

Method	R ₁	R ₂	R ₃	R ₄	ΔR ₁	ΔR ₂	ΔR ₃	ΔR ₄	RMS(R)	A ₁	A ₂	A ₃	ΔA ₁	ΔA ₂	ΔA ₃	RMS(A)
RHF(1)(2)	1.672	1.615	2.361	1.486	0.023	0.027	-0.005	0.034	0.025	97.79	128.29	129.73	1.67	-2.05	-0.32	1.54
MP2(1)(2)	1.704	1.653	2.359	1.533	-0.009	-0.012	-0.003	-0.012	0.010	100.39	125.31	129.52	-0.93	0.94	-0.10	0.76
QCISD(1)(2)	1.695	1.642	2.356	1.521	0.000	0.000	0.000	0.000	0.000	99.46	126.24	129.41	0.00	0.00	0.00	0.00
B3LYP(1)(3)	1.703	1.647	2.365	1.520	-0.008	-0.006	-0.009	0.000	0.007	99.52	126.14	129.25	-0.06	0.11	0.16	0.12
MNDO (4)	1.644	1.643	2.131	1.494	0.051	-0.002	0.225	0.027	0.116	92.16	129.80	117.82	7.30	-3.55	11.59	8.17
AM1 (4)	1.718	1.731	2.456	1.586	-0.023	-0.089	-0.100	-0.066	0.076	86.41	138.52	122.00	13.05	-12.28	7.41	11.19
PM3 (4)	1.649	1.660	2.468	1.515	0.046	-0.018	-0.112	0.006	0.061	102.99	126.56	121.72	-3.53	-0.32	7.69	4.89
PDDG/PM3 (5)	1.632	1.636	2.273	1.480	0.063	0.005	0.083	0.040	0.056	86.34	137.49	131.27	13.12	-11.24	-1.85	10.03
MNDOD (6)	1.760	1.714	2.353	1.531	-0.065	-0.073	0.003	-0.010	0.049	98.16	125.78	129.02	1.30	0.47	0.39	0.83
SAM1 (7)	1.623	1.618	2.468	1.525	0.072	0.023	-0.112	-0.005	0.067	98.19	131.16	124.82	1.27	-4.91	4.59	3.95
MSINDO (8)	1.662	1.635	2.346	1.512	0.033	0.007	0.010	0.009	0.018	108.36	119.67	125.25	-8.90	6.57	4.16	6.82
PM5 (9)	1.742	1.741	2.265	1.596	-0.047	-0.099	0.091	-0.075	0.081	97.38	125.50	117.43	2.08	0.74	11.98	7.04
MINDO/3 (10)	1.644	1.674	2.405	1.508	0.051	-0.032	-0.049	0.012	0.039	100.39	127.73	124.75	-0.93	-1.48	4.66	2.88

- (1) Basis set: aug-CC-pVTZ
- (2) MOLPRO 2002.6
- (3) GAUSSIAN 03 C.02
- (4) MOPAC 6
- (5) Modified MOPAC 6 <http://zarbi.chem.yale.edu/doc/pddg/>
- (6) MOPAC 97
- (7) AMPAC 8.15.9
- (8) MSINDO 3.1
- (9) MOPAC 2002 2.5.0
- (10) ViewMol3D 4.34, Si-O parameters from Edwards and Fowler (1985)

MP2/aug-CC-pVTZ
geometry

