Bindungsabstände - Originalquelle:
http://home.att.net/~mopacmanual/node660.html

20V-CT.htm

Notes on the Table

- The AM1 results for P_4O_6 and P_4O_{10} are incorrect. The experimental geometry was used to start the calculation. In order to generate the lowest energy geometry, the systems must first be distorted.
- For salicylaldoxim, the bonds reported are the internal hydrogen bond and a non-bonding O-N interaction.
- Several 180° angles are reported. Most of these correspond to symmetry-defined angles. In some instances, e.g., $MgCl_2$, the calculated angle is incorrect. The protocols for this Chapter require *all* such results to be reported.
- The PM3 prediction for the bond-length in HgI is in error by over 10Å. HgI is predicted, by PM3, to consist of a mercury and an iodine atom. The fault can be traced to the incorrect PM3 prediction for the ground state of the iodine atom. Removal of this one error would lower the average errors in Hg bond lengths from 0.586Å to 0.054Å, and the average error in I bond lengths from 0.371Å to 0.091Å. These, in turn, result in the average bond-length error in PM3 dropping from 0.045Å. If that were done, then PM3 would become the most accurate method for the prediction of bond-lengths. Again, the protocols involved preclude this being done at this time.

Table 9.52: Comparison of Calculated and Observed Geometries for MNDO, AM1, and PM3

Empirical	Chemical Name	Geometric	Exp.	Errors			
Formula		Variable		PM3	MNDO	AM1	Ref.
H_2	Hydrogen	HH	0.741	-0.042	-0.078	-0.064	a
CH_2	Methylene, singlet	CH	1.110	-0.018	-0.019	-0.007	a
		HCH	102.4	1.3	8.7	8.1	
CH_2	Methylene, triplet	CH	1.029	0.033	0.023	0.034	a
		HCH	136.0	9.1	13.7	12.4	
CH_4	Methane	CH	1.094	-0.007	0.010	0.018	b
C_2	Carbon, dimer	CC	1.242	-0.053	-0.073	-0.078	a
C_2H_2	Acetylene	CC	1.203	-0.013	-0.008	-0.008	b
		CH	1.060	0.004	-0.009	0.001	
C_2H_4	Ethylene	CC	1.339	-0.017	-0.004	-0.013	b
		CH	1.086	0.000	0.003	0.012	
		HCC	121.2	1.9	2.0	1.5	

C_2H_6	Ethane	CC	1.536	-0.032	-0.015	-0.036	b
		CH	1.091	0.007	0.018	0.026	
		HCC	110.9	0.7	0.3	-0.2	
C_3H_4	Allene	CC	1.308	-0.012	-0.002	-0.010	c
		CH	1.087	-0.001	0.003	0.013	
		HCC	120.9	1.3	1.9	1.2	
C_3H_4	Cyclopropene	C2C3	1.509	-0.025	0.003	-0.020	d
		C1C2	1.296	0.018	0.032	0.023	
		C1H	1.072	0.001	-0.010	-0.003	
		HC1C2	149.9	1.6	1.7	2.0	
C_3H_4	Propyne	C2C1	1.206	-0.014	-0.009	-0.009	e
		C1H	1.056	0.008	-0.005	0.004	
		C3C3	1.459	-0.026	-0.014	-0.032	
		C3H	1.105	-0.007	0.006	0.016	
		HCC	111.0	-0.3	0.0	-0.5	
C_3H_6	Cyclopropane	CC	1.510	-0.011	0.016	-0.009	f
		CH	1.089	0.006	0.007	0.015	
C_3H_6	Propene	C=C	1.336	-0.008	0.004	-0.005	g
		C-C	1.501	-0.021	-0.005	-0.025	
		CCC	124.3	-0.9	2.6	0.0	
		C3H	1.085	0.013	0.024	0.033	
		HC3C2	111.2	1.7	1.9	0.7	
		C2H	1.090	0.006	0.006	0.014	
		HC2C1	119.0	1.8	0.3	1.9	
		HC1	1.081	0.005	0.008	0.017	
		HC1C2	121.5	1.1	0.8	0.8	
C_3H_8	Propane	CC	1.526	-0.014	0.004	-0.019	g
		CCC	112.4	-0.6	3.0	-0.5	
		C2H	1.115	-0.007	0.000	0.007	
		HC2C1	109.5	0.3	-0.7	-0.1	
		C1H	1.096	0.001	0.014	0.021	
		HC1C2	111.8	-0.4	-1.5	-1.3	

Table 9.53: Comparison of Calculated and Observed Geometries for MNDO, AM1, and PM3 (contd.)

Empirical	Chemical Name	Geometric	Exp.	Errors			
Formula		Variable		PM3	MNDO	AM1	Ref.
C_4H_2	Diacetylene	C1C2	1.205	-0.012	-0.006	-0.006	h
		C2C3	1.376	-0.005	-0.008	-0.020	
		CH	1.046	0.019	0.004	0.014	
C_4H_4	CH2=C=C=CH2	CH	1.083	0.004	0.007	0.017	i
		C1C2	1.318	-0.017	-0.008	-0.016	
		C2C3	1.283	-0.016	-0.013	-0.017	
C_4H_4	Vinylacetylene	C3C4	1.341	-0.009	0.004	-0.005	j
		C2C3	1.431	-0.017	-0.014	-0.026	
		C2C3C4	123.1	-0.5	2.3	1.0	
		C1C2	1.208	-0.015	-0.010	-0.010	
C_4H_6	Bicyclobutane	C1C2	1.498	0.008	0.029	0.012	k
		C1C3	1.497	-0.016	0.040	-0.002	
		C2C3C1C4	121.7	-1.7	1.0	0.3	
		C1H	1.071	0.012	0.003	0.008	
		C2H	1.093	0.003	0.005	0.012	
C_4H_6	2-Butyne	C2C3	1.213	-0.020	-0.013	-0.015	j
		C1C2	1.467	-0.035	-0.023	-0.042	
		CH	1.115	-0.017	-0.004	0.006	
		HCC	110.7	0.0	0.3	-0.1	
C_4H_6	1,3-Butadiene	C1C2	1.344	-0.013	0.000	-0.009	l
		C2C3	1.467	-0.011	-0.002	-0.016	
		CCC	122.9	-0.5	2.8	0.6	
C_4H_8	1-Butene	C2C3	1.347	-0.019	-0.006	-0.016	m
		C1C2	1.508	-0.019	-0.003	-0.024	
		CCC	123.8	-1.2	1.6	-0.4	
C_4H_8	Cyclobutane	CC	1.548	-0.006	0.001	-0.005	n
		C1C2C4C3	153.0	27.0	27.1	26.9	
		CH	1.105	-0.005	0.000	0.005	
C_4H_8	Isobutene	C1C2	1.330	0.003	0.018	0.006	o

		C2C3	1.507	-0.020	0.002	-0.023	
		C1C2C3	122.4	-0.3	-0.5	0.0	
C_4H_{10}	n-Butane	C1C2	1.533	-0.021	-0.002	-0.026	e
		C2C3	1.533	-0.013	0.006	-0.019	
		CCC	112.8	-1.2	2.0	-1.2	
C_4H_{10}	Isobutane	CC	1.525	-0.005	0.016	-0.011	p
C_5H_8	1,4-Pentadiene C1	C=C	1.339	-0.011	0.001	-0.008	q
		C-C	1.511	-0.022	-0.005	-0.027	
		C-C=C	115.5	7.6	11.1	8.4	
		C-C-C	113.1	1.3	-0.4	1.2	
C_5H_8	1,4-Pentadiene C2	C=C	1.339	-0.011	0.001	-0.008	q
		C-C	1.511	-0.021	-0.005	-0.025	
		C-C=C	115.5	7.6	11.2	8.3	
		C-C-C	108.9	1.9	3.7	2.9	
C_5H_8	1,4-Pentadiene Cs	C=C	1.339	-0.011	0.001	-0.008	q
		C-C	1.511	-0.021	-0.005	-0.025	
		C-C=C	115.5	7.6	11.1	8.4	
		C-C-C	108.9	2.0	3.7	2.8	
C_5H_{12}	Neopentane	CC	1.539	-0.012	0.015	-0.018	f
		CH	1.120	-0.022	-0.011	-0.004	
		HCC	110.0	1.3	1.7	0.3	

Table 9.54: Comparison of Calculated and Observed Geometries for MNDO, AM1, and PM3 (contd.)

Empirical	Chemical Name	Geometric	Exp.	Errors			
Formula		Variable		PM3	MNDO	AM1	Ref.
C_6H_6	Benzene	CC	1.399	-0.008	0.008	-0.004	r
		CH	1.084	0.011	0.006	0.016	
C_6H_6	Fulvene	C3C4	1.476	-0.005	0.001	0.000	s
		C2C3	1.355	0.000	0.011	0.008	
		C1C2	1.470	0.008	0.021	0.013	
		C1C6	1.349	-0.018	-0.004	-0.017	
C_6H_{10}	Cyclohexene	C1C2	1.335	-0.001	0.011	0.002	t
		C2C3	1.504	-0.017	0.000	-0.020	

		C3C4	1.515	0.006	0.026	0.002	
		C4C5	1.550	-0.031	-0.011	-0.036	
		C5C4C2C1	21.8	6.0	-0.5	5.4	
C_6H_{12}	Cyclohexane	CC	1.536	-0.015	0.005	-0.021	u
		CCC	111.4	-0.4	3.3	0.0	
		CCCC	46.3	9.7	-0.6	8.7	
H_2O	Water	OH	0.957	-0.006	-0.014	0.004	b
		HOH	104.5	3.2	2.3	-1.0	
CO	Carbon monoxide	CO	1.128	0.007	0.035	0.043	v
CH_2O	Formaldehyde	CO	1.208	-0.006	0.009	0.019	w
		CH	1.116	-0.025	-0.010	-0.006	
		HCO	121.7	0.1	1.8	0.5	
CH_4O	Methanol	CO	1.425	-0.030	-0.034	-0.014	x
		CH	1.094	0.003	0.025	0.025	
		HCO	108.5	3.6	3.8	2.4	
		OH	0.945	0.004	0.002	0.019	
		COH	107.0	0.5	4.6	0.2	
C_2H_2O	Ketene	CO	1.161	0.014	0.023	0.032	y
		CC	1.314	-0.006	0.005	-0.007	
		CH	1.083	0.001	0.002	0.012	
		HCC	118.7	3.3	3.0	2.7	
C_2H_4O	Acetaldehyde	C1-C2	1.501	-0.002	0.016	-0.011	z
		C2-O	1.210	0.000	0.011	0.022	
		O-C2-C1	123.9	-0.6	1.1	-0.4	
		C2-H	1.114	-0.012	-0.002	0.000	
		C1-C2-H	117.5	-0.7	-3.5	-2.2	
C_2H_6O	Dimethyl ether	CC	1.410	-0.004	-0.014	0.007	aa
		COC	111.3	2.8	8.7	1.6	
C_3H_4O	Acrolein	C3C2	1.335	-0.005	0.008	-0.001	bb
		C2C1	1.478	0.001	0.007	-0.010	
		CCC	121.0	2.6	6.3	2.2	
		CO	1.208	0.003	0.016	0.026	
		OCC	124.0	0.0	1.5	0.1	
C_3H_6O	Acetone	C=O	1.222	-0.006	0.005	0.013	cc

		C-C	1.507	-0.002	0.020	-0.012	
		C-C=O	121.4	0.9	-0.1	0.9	
C_4H_4O	Furan	CO	1.362	0.016	0.005	0.033	dd
		CCO	106.6	0.3	1.0	0.0	
		C3C2	1.361	0.012	0.029	0.019	
		CCC	110.7	-0.5	-0.4	-0.6	

Table 9.55: Comparison of Calculated and Observed Geometries for MNDO, AM1, and PM3 (contd.)

Empirical	Chemical Name	Geometric	Exp.	Errors			
Formula		Variable		PM3	MNDO	AM1	Ref.
O_2	Oxygen, triplet state	OO	1.216	-0.047	-0.082	-0.131	v
H_2O_2	Hydrogen peroxide	OO	1.475	0.006	-0.180	-0.177	ee
		OH	0.950	-0.005	0.011	0.034	
		HOO	94.8	1.8	12.5	11.5	
		HOOH	119.8	60.4	36.8	1.7	
		HOOH	119.8	60.4	36.8	1.7	ee
CO_2	Carbon dioxide	CO	1.162	0.019	0.024	0.027	b
CH_2O_2	Formic acid	C=O	1.202	0.009	0.025	0.028	ff
		C-O	1.343	0.001	0.011	0.014	
		OCO	124.9	-7.7	-4.3	-7.2	
		OH	0.972	-0.019	-0.023	-0.001	
		HOC	106.3	5.5	10.0	4.3	
		CH	1.097	-0.002	0.008	0.006	
		HC-O	124.1	6.3	2.6	6.0	
$C_2H_2O_2$	trans Glyoxal	CO	1.207	0.000	0.013	0.022	bb
		CC	1.525	0.001	0.004	-0.016	
		CCO	121.2	-0.7	0.8	-0.2	
$C_2H_4O_2$	Methyl formate	C=O	1.200	0.008	0.024	0.029	gg
		C-O	1.334	0.022	0.023	0.028	
		O-C=O	125.9	-5.3	-3.9	-6.7	
		O-CH3	1.437	-0.024	-0.033	-0.009	
		C-O-C	114.8	4.8	10.8	2.5	
$C_6H_4O_2$	p-Benzoquinone	C1C2	1.477	0.010	0.024	0.002	hh

		C2C3	1.322	0.013	0.027	0.016	
		CCC	121.1	0.5	1.0	0.8	
		CO	1.222	-0.005	0.004	0.014	
O_3	Ozone	O-O	1.198	0.025	-0.007	-0.038	b
		O-O-O	114.9	-0.8	2.7	6.0	
H_3N	Ammonia	NH	1.012	-0.013	-0.005	-0.014	a
		HNH	106.7	1.4	-1.4	2.4	
CN	Cyanide (+)	CN	1.290	0.065	-0.149	-0.164	a
CN	Cyanide	CN	1.175	-0.018	-0.022	-0.027	a
CHN	Hydrogen cyanide	CN	1.154	0.002	0.006	0.006	ii
		CH	1.063	0.007	-0.008	0.006	
CH_5N	Methylamine	CN	1.474	-0.005	-0.014	-0.041	jj
		NH	1.011	-0.012	-0.003	-0.010	
		HNC	112.0	-2.2	-2.2	-0.9	
		HNH	105.9	2.8	-0.3	3.0	
C_2H_3N	Acetonitrile	CC	1.458	-0.018	-0.006	-0.019	kk
		CH	1.104	-0.006	0.006	0.016	
		HCC	109.5	0.9	1.1	0.6	
		CN	1.157	0.002	0.005	0.006	
C_2H_3N	Methyl isocyanide	CN-	1.424	0.009	0.000	-0.029	kk
		CH	1.101	-0.004	0.014	0.024	
		HCN	109.1	0.6	1.1	1.0	
		-CN	1.166	0.015	0.025	0.015	

Table 9.56: Comparison of Calculated and Observed Geometries for MNDO, AM1, and PM3 (contd.)

