SUPPORTING INFORMATION

Octahedral Aromaticity in ${}^{2S+1}A_{1g} X_6^q$ Clusters (X = Li–C and Be–Si, S = 0–3, and q = -2–+4)

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Table S1. Cartesian coordinates of optimized ${}^{2S+1}A_{1g} X_6^{q}$ clusters which are minima in the potential energy surface.

Table S2. Cartesian coordinates of optimized ${}^{2S+1}A_{1g}X_6^q$ clusters that are saddle-points in the potential energy surface. The number of imaginary frequencies is included.

Table S3. Linear correlation coefficients between the different computed indices including all the possible combinations.

Table S4. Relative energies of Li_{6^+} , $\text{Na}_{6^{2^-}}$, $\text{Mg}_{6^{2^-}}$ and $\text{Al}_{6^{2^-}}$ between two electronic states. Values in kcal/mol.

Table S5. Molecular structures of octahedral clusters ${}^{2S+1}A_{1g}X_6^q$ that are saddle-points in the potential surface. Values of X–X bond distance in Å, MCI and PDI in electrons and NICS in ppm.

Figure S1. Energetic order of molecular orbitals for studied $O_h^{2S+1}A_{1g}X_6^q$ clusters that are minima (Table S1).

Figure S2. CMO-NICS for Na_6^{2-} , Be_6^{2+} , Mg_6^{2-} , Mg_6 , B_6^{2+} , B_6^{4+} , Al_6^{2-} and Si_6^{2-} in the ${}^1A_{1g}$ electronic state.

Table S1.	Cartesian coordinates	of optimized ²	$^{2S+1}A_{1g}X_{6}^{q}c$	lusters that are	e minima in tl	he potential	energy
surface.							

