Methylgermane CH_3GeH_3	C—H 1.083 C—Ge 1.945 ∠HGeH 109.3	Ge—H 1.529 ∠HCH 108.4			MW
Methyl hypochlorite CH_3OCl	C—H 1.103 O—C 1.389 ∠COCl 112.8	O—Cl 1.674 ∠HCH 109.6			MW
Methylidyne radical :ĊH	C—H (r_e) 1.1198				UV
Methylidyne phosphide HCP	H—C (r_e) 1.0692	C—P (r_e) 1.5398			MW
Methyl iodide CH_3I	C—H (r_e) 1.084 ∠HCH (θ_e) 111.2	C—I (r_e) 2.132 (C_{3v})			MW, IR
Methyl isocyanide	C_aH_3—N≡C_b	C_a—H 1.102	C_a—N 1.424		MW
	N—C_b 1.166	∠NC_aH 109.12			
Methylketene		O—C_a 1.171 C_b—C_c 1.518 C_c—H 1.10			MW
	C_a—C_b 1.306 ∠OC_aC_b 180.5 ∠C_aC_bH 113.7 ∠HCH 109.2	C_b—H 1.083 ∠$C_aC_bC_c$ 122.6 ∠C_cC_bH 123.7			
Methylmercury chloride CH_3HgCl	Hg—Cl 2.282 Hg—C 1.99	C—H 1.15 (C_{3v})			MW, NMR
Methyl nitrate		C—H_a 1.10 C—H_b 1.09 C—O 1.437 O—N 1.402			MW
	N—O_a 1.205 ∠OCH_a 110 ∠CON 112.7 ∠ONO_b 112.4	N—O_b 1.208 ∠OCH_b 103 ∠ONO_a 118.1			

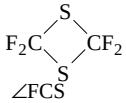
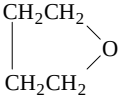
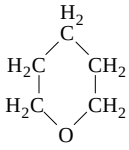
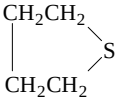
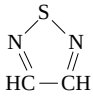
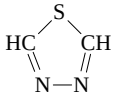
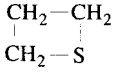
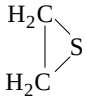
Compound	Structure						Method
Methylphosphine CH_3PH_2	C—P	1.858		C—H	1.094		ED
2-Methylpropane → Isobutane							
2-Methylpropene				C_a—H C_c—H_c C_a—C_b C_b—C_c	1.119 1.10 1.508 1.342		ED, MW
	$\angle HC_aC_b$ (average)	111.4		$\angle H_cC_cH_c$	118.5		
	$\angle C_aC_bC_a$	115.6		$\angle C_aC_bC_c$	122.2		
	$\angle HC_aH$	107.9		$\angle C_bC_cH$	121		
Methylsilane CH_3SiH_3	C—H Si—H $\angle$HSiH	1.093 1.485 108.3		C—Si $\angle$HCH (C_{3v})	1.867 107.7		MW
Methylstannane CH_3SnH_3	C—Sn	2.143		Sn—H (C_{3v})	1.700		MW
Methyl thiocyanate			S—C_b C_b—N	1.684 1.170	S—C_a C—H	1.824 1.081	MW
	$\angle C_aSC_b$	99.0	$\angle$HCH	110.6	$\angle$HCS	108.3	
Naphthalene				C_a—C_b C_b—C_b C_a—C_c C_c—C_c C—C (average) $\angle C_aC_cC_c$	1.37 1.41 1.42 1.42 1.40 119.4		ED
Neopentane $C(CH_3)_4$	C—C $\angle$CCH	1.537 112		C—H	1.114		ED
Nickelocene → Bis (cyclopentadienyl) nickel							
Nitromethane CH_3NO_2	C—H N—O $\angle$ONO	1.088 (assumed) 1.224 125.3		C—N $\angle$NCH	1.489 107		MW
N-Nitrosodimethylamine $(CH_3)_2NNO$	N—O C—N $\angle$CNC	1.235 1.461 123.2		N—N $\angle$ONN $\angle$CNN	1.344 113.6 116.4		ED
Nitrosomethane CH_3NO	C—N C—H $\angle$NCH	1.49 1.084 109.0		N—O $\angle$CNO	1.22 112.6		MW
Norbornane → Bicyclo[2.2.1]heptane							
Norbornadiene → Bicyclo[2.2.1]hepta-2,5-diene							
1,2,5-Oxadiazole			O—N C—N C—C C—H $\angle$NCH	1.380 1.300 1.421 1.076 120.9	$\angle$NON $\angle$ONC $\angle$CCN $\angle$CCH planar	110.4 105.8 109.0 130.2	MW
1,3,4-Oxadiazole			O—C C—N N—N C—H $\angle$NCH	1.348 1.297 1.399 1.075 128.5	$\angle$COC $\angle$OCN $\angle$CNN $\angle$OCH planar	102.0 113.4 105.6 118.1	MW
Oxalic acid				C—C C—O_a C—O_b O_b—H $\angle CCO_a$ $\angle O_aCO_b$ $\angle CO_bH$	1.544 1.205 1.336 1.05 123.1 125.0 104		ED