Empirical	Chemical Name	Geometric	Exp.	Errors			
Formula		Variable		PM3	MNDO	AM1	Ref.
C_2H_7N	Dimethylamine	C-N	1.462	0.012	0.000	-0.024	ll
		N-H	1.019	-0.021	-0.010	-0.016	
		H-N-C	108.9	0.6	0.5	1.5	
		C-N-C	112.2	1.1	5.3	2.1	
C_3H_9N	Trimethylamine	CN	1.451	0.029	0.014	-0.006	mm
		CNC	110.9	1.3	5.2	2.1	

C_4H_5N	Pyrrole	CN	1.370	0.027	0.028	0.022	l
		CNC	107.7	2.0	2.0	1.1	
		C3C2	1.382	0.008	0.013	0.020	
		CCC	109.8	-2.8	-2.4	-1.4	
		C4C3	1.417	-0.027	-0.022	-0.015	
NO	Nitrogen oxide	NO	1.151	-0.024	-0.029	-0.037	a
CHNO	Hydrogen isocyanate	NH	0.987	-0.001	0.014	0.000	a
		CN	1.207	0.044	0.043	0.025	
		CNH	128.1	-6.3	-10.3	-2.7	
		CO	1.171	0.011	0.014	0.031	
		OCN	180.0	0.0	0.0	0.0	
CH_3NO	Formamide	CN	1.376	0.015	0.013	-0.009	nn
		NH	1.002	-0.012	-0.010	-0.016	
		CH	1.102	-0.001	0.006	0.012	
		CO	1.193	0.027	0.034	0.050	
		OCN	123.8	-6.1	-2.9	-1.8	
NO_2	Nitrogen dioxide	NO	1.197	-0.016	-0.023	-0.038	a
		ONO	136.0	1.7	-2.8	0.5	
HNO_2	Nitrous acid (cis)	N-O	1.460	-0.122	-0.163	-0.169	a
		N=O	1.200	-0.025	-0.031	-0.038	
		ONO	114.0	-0.7	3.1	2.6	
		OH	0.980	-0.020	-0.017	0.003	
		HON	103.0	6.8	16.7	12.5	
HNO_2	Nitrous acid (trans)	N-O	1.460	-0.077	-0.148	-0.141	a
		N=O	1.200	-0.033	-0.034	-0.042	
		ONO	118.0	-8.9	-4.7	-5.2	
		OH	0.980	-0.029	-0.022	-0.005	
		HON	105.0	-0.4	5.0	2.0	
$C_7H_7NO_2$	Salicylaldoxime	N · · · H	1.834	0.013	0.450	0.303	oo
		O * * * N	2.626	0.058	0.350	0.298	
HNO_3	Nitric acid	N=O	1.206	-0.003	0.005	-0.011	a
		O=N=O	130.0	2.7	-3.5	-0.9	
		N-O	1.405	0.005	-0.065	-0.072	

		OH	0.960	-0.007	0.002	0.022	
		NOH	102.0	7.0	12.0	7.7	
N_2	Nitrogen	NN	1.094	0.004	0.010	0.012	v
H_4N_2	Hydrazine	NN	1.449	-0.009	-0.052	-0.071	a
		NH	1.022	-0.021	-0.001	-0.008	
		HNN	112.0	-5.5	-4.8	-4.4	
		HNNH	90.0	90.8	90.3	90.2	

Table 9.57: Comparison of Calculated and Observed Geometries for MNDO, AM1, and PM3 (contd.)

Empirical	Chemical Name	Geometric	Exp.	Errors			
Formula		Variable		PM3	MNDO	AM1	Ref.
C_2N_2	Cyanogen	CN	1.154	0.005	0.008	0.008	b
		CC	1.389	-0.007	-0.011	-0.005	
$C_2H_6N_2$	Dimethyldiazene	NN	1.254	-0.026	-0.032	-0.030	b
		CN	1.474	-0.007	0.000	-0.022	
		CNN	111.9	7.4	5.0	7.9	
$C_4H_4N_2$	Pyrimidine	C4C5	1.393	0.003	0.016	0.015	pp
		N3C4	1.350	0.004	0.003	0.000	
		N3C4C5	121.2	-0.5	0.1	1.1	
		C2N3	1.328	0.029	0.029	0.033	
		C2H	1.082	0.016	0.016	0.028	
		C5H	1.087	0.007	0.000	0.008	
		C6H	1.079	0.017	0.016	0.026	
N_2O	Nitrous oxide	NN	1.128	-0.004	0.000	0.000	a
		NO	1.184	0.013	-0.003	-0.009	
$H_2N_2O_2$	NH2-NO2	NN	1.427	0.004	-0.020	-0.060	qq
		NO	1.206	0.005	0.003	-0.002	
		NH	1.005	-0.005	0.013	-0.003	
		ONO	130.1	-3.0	-6.0	-6.1	
N_2O_3	Dinitrogen trioxide	NN	2.080	-0.383	-0.550	-0.498	a
		NO	1.120	0.031	0.018	0.008	

		NNO	110.0	6.7	6.1	6.2	
		NO'	1.180	0.022	0.028	0.019	
		O'NO'	134.0	-4.6	-9.1	-9.2	
N_2O_4	Dinitrogen tetroxide	NN	1.750	0.009	-0.135	0.068	a
		NO	1.180	0.015	0.009	-0.008	
		ONN	113.1	1.5	2.2	1.1	
N_3	Azide	NN	1.181	-0.008	-0.007	-0.004	a
$C_3H_3N_3$	s-Triazine	CN	1.338	0.020	0.019	0.026	rr
		NCN	126.8	-5.2	-3.4	-1.1	
CHN_3O_6	Trinitromethane	C-N	1.505	0.078	0.053	0.055	ss
		N-C-N	110.7	-4.0	-1.1	-3.9	
		N=O	1.219	-0.018	-0.014	-0.027	
H_2S	Hydrogen sulfide	HS	1.328	-0.038	-0.029	-0.005	a
		HSH	92.2	1.3	5.8	3.3	
CS	Carbon sulfide	CS	1.534	-0.087	-0.050	-0.105	tt
CH_2S	Thioformaldehyde	CS	1.611	-0.072	-0.074	-0.099	nn
		CH	1.093	0.002	0.000	0.013	
		HCS	121.6	4.5	2.4	3.7	
CH_4S	Thiomethanol	CS	1.818	-0.018	-0.101	-0.064	uu
		SH	1.329	-0.022	-0.027	-0.008	
		HSC	100.3	-0.4	2.0	-0.8	
		HCSH	180.0	0.0	0.0	0.0	
C_2H_6S	Dimethyl thioether	CS	1.802	0.000	-0.079	-0.050	ss
		CSC	98.9	3.2	9.4	3.0	
		HCS	106.6	3.8	3.1	2.6	
		H'CS	106.6	0.0	0.0	0.0	

Table 9.58: Comparison of Calculated and Observed Geometries for MNDO, AM1, and PM3 (contd.)

Empirical	Chemical Name	Geometric	Exp.	Errors			
Formula		Variable		PM3	MNDO	AM1	Ref.
C_4H_4S	Thiophene	CS	1.714	0.011	-0.035	-0.042	vv
		CCS	92.2	-0.8	1.4	1.6	
		C3C2	1.370	-0.004	0.005	0.007	

		CCC	111.5	0.6	0.4	0.1	
CSO	Carbon oxysulfide	CO	1.159	0.017	0.022	0.042	ww
		CS	1.559	-0.055	-0.049	-0.101	
SO_2	Sulfur dioxide	SO	1.432	0.010	0.044	-0.003	a
		OSO	119.5	-13.4	-12.7	-11.6	
SO_3	Sulfur trioxide	SO	1.430	-0.046	0.061	-0.080	a
H_2SO_4	Sulfuric acid	S-O	1.550	0.118	0.079	0.072	a
		OH	0.970	-0.023	-0.023	-0.015	
		SOH	105.0	12.7	12.2	15.9	
		S=O	1.420	-0.013	0.095	-0.062	
NS	Sulfur nitride	SN	1.495	-0.044	-0.055	-0.105	a
C_2H_3NS	Methyl isothiocyanate	CS	1.597	-0.099	-0.087	-0.125	xx
		C=N	1.192	0.039	0.026	0.029	
		C-N	1.479	-0.039	-0.043	-0.075	
		C-N=C	141.6	-2.0	0.4	-0.4	
C_2N_2S	Sulfur dicyanide	CN	1.157	0.007	0.007	0.012	yy
		CS	1.701	-0.037	-0.071	-0.083	
		NCS	170.0	6.4	6.9	6.5	
		CSC	98.4	3.2	5.1	4.8	
S_2	Sulfur dimer	SS	1.889	-0.032	-0.114	-0.053	a
H_2S_2	H2S2	SS	2.055	-0.022	-0.132	0.052	zz
		SH	1.327	-0.017	-0.023	-0.001	
		HSS	91.3	12.0	11.2	7.4	
		HSSH	90.5	1.9	9.0	8.9	
CS_2	Carbon disulfide	CS	1.553	-0.072	-0.061	-0.094	ss
$C_2H_6S_2$	2,3-Dithiabutane	CS	1.810	-0.006	-0.085	-0.060	aaa
		SS	2.038	-0.001	-0.102	0.072	
		CSS	102.8	6.4	5.2	3.4	
		CSSC	84.7	5.5	23.1	9.8	
		CS	1.810	-0.006	-0.085	-0.060	ss
		SS	2.038	-0.001	-0.102	0.072	
		SSC	102.8	5.8	5.2	3.2	
		CSSC	84.7	5.5	23.1	9.8	
S_6	S6	SS	2.057	-0.009	-0.110	0.052	bbb

		SSS	102.2	5.3	2.9	0.3	
		SSSS	74.5	-9.9	-5.1	-0.6	
S_8	S8	SS	2.048	-0.075	-0.113	-0.042	ccc
		SSS	107.9	8.1	0.4	3.7	
		SSSS	98.6	-11.0	-0.2	-4.4	
HF	Hydrogen fluoride	HF	0.917	0.021	0.039	-0.091	ddd
CF	Fluoromethylidyne	CF	1.266	-0.008	-0.003	-0.008	a
CHF	Fluoromethylene	CH	1.121	-0.021	-0.001	0.006	a
		CF	1.314	-0.030	-0.029	-0.023	
		FCH	101.6	4.0	9.5	9.0	

Table 9.59: Comparison of Calculated and Observed Geometries for MNDO, AM1, and PM3 (contd.)

