

Table 3.5: (OC)(HF)

method	D_e^{cpc}	BSSE	D_0^{h}	$r_{\text{C}\cdots\text{F}}$	$\Delta r_{\text{H-F}}(\text{d})$	$\Delta\omega(\text{d})$
HF	8.83	0.92	2.38	3.1798	0.0031	−79
MP2	14.34	2.72	6.97	2.9915	0.0066	−153
B3LYP	14.58	2.30	7.46	2.9644	0.0083	−194
B97-1	16.22	2.08	9.13	2.9586	0.0084	−199
PBE0	16.58	2.12	9.25	2.9273	0.0094	−224
HCTH	8.54	2.39	2.25	3.0818	0.0067	−168
HCTH38	15.13	2.57	8.43	2.9785	0.0089	−214
BLYP	14.33	2.95	7.44	2.9566	0.0098	−220
PBE	18.54	2.94	11.46	2.8949	0.0122	−275
LDA	31.97	3.17	24.32	2.7517	0.0188	−393
Best <i>ab initio</i> ^a	14.62	2.02		2.9871	0.0066	

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