

Table 3.1: $(\text{HF})_2$

method	D_e^{cpc}	BSSE	D_0^{h}	$r_{\text{F}\dots\text{F}}$	$\Delta r_{\text{H}-\text{F}}(\text{d})$	$\Delta\omega(\text{d})$
HF	16.01	1.03	8.88	2.8072	0.0039	-89
MP2	17.70	2.76	9.99	2.7390	0.0057	-121
B3LYP	19.79	2.31	11.98	2.7094	0.0076	-162
B97-1	20.49	2.04	12.85	2.7179	0.0074	-162
PBE0	20.57	2.12	12.72	2.6911	0.0080	-177
HCTH	11.68	2.30	4.99	2.8709	0.0051	-117
HCTH38	18.50	2.48	11.20	2.7580	0.0073	-162
BLYP	18.78	2.89	11.13	2.7295	0.0086	-176
PBE	21.37	2.88	13.62	2.6948	0.0098	-207
LDA	35.77	3.11	27.09	2.5419	0.0163	-318
Best <i>ab initio</i>	19.1 ^a		12.84 ^b	2.732 ^c	0.0056 ^b	-114 ^b

^alimit of the MP2 limit corrected CCSD(T)/aug-cc-pVxZ series (frozen core, fixed dimer and monomer geometries), [29].

^bCCSD(T)/cc-pVQZ (frozen core), [33].

^cCCSD(T)/aug-cc-pVQZ (frozen core, constrained optimisation), [34].