Empirical	Chemical Name	Geometric	Exp.	Errors			
Formula		Variable		PM3	MNDO	AM1	Ref.
CH_3F	Fluoromethane	CH	1.098	-0.006	0.019	0.023	eee
		CF	1.382	-0.032	-0.033	-0.007	
		FCH	108.5	1.2	0.8	1.0	
C_2HF	Fluoroacetylene	H-C	1.053	0.012	-0.004	0.006	fff
		C-C	1.198	-0.010	-0.005	-0.004	
		C-F	1.279	0.020	-0.002	0.018	
C_2H_3F	Fluoroethylene	CC	1.333	0.000	0.018	0.007	ggg
		CH(g)	1.076	0.017	0.023	0.028	
		CCH(g)	127.7	-1.6	-4.7	-3.9	
		CH(t)	1.085	0.000	0.002	0.011	
		CCH(t)	123.9	-2.6	-3.0	-3.0	
		CH(c)	1.090	-0.004	-0.003	0.006	
		CCH(c)	121.4	2.3	3.1	1.5	
		CF	1.348	-0.010	-0.024	0.003	
		FCC	121.0	1.1	2.3	2.2	
C_3H_3F	Fluoroallene	C1C2	1.301	0.009	0.019	0.012	hhh
		C1H	1.083	0.011	0.016	0.022	
		HC1C2	124.3	0.5	-1.4	-1.4	
		C1F	1.360	-0.020	-0.035	-0.007	

		FC1C2	121.9	0.4	1.0	1.8	
		C2C3	1.309	-0.015	-0.006	-0.014	
		C3H	1.086	0.001	0.005	0.015	
		HC3C2	120.8	1.5	2.1	1.5	
CNF	Cyanogen fluoride	CN	1.159	0.000	0.001	0.006	fff
		CF	1.262	0.035	0.011	0.045	
NOF	Nitrosyl fluoride	NF	1.520	-0.153	-0.215	-0.153	a
		NO	1.130	0.032	0.031	0.018	
		FNO	110.2	1.4	3.6	2.1	
CH_3SO_3F	Methyl fluorosulfate	S=O	1.410	-0.005	0.101	-0.051	iii
		O=S=O	124.4	-0.6	-2.0	-0.5	
		S-F	1.545	-0.009	0.064	-0.038	
		F-S=O	106.8	1.6	0.4	2.3	
		S-O	1.558	0.125	0.075	0.084	
		O-S=O	109.5	0.5	0.3	-1.6	
		C-O	1.420	-0.019	-0.017	-0.012	
		C-O-S	116.5	7.1	9.5	7.1	
F_2	Fluorine	FF	1.412	-0.062	-0.146	0.015	a
H_2F_2	Hydrogen fluoride dimer	HF	0.920	0.019	0.036	-0.093	a
		H'F	1.870	-0.126	1.199	0.430	
		H'FH	108.0	39.3	36.1	-18.3	
CF_2	Difluoromethylene	CF	1.300	-0.002	0.004	0.012	a
		FCF	104.9	1.4	3.4	1.1	
OF_2	F2O	OF	1.412	-0.034	-0.131	-0.058	a
		FOF	103.2	-2.2	5.9	-0.7	
COF_2	Carbonyl difluoride	CO	1.174	0.025	0.045	0.046	a
		CF	1.312	0.010	0.004	0.016	
		FCO	126.0	-1.4	-1.9	-1.5	

Table 9.60: Comparison of Calculated and Observed Geometries for MNDO, AM1, and PM3 (contd.)

Empirical	Chemical Name	Geometric	Exp.	Errors			
Formula		Variable		PM3	MNDO	AM1	Ref.
SF_2	Sulfur difluoride	SF	1.592	-	-0.020	-	a

				0.032		0.036	
		FSF	98.2	-1.7	1.4	0.8	
CSF_2	Thiocarbonyl difluoride	CS	1.589	0.011	-0.014	-0.029	ss
		CF	1.315	0.023	0.006	0.031	
		FCS	126.4	2.5	-0.4	2.4	
SOF_2	Thionyl fluoride	SO	1.412	0.055	0.068	0.021	a
		SF	1.585	-0.010	0.023	-0.037	
		FSO	106.8	-5.8	-4.0	-4.2	
		FSF	92.8	1.0	4.2	3.7	
SO_2F_2	Sulfuryl fluoride	SF	1.530	0.017	0.080	-0.015	a
		FSF	96.1	-0.8	1.6	1.2	
		SO	1.405	-0.005	0.103	-0.046	
		OSO	124.0	2.5	0.9	0.9	
S_2F_2	FSSF	SF	1.635	-0.051	-0.063	-0.071	a
		SS	1.888	0.121	0.077	0.243	
		FSS	108.3	3.7	-1.8	0.8	
		FSSF	87.9	-0.2	-0.4	1.7	
S_2F_2	SSF2	SS	1.860	0.059	0.034	-0.027	a
		SF	1.598	-0.006	0.003	-0.047	
		FSS	107.5	7.0	1.4	12.4	
		FSF	92.5	-1.6	4.0	1.0	
CHF_3	Trifluoromethane	CH	1.098	0.013	0.038	0.032	a
		CF	1.333	0.013	0.020	0.035	
		FCH	110.3	2.8	1.2	2.7	
NF_3	Nitrogen trifluoride	NF	1.371	-0.017	-0.056	-0.011	a
		FNF	102.2	2.8	4.0	0.4	
C_2NF_3	Trifluoroacetonitrile	CC	1.461	0.026	0.037	0.025	a
		CF	1.335	0.015	0.020	0.036	

		CCF	111.4	2.0	0.5	2.1	
		CN	1.153	0.002	0.006	0.006	
CF_4	Carbon tetrafluoride	CF	1.321	0.016	0.026	0.037	jjj
C_2F_4	Tetrafluoroethylene	CC	1.311	0.044	0.070	0.057	ggg
		CF	1.319	0.007	-0.001	0.021	
		FCC	123.8	1.3	0.4	1.6	
SF_4	Sulfur tetrafluoride	SF	1.545	0.051	0.052	0.001	a
		FSF	101.5	19.7	0.6	2.4	
		SF'	1.646	-0.024	0.025	-0.073	
		FSF'	87.8	-6.9	0.6	-0.8	
$CNSOF_5$	Pentafluoro(isocyanato)sulfur	S-F	1.567	-0.004	0.089	-0.007	iii
		S-N	1.668	0.085	0.061	0.000	
		N=C	1.234	0.011	0.026	-0.022	
		S-N=C	124.9	27.9	10.7	55.1	
		C=O	1.179	-0.005	-0.006	0.015	
		N=C=O	173.8	0.6	-3.9	6.1	
C_2F_6	C2F6	C-C	1.545	0.062	0.129	0.077	kkk
		C-F	1.314	0.027	0.032	0.049	
		F-C-C	109.8	1.7	0.9	2.3	

Table 9.61: Comparison of Calculated and Observed Geometries for MNDO, AM1, and PM3 (contd.)

Empirical	Chemical Name	Geometric	Exp.	Errors			
Formula		Variable		PM3	MNDO	AM1	Ref.
SF_6	Sulfur hexafluoride	SF	1.564	-0.003	0.091	-0.024	a
C_3F_8	Perfluoropropane	C-C	1.551	0.050	0.121	0.063	kkk
		C-C-C	115.7	-4.9	-1.7	-5.6	
		C-F	1.314	0.029	0.033	0.050	
		F-C-C	110.7	1.2	0.6	1.8	
$C_3O_2F_8$	CF3-O-CF2-O-CF3	C1-O	1.358	0.035	0.049	0.049	kkk

		O-C2	1.357	0.036	0.046	0.043	
		C1-O-C2	123.3	-4.4	7.6	-1.5	
		C1-F	1.305	0.027	0.038	0.047	
C_4F_{10}	Perfluoro-n-butane	C1-C2	1.554	0.053	0.123	0.063	kkk
		C2-C3	1.554	0.039	0.112	0.051	
		C-C-C	115.0	-3.9	-1.1	-5.1	
		C1-F	1.314	0.028	0.033	0.050	
		F-C1-C2	108.5	2.5	1.6	3.2	
S_2F_{10}	S2F10	S-S	2.210	0.680	3.395	1.819	a
		S-F	1.560	0.021	2.399	-0.006	
$C_5O_2F_{12}$	CF3-O-CF2-O-CF(CF3)-O-CF3	C1-O	1.355	0.042	0.057	0.057	kkk
		C1-F	1.305	0.026	0.036	0.046	
		F-C1-O	107.0	-4.5	-1.1	-3.2	
HCl	Hydrogen chloride	HCl	1.275	-0.007	0.073	0.009	a
CHCl	Chloromethylene	CH	1.120	-0.020	-0.020	-0.010	a
		CCl	1.689	-0.135	0.050	-0.042	
		ClCH	103.4	12.1	6.0	7.7	
CH_3Cl	Chloromethane	CCl	1.781	-0.017	0.014	-0.040	a
		CH	1.096	-0.002	0.006	0.016	
		HCCl	110.9	-1.0	-2.8	-2.6	
C_2HCl	Chloroacetylene	H-C	1.055	0.009	-0.004	0.005	lll
		C-C	1.203	-0.009	-0.010	-0.007	
		C-Cl	1.637	-0.065	0.024	-0.039	
OCl	Chlorine monoxide	ClO	1.546	0.002	0.073	0.089	a
NOCl	NOCl	ClN	1.950	-0.186	-0.167	-0.219	a
		NO	1.170	-0.014	-0.033	-0.033	

		CNCl	114.0	4.9	3.5	5.3	
NO_2Cl	NO2Cl	ClN	1.830	-0.012	-0.020	-0.060	a
		NOCl	1.210	-0.013	-0.019	-0.024	
FCl	Chlorine fluoride	ClF	1.628	-0.045	0.022	0.019	a
O_3FCl	ClO3F	ClF	1.630	0.060	0.105	0.051	a
		ClO	1.460	-0.007	0.270	0.328	
		OClF	95.2	7.6	11.0	3.0	
CHF_2Cl	Chlorodifluoromethane	CH	1.090	0.018	0.036	0.037	mmm
		CCl	1.740	0.082	0.100	0.070	
		ClCH	107.0	2.9	-2.1	-1.8	
		CF	1.350	-0.004	-0.009	0.019	
		FCCl	110.5	-0.3	-0.3	1.9	
		FCClH	120.0	2.5	1.0	2.0	
F_3Cl	Chlorine trifluoride C2v	ClF	1.598	0.073	0.101	0.085	a
		ClF'	1.698	-0.027	0.001	-0.015	
		FClF'	87.5	32.5	32.5	32.5	

Table 9.62: Comparison of Calculated and Observed Geometries for MNDO, AM1, and PM3 (contd.)

Empirical	Chemical Name	Geometric	Exp.	Errors			
Formula		Variable		PM3	MNDO	AM1	Ref.
Cl_2	Chlorine	ClCl	1.986	0.049	0.010	-0.068	a
CH_2Cl_2	Dichloromethane	CCl	1.772	-0.014	0.014	-0.031	jjj
		ClCCl	111.8	-3.9	-0.6	1.1	
		CH	1.103	-0.001	0.000	0.010	
OCl_2	Cl2O	ClO	1.701	-0.001	-0.018	0.032	a
		ClOCl	110.8	-1.6	2.2	0.3	
$COCl_2$	Carbonyl chloride	CO	1.166	0.032	0.034	0.056	a

		CCl	1.746	-0.009	0.014	-0.027	
		ClCO	124.3	-0.1	-0.4	-1.0	
SCl_2	Sulfur dichloride	SCl	2.015	0.016	-0.044	-0.057	a
		ClSCl	102.7	-1.1	3.6	3.6	
$SOCl_2$	Thionyl chloride	SO	1.443	0.035	0.025	0.007	nnn
		SCl	2.076	0.005	-0.039	-0.069	
		ClSO	106.3	-1.6	0.4	1.8	
SO_2Cl_2	Sulfuryl chloride	S=O	1.418	-0.017	0.089	-0.024	iii
		S-Cl	2.012	0.063	0.044	0.032	
		O=S-Cl	108.0	0.7	1.3	1.3	
S_2Cl_2	ClSSCl	SCl	2.057	-0.014	-0.081	-0.098	a
		SS	1.931	0.033	-0.011	-0.014	
		ClSSCl	108.2	5.0	0.0	8.9	
CF_2Cl_2	Dichlorodifluoromethane	CCl	1.770	0.038	0.055	0.037	a
		ClCCl	108.5	-1.9	-1.7	-1.8	
		CF	1.330	0.015	0.007	0.040	
		FCCl	109.8	1.6	0.8	2.1	
$CHCl_3$	Chloroform	CCl	1.782	-0.029	0.000	-0.034	jjj
		ClCH	107.5	2.9	1.1	0.2	
$CFCl_3$	Trichlorofluoromethane	CF	1.330	0.019	-0.003	0.046	a
		CCl	1.760	0.019	0.046	0.026	
CCl_4	Carbon tetrachloride	CCl	1.760	-0.013	0.022	0.000	jjj
C_2Cl_6	Hexachloroethane	CC	1.550	-0.038	0.016	0.007	a
		CCl	1.740	0.014	0.050	0.020	
		ClCC	109.0	1.2	2.4	0.7	
SCl_6	Sulfur hexachloride	SCl	2.030	0.110	0.112	0.118	ooo
HBr	Hydrogen bromide	HBr	1.415	0.056	0.025	0.006	ppp
CH_3Br	Bromomethane	CBr	1.933	0.018	-0.055	-0.028	ss
		CH	1.086	0.004	0.016	0.024	
		HCBr	107.7	0.7	0.8	1.1	
C_2HBr	Bromoacetylene	H-C	1.055	0.010	-0.004	0.006	qqq
		C-C	1.204	-0.016	-0.009	-0.005	
		C-Br	1.792	-0.007	-0.051	-0.049	
C_2HOBr	Bromoketene	C-Br	1.880	-0.003	-0.063	-0.042	rrr

		C-H	1.082	0.005	0.001	0.015	
		H-C-Br	124.4	-6.9	-8.9	-8.6	
		C=C	1.316	-0.005	0.006	-0.003	
		Br-C=C	118.4	-2.5	3.0	5.4	
		C=O	1.161	0.011	0.020	0.027	

Table 9.63: Comparison of Calculated and Observed Geometries for MNDO, AM1, and PM3 (contd.)

