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Erratum

Implementation and Performance of DFT-D with Respect to Basis Set and Functional for Study of Dispersion Interactions in Nanoscale Aromatic Hydrocarbons. [*J. Chem. Theory Comput. 4,* 2030–2048 (2008)]. By Roberto Peverati and Kim K. Baldridge*.

Page 2046. A typographical error occurred in Table 9 of this manuscript with the s_6 values of the B2PLYP DFT functional. Values reported as 1.55 should be 0.55, as also correctly reported in the original Figure 4, and the associated analysis in the main text.

Table 9. Summary of Density Functional Plus s_R/s_6 Coefficient Combinations Proposed for a Variety of Basis Sets, As Determined from Predictions of S22 Complexes

DFT functional	basis set	s_R value	optimized s_6 value	MAD (kcal/mol)
B97D	cc-pVDZ	1.1	1.00	1.075
	cc-pVDZ+CP	1.1	1.39	0.518
	cc-pVTZ	1.1	1.18	0.337
	cc-pVTZ+CP	1.1	1.41	0.454
	cc-pVQZ	1.1	1.26	0.330
	cc-pVQZ+CP	1.1	1.39	0.441
	TZV(2d,2p)	1.1	1.25	0.375
	TZV(2d,2p)+CP	1.1	1.38	0.425
B3LYP	cc-pVDZ	1.1	0.73	1.709
	cc-pVTZ	1.1	0.88	0.853
	cc-pVQZ	1.1	0.96	0.612
PBE	cc-pVDZ	1.1	0.50	2.579
	cc-pVTZ	1.1	0.64	1.030
	cc-pVQZ	1.1	0.65	0.798
revPBE	cc-pVDZ	1.1	1.66	0.826
	cc-pVTZ	1.1	1.87	1.326
	cc-pVQZ	1.1	1.90	1.536
	cc-pVTZ (8−22)	1.1	1.87	0.393
	cc-pVQZ (8−22)	1.1	1.90	0.355
B2PLYP	cc-pVDZ	1.3	0.55	1.394
	cc-pVTZ	1.3	0.55	0.517

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