

Supplementary Material

Counterpoise correction from a practical perspective: is the result worth the cost?

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Table S1. Mean unsigned deviation (kJ mol^{-1}), mean signed deviation (MSD), standard deviation of the deviations (SDD), and maximum deviation (MAX) from benchmark M06-2X/QZVPD' values for relative energies obtained with smaller basis sets for the cast-study-2 set of 29 reactions in the insertion of CO_2 into epoxide, and total wall times (s) used in the computations

basis set	MUD	MSD	SDD	MAX	Time
TZVPD'	1.2	-0.4	1.4	-2.3	70312
SVPD'	6.6	-4.3	7.4	-17.9	23840
(CP)SVPD'	7.0	-2.8	8.7	-21.3	36165
TZVPD':CP-SVPD'	5.5	-2.1	8.1	-21.3	91776
SVPD'+gCP	7.6	-1.1	9.3	-18.0	23840
vDZP	6.1	-3.9	7.8	-20.3	20416

The n VPD' basis set ($n = \text{S, TZ, QZ}$) combines def2- n VP for hydrogen and def2- n VPD for other atoms. The (CP)SVPD' notation represents SVPD' values obtained with CP corrections applied to the complexation reactions. The TZVPD':CP-SVPD' notation signifies CP-corrected SVPD' for the complexation reactions and TZVPD' for other relative energies. The gCP values for SVPD' are obtained as the average of the "dft/svp" and "dft/tzvp" values. The total time for M06-2X/QZVPD' is 248480.