

Table 3.2: $(\text{HCl})_2$

method	D_e^{cpc}	BSSE	D_0^{h}	$r_{\text{Cl}\cdots\text{Cl}}$	$\Delta r_{\text{H}-\text{Cl}}(\text{d})$	$\Delta\omega(\text{d})$
HF	3.55	0.35	0.58	4.1851	0.0016	−19
MP2	7.13	1.18	3.29	3.8281	0.0043	−57
B3LYP	5.73	0.66	1.82	3.8505	0.0059	−80
B97-1	8.32	0.60	4.30	3.8006	0.0068	−86
PBE0	7.79	0.62	3.68	3.7563	0.0073	−103
HCTH	2.61	0.52	−0.25	4.2484	0.0023	−32
HCTH38	7.41	0.72	3.73	3.8774	0.0058	−83
BLYP	5.24	0.80	1.33	3.8577	0.0072	−98
PBE	9.12	0.82	4.91	3.7148	0.0104	−142
LDA	20.31	0.98	15.48	3.4638	0.0206	−254
Best <i>ab initio</i> ^a	7.75	0.75				

^aCCSD(T)/aug-cc-pVQZ (frozen core, fixed geometry from ref. [55]), this work.