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CORRECTION

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

Thomas Gasevic,[c] Markus Bursch,*[ad] Qianli Ma,[b] Stefan Grimme,[c] Hans-Joachim Werner*[b] and Andreas Hansen*[c]

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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 ($RMSD_{cov}$ = 7.5 *vs.* 8.0 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 ($RMSD_{cov}$ = 3.4 kcal mol^{-1}; $RMSD_{wda}$ = 0.8 kcal mol^{-1}).

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

[a] *Max-Planck-Institut für Kohlenforschung, Kaiser-Wilhelm-Platz 1, 45470 Mülheim an der Ruhr, Germany. E-mail: bursch@kofo.mpg.de*
[b] *Institut für Theoretische Chemie, Universität Stuttgart, Pfaffenwaldring 55, D-70569 Stuttgart, Germany. E-mail: werner@theochem.uni-stuttgart.de*
[c] *Mulliken Center for Theoretical Chemistry, Rheinische Friedrich-Wilhelms-Universität Bonn, Beringstr. 4, 53115 Bonn, Germany. E-mail: hansen@thch.uni-bonn.de*
[d] *FACCTs GmbH, 50677, Koeln, Germany*

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

		RMSD/kcal mol^{-1}							
		Covalent				Weak donor–acceptor			
Class	Method	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		
	GFN0-xTB			52.0				6.9	
	GFN1-xTB[8]		46.7				7.6		
	GFN2-xTB[9]			36.8				6.7	
Composite	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		
	ωB97X-3c[14]			8.0				1.1	
	HF-3c[15]		33.6				9.0		
(meta-)GGA	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	0.6
	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 PM*x* methods are not parameterized for Po, no data for Po-containing systems are included.

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