

Table 3.8: (H₂O)(NH₃)

method	D _e ^{cpc}	BSSE	D ₀ ^h	r _{O...N}	Δr _{O-H} (d)	Δω(d)
HF	19.59	1.15	10.46	3.0876	0.0071	-162
MP2	25.07	4.13	15.31	2.9261	0.0130	-283
B3LYP	25.69	2.53	15.92	2.9406	0.0143	-300
B97-1	27.84	2.31	18.15	2.9383	0.0142	-299
PBE0	28.37	2.33	18.53	2.9015	0.0160	-337
HCTH	17.37	2.51	8.28	3.0383	0.0122	-267
HCTH38	25.21	2.81	15.79	2.9606	0.0147	-315
BLYP	24.55	3.12	14.92	2.9535	0.0158	-319
PBE	29.47	3.07	19.75	2.8978	0.0189	-382
LDA	46.33	3.38	36.13	2.7572	0.0287	-540
Best <i>ab initio</i> ^a	25.24	2.47				

^aMP4/6-311++G(3df,2pd) (fixed geometry), [44].