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Correction: The p-block challenge: assessing quantum chemistry methods for inorganic heterocycle dimerizations

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 Correction for 'The p-block challenge: assessing quantum chemistry methods for inorganic heterocycle dimerizations' by Thomas Gasevic *et al.*, *Phys. Chem. Chem. Phys.*, 2024, **26**, 13884–13908, <https://doi.org/10.1039/D3CP06217A>.

The root mean square deviations (RMSDs) reported in Table 4 of the original publication are incorrect for revDSD-PBEP86-D3(BJ) and B2NC-PLYP due to faulty inputs in the calculations. The correct values are now provided here in Table 1. Further, PM6-D3H4X was used instead of PM6-D3H4.

In our manuscript, we used the final single point energies of revDSD-PBEP86-D4(2021) and replaced the D4 London dispersion correction with the D3(BJ) correction of the original revDSD-PBEP86-D3(BJ) publication. However, as the density functional itself was also re-parameterized in 2021, this approach is not valid.^{1,2} The correct parameters for revDSD-PBEP86-D3(BJ) yield slightly larger deviations ($\text{RMSD}_{\text{cov}} = 7.5$ vs. $8.0 \text{ kcal mol}^{-1}$).

In the calculations with B2NC-PLYP, Hartree Fock was applied instead of Density Functional Theory (DFT). Using the correct settings significantly reduces the errors for this test set, making B2NC-PLYP a viable choice for the computation of inorganic heterocycle dimerizations ($\text{RMSD}_{\text{cov}} = 3.4 \text{ kcal mol}^{-1}$; $\text{RMSD}_{\text{wda}} = 0.8 \text{ kcal mol}^{-1}$).

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.

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Table 1 Root mean square deviations (RMSDs) for all tested methods in kcal mol⁻¹. Except for the FF, SQM, and DFT composite methods, the def2-QZVPP basis set was applied. The values of further statistical descriptors are given in the ESI

Class	Method	RMSD/kcal mol ⁻¹							
		Covalent				Weak donor-acceptor			
		Plain	D3	D4	NL	Plain	D3	D4	NL
FF	GFN-FF ³			184.3				9.1	
	UFF ⁴	1416.3				1.0			
SQM	PM6-D3H4X ^{5,6 a}		158.8				33.2		
	PM7 ^{7 a}		162.7				17.9		
Composite	GFN0-xTB			52.0				6.9	
	GFN1-xTB ⁸		46.7				7.6		
	GFN2-xTB ⁹			36.8				6.7	
	B97M-V-C ¹⁰				12.7				4.1
	B97-3c ¹¹		9.3				6.8		
	r ² SCAN-3c ¹²			5.7				1.5	
	PBEh-3c ¹³		10.0				1.8		
(meta-)GGA	ωB97X-3c ¹⁴			8.0				1.1	
	HF-3c ¹⁵		33.6				9.0		
	PBE ¹⁶	16.3	7.3	7.4		8.3	1.0	2.2	
	BP86 ^{17,18}	23.3	11.6	8.6		10.9	10.3	7.7	
	B97M ¹⁹				8.8				2.2
	TPSS ²⁰	14.9	7.0	9.6		9.5	3.9	4.7	
	r ² SCAN ²¹⁻²⁴	8.1	4.3	4.8		4.7	1.0	1.5	
	M06-L ²⁵	12.9	12.7	11.7		1.8	1.7	1.6	
	MN15-L ²⁶	14.4	14.4			3.2	3.2		
	Hybrid	PBE0 ²⁷	7.4	9.1	9.7	9.2	7.2	2.9	3.2
B3LYP ^{28,29}		33.5	8.2	9.6		12.9	4.2	3.9	
TPSSH ³⁰		11.4	8.7	9.6		9.0	4.8	4.6	
r ² SCAN0 ³¹		5.0	5.6	5.1	6.2	4.5	1.3	1.0	1.0
M06 ³²		7.7	6.8	5.8		1.2	1.6	2.2	
M06-2X ³²		6.9	6.7			1.7	2.0		
MN15 ³³		12.9	12.9			2.2	2.2		
PW6B95 ³⁴		9.8	5.8	8.0		6.1	3.4	3.6	
ωB97X ³⁵					8.7				1.1
ωB97M ³⁶					4.8				2.1
Double-hybrid		revDSD-PBEP86-D3(BJ) ¹		8.0				3.7	
	revDSD-PBEP86-D4(2021) ²	4.8		2.8		2.4		0.8	
	PWPB95 ³⁷	3.8	13.1	3.6		3.4	4.8	1.7	
	ωB97M(2) ³⁸				9.7				3.0
	ωB97X-2 ³⁹				7.0				2.1
	Pr ² SCAN50 ⁴⁰			5.0	6.7			1.1	1.0
	κPr ² SCAN50 ⁴⁰			7.2				1.0	
	ωPr ² SCAN50 ⁴⁰			7.1	6.9			1.6	0.5
	SOS0-PBE0-2 ^{41,42}	7.6	11.2			1.8	1.7		
	B2NC-PLYP ^{42,43}	3.4	4.5			0.8	1.7		

^a As the PMx methods are not parameterized for Po, no data for Po-containing systems are included.

Notes and references

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