1 x 1 g	Li_6^+	${}^{4}A_{1g}$	Be ₆ -		
3	0.000000 0.000000 2.126102	4	0.000000	0.000000	1.431286
3	2.126102 0.000000 0.000000	4	0.000000	1.431286	0.000000
3	0.000000 -2.126102 0.000000	4	1.431286	0.000000	0.000000
3	-2.126102 0.000000 0.000000	4	0.000000	-1.431286	0.000000
3	0.000000 2.126102 0.000000	4	-1.431286	0.000000	0.000000
3	0.000000 0.000000 -2.126102	4	0.000000	0.000000	-1.431286
${}^{6}A_{1g}$	Li ₆ ⁺	${}^{5}A_{1g}$	Be ₆		
3	0.000000 0.000000 2.200515	4	0.000000	0.000000	1.442232
3	2.200515 0.000000 0.000000	4	1.442232	0.000000	0.000000
3	0.000000 -2.200515 0.000000	4	0.000000	-1.442232	0.000000
3	-2.200515 0.000000 0.000000	4	-1.442232	0.000000	0.000000
3	0.000000 2.200515 0.000000	4	0.000000	1.442232	0.000000
3	0.000000 0.000000 -2.200515	4	0.000000	0.000000	-1.442232
${}^{1}A_{1g}$	Na_{6}^{2}	${}^{1}A_{1g}$	${\rm Be_6}^{2+}$		
11	0.000000 0.000000 2.549470	4	0.000000	0.000000	1.509343
11	2.549470 0.000000 0.000000	4	1.509343	0.000000	0.000000
11	0.000000 -2.549470 0.000000	4	0.000000	-1.509343	0.000000
11	-2.549470 0.000000 0.000000	4	-1.509343	0.000000	0.000000
11	0.000000 2.549470 0.000000	4	0.000000	1.509343	0.000000
11	0.000000 0.000000 -2.549470	4	0.000000	0.000000	-1.509343
$^{7}A_{1g}$	Na_{6}^{2}	$^{2}A_{1g}$	${\rm Be_6}^{3+}$		
⁷ A _{1g} 11	Na ₆ ²⁻ 0.000000 0.000000 2.750779	² A _{1g} 4	$\frac{\mathrm{Be_6}^{3+}}{0.000000}$	0.000000	1.603276
⁷ A _{1g} 11 11	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	$^{2}A_{1g}$ 4 4	Be ₆ ³⁺ 0.000000 1.603276	0.000000 0.000000	1.603276 0.000000
⁷ A _{1g} 11 11 11	$\begin{array}{ccccccc} Na_6^{2-} \\ 0.000000 & 0.000000 & 2.750779 \\ 2.750779 & 0.000000 & 0.000000 \\ 0.000000 & -2.750779 & 0.000000 \end{array}$	$^{2}A_{1g}$ 4 4 4	Be ₆ ³⁺ 0.000000 1.603276 0.000000	0.000000 0.000000 -1.603276	1.603276 0.000000 0.000000
⁷ A _{1g} 11 11 11 11	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$^{2}A_{1g}$ 4 4 4 4 4	Be ₆ ³⁺ 0.000000 1.603276 0.000000 -1.603276	0.000000 0.000000 -1.603276 0.000000	1.603276 0.000000 0.000000 0.000000
⁷ A _{1g} 11 11 11 11 11	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	${}^{2}A_{1g}$ 4 4 4 4 4 4	Be ₆ ³⁺ 0.000000 1.603276 0.000000 -1.603276 0.000000	0.000000 0.000000 -1.603276 0.000000 1.603276	1.603276 0.000000 0.000000 0.000000 0.000000
⁷ A _{1g} 11 11 11 11 11 11 11	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	${}^{2}A_{1g}$ 4 4 4 4 4 4 4	$\begin{array}{c} \text{Be}_{6}{}^{3+}\\ 0.000000\\ 1.603276\\ 0.000000\\ -1.603276\\ 0.000000\\ 0.000000\\ \end{array}$	0.000000 0.000000 -1.603276 0.000000 1.603276 0.000000	1.603276 0.000000 0.000000 0.000000 0.000000 -1.603276
⁷ A _{1g} 11 11 11 11 11 11 11 4A _{1g}	$\begin{array}{l} Na_6^{2-} \\ 0.000000 & 0.000000 & 2.750779 \\ 2.750779 & 0.000000 & 0.000000 \\ 0.000000 & -2.750779 & 0.000000 \\ -2.750779 & 0.000000 & 0.000000 \\ 0.000000 & 2.750779 & 0.000000 \\ 0.000000 & 0.000000 & -2.750779 \\ Na_6^+ \end{array}$	$^{2}A_{1g}$ 4 4 4 4 4 4 1 $^{1}A_{1g}$	Be ₆ ³⁺ 0.000000 1.603276 0.000000 -1.603276 0.000000 0.000000 Mg ₆ ²⁻	0.000000 0.000000 -1.603276 0.000000 1.603276 0.000000	1.603276 0.000000 0.000000 0.000000 0.000000 -1.603276
