SUPPORTING INFORMATION

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 the isomerisation energies through the turn-upside-down approach

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Table S1. Cartesian coordinates of all systems analysed.

Table S2. Energy decomposition analysis (EDA) of B_6^{2-} metal cluster with D_{2h} and O_h symmetries (in kcal mol^{-1}), from two B_3^- fragments at their quintuplet state, computed at the BLYP-D3(BJ)/TZ2P level.

Table S3. Energy decomposition analysis (EDA) of Al_6^{2-} metal cluster with D_{2h} and O_h symmetries (in kcal mol^{-1}), from two Al_3^- fragments at their quintuplet state, computed at the BLYP-D3(BJ)/TZ2P level.

Table S4. Energy decomposition analysis (EDA) of Ga_6^{2-} metal cluster with D_{2h} and O_h symmetries (in kcal mol^{-1}), from two Ga_3^- fragments at their quintuplet state, computed at the BLYP-D3(BJ)/TZ2P level.

Table S5. Energy decomposition analysis (EDA) of B_6^{2-} metal cluster with D_{2h} and O_h symmetries (in kcal mol^{-1}), from two B_3^- fragments at their triplet state, computed at the BLYP-D3(BJ)/TZ2P level.

Table S1. Cartesian coordinates of all systems analysed.

$B_6^{2-}(D_{2h})$

B	-0.890490	-0.830846	0.000000
B	0.000000	-2.082890	0.000000
B	0.890490	-0.830846	0.000000
B	-0.890490	0.830846	0.000000
B	0.890490	0.830846	0.000000
B	0.000000	2.082890	0.000000

$B_6^{2-}(O_h)$

B	0.000000	0.000000	1.249985
B	0.000000	1.249985	0.000000
B	0.000000	0.000000	-1.249985
B	0.000000	-1.249985	0.000000
B	-1.249985	0.000000	0.000000
B	1.249985	0.000000	0.000000

$Al_6^{2-}(D_{2h})$

Al	-1.437928	-1.286828	0.000000
Al	0.000000	-3.819606	0.000000
Al	1.437928	-1.286828	0.000000
Al	-1.437928	1.286828	0.000000
Al	1.437928	1.286828	0.000000
Al	0.000000	3.819606	0.000000

$Al_6^{2-}(O_h)$

Al	0.000000	0.000000	1.941805
Al	0.000000	1.941805	0.000000
Al	0.000000	0.000000	-1.941805
Al	0.000000	-1.941805	0.000000
Al	-1.941805	0.000000	0.000000
Al	1.941805	0.000000	0.000000

$Ga_6^{2-}(D_{2h})$

Ga	-1.415706	-1.263017	0.000000
Ga	0.000000	-3.791914	0.000000
Ga	1.415706	-1.263017	0.000000
Ga	-1.415706	1.263017	0.000000
Ga	1.415706	1.263017	0.000000
Ga	0.000000	3.791914	0.000000

$Ga_6^{2-}(O_h)$

Ga	0.000000	0.000000	1.950378
Ga	0.000000	1.950378	0.000000
Ga	0.000000	0.000000	-1.950378
Ga	0.000000	-1.950378	0.000000
Ga	-1.950378	0.000000	0.000000
Ga	1.950378	0.000000	0.000000

$B_2Al_4^{2-}$ (D_{2h})

Al	-1.377132	-1.351418	0.000000
B	0.000000	-2.890830	0.000000
Al	1.377132	-1.351418	0.000000
Al	-1.377132	1.351418	0.000000
Al	1.377132	1.351418	0.000000
B	0.000000	2.890830	0.000000

$B_2Al_4^{2-}$ (O_h)

B	0.000000	1.304474	0.000000
Al	0.000000	0.000000	-1.735715
B	0.000000	-1.304474	0.000000
Al	0.000000	0.000000	1.735715
B	-1.304474	0.000000	0.000000
B	1.304474	0.000000	0.000000

$Al_2B_4^{2-}$ (D_{2h})

B	-0.897799	-0.785648	0.000000
Al	0.0000000	-2.763150	0.000000
B	0.897799	-0.785648	0.000000
B	-0.897799	0.785648	0.000000
B	0.897799	0.785648	0.000000
Al	0.000000	2.763150	0.000000

