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Erratum

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Erratum to "S66: A Well-balanced Database of Benchmark Interaction Energies Relevant to Biomolecular Structures"

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SUMMARY

Recently, we have discovered an error in our paper "S66: A Well-balanced Database of Benchmark Interaction Energies Relevant to Biomolecular Structures" (*J. Chem. Theory Comput.* **2011**, 7, 2427−2438) which we would like to correct here. The results from one of the methods tested, corrected MP2 (MP2C), were processed incorrectly. Correcting this mistake makes MP2C results much better: the RMSE in the S66 data set drops to 0.13 kcal/mol (the previously reported erroneous value was 0.71 kcal/mol). This results moves MP2C among the best methods we have tested (it ranks second after the more expensive SCS-MI-CCSD, which has an RMSE of 0.08 kcal/mol).

We sincerely apologize to the authors of MP2C as well as to others who might have been affected by this mistake.

CHANGES TO RESULTS AND DISCUSSION

The MP2C/CBS results discussed here were obtained by combining MP2/CBS calculations with the MP2 correction calculated in the aug-cc-pVDZ basis set as described in the original work. The errors reported in Table 3, shown in the plots, and discussed in the text were incorrect. The correct MP2C/CBS interaction energies are listed in Table E1.

Table E1. Correct MP2C/CBS Interaction Energies in the S66 Data Set

	hydrogen bonds	Δ*E*		hydrogen bonds	Δ*E*
1	water···water	−4.97	13	peptide···MeOH	−6.29
2	water···MeOH	−5.68	14	peptide···MeNH2	−7.74
3	water···MeNH2	−7.15	15	peptide···peptide	−8.58
4	water···peptide	−8.00	16	peptide···water	−5.17
5	MeOH···MeOH	−5.83	17	uracil···uracil (BP)	−16.98
6	MeOH···MeNH2	−7.81	18	water···pyridine	−6.95
7	MeOH···peptide	−8.15	19	MeOH···pyridine	−7.50
8	MeOH···water	−5.04	20	AcOH···AcOH	−18.98
9	MeNH2···MeOH	−3.08	21	AcNH2···AcNH2	−16.17
10	MeNH2···MeNH2	−4.33	22	AcOH···Uracil	−19.31
11	MeNH2···peptide	−5.41	23	AcNH2···uracil	−19.01
12	MeNH2···water	−7.53			
	dispersion	Δ*E*		dispersion	Δ*E*
24	benzene···benzene (*π*−*π*)	−2.78	36	neopentane···neopentane	−1.80
25	pyridine···pyridine (*π*−*π*)	−3.91	37	cyclopentane···neopentane	−2.46
26	uracil···uracil (*π*−*π*)	−9.37	38	cyclopentane···cyclopentane	−3.09
27	benzene···pyridine (*π*−*π*)	−3.40	39	benzene···cyclopentane	−3.68
28	benzene···uracil (*π*−*π*)	−5.45	40	benzene···neopentane	−3.00
29	pyridine···uracil (*π*−*π*)	−6.55	41	uracil···pentane	−4.75
30	benzene···ethene	−1.44	42	uracil···cyclopentane	−4.05
31	uracil···ethene	−3.27	43	uracil···neopentane	−3.64
32	uracil···ethyne	−3.62	44	ethene···pentane	−2.08
33	pyridine···ethene	−1.90	45	ethyne···pentane	−1.87
34	pentane···pentane	−3.88	46	peptide···pentane	−4.27
35	neopentane···pentane	−2.66			
	others	Δ*E*		others	Δ*E*
47	benzene···benzene (TS)	−2.96	57	benzene···peptide (NH···*π*)	−5.43
48	pyridine···pyridine (TS)	−3.64	58	pyridine···pyridine (CH···N)	−4.18
49	benzene···pyridine (TS)	−3.41	59	ethyne···water (CH···O)	−2.86
50	benzene···ethyne (CH···*π*)	−2.96	60	ethyne···AcOH (OH···*π*)	−4.91
51	ethyne···ethyne (TS)	−1.59	61	pentane···AcOH	−2.88
52	benzene···AcOH (OH···*π*)	−4.72	62	pentane···AcNH2	−3.48
53	benzene···AcNH2 (NH···*π*)	−4.39	63	benzene···AcOH	−3.75
54	benzene···water (OH···*π*)	−3.26	64	peptide···ethene	−3.00
55	benzene···MeOH (OH···*π*)	−4.25	65	pyridine···ethyne	−4.08
56	benzene···MeNH2 (NH···*π*)	−3.28	66	MeNH2···pyridine	−4.03

The errors, as listed in Table 3, are corrected to RMSE 0.13 kcal/mol, MUE 0.10 kcal/mol, AVG −0.01 kcal/mol, and MAX 6.65%.

In the discussion, we expressed our surprise that the theoretically well justified MP2C does not bring any substantial improvement over uncorrected MP2. This was based on the erroneous results; MP2C indeed works well. Not only it is

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the best method among those based on MP2, it outperforms the other MP2-based approaches tested by a large margin. Additionally, the correction does increase the scaling of the calculations and might be therefore applied to rather large systems. The MP2C method has, however, one limitation—it is designed specifically for noncovalent interactions and cannot be applied to other properties than the interaction energy.

CHANGES TO CONCLUSIONS

In the conclusions, we recommended MP2.5 and SCS-MI-CCSD as the most accurate methods with scaling better than CCSD(T). MP2C has to be added to this list not only because it yields very accurate results but also because it is the least expensive approach among the methods that are able to reproduce the CCSD(T) benchmarks closely.

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