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CORRECTION

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Correction: Planar *vs.* three-dimensional X_6^{2-}, $X_2Y_4^{2-}$, and $X_3Y_3^{2-}$ (X, Y = B, Al, Ga) metal clusters: an analysis of their relative energies through the turn-upside-down approach

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Correction for 'Planar *vs.* three-dimensional X_6^{2-}, $X_2Y_4^{2-}$, and $X_3Y_3^{2-}$ (X, Y = B, Al, Ga) metal clusters: an analysis of their relative energies through the turn-upside-down approach by Ouissam El Bakouri *et al.*, *Phys. Chem. Chem. Phys.*, 2016, **18**, 21102–21110.

In the Computational methods section of our published article, we stated: ''To facilitate a straightforward comparison, the EDA results were scaled to match exactly the regular bond energies''. However, the referred scaling factor (or correction factor) was inadvertently not applied to the values of Tables 2 and 3. The new Tables 2 and 3 included in this Erratum now contain the scaled values. Changes in the values of these two tables do not affect the conclusions of the work.

As to the discussion, there are only two paragraphs affected:

(1) Last paragraph on page 21105 that now reads:

The different terms of the EDA analysis for B_6^{2-}, Al_6^{2-}, and Ga_6^{2-} clusters are enclosed in Table 2. First, we notice that the total bonding energies (ΔE) are much larger for B_6^{2-} than for Al_6^{2-} or Ga_6^{2-}. For the former, ΔE are −95.4 (O_h) and −162.9 kcal mol^{-1} (D_{2h}), whereas for the two latter are in between −17.8 and −35.8 kcal mol^{-1}. This trend correlates with the shorter B–B bond lengths mentioned above. Table 2 also encloses the relative EDA energies between the two clusters. The B_3^- fragment taken from B_6^{2-} system in its D_{2h} symmetry is the one that suffers the largest deformation, *i.e.* the largest change in geometry with respect to the fully relaxed B_3^- cluster in the quintet state (ΔE_{dist} = 25.1 kcal mol^{-1}), whereas the rest of the systems present small values of ΔE_{dist} (0.0–3.0 kcal mol^{-1}). However, differences in ΔE are not due to distortion energies (indeed ΔE_{dist} values follow the opposite trend as ΔE), but to interaction energies (ΔE_{int}).

(2) First paragraph on page 21106 that now reads:

Thus, we focus on the decomposition of ΔE_{int} into ΔE_{Pauli}, ΔV_{elstat}, ΔE_{oi}, and ΔE_{disp} terms. As a general trend, in all three X_6^{2-} clusters ΔE_{Pauli} is larger for the O_h than the D_{2h} cluster ($\Delta(\Delta E_{Pauli})$ = −188.0, −121.1, and −116.5 kcal mol^{-1} for B_6^{2-}, Al_6^{2-}, and Ga_6^{2-}, respectively), so making it less stable. The overlaps between doubly occupied MOs are larger in the more compact O_h structure that, consequently, has larger ΔE_{Pauli}. The larger difference in ΔE_{Pauli} between the O_h and D_{2h} structures in the case of B_6^{2-} as compared to Al_6^{2-} and Ga_6^{2-} is attributed to the particularly short B–B distances that increases the overlap between doubly occupied MOs of each B_3^- fragment. At the same time, the O_h form presents larger (more negative) electrostatic interactions ($\Delta(\Delta V_{elstat})$ = 48.0, 69.2, and 69.9 kcal mol^{-1} for B_6^{2-}, Al_6^{2-}, and Ga_6^{2-}, respectively). It is usually the case that higher destabilising Pauli repulsions goes with larger stabilising electrostatic interactions. The reason has to be found in the fact that both interactions increase in absolute value when electrons and nuclei are confined in a relatively small space. The electrostatic interaction together with orbital interaction ($\Delta(\Delta E_{oi})$ = 51.1, 70.0, and 57.8 kcal mol^{-1} for B_6^{2-}, Al_6^{2-}, and Ga_6^{2-}, respectively) terms favour the O_h structure. In the case of O_h B_6^{2-}, however, $\Delta(\Delta V_{elstat})$ and $\Delta(\Delta E_{oi})$ cannot compensate $\Delta(\Delta E_{Pauli})$, which causes the D_{2h} system to be the lowest in energy. The opposite happens for Al_6^{2-} and Ga_6^{2-}. Finally, the dispersion term does almost not affect the relative energies, as the difference in dispersion is only in the order of *ca.* 1.0 kcal mol^{-1}. Therefore, what causes the different trend