$Al_2B_4^{2-}$ (O_h)

Al	0.000000	1.802815	0.000000
B	0.000000	0.000000	-1.455322
Al	0.000000	-1.802815	0.000000
B	0.000000	0.000000	1.455322
Al	-1.802815	0.000000	0.000000
Al	1.802815	0.000000	0.000000

$Al_2Ga_4^{2-}$ (D_{2h})

Ga	-1.425711	-1.256714	0.000000
Al	0.000000	-3.754547	0.000000
Ga	1.425711	-1.256714	0.000000
Ga	-1.425711	1.256714	0.000000
Ga	1.425711	1.256714	0.000000
Al	0.000000	3.754547	0.000000

$Al_2Ga_4^{2-}$ (O_h)

Ga	0.000000	1.936152	0.000000
Al	0.000000	0.000000	-1.950434
Ga	0.000000	-1.936152	0.000000
Al	0.000000	0.000000	1.950434
Ga	-1.936152	0.000000	0.000000
Ga	1.936152	0.000000	0.000000

$Ga_2Al_4^{2-}$ (D_{2h})

Al	-1.428358	-1.293707	0.000000
Ga	0.000000	-3.835594	0.000000
Al	1.428358	-1.293707	0.000000
Al	-1.428358	1.293707	0.000000
Al	1.428358	1.293707	0.000000
Ga	0.000000	3.835594	0.000000

$Ga_2Al_4^{2-}$ (O_{2h})

Al	0.000000	1.949081	0.000000
Ga	0.000000	0.000000	-1.912150
Al	0.000000	-1.949081	0.000000
Ga	0.000000	0.000000	1.912150
Al	-1.949081	0.000000	0.000000
Al	1.949081	0.000000	0.000000

$Ga_2B_4^{2-}$ (D_{2h})

B	-0.891736	-0.787322	0.000000
Ga	0.000000	-2.828659	0.000000
B	0.891736	-0.787322	0.000000
B	-0.891736	0.787322	0.000000
B	0.891736	0.787322	0.000000
Ga	0.000000	2.828659	0.000000

$Ga_2B_4^{2-}$ (O_h)

B	0.000000	1.323781	0.000000
Ga	0.000000	0.000000	-1.766260
B	0.000000	-1.323781	0.000000
Ga	0.000000	0.000000	1.766260
B	-1.323781	0.000000	0.000000
B	1.323781	0.000000	0.000000

$Al_3Ga_3^{2-}$ (D_{2h})

Ga	0.000000	-1.431932	1.229977
Ga	0.000000	0.000000	3.727810
Ga	0.000000	1.431932	1.229977
Al	0.000000	-1.421171	-1.309089
Al	0.000000	1.421171	-1.309089
Al	0.000000	0.000000	-3.874624

$Al_3Ga_3^{2-}$ (O_h)

Al	1.580083	0.000000	1.112352
Al	-0.790042	1.368392	1.112352
Ga	-1.600688	0.000000	-1.117676
Ga	0.800344	-1.386237	-1.117676
Al	-0.790042	-1.368392	1.112352
Ga	0.800344	1.386237	-1.117676

Table S2. Energy decomposition analysis (EDA) of B_6^{2-} metal cluster with D_{2h} and O_h symmetries (in kcal mol^{-1}), from two B_3^- fragments at their quintuplet state, computed at the BLYP-D3(BJ)/TZ2P level.

B_6^{2-}	D_{2h} + D_{2h} ➔ D_{2h}	O_h + O_h ➔ O_h	*ΔE* *D_{2h} - O_h*	O_h + O_h ➔ D_{2h}	*ΔE* *D_{2h}*	D_{2h} + D_{2h} ➔ O_h	*ΔE* *O_h*
ΔE_{int}	-192.0	-101.4	*-90.6*	-125.3	*66.7*	-81.2	*20.2*
ΔE_{Pauli}	533.5	735.3	*-201.8*	519.1	*-14.4*	724.4	*-10.9*
ΔV_{elstat}	-239.0	-291.9	*52.9*	-206.1	*32.9*	-286.2	*5.7*
ΔE_{oi}	-483.4	-542.8	*59.4*	-435.6	*47.8*	-516.6	*26.2*
ΔE_{disp}	-3.2	-2.1	*-1.1*	-2.7	*0.5*	-1.9	*0.2*
ΔE_{prep}	12.5	1.3	*11.2*	1.3	*-11.2*	12.5	*11.2*
ΔE	-179.5	-100.2	*-79.3*	-124.0	*55.5*	-68.7	*31.5*

