Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

SUPPORTING INFORMATION

Molecular Structures of $M_2N_2^{2-}$ (M and N = B, Al, and Ga) Clusters Using the Gradient Embedded Genetic Algorithm

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Table S1. Cartesian coordinates of the MP2/6-311G* optimized geometries of all studied species.

Table S2. MCI values of Al_4^{2-} obtained with the B3LYP method using different basis sets.

Figure S1. NICS profiles of Al_4^{2-} obtained at the B3LYP level with different basis sets.

Table S1. Cartesian coordinates of the MP2/6-311G* optimized geometries of all studied species.

B_4^{2-} D_{4h}

1	5	0	0.000000	1.190879	0.000000
2	5	0	0.000000	-1.190879	0.000000
3	5	0	1.190879	0.000000	0.000000
4	5	0	-1.190879	0.000000	0.000000

B_4^{2-} $D_{\infty h}$

1	5	0	0.000000	0.000000	2.399749
2	5	0	0.000000	0.000000	0.782526
3	5	0	0.000000	0.000000	-0.782526
4	5	0	0.000000	0.000000	-2.399749

Al_4^{2-} D_{4h}

1	13	0	0.000000	1.823500	0.000000
2	13	0	0.000000	-1.823500	0.000000
3	13	0	1.823500	0.000000	0.000000
4	13	0	-1.823500	0.000000	0.000000

Al_4^{2-} $D_{\infty h}$

1	13	0	0.000000	0.000000	3.883931
2	13	0	0.000000	0.000000	1.312796
3	13	0	0.000000	0.000000	-1.312796
4	13	0	0.000000	0.000000	-3.883931

Ga_4^{2-} D_{4h}

1	31	0	0.000000	1.836000	0.000000
2	31	0	0.000000	-1.836000	0.000000
3	31	0	1.836000	0.000000	0.000000
4	31	0	-1.836000	0.000000	0.000000

$Al_2B_2^{2-}$ C_{2v}

1	5	0	0.785171	1.431401	0.000157
2	5	0	-0.785077	1.431412	0.000094

3	13	0	1.383376	-0.550566	0.000011
4	13	0	-1.383412	-0.550516	-0.000107

$Al_2B_2^{2-}$ D_{2h}

1	5	0	-0.000006	0.000000	1.529623
2	5	0	-0.000006	0.000000	-1.529623
3	13	0	0.000011	1.478827	0.000000
4	13	0	-0.000006	-1.478827	0.000000

$Al_2B_2^{2-}$ $D_{\infty h}$

1	13	0	0.000000	0.000000	2.840949
2	5	0	0.000000	0.000000	0.781571
3	5	0	0.000000	0.000000	-0.781571
4	13	0	0.000000	0.000000	-2.840949

$Ga_2B_2^{2-}$ C_{2v}

1	5	0	0.788738	1.724083	0.000223
2	5	0	-0.788680	1.724080	0.000079
3	31	0	1.419373	-0.278084	0.000012
4	31	0	-1.419383	-0.278071	-0.000061

$Ga_2B_2^{2-}$ D_{2h}

1	5	0	0.000000	0.000000	1.540947
2	5	0	0.000000	0.000000	-1.540947
3	31	0	0.000000	-1.503316	0.000000
4	31	0	0.000000	1.503316	0.000000

$Ga_2B_2^{2-}$ $D_{\infty h}$

1	31	0	0.000000	0.000000	2.851137
2	5	0	0.000000	0.000000	0.780880
3	5	0	0.000000	0.000000	-0.780880
4	31	0	0.000000	0.000000	-2.851137

$Ga_2Al_2^{2-}$ C_{2v}

1	13	0	1.294614	1.817919	0.000239

2	13	0	-1.294455	1.818014	0.000080
3	31	0	1.290786	-0.762420	0.000018
4	31	0	-1.290853	-0.762326	-0.000152

$Ga_2Al_2^{2-}$ D_{2h}

1	13	0	-0.000001	0.000000	1.842621
2	13	0	-0.000001	0.000000	-1.842621
3	31	0	-0.000001	1.808474	0.000000
4	31	0	0.000003	-1.808474	0.000000

$Al_2B_2^{2-}$ C_{2v} + Li^+

1	5	0	0.150544	1.318651	0.794424
2	5	0	0.150544	1.318651	-0.794424
3	13	0	0.150544	-0.696139	1.361030
4	13	0	0.150544	-0.696139	-1.361030
5	3	0	-1.806525	1.637704	0.000000

$Al_2B_2^{2-}$ D_{2h} + Li^+

1	5	0	0.000000	1.457170	-0.016678
2	5	0	0.000000	-1.457170	-0.016678
3	13	0	1.557653	0.000000	-0.214598
4	13	0	-1.557653	0.000000	-0.214598
5	3	0	0.000000	0.000000	1.915442

$Ga_2B_2^{2-}$ C_{2v} + Li^+

1	5	0	0.076424	1.669677	0.800044
2	5	0	0.076424	1.669677	-0.800044
3	31	0	0.076424	-0.375334	1.369721
4	31	0	0.076424	-0.375334	-1.369721
5	3	0	-1.834187	2.191316	0.000000

$Ga_2B_2^{2-}$ D_{2h} + Li^+

1	5	0	0.000000	1.482180	0.057804
2	5	0	0.000000	-1.482180	0.057804

3	31	0	-1.576741	0.000000	-0.106815
4	31	0	1.576741	0.000000	-0.106815
5	3	0	0.000000	0.000000	2.014834

$Ga_2Al_2^{2-}$ C_{2v} + Li^+

1	13	0	1.310723	1.813514	-0.127381
2	13	0	-1.310715	1.813521	-0.127373
3	31	0	1.301363	-0.789907	-0.046100
4	31	0	-1.301369	-0.789899	-0.046099
5	3	0	0.000033	0.607513	2.056658

$Ga_2Al_2^{2-}$ D_{2h} + Li^+

1	13	0	0.000000	1.853603	-0.087330
2	13	0	0.000000	-1.853603	-0.087330
3	31	0	1.833140	0.000000	-0.063882
4	31	0	-1.833140	0.000000	-0.063882
5	3	0	0.000000	0.000000	2.077075

Table S2. MCI values of Al_4^{2-} obtained with the B3LYP method using different basis sets.

	6-311G*	6-311+G*	aug-cc-pVTZ
MCI	0.356	0.357	0.359
MCI(σ)	0.187	0.188	0.188
MCI(π)	0.169	0.169	0.169

Figure S1. NICS profiles of Al_4^{2-} obtained at the B3LYP level with different basis sets.