

Dataset for Accuracy Validation of Quantum Mechanical Calculation--Bond length

Compound	Bond label	This calculated length (Å)	Experimental length (Å)	Error
a1	O1-O2	1.206	1.208	-0.17%
a2	N1-O1	1.148	1.151	-0.26%
a3	O1-O2	1.256	1.278	-1.72%
a4	N1-O1	1.193	1.197	-0.33%
a5	N1-N2	1.122	1.126	-0.36%
a6	N2-O1	1.179	1.186	-0.59%
	N1-O1	1.149	1.150	-0.09%
a7	N2-N3	1.881	1.864	0.91%
	N2-O1	1.133	1.142	-0.79%
	N3-O4	1.201	1.202	-0.08%
	N3-O5	1.201	1.217	-1.31%
a8	N1-N2	1.810	1.780	1.69%
	N1-O1	1.187	1.190	-0.25%
	O1-N2	1.164	1.204	-3.32%
a10	N2-N3	1.528	1.484	2.96%
	N3-N4	1.245	1.270	-1.97%
	N4-N5	1.129	1.154	-2.17%
	O1-N1	1.211	1.235	-1.94%
a11	O2-N1	1.200	1.226	-2.12%
	N1-N2	1.491	1.462	1.98%
	N2-N3	1.254	1.235	1.54%
	N3-N4	1.123	1.151	-2.43%
Compound	Bond label	This calculated length (Å)	Reported calculated length (Å)	Error
a6	N1-N2	1.871	1.871	0.00%
	N1-O1	1.155	1.155	0.00%
a7	N2-N3	1.881	1.880	0.05%
	N2-O1	1.133	1.133	0.00%

a8	N3-O4	1.201	1.202	-0.08%
	N3-O5	1.201	1.201	0.00%
	N1-N2	1.810	1.798	0.67%
	N1-O1	1.187	1.188	-0.08%
a9	O1-N2\O4-N5	1.155	1.155	-0.04%
	N2-O3\O3-N4	1.494	1.494	0.00%
a10	O1-N2	1.164	1.164	0.00%
	N2-N3	1.528	1.529	-0.07%
	N3-N4	1.245	1.245	0.00%
	N4-N5	1.129	1.129	0.00%
a13	O1-N2	1.205	1.203	0.17%
	N2-O3	1.422	1.426	-0.28%
	O3-N4	1.639	1.626	0.80%
	N4-O5	1.130	1.130	0.00%
a14	N2-O6	1.200	1.199	0.08%
	O1-N2	1.148	1.150	-0.17%
	N2-O3	1.547	1.540	0.48%
	O3-O4	1.383	1.384	-0.07%
	O4-N5	1.560	1.561	-0.06%
	N5-O6	1.145	1.146	-0.09%
d7	O1-N2	1.378	1.378	0.00%
	N2-N5	1.243	1.243	0.00%
	N4-N5	1.413	1.413	0.00%

Dataset for Accuracy Validation of Quantum Mechanical Calculation--Bond angle

Compound	Bond angle label	This calculated angle (°)	Experimental angle (°)	Error
a3	O1-O2-O3	118.495	116.800	1.45%
a4	O1-N1-O2	134.347	134.300	0.03%
a6	O1-N1-N2	101.478	101.000	0.47%
a7	O1-N2-N3	106.273	105.000	1.21%

a8	O4-N3-N2	112.083	112.700	-0.55%
	O5-N3-N2	116.614	117.500	-0.75%
	O4-N3-O5	131.303	129.800	1.16%
	O1-N1-N2	112.635	112.000	0.57%
	O1-N1-O2	134.775	135.000	-0.17%
a10	N3-N4-N5	177.039	174.300	1.57%
a12	N2-O3-N4	114.968	114.000	0.85%
	O3-N2-O6	133.446	133.000	0.34%

Compound	Bond angle label	This calculated angle (°)	Reported calculated angle (°)	Error
a6	O1-N1-N2	108.585	108.600	-0.01%
a8	O1-N1-N2	112.635	112.600	0.03%
	O1-N1-O2	134.775	134.800	-0.02%
a10	O1-N2-N3	111.350	111.300	0.04%
	N2-N3-N4	108.275	108.200	0.07%
	N3-N4-N5	177.039	177.100	-0.03%
	O1-N2-O6	130.034	130.300	-0.20%
a13	N2-O3-N4	111.719	111.600	0.11%
	O3-N4-O5	107.563	107.500	0.06%
	O1-N2-O3	108.961	108.900	0.06%
a14	O4-N5-O6	108.074	107.500	0.53%
d7	N2-O1-N3	106.543	106.600	-0.05%