⁷ A _{1g} 11 11 11 11 11 11 11 11 4A _{1g} 11	$\begin{array}{l} Na_6^{2-} \\ 0.000000 & 0.000000 & 2.750779 \\ 2.750779 & 0.000000 & 0.000000 \\ 0.000000 & -2.750779 & 0.000000 \\ -2.750779 & 0.000000 & 0.000000 \\ 0.000000 & 2.750779 & 0.000000 \\ 0.000000 & 0.000000 & -2.750779 \\ \end{array}$	$^{2}A_{1g}$ 4 4 4 4 4 4 4 1 4 1 2	$\begin{array}{c} Be_{6}{}^{3+}\\ 0.000000\\ 1.603276\\ 0.000000\\ -1.603276\\ 0.000000\\ 0.000000\\ Mg_{6}{}^{2-}\\ 0.000000\\ \end{array}$	0.000000 0.000000 -1.603276 0.000000 1.603276 0.000000	1.603276 0.000000 0.000000 0.000000 -1.603276 2.432066
⁷ A _{1g} 11 11 11 11 11 11 11 11 4A _{1g} 11 11	$\begin{array}{l} Na_6^{2-} \\ 0.000000 & 0.000000 & 2.750779 \\ 2.750779 & 0.000000 & 0.000000 \\ 0.000000 & -2.750779 & 0.000000 \\ -2.750779 & 0.000000 & 0.000000 \\ 0.000000 & 2.750779 & 0.000000 \\ 0.000000 & 0.000000 & -2.750779 \\ \end{array}$	² A _{1g} 4 4 4 4 4 4 4 1 4 12 12	$\begin{array}{c} \text{Be}_{6}{}^{3+}\\ 0.000000\\ 1.603276\\ 0.000000\\ -1.603276\\ 0.000000\\ 0.000000\\ 0.000000\\ \text{Mg}_{6}{}^{2-}\\ 0.000000\\ 2.432066 \end{array}$	0.000000 0.000000 -1.603276 0.000000 1.603276 0.000000 0.000000	1.603276 0.000000 0.000000 0.000000 -1.603276 2.432066 0.000000
⁷ A _{1g} 11 11 11 11 11 11 11 11 11 11 11	$\begin{array}{llllllllllllllllllllllllllllllllllll$	$^{2}A_{1g}$ 4 4 4 4 4 1 $^{1}A_{1g}$ 12 12 12	$\begin{array}{c} Be_{6}{}^{3+}\\ 0.000000\\ 1.603276\\ 0.000000\\ -1.603276\\ 0.000000\\ 0.000000\\ 0.000000\\ Mg_{6}{}^{2-}\\ 0.000000\\ 2.432066\\ 0.000000\\ \end{array}$	0.000000 0.000000 -1.603276 0.000000 1.603276 0.000000 0.000000 -2.432066	1.603276 0.000000 0.000000 0.000000 -1.603276 2.432066 0.000000 0.000000
⁷ A _{1g} 11 11 11 11 11 11 11 11 11 11 11	$\begin{array}{llllllllllllllllllllllllllllllllllll$	$^{2}A_{1g}$ 4 4 4 4 4 4 1 1 A_{1g} 12 12 12 12	$\begin{array}{c} Be_{6}{}^{3+}\\ 0.000000\\ 1.603276\\ 0.000000\\ -1.603276\\ 0.000000\\ 0.000000\\ 0.000000\\ Mg_{6}{}^{2-}\\ 0.000000\\ 2.432066\\ 0.000000\\ -2.432066\end{array}$	0.000000 0.000000 -1.603276 0.000000 1.603276 0.000000 0.000000 -2.432066 0.000000	1.603276 0.000000 0.000000 0.000000 -1.603276 2.432066 0.000000 0.000000 0.000000
⁷ A _{1g} 11 11 11 11 11 11 11 11 11 11 11 11	$\begin{array}{llllllllllllllllllllllllllllllllllll$	$^{2}A_{1g}$ 4 4 4 4 4 4 1 1 1 2 1 2 1 2 1 2 1 2 1 2	$Be_{6}^{3+} \\ 0.000000 \\ 1.603276 \\ 0.000000 \\ -1.603276 \\ 0.000000 \\ 0.000000 \\ Mg_{6}^{2-} \\ 0.000000 \\ 2.432066 \\ 0.000000 \\ -2.432066 \\ 0.000000 \\ -2.432066 \\ 0.000000 \\ 0.000000 \\ -2.432066 \\ 0.000000 \\ 0.000000 \\ -2.432066 \\ 0.000000 \\ 0.000000 \\ -2.432066 \\ 0.000000 \\ -2.43206 \\ -2.43200 \\ -2.4300 \\ -2.4300 \\ -2.4300 \\ -2.4300 $	0.000000 0.000000 -1.603276 0.000000 1.603276 0.000000 0.000000 -2.432066 0.000000 2.432066	1.603276 0.000000 0.000000 0.000000 -1.603276 2.432066 0.000000 0.000000 0.000000 0.000000
