

Table 3.6: (FH)(NH₃)

method	D _e ^{cp}	BSSE	D ₀ ^h	r _{F...N}	Δr _{H-F} (d)	Δω(d)
HF	42.16	1.77	29.26	2.7334	0.0206	-520
MP2	49.36	6.36	36.14	2.6399	0.0327	-731
B3LYP	54.37	3.58	41.65	2.6378	0.0377	-806
B97-1	55.75	3.30	43.11	2.6340	0.0374	-814
PBE0	57.66	3.31	44.90	2.6088	0.0401	-869
HCTH	43.45	3.75	31.17	2.6578	0.0384	-825
HCTH38	53.02	4.00	40.67	2.6352	0.0406	-855
BLYP	53.64	4.33	41.25	2.6492	0.0418	-835
PBE	59.85	4.23	47.46	2.6115	0.0466	-924
LDA	82.61	4.51	69.88	2.5342	0.0586	-1078
Best <i>ab initio</i> ^a	52.69					

^aQCISD(T)/6-311+G** (frozen core, fixed geometry, corrected by the difference of MP2/6-311+G** and MP2/6-311+G(3df,2p), not cp-corrected), [58].