Empirical	Chemical Name	Geometric	Exp.	Errors			
Formula		Variable		PM3	MNDO	AM1	Ref.
C_2H_3OBr	Acetyl bromide	CC	1.516	-0.039	-0.001	-0.026	ss
		CBr	1.973	-0.007	-0.087	-0.026	
		BrCC	111.0	-4.7	2.0	2.3	
		CO	1.183	0.002	0.026	0.042	
		CCO	127.1	7.2	0.2	-3.0	
CNBr	Cyanogen bromide	BrC	1.789	0.007	-0.046	-0.028	a
		CN	1.158	-0.003	0.003	0.006	
NOBr	BrNO	BrN	2.140	-0.252	-0.271	-0.218	ss
		NO	1.146	0.001	-0.007	-0.011	
		BrNO	114.5	6.3	4.4	8.0	
FBr	BrF	BrF	1.756	0.018	-0.029	0.021	a
F_3Br	Bromine trifluoride	BrF	1.721	0.065	0.036	0.087	a
		BrF'	1.806	-0.020	-0.049	0.010	
		FBrF'	86.2	33.8	33.8	-4.8	
CF_3Br	Trifluorobromomethane	CBr	1.909	0.051	0.029	0.134	a
		CF	1.328	0.007	0.019	0.039	
		FCBr	110.3	0.5	0.8	3.4	
F_5Br	Bromine pentafluoride	BrF(ax)	1.697	0.058	0.069	0.126	iii
		BrF(eq)	1.768	0.006	0.003	0.031	

SF_5Br	Sulfur bromide pentafluoride	S-F(ax)	1.520	0.019	0.125	0.022	iii
		S-F(eq)	1.646	-0.105	0.020	-0.101	
		S-Br	2.133	0.293	0.224	0.461	
ClBr	Bromine chloride	BrCl	2.136	0.040	-0.056	-0.072	a
CH_2ClBr	Bromochloromethane	C-Cl	1.768	-0.050	0.015	-0.035	sss
		C-Br	1.930	0.009	-0.058	-0.014	
		Br-C-Cl	112.3	-9.8	-0.7	1.6	
		C-H	1.074	0.026	0.028	0.038	
Br_2	Bromine	BrBr	2.283	0.160	-0.115	-0.099	a
CH_2Br_2	Dibromomethane	CH	1.079	0.015	0.023	0.031	ss
		HCH	113.6	-2.4	-2.8	-3.5	
		CBr	1.927	-0.015	-0.059	-0.025	
		BrCH	106.5	6.0	2.1	1.7	
$C_4O_2Br_2$	1,2-Dibromocyclobutene-3,4-dione	C=C2	1.356	-0.013	0.008	0.015	ttt
		C2-C3	1.518	-0.005	-0.001	0.000	
		C=C2-C3	94.4	0.1	-0.9	-1.2	
		C-Br	1.831	-0.004	-0.044	-0.028	
		Br-C=C	133.0	-0.1	2.4	2.5	
		C-O	1.185	0.006	0.020	0.024	
		O-C3-C2	135.0	1.7	1.6	1.1	
$SOBr_2$	Thionyl bromide	S=O	1.449	-0.002	0.025	0.016	iii
		S-Br	2.255	0.066	-0.120	-0.048	
		Br-S-O	107.6	-4.2	0.5	3.4	
		Br-S-Br	2.255	0.066	-0.120	-0.048	
C_2Br_4	Tetrabromoethylene	CC	1.362	-0.065	-0.020	-0.018	ss

		CBr	1.881	-0.043	-0.060	-0.024	
		BrCC	122.4	6.2	1.3	0.0	
SBr_6	Sulfur hexabromide	SBr	2.190	0.238	0.052	0.108	ooo

Table 9.64: Comparison of Calculated and Observed Geometries for MNDO, AM1, and PM3 (contd.)

Empirical	Chemical Name	Geometric	Exp.	Errors			
Formula		Variable		PM3	MNDO	AM1	Ref.
HI	Hydrogen iodide	HI	1.609	0.068	-0.042	-0.022	ppp
CH_3I	Iodomethane	CH	1.084	0.009	0.020	0.025	ss
		CI	2.132	-0.104	-0.117	-0.082	
		HCH	111.2	-1.2	-2.8	-1.4	
C_2HI	Iodoacetylene	H-C	1.056	0.009	-0.004	0.006	uuu
		C-C	1.206	-0.018	-0.007	-0.008	
		C-I	1.989	-0.084	-0.106	-0.077	
FI	Iodine fluoride	IF	1.906	-0.017	-0.004	-0.025	a
CF_3I	Trifluoroiodomethane	CI	2.130	-0.078	-0.005	0.045	a
		CF	1.332	0.008	0.022	0.037	
		FCI	110.6	1.5	1.9	3.5	
F_5I	Iodine pentafluoride	IF(ax)	1.844	0.023	0.139	0.087	vvv
		IF(eq)	1.869	0.013	0.088	0.029	
F_7I	Iodine heptafluoride	IF(ax)	1.760	1.034	0.731	0.866	www
		IF(eq)	1.860	0.042	0.218	0.114	
ClI	Iodine chloride	ICl	2.327	-0.135	-0.065	-0.109	a
BrI	Iodine bromide	IBr	2.485	0.076	-0.135	-0.131	a
I_2	Iodine	II	2.666	0.002	-0.151	-0.128	a
BeH	Beryllium hydride (+)	Be-H	1.312	-	-0.065	-	a

				0.039		0.045	
BeH	Beryllium hydride	Be-H	1.343	-0.036	-0.053	-0.033	a
BeO	Beryllium oxide	Be-O	1.331	-0.027	0.004	0.071	a
BeS	Beryllium sulfide	Be-S	1.742	-0.090	-0.118	-0.057	a
BeF	Beryllium fluoride	Be-F	1.361	0.012	0.098	0.121	a
BeF_2	Beryllium difluoride	Be-F	1.400	0.002	0.060	0.090	a
C_5BeH_5Cl	Cyclopentadienylberyllium chloride	C-H	1.090	-0.006	-0.005	0.000	xxx
		Be-ring	1.485	0.198	0.068	0.262	
		Be-Cl	1.839	-0.068	0.117	0.017	
$BeCl_2$	Beryllium dichloride	Be-Cl	1.770	-0.026	0.143	0.067	a
$BeBr_2$	Beryllium dibromide	Be-Br	1.910	-0.096	0.102	-0.013	a
BeI	Beryllium iodide	Be-I	2.132	0.090	0.023	0.006	a
BeI_2	Beryllium diiodide	Be-I	2.120	-0.051	0.001	-0.019	a
MgH	Magnesium hydride	Mg-H	1.730	-0.043			a
MgO	Magnesium oxide	Mg-O	1.749	0.031			a
MgS	Magnesium sulfide	Mg-S	2.143	0.215			a
MgF	Magnesium fluoride	Mg-F	1.750	0.004			a
MgF_2	Magnesium difluoride	Mg-F	1.771	-0.009			yyy
MgCl	Magnesium chloride	Mg-Cl	2.199	-0.324			a
$MgCl_2$	Magnesium dichloride	Mg-Cl	2.186	-0.299			yyy
		Cl-Mg-Cl	180.0	23.7			
MgBr	Magnesium bromide	Mg-Br	2.360	-0.006			a
$MgBr_2$	Magnesium dibromide	Mg-Br	2.340	0.013			a
MgI_2	Magnesium diiodide	Mg-I	2.520	-0.100			a

Mg_2	Magnesium, dimer	Mg-Mg	3.9	3.1			a
BH	BH	BH	1.236		-0.058	-0.016	xxx
BH_2	BH2	BH	1.180		-0.022	0.016	aaa
		HBH	131.0		-4.6	-3.0	
C_3BH_9	Trimethylboron	B-C	0.850		0.000	0.000	ooo

Table 9.65: Comparison of Calculated and Observed Geometries for MNDO, AM1, and PM3 (contd.)

Empirical	Chemical Name	Geometric	Exp.	Errors			
Formula		Variable		PM3	MNDO	AM1	Ref.
BO	BO	BO	1.204		-0.034	-0.036	xxx
CBH_3O	BH3CO	C-B	1.534		-0.039	-0.004	iii
		B-H	1.222		-0.046	-0.017	
		C-B-H	103.8		3.0	-0.5	
		C-O	1.135		0.028	0.036	
$C_3BH_9O_3$	Trimethoxyborane	B-O	1.380		-0.008	-0.020	ooo
CBH_3S	CH3-B=S	B-C	1.535		-0.025	-0.029	iii
		C-H	1.109		0.002	0.003	
		H-C-B	110.3		0.1	-1.7	
		B=S	1.603		-0.118	-0.131	
$C_6BH_5F_2$	PhBF2	B-F	1.330		-0.007	-0.020	bbb
		F-B-F	116.0		-3.7	-3.6	
		B-C	1.550		0.007	0.000	
$C_2B_4H_6$	C2B4H6	C-C	1.540		0.055	0.010	ggg
		C-B3	1.627		0.023	-0.004	
		C-B4	1.605		0.072	0.043	
		B3-B4	1.721		0.031	0.003	
		B4-B6	1.752		0.006	-0.013	
B_6H_{10}	B6H10	B1-B2	1.757		0.043	-0.029	jjj
		B2-B3	1.755		-0.001	-0.058	
		BBB	58.7		0.6	1.5	
		BB	1.808		0.096	0.021	
		BBB	58.7		0.6	1.5	

HAl	AlH	AlH	1.648	0.015	-0.222	-0.186	a
AlO	AlO	AlO	1.618	0.003	-0.143	-0.068	a
AlF	Aluminum fluoride	AlF	1.654	-0.002	-0.094	-0.096	a
AlF_3	Aluminum trifluoride	AlF	1.630	0.015	-0.041	-0.052	a
AlF_4	AlF4(-)	AlF	1.690	-0.002	-0.041	-0.070	a
AlCl	Aluminum chloride	AlCl	2.130	-0.183	-0.055	-0.294	a
$AlCl_3$	Aluminum trichloride	AlCl	2.060	-0.094	0.005	-0.186	a
AlBr	Aluminum bromide	AlBr	2.295	-0.003	-0.093	-0.031	a
$AlBr_3$	Aluminum tribromide	AlBr	2.270	-0.395	-0.095	-0.026	a
AlI_3	Aluminum triiodide	AlI	2.499	-0.012	-0.174	-0.111	a
Al_2	Al2	AlAl	2.467	0.073	-0.175	-0.060	a
Al_2O	Al2O	AlO	1.730	-0.053	-0.124	-0.065	a
GaH	Gallium hydride	Ga-H	1.663	-0.015			ppp
GaF	Gallium fluoride	Ga-F	1.774	0.009			ppp
GaF_3	Gallium trifluoride	Ga-F	1.725	-0.012			yyy
GaCl	Gallium chloride	Ga-Cl	2.202	0.104			ppp
GaH_3NCl_3	Gallium trichloride-ammonia	Ga-N	2.057	0.358			iii
		Ga-Cl	2.142	0.233			
		Cl-Ga-Cl	116.4	4.0			
$GaCl_4$	GaCl4(-)	Ga-Cl	2.170	0.046			kkk
GaBr	Gallium bromide	Ga-Br	2.352	0.042			ppp
GaH_3NBr_3	Gallium tribromide-ammonia	Ga-N	2.081	-0.230			iii
		Ga-Br	2.288	0.048			
		Br-Ga-Br	116.1	-1.7			

Table 9.66: Comparison of Calculated and Observed Geometries for MNDO, AM1, and PM3 (contd.)

Empirical	Chemical Name	Geometric	Exp.	Errors			
Formula		Variable		PM3	MNDO	AM1	Ref.
GaI	Gallium iodide	Ga-I	2.575	-0.036			ppp
GaI_3	Gallium triiodide	Ga-I	2.458	0.119			yyy
Ga_2O	Gallium(I) oxide	Ga-O	1.824	-0.028			iii

		Ga-O-Ga	142.9	37.1			
$Ga_2H_4Cl_2$	Ga2Cl2H4	Ga-Ga	3.241	0.583			lll
		Ga-Cl	2.349	0.059			
		Ga-H	1.559	0.039			
Ga_2Cl_6	Ga2Cl6	Ga-Cl(b)	2.300	0.061			ooo
		Ga-Cl(t)	2.100	-0.211			
Ga_2Br_6	Ga2Br6	Ga-Br(b)	2.450	-0.016			ooo
		Ga-Br(t)	2.250	-0.017			
InH	Indium hydride	In-H	1.838	-0.104			ppp
InF	Indium fluoride	In-F	1.985	0.001			ppp
InCl	Indium chloride	In-Cl	2.401	0.002			ppp
InBr	Indium bromide	In-Br	2.543	-0.253			ppp
InI	Indium iodide	In-I	2.729	-0.019			mmm
InI_3	Indium triiodide	In-I	2.641	0.004			yyy
In_2O	Indium(I) oxide	In-O	2.020	-0.021			iii
		In-O-In	145.0	35.0			
C_5TlH_5	Cyclopentadienyl thallium	Tl-C	2.705	0.007			xxx
TlF	Thallium fluoride (TlF)	Tl-F	2.084	0.050			ooo
TlCl	Thallium chloride	Tl-Cl	2.485	0.004			xxx
TlBr	Thallium bromide	Tl-Br	2.618	-0.059			xxx
TlI	Thallium iodide	Tl-I	2.814	-0.090			xxx
Tl_2F_2	Thallium fluoride dimer	Tl-F	2.290	-0.005			iii
		F-Tl-F	90.0	23.1			
HSi	SiH	SiH	1.520	-0.015	-0.146	-0.066	a
H_2Si	Silylene (singlet)	SiH	1.519	-0.006	-0.139	-0.062	nnn
		HSiH	92.1	2.8	5.2	8.9	
H_4Si	Silane	SiH	1.481	0.007	-0.105	-0.020	a
CH_6Si	Methylsilane	SiH	1.485	0.008	-0.106	-0.022	ss
		HSiH	108.3	-0.1	0.5	-0.4	
		SiC	1.867	0.001	-0.064	-0.058	
$C_4H_{12}Si$	Tetramethylsilane	SiC	1.875	0.015	-0.060	-0.046	ss
SiN	Silicon nitride	SiN	1.572	-0.108	-0.092	-0.087	a
CH_6SiS	CH3-S-SiH3	C-S	1.819	-0.019	-0.111	-0.058	ooo

		S-Si	2.134	0.105	-0.070	0.176	
		C-S-Si	98.3	3.9	16.8	10.5	
		Si-H	1.481	0.009	-0.112	-0.020	
		C-H	1.091	0.007	0.016	0.026	
CH_5SiF	CH3-SiH2F	Si-F	1.602	0.001	-0.004	0.021	ppp
		Si-C	1.845	0.028	-0.038	-0.043	
		C-Si-F	109.2	-0.1	0.1	2.8	
		Si-H	1.478	0.025	-0.097	-0.019	
		C-Si-H	112.4	-2.3	-1.5	-3.1	
SiF_2	Difluorosilylene	SiF	1.591	-0.016	-0.013	0.021	a
		FSiF	101.0	-5.7	-4.1	-4.0	

Table 9.67: Comparison of Calculated and Observed Geometries for MNDO, AM1, and PM3 (contd.)