⁷ A _{1g} 11 11 11 11 11 11 11 11 11 11 11 11 11	$\begin{array}{l} Na_6^{2-} \\ 0.000000 & 0.000000 & 2.750779 \\ 2.750779 & 0.000000 & 0.000000 \\ 0.000000 & -2.750779 & 0.000000 \\ -2.750779 & 0.000000 & 0.000000 \\ 0.000000 & 2.750779 & 0.000000 \\ 0.000000 & 0.000000 & -2.750779 \\ \end{array}$	² A _{1g} 4 4 4 4 4 4 4 4 4 4 4 1 2 12 12 12 12 12 12	$Be_{6}^{3+} \\ 0.000000 \\ 1.603276 \\ 0.000000 \\ -1.603276 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ 2.432066 \\ 0.000000 \\ -2.432066 \\ 0.0000000 \\ 0.0000000 \\ 0.000000 \\ 0.0000000 \\ 0.0000000 \\ 0.00000000$	0.000000 0.000000 -1.603276 0.000000 1.603276 0.000000 0.000000 -2.432066 0.000000 2.432066 0.000000	1.603276 0.000000 0.000000 0.000000 -1.603276 2.432066 0.000000 0.000000 0.000000 0.000000 -2.432066
⁷ A _{1g} 11 11 11 11 11 11 11 11 11 11 11 11 11	$\begin{array}{l} {\rm Na_6^{2-}} \\ 0.000000 & 0.000000 & 2.750779 \\ 2.750779 & 0.000000 & 0.000000 \\ 0.000000 & -2.750779 & 0.000000 \\ -2.750779 & 0.000000 & 0.000000 \\ 0.000000 & 2.750779 & 0.000000 \\ 0.000000 & 0.000000 & -2.750779 \\ \end{array}$	$^{2}A_{1g}$ 4 4 4 4 4 4 4 $^{1}A_{1g}$ 12 12 12 12 12 12 12 $^{7}A_{1g}$	Be_{6}^{3+} 0.000000 1.603276 0.000000 -1.603276 0.000000 0.000000 Mg_{6}^{2-} 0.000000 2.432066 0.000000 -2.432066 0.000000 0.000000 Mg_{6}^{2-}	0.000000 0.000000 -1.603276 0.000000 1.603276 0.000000 0.000000 -2.432066 0.000000 2.432066 0.000000	1.603276 0.000000 0.000000 0.000000 -1.603276 2.432066 0.000000 0.000000 0.000000 0.000000 -2.432066
⁷ A _{1g} 11 11 11 11 11 11 11 11 11 11 11 11 11	$\begin{array}{l} {\rm Na_6^{2-}} \\ 0.000000 & 0.000000 & 2.750779 \\ 2.750779 & 0.000000 & 0.000000 \\ 0.000000 & -2.750779 & 0.000000 \\ -2.750779 & 0.000000 & 0.000000 \\ 0.000000 & 2.750779 & 0.000000 \\ 0.000000 & 0.000000 & -2.750779 \\ \end{array}$	$^{2}A_{1g}$ $^{4}A_{4}$ $^{4}A_{4}$ $^{1}A_{1g}$ $^{12}12$	$Be_{6}^{3+} \\ 0.000000 \\ 1.603276 \\ 0.000000 \\ -1.603276 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ 2.432066 \\ 0.000000 \\ -2.432066 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ Mg_{6}^{2-} \\ 0.000000 \\ Mg_{6}^{2-} \\ 0.000000 \\ 0.00000 \\ Mg_{6}^{2-} \\ 0.0$	0.000000 0.000000 -1.603276 0.000000 1.603276 0.000000 0.000000 -2.432066 0.000000 2.432066 0.000000	1.603276 0.000000 0.000000 0.000000 -1.603276 2.432066 0.000000 0.000000 0.000000 -2.432066 2.189541
⁷ A _{1g} 11 11 11 11 11 11 11 11 11 11 11 11 11	$\begin{split} &\text{Na}_{6}^{2-} \\ & 0.000000 & 0.000000 & 2.750779 \\ & 2.750779 & 0.000000 & 0.000000 \\ & 0.000000 & -2.750779 & 0.000000 \\ & -2.750779 & 0.000000 & 0.000000 \\ & 0.000000 & 2.750779 & 0.000000 \\ & 0.000000 & 0.000000 & -2.750779 \\ \end{split}$	$^{2}A_{1g}$ 4 4 4 4 4 4 4 4 $^{1}A_{1g}$ 12 $^{$	$Be_{6}^{3+} \\ 0.000000 \\ 1.603276 \\ 0.000000 \\ -1.603276 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ 2.432066 \\ 0.000000 \\ -2.432066 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ Mg_{6}^{2-} \\ 0.000000 \\ 2.189541 \\ 0.000000 \\ 0.189541 \\ 0.0000000 \\ $	0.000000 0.000000 -1.603276 0.000000 1.603276 0.000000 0.000000 -2.432066 0.000000 2.432066 0.000000 0.000000 0.000000	1.603276 0.000000 0.000000 0.000000 -1.603276 2.432066 0.000000 0.000000 0.000000 -2.432066 2.189541 0.000000
