Table 3.3: $(H_2O)_2$

method	D_e^{cpc}	BSSE	D_0^h	$r_{O\cdots O}$	$\Delta r_{O-H}(d)$	$\Delta\omega(d)$
HF	16.31	0.83	7.80	3.0238	0.0041	−101
MP2	19.69	2.87	10.48	2.9021	0.0070	−163
B3LYP	20.10	1.93	10.83	2.9053	0.0081	−175
B97-1	21.72	1.75	12.50	2.9081	0.0081	−175
PBE0	21.86	1.77	12.47	2.8747	0.0091	−199
HCTH	12.31	1.84	4.05	3.0608	0.0059	−143
HCTH38	19.27	2.14	10.51	2.9517	0.0079	−181
BLYP	18.74	2.41	9.65	2.9283	0.0090	−187
PBE	22.49	2.38	13.22	2.8798	0.0109	−227
LDA	37.52	2.77	27.45	2.7154	0.0184	−351
Best *ab initio*	21.1[a]		11.5[b]	2.925[c]	0.0065[d]	−121[d]

[a]estimation from the limit of the MP2 limit corrected CCSD(T)/aug-cc-pCVxZ series (frozen core, fixed dimer and monomer geometries) and from additional core correlation and geometry relaxation effects, [29].
[b]D_e^{cpc} corrected by ΔZPE=9.6 kJ/mol, MP4/VTZ(2df) on O and VTZ(2p) on H, [42].
[c]cp-corrected CCSD(T) PES, [43].
[d]MP4/VTZ(2df) on O and VTZ(2p) on H, [42].