Empirical	Chemical Name	Geometric	Exp.	Errors			
Formula		Variable		PM3	MNDO	AM1	Ref.
$HSiF_3$	Trifluorosilane	SiH	1.447	0.061	-0.072	-0.007	a
		SiF	1.562	0.028	0.031	0.047	
		FSiH	110.6	1.8	3.0	1.2	
SiF_4	Tetrafluorosilane	SiF	1.552	0.028	0.032	0.052	a
SiCl	Chlorosilylidyne	SiCl	2.063	-0.117	0.009	-0.077	a
$SiCl_2$	Dichlorosilylene	ClSiCl	109.7	-7.8	-4.2	-5.3	qqq
CH_3SiCl_3	Trichloromethylsilane	Si-C	1.848	-0.002	-0.053	-0.060	iii
		Si-Cl	2.026	0.038	0.065	0.035	
		C-Si-Cl	110.3	1.0	1.5	0.9	
$SiCl_4$	Silicon tetrachloride	SiCl	2.017	0.024	0.063	0.022	a
SiF_3Br	Trifluorobromosilane	Si-Br	2.156	-0.282	0.063	0.139	rrr
		Si-F	1.559	0.013	0.026	0.048	
		F-Si-Br	110.4	-2.2	1.8	1.8	
$SiBr_4$	Silicon tetrabromide	SiBr	2.150	-0.354	0.040	0.093	a
H_3SiI	Iodosilane	SiI	2.437	-0.425	-0.051	-0.003	a
		SiH	1.486	0.006	-0.116	-0.020	

		HSiI	108.5	-0.5	-0.1	1.3	
SiI_4	Silicon tetraiodide	SiI	2.430	0.037	-0.097	-0.005	a
Si_2	Silicon dimer	SiSi	2.246	0.050	-0.260	-0.458	a
H_6Si_2	Disilane	SiSi	2.331	0.063	-0.166	0.081	sss
		SiH	1.492	-0.004	-0.118	-0.026	
		HSiSi	110.3	-0.8	2.3	-0.7	
$H_{10}Si_5$	Cyclopentasilane	Si-Si	2.342	0.040	-0.179	0.050	iii
GeH_4	Germane	Ge-H	1.527	-0.022	-0.046	0.019	ttt
$CGeH_6$	Methylgermane	Ge-C	1.945	0.010	-0.018	0.042	ss
		Ge-H	1.529	-0.024	-0.045	0.016	
		C-H	1.083	0.007	0.024	0.022	
C_2GeH_8	Ethylgermane	Ge-C	1.949	0.008	-0.008	0.055	xxx
		C-C	1.545	-0.052	-0.025	-0.056	
		Ge-C-C	112.2	-7.0	5.0	-1.0	
		Ge-H	1.522	-0.016	-0.039	0.023	
		H-Ge-C	109.7	-0.1	0.2	-2.2	
C_2GeH_8	Dimethylgermane	Ge-H	1.532	-0.027	-0.046	0.012	uuu
		H-Ge-H	108.7	0.0	0.7	5.2	
		Ge-C	1.950	0.007	-0.019	0.034	
		C-Ge-C	110.0	-0.4	0.8	-3.3	
C_3GeH_{10}	Trimethylgermane	Ge-H	1.522	-0.017	-0.034	0.021	xxx
		Ge-C	1.947	0.012	-0.013	0.035	
		H-Ge-C	109.3	0.3	-0.5	1.6	
C_4GeH_{12}	Tetramethylgermanium	Ge-C	1.945	0.015	-0.006	0.036	vvv
		C-H	1.120	-0.030	-0.013	-0.014	
GeO	Germanium oxide	Ge-O	1.625	0.012	-0.055	-0.002	ppp
$CGeH_3N$	Cyanogermane	Ge-C	1.919	-0.084	-0.060	-0.031	xxx
		C-N	1.155	0.003	0.011	0.008	
$CGeH_3NO$	Germyl isocyanate	Ge-H	1.532	-0.017	-0.048	0.007	www
		Ge-N	1.831	0.010	-0.001	-0.030	
GeH_3N_3	Germylazide	Ge-H	1.497	0.019	-0.012	0.057	xxx
		Ge-N	1.866	-0.035	0.010	-0.008	

Table 9.68: Comparison of Calculated and Observed Geometries for MNDO, AM1, and PM3 (contd.)

Empirical	Chemical Name	Geometric	Exp.	Errors			
Formula		Variable		PM3	MNDO	AM1	Ref.
GeS	Germanium sulfide	Ge-S	2.012	-0.039	-0.087	0.020	ppp
$CGeH_3NS$	Germyl isothiocyanate	Ge-H	1.520	-0.002	-0.037	0.021	iii
		Ge-N	1.817	0.015	0.028	-0.010	
		H-Ge-N	106.9	3.6	1.0	1.3	
		C-N	1.144	0.069	0.054	0.054	
GeF	Germanium fluoride	Ge-F	1.750	-0.039	-0.046	-0.093	yyy
GeH_3F	Fluorogermane	Ge-F	1.734	0.004	0.003	-0.019	iii
		Ge-H	1.523	-0.011	-0.039	0.017	
		F-Ge-H	106.0	3.9	2.6	2.3	
$CGeH_5F$	Methylgermanium fluoride dihydride	Ge-F	1.739	-0.003	0.003	-0.023	ppp
		Ge-C	1.927	0.034	0.004	0.044	
		C-Ge-F	106.0	1.5	1.7	-1.7	
		Ge-H	1.523	-0.012	-0.038	0.015	
		C-Ge-H	113.9	-4.3	-2.5	-3.1	
GeF_2	Germanium difluoride	Ge-F	1.732	-0.037	-0.017	-0.062	yyy
		F-Ge-F	97.2	14.5	-2.0	-1.7	
$C_2GeH_6F_2$	Dimethylgermanium difluoride	Ge-F	1.739	-0.015	0.004	-0.029	zzz
		F-Ge-F	105.4	-1.7	-3.7	-4.2	
		Ge-C	1.928	0.027	0.008	0.038	
		C-Ge-F	107.4	2.3	2.3	1.8	
$CGeH_3F_3$	Trifluoromethylgermane	Ge-C	1.904	0.046	0.032	0.065	iii
		Ge-F	1.714	0.000	0.024	-0.007	
		F-Ge-C	113.2	0.0	0.8	1.3	

GeH_3Cl	Chlorogermane	Ge-Cl	2.150	0.046	0.098	-0.018	ss
		Ge-H	1.537	-0.033	-0.060	0.009	
		H-Ge-H	111.0	-0.9	1.3	1.1	
C_3GeH_9Cl	Trimethylchlorogermane	Ge-Cl	2.170	0.033	0.088	-0.026	A
		Ge-C	1.940	0.011	-0.010	0.040	
		C-Ge-Cl	106.6	0.5	0.0	1.4	
GeF_3Cl	Chlorotrifluorogermane	Ge-Cl	2.067	0.067	0.189	0.105	xxx
		Ge-F	1.688	0.014	0.040	0.015	
		F-Ge-F	107.5	0.1	-0.7	-2.0	
$GeCl_2$	Germanium dichloride	Ge-Cl	2.186	-0.198	0.027	-0.089	yyy
		Cl-Ge-Cl	100.4	79.6	4.3	13.6	
$C_2GeH_6Cl_2$	Dimethylgermanium dichloride	Ge-Cl	2.143	0.039	0.099	-0.004	B
		Cl-Ge-Cl	105.0	1.9	1.1	3.3	
		Ge-C	1.928	0.014	-0.002	0.054	
		C-Ge-Cl	108.0	0.8	0.7	0.9	
$GeHCl_3$	Trichlorogermane	Ge-Cl	2.114	0.040	0.108	0.015	xxx
$CGeH_3Cl_3$	Trichloromethylgermane	Ge-Cl	2.135	0.028	0.097	0.001	xxx
		C-Ge-Cl	106.0	4.6	5.6	4.2	
$GeCl_4$	Germanium tetrachloride	Ge-Cl	2.113	0.037	0.112	0.024	C
GeH_3Br	Bromogermane	Ge-Br	2.297	0.035	0.069	-0.041	iii
		Ge-H	1.527	-0.026	-0.051	0.025	
		H-Ge-Br	106.3	1.6	0.7	3.2	
C_3GeH_9Br	Bromotrimethylgermane	Ge-Br	2.323	0.039	0.051	-0.055	xxx
		Ge-C	1.936	0.012	-0.006	0.055	
		Br-Ge-C	106.3	0.1	0.6	4.2	

Table 9.69: Comparison of Calculated and Observed Geometries for MNDO, AM1, and PM3 (contd.)

Empirical	Chemical Name	Geometric	Exp.	Errors			
Formula		Variable		PM3	MNDO	AM1	Ref.
$GeBr_2$	Germanium dibromide	Ge-Br	2.337	-0.015	-0.016	-0.157	D
		Br-Ge-Br	101.2	11.3	4.2	78.7	
$CGeH_3Br_3$	Tribromomethylgermane	Ge-C	1.889	0.047	0.036	0.133	iii
		Ge-Br	2.276	0.056	0.075	-0.010	
		C-Ge-Br	111.6	-1.0	-1.4	-5.8	
		C-H	1.120	-0.028	-0.014	-0.015	
$GeBr_4$	Germanium tetrabromide	Ge-Br	2.272	0.041	0.067	-0.003	E
GeH_3I	Iodogermane	Ge-I	2.508	-0.036	0.023	-0.075	xxx
GeI_4	Germanium tetraiodide	Ge-I	2.500	-0.032	-0.003	-0.090	ooo
GeH_6Si	Germylsilane	Ge-Si	2.357	0.047	-0.017	0.002	xxx
		Ge-H	1.529	-0.031	-0.047	0.020	
		Si-H	1.483	0.005	-0.104	-0.025	
Ge_2H_6	Digermane	GeGe	2.403	-0.010	0.121	-0.037	ss
		GeH	1.541	-0.038	-0.059	0.007	
		HGeH	106.4	4.0	1.4	2.0	
$C_6Ge_2H_{18}O$	Bis(trimethylgermanium) oxide	Ge-O	1.770	0.016	-0.016	0.079	F
		Ge-O-Ge	141.0	-15.8	38.9	-19.4	
		Ge-C	1.980	-0.005	-0.038	-0.011	
SnH_4	Tin tetrahydride (stannane)	Sn-H	1.701	0.000	-0.115		G
$CSnH_6$	Methyltin trihydride	Sn-C	2.140	0.047	-0.083		iii
		Sn-H	1.708	-0.007	-0.122		
		H-Sn-C	109.4	0.7	1.2		
C_2SnH_8	Dimethyltin dihydride	Sn-H	1.680	0.019	-0.092		H

		Sn-C	2.150	0.027	-0.091		
		H-Sn-C	108.0	1.8	1.4		
		C-Sn-C	104.8	4.5	7.6		
C_3SnH_{10}	Trimethyltin hydride	Sn-H	1.705	-0.008	-0.117		I
		Sn-C	2.147	0.018	-0.086		
		H-Sn-C	111.5	-1.8	-3.6		
C_4SnH_{12}	Tetramethyltin	Sn-C	2.134	0.014	-0.071		J
SnO	Tin oxide	SnO	1.833	0.006	-0.084		ppp
SnS	Tin sulfide	SnS	2.209	-0.071	-0.208		ppp
SnH_3Cl	Tin chloride trihydride	Sn-Cl	2.327	0.069	-0.018		xxx
$SnCl_2$	Tin dichloride	Sn-Cl	2.346	-0.006	-0.075		yyy
		Cl-Sn-Cl	99.0	-0.1	3.5		
$C_2SnH_6Cl_2$	Dimethyltin dichloride	Sn-Cl	2.327	0.037	-0.020		H
		Cl-Sn-Cl	106.2	-0.3	-2.1		
		Sn-C	2.109	0.000	-0.034		
		S-Sn-Cl	108.5	-0.2	-0.9		
$SnCl_4$	Tin tetrachloride	Sn-Cl	2.280	0.075	0.004		K
SnH_3Br	Tin bromide trihydride	Sn-Br	2.469	-0.016	-0.068		ss
		Sn-H	1.767	-0.075	-0.178		
		H-Sn-H	112.8	1.2	-0.4		
C_3SnH_9Br	Trimethyltin bromide	Sn-Br	2.490	-0.039	-0.074		L
		Sn-C	2.170	-0.056	-0.105		

Table 9.70: Comparison of Calculated and Observed Geometries for MNDO, AM1, and PM3 (contd.)

