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Erratum

Efficient Diffuse Basis Sets: cc-pV*x*Z+ and maug-cc-pV*x*Z. [*J. Chem. Theory Comput. 5,* 1197–1202 (2009)]. By Ewa Papajak, Hannah R. Leverentz, Jingjing Zheng, and Donald G. Truhlar*.

Pages 1199. Some data in Tables 3-6 are corrected. These corrections do not change any of our discussion or conclusions in the paper. In the second paragraph of Section 4, "cc-pVDZ+" should be "cc-pVTZ+".

Table 3. Mean Unsigned Errors (MUEs) (in kcal/mol) in Ionization Potentials

	B3LYP	M06-2X	CCSD(T)
cc-pVDZ+	4.88	3.09	8.57
aug-cc-pVTZ		2.70	

Table 4. Mean Unsigned Errors (MUEs) (in kcal/mol) in Electron Affinities

	B3LYP	M06-2X	CCSD(T)
cc-pVDZ		20.10	
cc-pVDZ+	3.17	2.66	9.77
aug-cc-pVDZ		2.37	
cc-pVTZ		9.85	
cc-pVTZ+		1.92	
aug-cc-pVTZ		1.55	

Table 5. Mean Unsigned Errors Per Bond (MUEPBs) in (kcal/mol) in Atomization Energies

	B3LYP	M06-2X	CCSD(T)
cc-pVDZ+	3.15	2.40	8.88

Table 6. Mean Unsigned Errors (MUEs) (in kcal/mol) in the Barrier Heights of the DBH24/08 Database

	HATBH6	NSBH6	UABH6	HTBH6	DBH24
B3LYP/cc-pVDZ+	7.57	3.79		5.81	4.80
M06-2X/cc-pVDZ+	2.02	1.17		1.37	1.45
CCSD(T)/cc-pVDZ+	4.15	0.82		1.79	2.05

Addendum. We also present here some further calculations that do not correct an error in the original article but that provide further relevant information. In particular, we note that the article tested the new plus basis sets for ionization potentials, electron affinities, atomization energies, barrier heights, and basis set superposition errors. We then presented tests of another set of basis sets, called maug basis sets, obtained by truncating the aug basis sets to the same size as the plus basis sets. The maug basis sets were tested only for barrier heights and basis set superposition errors, and we found very similar performance to the plus basis sets. As an example of the differences in the basis sets, diffuse functions on O in maug-cc-pVTZ have exponential parameters of 0.07376 for *s* functions and 0.05974 for *p*; these exponential parameters are smaller than those in the plus basis set, where both parameters are 0.0845. The most difficult tests of the adequacy of a scheme for diffuse basis functions are provided by electron affinities. We have now tested maug-cc-pV*x*Z against cc-pV*x*Z+ with both $x = D$ and $x = T$ for electron affinities, and we found better performance with the maug basis sets for M06-2X (better on average) and CCSD(T) (always better), especially for systems containing oxygen atoms (and to a lesser extent for Si^- and C^-), but better performance (on average) with the plus basis set for B3LYP. However, in all 78 cases the anion energies are lower for the maug basis set than the corresponding plus one, so the improvement of the plus basis sets for B3LYP electron affinities is presumably due to cancellation of basis set error with a large error in the opposite direction from the functional itself. Table A1 gives two additional rows for the original Table 4 that show the mean unsigned errors in electron affinities with two maug basis sets. The conclusion is that anion energies and electron affinities are more sensitive than barrier heights and basis set superposition errors to the precise values of the diffuse exponents, and the maug basis sets are more accurate for such calculations, probably because the exponents were optimized for atomic anions.[1]

Table A1. Mean Unsigned Errors (MUEs) (in kcal/mol) in Electron Affinities

	B3LYP	M06-2X	CCSD(T)
maug-cc-pVDZ	3.19	2.46	9.41
maug-cc-pVTZ	2.49	1.57	4.88

Reference

(1) Kendall, R. A.; Dunning, Jr., T. H., Jr.; Harrison, R. J. *J. Chem. Phys.* **1992**, *96*, 6796.

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