

Table 3.7: (ClH)(NH₃)

method	D _e ^{cpc}	BSSE	D ₀ ^h	r _{Cl...N}	Δr _{H-Cl} (d)	Δω(d)
HF	23.05	1.13	14.06	3.3352	0.0207	−305
MP2	33.19	5.32	23.61	3.0771	0.0519	−727
B3LYP	35.88	2.53	26.20	3.0812	0.0625	−801
B97-1	40.35	2.43	30.73	3.0389	0.0731	−911
PBE0	42.27	2.47	32.49	3.0009	0.0801	−1010
HCTH	28.49	2.70	18.86	3.0700	0.0684	−861
HCTH38	37.82	2.98	28.14	3.0450	0.0728	−900
BLYP	36.05	3.10	26.47	3.0824	0.0717	−849
PBE	46.00	3.21	36.22	2.9922	0.0954	−1074
LDA	71.65	3.60	61.33	2.8958	0.1363	−1321
Best <i>ab initio</i> ^a	35.08					

^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].