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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 ( $\Delta E$ ) are much larger for  $B_6^{2-}$  than for  $Al_6^{2-}$  or  $Ga_6^{2-}$ . For the former,  $\Delta E$  are  $-95.4$  ( $O_h$ ) and  $-162.9$  kcal mol<sup>-1</sup> ( $D_{2h}$ ), whereas for the two latter are in between  $-17.8$  and  $-35.8$  kcal mol<sup>-1</sup>. 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 ( $\Delta E_{\text{dist}} = 25.1$  kcal mol<sup>-1</sup>), whereas the rest of the systems present small values of  $\Delta E_{\text{dist}}$  (0.0–3.0 kcal mol<sup>-1</sup>). However, differences in  $\Delta E$  are not due to distortion energies (indeed  $\Delta E_{\text{dist}}$  values follow the opposite trend as  $\Delta E$ ), but to interaction energies ( $\Delta E_{\text{int}}$ ).

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

Thus, we focus on the decomposition of  $\Delta E_{\text{int}}$  into  $\Delta E_{\text{Pauli}}$ ,  $\Delta V_{\text{elstat}}$ ,  $\Delta E_{\text{oi}}$ , and  $\Delta E_{\text{disp}}$  terms. As a general trend, in all three  $X_6^{2-}$  clusters  $\Delta E_{\text{Pauli}}$  is larger for the  $O_h$  than the  $D_{2h}$  cluster ( $\Delta(\Delta E_{\text{Pauli}}) = -188.0$ ,  $-121.1$ , and  $-116.5$  kcal mol<sup>-1</sup> 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  $\Delta E_{\text{Pauli}}$ . The larger difference in  $\Delta E_{\text{Pauli}}$  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 ( $\Delta(\Delta V_{\text{elstat}}) = 48.0$ ,  $69.2$ , and  $69.9$  kcal mol<sup>-1</sup> 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 ( $\Delta(\Delta E_{\text{oi}}) = 51.1$ ,  $70.0$ , and  $57.8$  kcal mol<sup>-1</sup> 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,  $\Delta(\Delta V_{\text{elstat}})$  and  $\Delta(\Delta E_{\text{oi}})$  cannot compensate  $\Delta(\Delta E_{\text{Pauli}})$ , 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<sup>-1</sup>. 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  $\text{kcal mol}^{-1}$ ), from two  $X_3^-$  fragments at their quintet state, computed at the BLYP-D3(BJ)/TZ2P level. Units are  $\text{kcal mol}^{-1}$ 

	$B_6^{2-}$			$Al_6^{2-}$			$Ga_6^{2-}$		
	$D_{2h} + D_{2h} \rightarrow D_{2h}$	$O_h + O_h \rightarrow O_h$	$\Delta(E)$	$D_{2h} + D_{2h} \rightarrow D_{2h}$	$O_h + O_h \rightarrow O_h$	$\Delta(E)$	$D_{2h} + D_{2h} \rightarrow D_{2h}$	$O_h + O_h \rightarrow O_h$	$\Delta(E)$
$\Delta E_{\text{int}}$	−188.0	−98.0	−90.0	−20.0	−38.8	18.8	−18.0	−29.8	11.9
$\Delta E_{\text{Pauli}}$	522.4	710.4	−188.0	218.1	339.2	−121.1	253.5	370.0	−116.5
$\Delta V_{\text{elstat}}$	−234.0	−282.0	48.0	−93.0	−162.3	69.2	−129.7	−199.7	69.9
$\Delta E_{\text{oi}}$	−473.4	−524.4	51.1	−141.9	−211.9	70.0	−137.9	−195.7	57.8
$\Delta E_{\text{disp}}$	−3.1	−2.0	−1.1	−3.1	−3.8	0.7	−3.8	−4.5	0.7
$\Delta E_{\text{dist}}$	25.1	2.6	22.5	0.0	3.0	−3.0	0.2	2.8	−2.6
$\Delta E$	−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  $\text{kcal mol}^{-1}$ ), from two fragments at their quintet states, computed at the BLYP-D3(BJ)/TZ2P level

		$\Delta E_{\text{int}}$	$\Delta E_{\text{Pauli}}$	$\Delta V_{\text{elstat}}$	$\Delta E_{\text{oi}}$	$\Delta E_{\text{disp}}$
$B_2Al_4^{2-}$	$D_{4h}$	−51.1	431.3	−198.6	−280.0	−3.8
	$D_{2h}$	−39.6	238.5	−96.1	−178.9	−3.2
	$\Delta E$	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
	$\Delta E$	−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
	$\Delta E$	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
	$\Delta E$	−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
	$\Delta E$	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
	$\Delta E$	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  $\Delta E_{\text{oi}}$  term, which combined with the  $\Delta V_{\text{elstat}}$  component does ( $Al_6^{2-}$  and  $Ga_6^{2-}$ ) or does not ( $B_6^{2-}$ ) compensate for the higher  $\Delta E_{\text{Pauli}}$  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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