

Table 3.4: (CO)(HF)

method	D_e^{cpc}	BSSE	D_0^{h}	$r_{\text{O}\cdots\text{F}}$	$\Delta r_{\text{H-F}}(\text{d})$	$\Delta\omega(\text{d})$
HF	6.12	0.76	1.59	3.0834	0.0012	−23
MP2	4.77	1.93	0.13	3.0042	0.0011	−20
B3LYP	5.87	1.58	1.33	2.9768	0.0018	−37
B97-1	7.00	1.39	2.59	2.9856	0.0018	−36
PBE0	6.41	1.42	1.90	2.9679	0.0019	−41
HCTH	2.05	0.95	−0.71	3.4201	0.0004	−8
HCTH38	5.85	1.43	2.27	3.0931	0.0013	−28
BLYP	4.67	1.82	0.49	3.0161	0.0017	−36
PBE	6.30	1.78	2.12	2.9762	0.0022	−46
LDA	14.23	2.35	8.86	2.7399	0.0054	−106
Best <i>ab initio</i> ^a	6.99	1.92		2.9517	0.0020	

^aCCSD(T)/aug-cc-pVQZ, this work.