BOND LENGTHS AND ANGLES IN GAS-PHASE MOLECULES (continued)

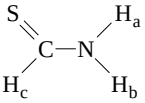
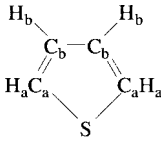
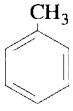
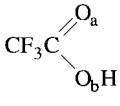
Compound	Structure						Method
Oxalyl dichloride			C—O	1.182			ED
			C—C	1.534			
			C—Cl	1.744			
	∠CCO	124.2	∠CCCl	111.7			
	fraction of the *trans* conformer at 0°C 68%, that of the *gauche* conformer 32%						
Oxetane			C—O	1.448			MW
			C—C	1.546			
			C—H (average)	1.090			
			∠COC	92			
	∠CCC	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	110.4			
			(C_{2h})				
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			

Compound	Structure						Method
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		
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		
	$∠C_aNC_a$	116.8		$∠NC_aC_b$	123.9		
	$∠C_aC_bC_c$	118.5		$∠C_bC_cC_b$	118.3		
	$∠NC_aH_a$	115.9		$∠C_cC_bH_b$	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		$∠C_aNC_a$	109.8		
	$∠NC_aC_b$	107.7		$∠C_aC_bC_b$	107.4		
	$∠NC_aH_a$	121.5		$∠C_bC_bH$	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		
	$∠C_aC_bO$	124.5		$∠C_aC_bC_c$	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		
				$∠C_bC_aC_b$	62		
	∠HCH	118		(D_{2d})			

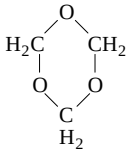
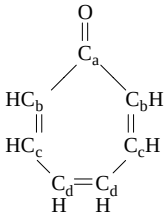
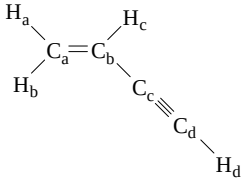
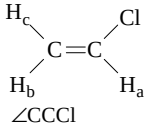
BOND LENGTHS AND ANGLES IN GAS-PHASE MOLECULES (continued)

Compound	Structure						Method
Succinonitrile	CH_2CN | CH_2CN	C—C	1.561	C—C(N)	1.465		ED
		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)				
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		

BOND LENGTHS AND ANGLES IN GAS-PHASE MOLECULES (continued)

Compound	Structure				Method
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	
	$\angle H_aNH_b$	121.7	$\angle H_aNC$	117.9	
	$\angle H_bNC$	120.4	∠NCS	125.3	
	$\angle NCH_c$	108	$\angle SCH_c$	127	
Thiolane → Tetrahydrothiophene					
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					

BOND LENGTHS AND ANGLES IN GAS-PHASE MOLECULES (continued)

Compound	Structure				Method
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	
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	