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Table 2 Energy decomposition analysis (EDA) of X_6^{2-} (X = B, Al, and Ga) metal clusters with D_{2h} and O_h symmetries (in kcal mol^{-1}), from two X_3^- fragments at their quintet state, computed at the BLYP-D3(BJ)/TZ2P level. Units are kcal mol^{-1}

	B_6^{2-}			Al_6^{2-}			Ga_6^{2-}		
	$D_{2h} + D_{2h} \rightarrow D_{2h}$	$O_h + O_h \rightarrow O_h$	$\Delta(\Delta E)$	$D_{2h} + D_{2h} \rightarrow D_{2h}$	$O_h + O_h \rightarrow O_h$	$\Delta(\Delta E)$	$D_{2h} + D_{2h} \rightarrow D_{2h}$	$O_h + O_h \rightarrow O_h$	$\Delta(\Delta E)$
ΔE_{int}	−188.0	−98.0	*−90.0*	−20.0	−38.8	*18.8*	−18.0	−29.8	*11.9*
ΔE_{Pauli}	522.4	710.4	*−188.0*	218.1	339.2	*−121.1*	253.5	370.0	*−116.5*
ΔV_{elstat}	−234.0	−282.0	*48.0*	−93.0	−162.3	*69.2*	−129.7	−199.7	*69.9*
ΔE_{oi}	−473.4	−524.4	*51.1*	−141.9	−211.9	*70.0*	−137.9	−195.7	*57.8*
ΔE_{disp}	−3.1	−2.0	*−1.1*	−3.1	−3.8	*0.7*	−3.8	−4.5	*0.7*
ΔE_{dist}	25.1	2.6	*22.5*	0.0	3.0	*−3.0*	0.2	2.8	*−2.6*
ΔE	−162.9	−95.4	*−67.5*	−20.0	−35.8	*15.8*	−17.8	−27.0	*9.3*

Table 3 Energy decomposition analysis (EDA) of all mixed metal clusters with planar and 3D symmetries (in kcal mol^{-1}), from two fragments at their quintet states, computed at the BLYP-D3(BJ)/TZ2P level

		ΔE_{int}	ΔE_{Pauli}	ΔV_{elstat}	ΔE_{oi}	ΔE_{disp}
$B_2Al_4^{2-}$	D_{4h}	−51.1	431.3	−198.6	−280.0	−3.8
	D_{2h}	−39.6	238.5	−96.1	−178.9	−3.2
	ΔE	11.5	−192.8	102.5	101.1	0.6
$Al_2B_4^{2-}$	D_{4h}	−72.8	566.5	−244.1	−392.0	−3.2
	D_{2h}	−136.8	545.5	−233.8	−445.4	−3.2
	ΔE	−64.0	−21.0	10.3	−53.4	0.0
$Al_2Ga_4^{2-}$	D_{4h}	−33.6	366.0	−193.0	−202.2	−4.4
	D_{2h}	−18.8	277.4	−144.2	−148.4	−3.7
	ΔE	14.8	−88.5	48.8	53.8	0.7
$Ga_2B_4^{2-}$	D_{4h}	−82.1	578.6	−257.3	−400.0	−3.4
	D_{2h}	−152.8	523.8	−218.8	−454.5	−3.1
	ΔE	−70.7	−54.8	38.4	−54.5	0.3
$Ga_2Al_4^{2-}$	D_{4h}	−37.6	362.7	−184.2	−211.8	−4.2
	D_{2h}	−20.2	213.6	−89.0	−141.5	−3.5
	ΔE	17.4	−149.1	95.3	70.3	0.7
$Al_3Ga_3^{2-}$	D_{3h}	−35.7	369.6	−191.9	−209.2	−4.1
	C_{3v}	−19.9	244.2	−117.9	−142.8	−3.5
	ΔE	15.8	−125.3	74.0	66.5	0.6

observed for B_6^{2-} on one side, and Al_6^{2-} and Ga_6^{2-} on the other side is basically the ΔE_{oi} term, which combined with the ΔV_{elstat} component does (Al_6^{2-} and Ga_6^{2-}) or does not (B_6^{2-}) compensate for the higher ΔE_{Pauli} of the O_h form.

As to the conclusions, the sentence "From one side the $D_{2h}{}^{\text{HOMO-1}}(b_{2u})$ formed from two tangential SOMO $\sigma^T(b_2)$ orbitals" should read "From one side the $D_{2h}{}^{\text{HOMO-2}}(b_{2u})$ formed from two tangential SOMO $\sigma^T(b_2)$ orbitals".

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

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