Empirical	Chemical Name	Geometric	Exp.	Errors			
Formula		Variable		PM3	MNDO	AM1	Ref.
$SnBr_2$	Tin dibromide	Sn-Br	2.512	-0.108	-0.149		yyy
		Br-Sn-Br	100.0	2.5	4.2		

$SnBr_4$	Tin tetrabromide	Sn-Br	2.440	0.000	-0.055		M
SnH_3I	Tin iodide trihydride	Sn-I	2.674	-0.051	-0.139		xxx
C_3SnH_9I	Trimethyltin iodide	Sn-I	2.720	-0.052	-0.168		L
SnI_2	Tin diiodide	Sn-I	2.706	-0.062	-0.210		yyy
		I-Sn-I	103.8	5.7	3.3		
PbH	Lead hydride	Pb-H	1.839	-0.110	-0.181		a
C_4PbH_{12}	Tetramethyllead	Pb-C	2.240	-0.054	-0.069		N
		C-H	1.080	0.013	0.022		
		H-C-Pb	104.6	6.0	4.5		
PbO	Lead oxide	Pb-O	1.920	0.016	-0.038		O
PbS	Lead sulfide	Pb-S	2.290	-0.138	-0.179		O
PbF	Lead fluoride	Pb-F	2.058	-0.030	-0.063		a
PbF_2	Lead difluoride	Pb-F	2.033	-0.007	-0.038		P
		F-Pb-F	97.2	-8.3	-5.8		
PbCl	Lead chloride	Pb-Cl	2.180	0.203	0.198		a
$PbCl_2$	Lead dichloride	Pb-Cl	2.444	0.014	-0.064		Q
		Cl-Pb-Cl	98.3	1.3	2.5		
$PbCl_4$	Lead tetrachloride	Pb-Cl	2.430	-0.154	-0.049		a
PbBr	Lead bromide	Pb-Br	2.546	0.017	-0.080		a
$PbBr_2$	Lead dibromide	Pb-Br	2.597	-0.032	-0.127		P
		Br-Pb-Br	99.2	3.4	2.7		
PbI	Lead iodide	Pb-I	2.736	0.037	-0.155		a
PbI_2	Lead diiodide	Pb-I	2.804	-0.026	-0.206		P
		I-Pb-I	99.7	8.2	4.4		
$C_6Pb_2H_{18}$	Hexamethyldiplumbane	Pb-Pb	2.880	-0.012	-0.110		R
		Pb-C	2.250	-0.050	-0.073		
		Pb-Pb-C	109.5	2.8	2.2		
H_3P	Phosphine	PH	1.420	-0.096	-0.080	-0.057	a
		HPH	93.8	3.3	2.3	2.6	
CP	Carbon phosphide	CP	1.562	-0.173	-0.145	-0.029	a
CHP	Methinophosphide	CP	1.542	-0.133	-0.114	-0.132	a
		HC	1.067	0.001	-0.010	-0.003	
CH_5P	Methylphosphine	CP	1.858	0.007	-0.108	-0.132	ss
		PH	1.423	-0.087	-0.080	-0.059	

		HPC	97.5	2.5	3.3	2.5	
		HPH	93.4	3.5	2.6	2.8	
C_3H_9P	Trimethylphosphine	CP	1.843	0.029	-0.081	-0.118	ss
		CPC	98.9	1.7	7.9	3.2	
C_5H_5P	Phosphole (?)	C1C2	1.384	-0.006	0.013	-0.005	ss
		CP	1.733	-0.042	-0.092	-0.133	
		C2C3	1.413	-0.034	-0.016	-0.034	
PO	Phosphorus oxide	PO	1.476	-0.018	-0.053	-0.039	a
NP	Phosphorus nitride	PN	1.491	-0.077	-0.093	-0.109	a
CH_2PF	CH2=P-F	P-F	1.598	-0.030	-0.049	-0.052	S
		C=P	1.644	-0.071	-0.064	-0.106	

Table 9.71: Comparison of Calculated and Observed Geometries for MNDO, AM1, and PM3 (contd.)

Empirical	Chemical Name	Geometric	Exp.	Errors			
Formula		Variable		PM3	MNDO	AM1	Ref.
PF_3	Phosphorus trifluoride	PF	1.570	-0.012	-0.014	-0.027	a
		FPF	97.8	-2.0	1.1	0.2	
POF_3	Phosphous oxyfluoride	PF	1.520	0.009	0.034	0.006	a
		FPF	102.5	-2.7	-0.6	-0.8	
		PO	1.450	0.001	0.036	0.001	
PSF_3	Phosphorus thiofluoride	PF	1.530	0.009	0.027	0.000	a
		FPF	100.3	-5.2	-0.9	-1.8	
		PS	1.870	0.064	0.106	0.004	
PF_5	Phosphorus pentafluoride	PF(ax)	1.577	-0.024	0.025	-0.028	a
		PF(eq)	1.534	-0.006	0.039	0.001	
PCl_3	Phosphorus trichloride	PCl	2.039	0.025	-0.050	-0.120	a
		ClPCl	100.3	-0.6	4.9	5.1	
PCl_5	Phosphorus pentachloride	PCl(ax)	2.190	-0.097	-0.078	-0.115	a
		PCl(eq)	2.040	0.012	-0.007	-0.069	

PBr_3	Phosphorus tribromide	PBR	2.220	-0.070	-0.131	-0.119	ss
		BrPBr	101.0	0.3	4.7	5.8	
$POBr_3$	Phosphorus oxybromide	P=O	1.455	-0.048	0.021	0.025	iii
		P-Br	2.174	-0.059	-0.046	-0.014	
		O=P-Br	114.2	2.3	-0.4	1.0	
$PSBr_3$	Phosphorus thiotribromide	P=S	1.894	-0.053	-0.042	-0.011	iii
		P-Br	2.193	-0.102	-0.077	-0.040	
		S=P-Br	116.2	12.0	-1.5	-1.0	
BH_3PF_3	PH3-BF3	P-B	1.836		2.386	0.321	xxx
		P-H	1.207		0.132	0.158	
		H-P-H	115.1		-18.8	-16.6	
GeH_3PSF_2	Difluoro(germylthio)phosphine	Ge-S	2.256	0.031	-0.072	0.058	iii
		P-S	2.115	-0.013	-0.163	-0.009	
		Ge-S-P	99.0	26.4	41.3	17.6	
		Ge-H	1.538	-0.032	-0.061	0.006	
		S-Ge-H	110.0	3.5	-3.2	-1.2	
		P-F	1.590	-0.035	-0.032	-0.052	
		S-P-F	99.9	13.4	5.4	9.3	
Ge_3H_9P	Trigermylphosphine	P-Ge	2.306	-0.070	-0.159	-0.204	iii
		Ge-P-Ge	95.7	13.5	24.3	24.3	
		Ge-H	1.490	0.016	-0.009	0.031	
		P-Ge-H	110.3	5.6	-3.0	-7.8	
P_2	Phosphorus dimer	PP	1.894	-0.179	-0.200	-0.271	a
$Ge_2H_6P_2F_2$	1,1-Difluoro-2,2-digermyldiphosphan	P-F	1.581	-0.032	-0.028	-0.052	iii
		P-P	2.177	-0.061	-0.209	-0.288	
		P-P-F	98.9	8.1	7.1	0.6	

		Ge-P	2.320	-0.110	-0.141	-0.166	
		Ge-P-F	95.7	33.6	31.9	30.5	
		Ge-P-Ge	98.6	12.3	19.8	12.3	
		Ge-H	1.512	0.000	-0.034	0.018	
P_4	Phosphorus tetramer	PP	2.210	-0.013	-0.158	-0.170	a
P_4O_6	Phosphorus trioxide	PO	1.650	0.058	-0.046	0.020	a
		OPO	99.0	-2.5	-3.0	-2.3	

Table 9.72: Comparison of Calculated and Observed Geometries for MNDO, AM1, and PM3 (contd.)

Empirical	Chemical Name	Geometric	Exp.	Errors			
Formula		Variable		PM3	MNDO	AM1	Ref.
P_4O_{10}	Phosphorus pentoxide	P-O	1.600	0.090	0.006	0.004	a
		O-P-O	101.0	-4.7	-3.1	14.2	
AsH_3	Arsine	As-H	1.513	0.007			T
		H-As-H	92.1	2.1			
C_3AsN_3	Arsenic tricyanide	As-C	1.900	-0.031			ooo
		C-As-C	92.0	6.3			
		As-C-N	171.0	4.9			
AsF_3	Arsenic trifluoride	As-F	1.706	0.000			ooo
		F-As-F	96.2	-0.3			
AsF_5	Arsenic pentafluoride	As-F(ax)	1.711	-0.026			ss
		As-F(eq)	1.656	0.005			
C_3AsF_9	Triperfluoromethylarsine	As-C	2.053	0.028			ooo
		C-As-C	100.0	-0.5			
$AsCl_3$	Arsenic trichloride	As-Cl	2.161	0.002			ooo
		Cl-As-Cl	98.7	1.1			
$AsBr_3$	Arsenic tribromide	As-Br	2.323	-0.008			iii
		Br-As-Br	99.8	0.5			
AsI_3	Arsenic triiodide	As-I	2.550	-0.041			ooo

		I-As-I	100.2	4.6			
AsH_9Si_3	Trisilylarsine	As-Si	2.353	0.018			iii
		Si-As-Si	94.1	-3.3			
		Si-H	1.470	0.024			
C_2ZnH_6	Dimethylzinc	Zn-C	1.930	0.007	-0.046	-0.031	U
		C-Zn-C	180.0	0.0	0.6	-0.1	
C_4ZnH_{10}	Diethylzinc	Zn-C	1.950	0.017	-0.046	-0.022	U
		C-C-Zn	114.5	-15.8	3.9	0.1	
		C-Zn-C	180.0	0.2	0.1	0.0	
C_6ZnH_8	Cyclopentadienylmethylzinc	C-C	1.438	-0.003	0.012	0.000	V
		C-Zn	2.280	0.061	-0.023	0.078	
		Zn-C(H3)	1.903	0.043	-0.025	-0.023	
C_6ZnH_{14}	Di-n-propylzinc	C-C-C	113.6	-0.8	1.8	-1.7	U
		Zn-C	1.952	0.021	-0.044	-0.020	
		Zn-C-C	114.5	-13.6	3.8	0.6	
		C-Zn-C	180.0	0.0	0.0	0.0	
ZnF_2	Zinc difluoride	Zn-F	1.742	-0.002	-0.062	0.006	yyy
		F-Zn-F	180.0	0.0	0.1	0.0	
$ZnCl_2$	Zinc dichloride	Zn-Cl	2.062	0.002	0.053	0.005	yyy
		Cl-Zn-Cl	180.0	0.0	0.0	0.0	
$ZnBr_2$	Zinc dibromide	Zn-Br	2.204	-0.107	0.031	-0.093	yyy
		Br-Zn-Br	180.0	0.0	0.0	0.0	
ZnI_2	Zinc diiodide	Zn-I	2.401	0.003	-0.019	-0.055	yyy
		I-Zn-I	180.0	0.0	-0.1	0.0	
C_2CdH_6	Dimethylcadmium	Cd-C	2.112	-0.077			xxx
$C_4CdN_4S_4$	Cd(NCS)3(SCN) (=)	Cd-N	2.240	-0.022			W
		Cd-S	2.570	-			

				0.001			
CdF_2	Cadmium difluoride	Cd-F	1.970	-0.004			ooo
$CdCl_2$	Cadmium dichloride	Cd-Cl	2.210	0.015			ooo

Table 9.73: Comparison of Calculated and Observed Geometries for MNDO, AM1, and PM3 (contd.)

Empirical	Chemical Name	Geometric	Exp.	Errors			
Formula		Variable		PM3	MNDO	AM1	Ref.
$CdBr_2$	Cadmium dibromide	Cd-Br	2.394	-0.034			X
CdI_2	Cadmium diiodide	Cd-I	2.550	0.038			ooo
HgH	Mercury hydride	Hg-H	1.740	-0.044	-0.190	-0.069	a
HgO	Mercury oxide	Hg-O	1.840	0.001	0.042	0.222	www
C_2HgH_3N	Methylmercuric cyanide	Hg-CN	2.082	-0.055	-0.148	-0.070	Y
		Hg-CH3	2.051	0.056	-0.069	-0.005	
		C-N	1.141	0.016	0.030	0.026	
HgF	Mercury fluoride	Hg-F	1.890	0.010	-0.019	0.003	www
HgF_2	Mercury difluoride	Hg-F	1.960	-0.032	-0.082	-0.052	www
C_2HgF_6	Ditrifluoromethyl mercury	Hg-C	2.101	-0.003	0.162	0.110	Z
		C-Hg-C	180.0	0.0	0.3	0.2	
HgCl	Mercury chloride	Hg-Cl	2.230	-0.036	0.049	0.010	a
$CHgH_3Cl$	Methylmercuric chloride	Hg-C	2.052	0.060	-0.070	-0.003	xxx
		Hg-Cl	2.285	-0.031	0.006	-0.031	
$HgCl_2$	Mercury dichloride	Hg-Cl	2.252	-0.007	0.016	-0.013	AA
HgBr	Mercury bromide	Hg-Br	2.330	-0.116	0.038	-0.101	www
$CHgH_3Br$	Methylmercuric bromide	Hg-C	2.062	0.028	-0.079	-0.012	iii
		Hg-Br	2.405	-0.114	-0.021	-0.148	
		C-H	1.095	-0.008	0.013	0.013	
		Hg-C-H	109.6	-0.1	0.1	-1.8	
$HgBr_2$	Mercury dibromide	Hg-Br	2.440	-0.215	-0.077	-0.190	BB
HgI	Mercury iodide	Hg-I	2.490	0.156	-0.024	0.036	www
$CHgH_3I$	Methylmercuric iodide	Hg-C	2.069	0.008	-0.082	-0.015	iii
		Hg-I	2.588	-0.087	-0.109	-0.094	
HgI_2	Mercury diiodide	Hg-I	2.554	-0.080	-0.079	-0.058	CC

SbH_3	Stibine	Sb-H	1.707	-0.005			ooo
		H-Sb-H	91.3	1.1			
SbF_5	Antimony pentafluoride	Sb-F(ax)	2.430	-0.455			ooo
		Sb-F(eq)	2.310	-0.348			
C_3SbF_9	Triperfluoromethylstibine	Sb-C	2.202	0.007			ooo
		C-Sb-C	100.0	-0.8			
$SbCl_3$	Antimony trichloride	Sb-Cl	2.323	-0.003			iii
		Cl-Sb-Cl	97.1	-0.1			
$SbCl_5$	Antimony pentachloride	Sb-Cl(ax)	2.338	0.035			yyy
		Sb-Cl(eq)	2.277	0.073			
$SbBr_3$	Antimony tribromide	Sb-Br	2.490	-0.019			ooo
		Br-Sb-Br	98.0	0.4			
SbH_9Si_3	Trisilylstibine	Sb-Si	2.555	-0.022			iii
		Si-Sb-Si	89.0	5.8			
		Si-H	1.470	0.018			
Sb_2	Antimony, dimer	Sb-Sb	2.590	-0.289			DD
SeH_2	Hydrogen selenide	SeH	1.460	0.010			ooo
		HSeH	91.0	2.6			
CSe	Selenium carbide	Se-C	1.676	-0.085			ppp
$CSeH_4$	Methylselenium hydride	CSe	1.959	-0.012			ss
		CH	1.088	0.005			
		SeH	1.473	-0.003			

Table 9.74: Comparison of Calculated and Observed Geometries for MNDO, AM1, and PM3 (contd.)