Table S3. Energy decomposition analysis (EDA) of Al_6^{2-} metal cluster with D_{2h} and O_h symmetries (in kcal mol^{-1}), from two Al_3^- fragments at their quintuplet state, computed at the BLYP-D3(BJ)/TZ2P level.

Al_6^{2-}	D_{2h} + D_{2h} ➔D_{2h}	O_h + O_h ➔O_h	*ΔE* *D_{2h} - O_h*	O_h + O_h ➔D_{2h}	*ΔE* *D_{2h}*	D_{2h} + D_{2h} ➔O_h	*ΔE* *O_h*
ΔE_{int}	-20.7	-39.8	*19.1*	-21.2	*-0.5*	-32.8	*7.0*
ΔE_{Pauli}	225.7	348.0	*-122.3*	230.3	*4.6*	338.1	*-9.9*
ΔV_{elstat}	-96.3	-166.5	*70.2*	-99.5	*-3.2*	-157.9	*8.6*
ΔE_{oi}	-146.9	-217.4	*70.5*	-149.3	*-2.4*	-213.8	*3.6*
ΔE_{disp}	-3.2	-3.9	*0.7*	-2.7	*0.5*	0.8	*4.7*
ΔE_{prep}	0.0	1.7	*-1.7*	1.7	*1.7*	0.0	*-1.7*
ΔE	-20.7	-38.1	*17.4*	-19.5	*1.2*	-32.8	*5.3*

Table S4. Energy decomposition analysis (EDA) of Ga_6^{2-} metal cluster with D_{2h} and O_h symmetries (in kcal mol^{-1}), from two Ga_3^- fragments at their quintuplet state, computed at the BLYP-D3(BJ)/TZ2P level.

Ga_6^{2-}	$D_{2h} + D_{2h}$ ➔D_{2h}	$O_h + O_h$ ➔O_h	*ΔE* *D_{2h} - O_h*	$O_h + O_h$ ➔D_{2h}	*ΔE* *D_{2h}*	D_{2h} + D_{2h} ➔O_h	*ΔE* *O_h*
ΔE_{int}	-19.1	-31.0	*11.9*	-20.3	*-1.2*	-26.4	*4.6*
ΔE_{Pauli}	269.6	384.5	*-114.9*	278.2	*8.6*	372.8	*-11.8*
ΔV_{elstat}	-138.0	-207.5	*69.5*	-144.0	*-6.0*	-198.2	*9.3*
ΔE_{oi}	-146.7	-203.4	*56.7*	-150.6	*-3.9*	-199.2	*4.2*
ΔE_{disp}	-4.0	-4.7	*0.6*	-3.9	*0.1*	-1.8	*2.9*
ΔE_{prep}	0.1	1.4	*-1.3*	1.4	*1.3*	0.1	*-1.3*
ΔE	-19.0	-29.6	*10.6*	-18.9	*0.1*	-26.3	*3.3*

Table S5. Energy decomposition analysis (EDA) of B_6^{2-} metal cluster with D_{2h} and O_h symmetries (in kcal mol^{-1}), from two B_3^- fragments at their triplet state, computed at the BLYP-D3(BJ)/TZ2P level.

B_6^{2-}	$D_{2h} + D_{2h}$ ➔D_{2h}	$O_h + O_h$ ➔O_h	ΔE D_{2h} - O_h
ΔE_{int}	-84.9	-50.5	-34.4
ΔE_{Pauli}	451.8	1169.5	-717.7
ΔV_{elstat}	-180.9	-447.6	266.7
ΔE_{oi}	-352.7	-770.4	417.7
ΔE_{disp}	-3.2	-2.1	-1.1
ΔE_{prep}	0.2	11.8	-11.7
ΔE	-84.8	-38.7	-46.1