Empirical	Chemical Name	Geometric	Exp.	Errors			
Formula		Variable		PM3	MNDO	AM1	Ref.
C_2SeH_6	Ethyl selanol (anti)	Se-H	1.440	0.026			EE
		Se-C	1.962	-0.006			
		H-Se-C	93.5	6.4			
		Se-C-C	108.7	-8.5			
C_2SeH_6	Dimethylselenium	Se-C	1.943	0.005			FF
		C-Se-C	96.2	4.6			

C_4SeH_4	Selenophene	Se-C2	1.855	0.032			xxx
		C5-Se-C2	87.8	0.1			
		C2-C3	1.369	-0.025			
		Se-C2-C3	111.6	-1.5			
		C2-H	1.070	0.014			
		Se-C2-H2	121.7	-0.6			
C_4SeH_8	Tetrahydroselenophene	Se-C2	1.963	-0.004			xxx
		C5-Se-C2	90.7	1.5			
		C2-C3	1.549	-0.043			
		Se-C2-C3	104.0	-0.1			
SeO	Selenium oxide	Se-O	1.663	-0.063			GG
SeO_2	Selenium dioxide	SeO	1.608	-0.003			ppp
		OSeO	113.8	-7.2			
SeO_3	Selenium trioxide	Se-O	1.688	-0.150			iii
CSeHN	Isoselenocyanic acid (Se=C=N-H)	Se=C	1.719	-0.079			iii
		C=N	1.191	0.005			
		Se=C=N	175.0	0.0			
		N-H	0.990	-0.014			
		C=N-H	140.0	15.1			
CSeS	Carbon sulfide selenide	C-S	1.533	-0.081			xxx
		C-Se	1.695	-0.110			
$CSeF_2$	Selenocarbonyl difluoride	C=Se	1.743	0.002			iii
		C-F	1.314	0.006			
		F-C-F	107.5	-2.2			
$SeOF_2$	Selenyl fluoride	SeO	1.576	0.049			ss
		SeF	1.730	-0.006			

		FSeO	104.8	-3.4			
		FSeF	92.2	2.3			
SeO_2F_2	Selenoyl fluoride	Se-F	1.685	0.020			iii
		F-Se-F	94.1	1.0			
		Se-O	1.575	-0.017			
		O-Se-O	126.2	3.7			
SeF_4	Selenium tetrafluoride	SeF	1.770	-0.034			ooo
		FSeF	169.2	-28.9			
		SeF'	1.680	0.028			
		F'SF'	100.5	11.5			
$CSeNOF_5$	Pentafluoro(isocyanato)selenium	Se-F	1.677	0.032			iii
		Se-N	1.789	0.053			
		N=C	1.260	0.007			
		Se-N=C	116.9	12.3			
		C=O	1.187	-0.020			
		N=C=O	172.9	-0.6			

Table 9.75: Comparison of Calculated and Observed Geometries for MNDO, AM1, and PM3 (contd.)

Empirical	Chemical Name	Geometric	Exp.	Errors			
Formula		Variable		PM3	MNDO	AM1	Ref.
SeF_6	Selenium hexafluoride	SeF	1.685	0.005			HH
C_2SeF_6	Diperfluoromethyl selenide	Se-C	1.960	0.047			ooo
		C-Se-C	104.0	-2.8			
$SeCl_2$	Selenium dichloride	Se-Cl	2.157	0.007			iii
		Cl-Se-Cl	99.6	0.0			
$SeOCl_2$	Selenyl chloride	Se=O	1.614	0.020			iii
		Se-Cl	2.205	-0.005			
		O=Se-Cl	106.0	-3.0			
		Cl-Se-Cl	96.9	1.2			
In_2Se	Indium(I) selenide	In-Se	2.650	-			iii

				0.070			
		In-Se-In	113.0	66.3			
SeSi	Silicon selenide	Se-Si	2.058	-0.084			xxx
SeH_6Si_2	Disilyl selenide	Se-Si	2.270	0.123			ooo
		Si-Se-Si	97.0	-0.1			
GeSe	Germanium selenide	Ge-Se	2.135	-0.208			xxx
SnSe	Tin selenide	Sn-Se	2.326	-0.002			xxx
PbSe	Lead selenide	Pb-Se	2.402	-0.041			xxx
$SeHPF_2$	Difluorophosphine selenide	P=Se	2.026	0.062			iii
		P-F	1.557	-0.006			
		Se=P-F	116.8	-1.0			
		P-H	1.422	-0.158			
		Se=P-H	118.6	-0.3			
		F-P-F	98.1	-4.3			
$C_2Se_2H_6$	Me-Se-Se-Me	Se-C	1.950	-0.005			ooo
		Se-Se	2.330	0.040			
		Se-Se-C	99.0	1.2			
Se_2OF_{10}	Bis(pentafluoroselenium)oxide	Se-O	1.679	0.048			iii
		Se-O-Se	142.4	-16.4			
		Se-F(eq)	1.683	0.008			
		Se-F(ax)	1.665	0.031			
$C_7GeSe_2H_1$	Tetramethyldiselenagermacyclohexane	Se-C	-10.8	-4.2			II
		Ge-Se	108.7	2.8			
		Ge-Se-C	116.3	-2.1			
		Se-Ge-Se	-114.7	0.5			
		Ge-C'	100.2	-0.4			
		Ge-C"	119.2	-0.5			
		C'-Ge-C"	-24.2	-4.5			

TeH_2	Hydrogen telluride	Te-H	1.658	0.017			JJ
		H-Te-H	90.3	-2.0			
TeO_2	Tellurium dioxide	Te-O	1.830	-0.128			iii
$CTeNOF_5$	Pentafluoro(isocyanato)tellurium	Te-F	1.826	-0.002			iii
		Te-N	1.859	-0.045			
		Te-N=C	126.5	53.6			
TeF_6	Tellurium hexafluoride	TeF	1.815	0.001			iii
$TeCl_4$	Tellurium tetrachloride	Te-Cl	2.330	0.072			tt
$TeBr_2$	Tellurium dibromide	Te-Br	2.510	0.000			ooo
		Br-Te-Br	98.0	1.5			

Table 9.76: Comparison of Calculated and Observed Geometries for MNDO, AM1, and PM3 (contd.)

Empirical	Chemical Name	Geometric	Exp.	Errors			
Formula		Variable		PM3	MNDO	AM1	Ref.
$TeBr_4$	Tellurium tetrabromide	Te-Br	2.680	-0.149			tt
In_2Te	Indium(I) telluride	In-Te	2.840	-0.004			iii
		In-Te-In	99.0	6.0			
GeTe	Germanium telluride	Ge-Te	2.340	-0.338			ppp
SnTe	Tin telluride	Sn-Te	2.523	0.049			ppp
PbTe	Lead telluride	Pb-Te	2.595	0.141			xxx
$C_9TeH_{13}PS$	MeOPh-Te-S-P(S)(OMe)2	Te-C	2.114	-0.027			KK
		Te-S	2.444	0.234			
		C-Te-S	94.9	10.8			
		S-P	2.051	0.052			
		P-S-Te	103.3	-13.9			
		P=S	1.933	0.061			
		S=P-S	107.9	-1.4			

Te_2	Tellurium, dimer	Te-Te	2.560	0.145			ppp
Te_2OF_{10}	Bis(pentafluorotellurium)oxide	Te-O	1.832	-0.057			iii
		Te-O-Te	145.5	10.4			
		Te-Feq	1.820	-0.009			
		Te-Fax	1.799	0.015			
		Fax-Te-Feq	89.9	4.4			
C_3BiH_9	Trimethylbismuth	Bi-C	2.270	-0.004			ooo
		C-Bi-C	96.7	0.3			
$BiCl_3$	Bismuth trichloride	Bi-Cl	2.425	-0.006			yyy
		Cl-Bi-Cl	97.3	2.7			
$BiBr_3$	Bismuth tribromide	Bi-Br	2.630	-0.026			ooo
		Br-Bi-Br	100.0	-1.4			

bf References

a: M. W. Chase, C. A. Davies, J. R. Downey, D. R. Frurip, R. A. McDonald, A. N. Syverud, JANAF Thermochemical Tables, Third Edition, J. Phys. Chem. Ref. Data 14, Suppl. 1 (1985).
b: G. Herzberg, "Molecular Spectra and Molecular Structure III. Electronic Spectra and Electronic Structure of Polyatomic Molecules", Van Nostrand, New York, N.Y., 1966.
c: A. G. Maki, R. A. Toth, J. Mol. Spectr., 17, 136 (1965).
d: W. M. Stigliani, V. W. Laurie, J. C. Li, J. Chem. Phys., 62, 1890 (1975).
e: R. A. Bonham, L. S. Bartell, J. Am. Chem. Soc., 81, 3491 (1959).
f: O. Bastiansen, F. N. Fritsch, K. Hedberg, Acta. Crystallogr., 17, 538 (1964).
g: D. R. Lide, D. Christensen, J. Chem. Phys., 35, 1374 (1961).
h: J. H. Callomon, B. P. Stoicheff, Can. J. Phys., 35, 373 (1957).
i: A. Almenningen, O. Bastiansen, M. Traetteberg, Acta Chem. Scand., 15, 1557 (1961).
j: T. Fukuyama, K. Kuchitsu, Y. Morino, Bull. Chem. Soc. Jap., 42, 379 (1969).
k: K. W. Cox, M. D. Harmony, G. Nelson, K. B. Wiburg, J. Chem. Phys., 50, 1976 (1969).
l: W. Haugen, M. Traetteberg, Acta Chem. Scand., 20, 1226 (1966).
m: A. Almenningen, I. M. Anfinsen, A. Haaland, Acta Chem. Scand., 24, 43 (1970).
n: S. Meiboom, L. C. Snyder, J. Chem. Phys., 52, 3857 (1970).
o: L. R. H. Scharpen, V. W. Laurie, J. Chem. Phys., 39, 1972 (1963).
p: D. R. Lide, J. Chem. Phys., 33, 1519 (1960).
q: B. W. McCelland, K. Hedberg, J. Am. Chem. Soc., 109, 7304 (1987)
r: K. Tamagawa, T. Iijima, M. Kimura, J. Mol. Struct., 30, 243 (1976).

s: P. A. Baron, R. D. Brown, F. R. Burden, P. J. Domaille, J. E. Kent, J. Mol. Spectrosc., 43, 401 (1970).
t: J. F. Chiang, S. H. Bauer, J. Am. Chem. Soc., 91, 1898 (1969).
u: O. Bastiansen, L. Fernholt, H. M. Seip, H. Kambara, K. Kuchitsu, J. Mol. Struct., 18, 163 (1973).
v: G. Herzberg, "Molecular Spectra and Molecular Structure I. Spectra of Diatomic Molecules", 2nd ed, Van Nostrand, New York, N.Y., 1950.
w: K. Takagi, T. Oka, J. Phys. Soc. Jap., 18, 1174 (1963).
x: R. M. Lees, J. G. Baker, J. Chem. Phys., 48, 5299 (1968).
y: A. P. Cox, L. F. Thomas, J. Sheridan, Spectrochim. Acta, 15, 542 (1959).
aa: U. Blukis, P. H. Kasai, R. J. Myers, J. Chem. Phys., 38, 2753 (1963).
bb: K. Kuchitsu, T. Fukuyama, Y. Marino, J. Mol. Struct., 1, 463 (1968).
cc: R. Nelson, L. Pierce, J. Mol. Spectrosc. 18, 344 (1965).
dd: B. Bak, D. Christensen, W. B. Dixon, L. Hansen-Nygarrd, J. Rastrup-Anderson, M. Shottlander, J. Mol. Spectrosc., 9, 124 (1962).
ee: W. C. Oelfke, W. Gordy, J. Chem. Phys., 51, 5336 (1969).
ff: G. H. Kwei, R. F. Curl, J. Chem. Phys., 32, 1592 (1960).
gg: R. F. Curl, Jr. J. Chem. Phys., 30, 1529 (1959).
hh: J. Trotter, Acta Crystallogr., 13, 86 (1960).
ii: D. G. Lister, J. K. Tyler, J. H. Hog, N. W. Larson, J. Mol. Struct., 23, 253 (1974).
jj: D. R. Lide, J. Chem. Phys., 27, 343 (1957).
kk: C. C. Costain, J. Chem. Phys., 29, 864 (1958).
ll: J. E. Wollrab, V. W. Laurie, J. Chem. Phys., 48, 5058 (1968).
mm: J. E. Wollrab, V. W. Laurie, J. Chem. Phys., 51, 1580 (1969).
nn: D. R. Johnson, F. J. Lovas, W. H. Kirchhoff, J. Phys. Chem. Ref. Data, 1, 1011 (1972).
oo: J. O. Morley, J. Chem. Soc. Perkin Trans. II, (1987), (in press).
pp: S. Cradock, P. B. Liescheski, D. W. H. Rankin, H. E. Robertson, J. Am. Chem. Soc., 110, 2758 (1988).
qq: J. K. Tyler, J. Mol. Spectrosc., 11, 39 (1963).
rr: J. E. Lancaster, B. J. Stoicheff, Can. J. Phys., 34, 1016 (1965).
ss: J. H. Callomon, E. Hirota, K. Kuchitsu, W. J. Lafferty, A. G. Maki, C. S. Pote, "Structure Data on Free Polyatomic Molecules", Landolt-Bornstein, New Series, Group II, Vol. 7, Springer, Berlin (1976).
tt: L.E. Sutton, "Tables of Interatomic Distances and Configurations in Molecules and Ions", Special Publication No. 11 + 18, Chem. Soc., London (1958), (1965).
uu: R. W. Kilb, J. Chem. Phys., 23, 1736 (1955).
vv: B. Bak, D. Christensen, L. Hansen-Nygarrd, J. Rastrup-Anderson, J. Mol. Spectrosc., 7, 58 (1961).
ww: J. K. G. Watson, J. Mol. Spectrosc., 48, 479 (1973).
xx: D. W. W. Anderson, D. W. H. Rankin, A. Robertson, J. Mol. Struct., 14 385 (1972).
yy: P. Rosmus, H. Stafast, H. Bock, Chem. Phys. Lett., 34, 275 (1975).
zz: G. Winnewisser, M. Winnewisser, W. Gordy, J. Chem. Phys., 49, 3465 (1968).
aaa: R. Sutter, H. Driezler, F. Z. Rudolph, Naturforschung A, 20 1676 (1965).
bbb: J. Donohue, A. Caron, E. Goldish, J. Am. Chem. Soc., 83, 3748 (1961).
ccc: A. Caron, J. Donohue, Acta Crystallogr., 18, 562 (1965).
ddd: G. A. Kuipers, D. F. Smith, A. N. Nielsen, J. Chem. Phys., 25, 275 (1956).
eee: J. L. Duncan, J. Mol. Struct., 6, 447 (1970).
fff: J. K. Tyler, J. Sheridan, Trans. Faraday Soc., 59, 2661 (1963).
ggg: J. L. Carlos, R. R. Karl, S. H. Bauer, J. Chem. Soc., Faraday Trans. 2, 177 (1974).

hhh: T. Ogata, K. Fujii, M. Yoshikawa, F. Hirota, J. Am. Chem. Soc., 109, 7639 (1987).
iii: J. H. Callomon, E. Hirota, T. Iijima, K. Kuchitsu, W. J. Lafferty, "Structure Data on Free Polyatomic Molecules", Landolt-Bornstein, New Series, Group II, Vol. 15, Springer, Berlin (1977).
jjj: A. S. Rodgers, J. Chao, R. C. Wilhoit, B. J. Zwolinski, J. Phys. Chem. Ref. Data, 3, 117 (1974).
kkk: Private Communication by Dr Dave Dixon, DuPont.
lll: H. Jones, M. Takami, J. Sheridan, Z. Naturforsch., A33, 156 (1978).
mmm: S. S. Chen, A. C. Wilhoit, B. J. Zwolinski, J. Phys. Chem. Ref. Data 5, 571 (1975).
nnn: I. Hargittai, Acta Chem. (Budapest), 49, 351 (1969).
ooo: "Structural Inorganic Chemistry", A. F. Wells, Clarendon Press, Oxford, 1984
ppp: K. P. Huber, G. Herzberg, "Molecular Spectra and Molecular Structure", IV. "Constants for Diatomic Molecules", Van Nostrand, Reinhold, New York, (1979).
qqq: H. Jones, J. Sheridan, O. Stiefvater, Z. Naturforsch., A32, 866 (1977).
rrr: N. P. C. Westwood, W. Lewis-Bevan, M. C. L. Gerry, J. Mol. Spectr., 136, 93 (1989).
sss: Y. Niide, I. Ohkoshi, J. Mol. Spectr., 136, 17 (1989).
ttt: K. Hagen, B. Lunelli, J. Phys. Chem., 93, 1326 (1989).
uuu: U. Anderson, N. Heineking, H. Dreizler, J. Mol. Struct. 137, 296 (1989).
vvv: N. N. Greenwood, A. Earnshaw, "Chemistry of the Elements", Pergamon Press, Oxford, p.976 (1984).
www: D. R. Stull, H. Prophet, Natl. Stand., Ref. Data Ser. (U.S., Natl. Bur. Stand.) NSRDS-NBS 37, 1971.
xxx: M. D. Harmony, V. W. Laurie, R. L. Kuczkowsky, R. H. Schwendeman, D. A. Ramsay, F. J. Lovas, W. J. Lafferty, A. G. Maki, J. Phys. Chem. Ref. Data 8, 3 (1979).
yyy: M. Hargittai, Coord. Chem. Rev., 91, 35 (1988).
zzz: L. J. Guggenberger, R. E. Rundle, J. Am. Chem. Soc., 86, 5344 (1964).
aaaa: G. Herzberg, J. W. C. Johns, Proc. R. Soc. London, Ser. A., 298, 142 (1967).
bbbb: D. Christen, D. G. Lister, J. Sheridom, J. Chem. Soc., Faraday Trans. 2, 70, 1953 (1974).
cccc: S. G. W. Ginn, J. K. Kennedy, J. Overend, J. Chem. Phys., 48, 1571 (1968).
dddd: L. A. Curtiss, J. A. Pople, J. Chem. Phys., 90, 4314 (1989).
eeee: C. H. Chang, R. F. Porter, S. H. Bauer, Inorg. Chem., 8, 1689 (1969).
ffff: W. Harshbarger, G. Lee, R. F. Porter, S. H. Bauer, Inorg. Chem. 8, 1683 (1969).
gggg: R. A. Beaudet, R. L. Poynter, J. Chem. Phys., 53, 1899 (1970).
hhhh: D. Schwock, A. B. Burg, R. A. Beaudet, Inorg. Chem. 16, 3219 (1977).
iiii: E. Switkes, I. R. Epstein, J. A. Tossell, R. M. Stevens, W. N. Lipscomb, J. Am. Chem. Soc., 92, 3837 (1970).
jjjj: nI. R. Epstein, J. A. Tossell, E. Switkes, I. R. M. Stevens, W. N. Lipscomb, Inorg. Chem., 10, 171, (1971).
llll: M. J. Goode, A. J. Downs, C. R. Pulham, D. W. H. Rankin, H. E. Robertson, J. Chem. Soc. Chem. Comm., 768 (1988).
mmmm: S. N. Vempati, W. E. Jones, J. Mol. Spect., 127, 232 (1988).
nnnn: J. H. Meadows, H. F. Schaefer III, J. Am. Chem. Soc., 98, 4383 (1976).
oooo: J. Nakagawa, Y. Shiko, M. Hayashi, J. Mol. Spect., 122, 1 (1987).
pppp: M. Hayashi, S. Kaminaka, M. Fujitake, S. Miyazaki, J. Mol. Spect., 135, 289 (1989).
qqqq: R. W. Davis, M. C. L. Gerry, J. Mol. Spectrosc. 60, 117 (1976).
rrrr: A. P. Cox, I. C. Ewart, T. R. Gayton, J. Mol. Spect., 125, 76 (1987).
ssss: K. C. Shotton, A. G. Lee, W. J. Jones, J. Raman Spectrosc., 1, 243 (1973).

tttt: R. A. Eades, D. A. Dixon, J. Chem. Phys., 72, 3309 (1980).
uuuu: J. Durig, M. M. Chen, Y. S. Li, J. Phys. Chem., 77, 227 (1973), and E. C. Thomas, V. W. Laurie, J. Chem. Phys., 50, 3512 (1969).
vvvv: J. L. Hencher, F. J. Mistoe, Can. J. Chem., 53, 3542 (1975).
wwww: J. D. Murdoch, D. W. H. Rankin, B. Beagley, J. Mol. Struct., 31, 291, (1976).
xxxx: P. Groner, G. M. Attia, A. B. Mohamad, J. F. Sullivan, Y. S. Li, J. R. Durig, J. Chem. Phys., 91, 1434 (1989).
yyyy: S. Saito, Y. Endo, E. Hirota, J. Mol. Spect., 116, 499 (1986).
zzzz: J. E. Drake, R. T. Hemmings, J. L. Hencher, F. M. Mustoe, Q. Shem, J. Chem. Soc., Dalton Trans., 394, (1976).
A: J. Durig, K. L. Hellams, J. Mol. Struct., 29, 349 (1975).
B: J. E. Drake, H. L. Hencher, Q. Shem, Can. J. Chem., 55, 1104 (1977).
C: Y. Morino, Y. Nakamura, T. Iijima, J. Chem. Phys., 32, 643 (1960).
D: G. Schultz, J. Tremmel, I. Hargittai, N. D. Kagramanov, A. K. Maltsev, O. M. Nefedov, J. Mol. Struct., 82, 107 (1982).
E: G. G. B. Souza, J. D. Wieser, J. Mol. Struct., 25, 442 (1975).
F: L. V. Vilkov, N. A. Tarensenko, Zh. Strukt. Khim., 10, 102 (1969).
G: G. R. Wilkinson, M. K. Wilson, J. Chem. Phys., 25, 784 (1956).
H: B. Beagley, K. McAloon, J. M. Freeman, Acta Crystallogr., Sect. B, B30, 444 (1974).
I: H. C. Clark, S. G. Furnival, J. T. Kwon, Can. J. Chem., 41, 2889 (1963).
J: H. Fujii, M. Kimura, Bull. Chem. Soc. Japan, 44, 2643 (1970)
K: H. Fujii, M. Kimura, Bull. Chem. Soc. Japan, 43, 1933 (1970)
L: H. A. Skinner, L. E. Sutton, Trans. Farad. Soc., 44, 164 (1944).
M: E. Coop, L. E. Sutton, J. Chem. Soc., 1269 (1938).
N: T. Oyamada, T. Iijima, M. Kimura, Bull. Chem. Soc. Japan, 44, 2638 (1971).
O: F. J. Lovas, E. Tiemann, J. Phys. Chem. Ref. Data 3, 609 (1974).
P: A. V. Demidov, A. G. Gershikov, E. Z. Zasorin, V. P. Spiridonov, A. A. Ivanov, J. Struct. Chem., 24, 9 (1983).
Q: I. Hargittai, J. Mol. Struct., 100, 129 (1983).
R: H. A. Skinner, L. E. Sutton, Trans. Farad. Soc., 36, 1209 (1940).
S: O. I. Osman, B. J. Whitaker, N. P. C. Simmons, D. R. M. Walton, J. F. Nixon, H. W. Krojo, J. Mol. Spect., 137, 373 (1989).
T: G. A. McRae, M. C. L. Gerry, M. Wong, I. Ozier, E. A. Cohen, J. Mol. Spect., 123, 321 (1987).
U: A. Almenningen, T. U. Halgaker, A. Haaland, S. Samdal, Acta Chem. Scand., Part A. A36, 159 (1982).
V: A. Haaland, S. Samdal, R. Seip, J. Organomet. Chem., 153, 187 (1978).
W: K. Ozutsumi, T. Takamuka, S. Ishiguko, H. Ohtaki, Bull. Chem. Soc. Japan, 62, 1875 (1989).
X: V. M. Petrov, A. N. Utkin, G. V. Girichev, A. A. Ivanov, Zh. Strukt. Khim., 26, 52 (1985).
Y: N. Iwasaki, Bull. Chem. Soc. Japan, 49, 2735 (1976).
Z: H. Oberhammer, J. Mol. Struct., 48, 389 (1978).
AA: K. Kashiwabara, S. Konaka, N. M. Kimura, Bull. Chem. Soc. Japan, 46, 410 (1973).
BB: P. W. Allen, L. E. Sutton, Acta. Crystallogr. 3, 46 (1950).
CC: V. P. Spiridonov, A. G. Gershikov, B. S. Butayev, J. Mol. Struct., 52, 53 (1979).
DD: K. Balasubramanian, J. Li, J. Mol. Spect., 135, 169 (1989).
EE: J. Nakagawa, H. Okutani, M. Hayashi, J. Mol. Spectrosc., 94, 410 (1982).
FF: J. F. Beecher, J. Mol. Spectrosc., 21, 414 (1966).
GG: E. H. Fink, K. D. Setzer, J. Mol. Spect., 125, 66 (1987).

HH: L. S. Bartell, A. Jin, J. Mol. Struct., 118, 47 (1984).
II: S. Tomoda, M. Shimoda, M. Sanami, Y. Takeuchi, Y. Litaka, J. Chem. Soc. Chem. Comm., 1304 (1989).
JJ: N. K. Moncur, P. D. Willson, T. H. Edwards, J. Mol. Spectrosc., 52, 380 (1974).
KK: S. Husebye, K. Maartmann-Moe, O. Mikalsen, Acta Chem. Scand., 43, 868 (1989)

J. J. P. Stewart
Fujitsu Ltd. 1999