⁷ A _{1g} 11 11 11 11 11 11 11 11 11 11 11 11 11	$\begin{array}{l} {\rm Na_6^{2-}} \\ 0.000000 & 0.000000 & 2.750779 \\ 2.750779 & 0.000000 & 0.000000 \\ 0.000000 & -2.750779 & 0.000000 \\ -2.750779 & 0.000000 & 0.000000 \\ 0.000000 & 2.750779 & 0.000000 \\ 0.000000 & 0.000000 & -2.750779 \\ \end{array}$	$^{2}A_{1g}$ 4 4 4 4 4 4 4 4 $^{1}A_{1g}$ 12 $^{$	$Be_{6}^{3+} \\ 0.000000 \\ 1.603276 \\ 0.000000 \\ -1.603276 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ 2.432066 \\ 0.000000 \\ -2.432066 \\ 0.000000 \\ -2.432066 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ Mg_{6}^{2-} \\ 0.000000 \\ 2.189541 \\ 0.000000 \\ 0.00000 \\ 0.0000 \\ 0.00000 \\ 0.00000 \\ 0.00000 \\ 0.00000 \\ 0$	0.000000 0.000000 -1.603276 0.000000 1.603276 0.000000 0.000000 -2.432066 0.000000 2.432066 0.000000 0.000000 0.000000 -2.189541	1.603276 0.000000 0.000000 0.000000 -1.603276 2.432066 0.000000 0.000000 0.000000 -2.432066 2.189541 0.000000 0.000000
$^{7}A_{1g}$ 11 11 11 11 11 11 11 11 11 1	$\begin{array}{l} {\rm Na_6^{2-}} \\ 0.000000 & 0.000000 & 2.750779 \\ 2.750779 & 0.000000 & 0.000000 \\ 0.000000 & -2.750779 & 0.000000 \\ -2.750779 & 0.000000 & 0.000000 \\ 0.000000 & 2.750779 & 0.000000 \\ 0.000000 & 0.000000 & -2.750779 \\ \end{array}$	$^{2}A_{1g}$ $^{4}A_{4}$ $^{4}A_{4}$ $^{4}A_{4}$ $^{1}A_{1g}$ $^{1}2_{12}$ $^{1}2_$	$Be_{6}^{3+} \\ 0.000000 \\ 1.603276 \\ 0.000000 \\ -1.603276 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ 2.432066 \\ 0.000000 \\ -2.432066 \\ 0.000000 \\ -2.432066 \\ 0.000000 \\ 0.000000 \\ -2.432066 \\ 0.000000 \\ -2.432066 \\ 0.000000 \\ -2.432066 \\ 0.000000 \\ -2.432066 \\ 0.000000 \\ -2.189541 \\ 0.0000000 \\ -2.189541 \\ 0.000000 \\ -2.189541 \\ 0.0000000 \\ -2.18954$	0.000000 0.000000 -1.603276 0.000000 1.603276 0.000000 0.000000 -2.432066 0.000000 2.432066 0.000000 0.000000 0.000000 -2.189541 0.000000	1.603276 0.000000 0.000000 0.000000 -1.603276 2.432066 0.000000 0.000000 0.000000 -2.432066 2.189541 0.000000 0.000000 0.000000
$^{7}A_{1g}$ 11 11 11 11 11 11 11 11 11 1	$\begin{array}{l} {\rm Na_6^{2-}} \\ 0.000000 & 0.000000 & 2.750779 \\ 2.750779 & 0.000000 & 0.000000 \\ 0.000000 & -2.750779 & 0.000000 \\ -2.750779 & 0.000000 & 0.000000 \\ 0.000000 & 2.750779 & 0.000000 \\ 0.000000 & 0.000000 & -2.750779 \\ \end{array}$	$^{2}A_{1g}$ $^{4}A_{4}$ $^{4}A_{4}$ $^{4}A_{4}$ $^{1}A_{1g}$ $^{1}2_{12}$ $^{1}2_$	$Be_{6}^{3+} \\ 0.000000 \\ 1.603276 \\ 0.000000 \\ -1.603276 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ 2.432066 \\ 0.000000 \\ -2.432066 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ 2.189541 \\ 0.000000 \\ -2.189541 \\ 0.000000 \\ 0.000000 \\ -2.189541 \\ 0.000000 \\ 0.000000 \\ -2.189541 \\ 0.000000 \\ 0.000000 \\ -2.189541 \\ 0.000000 \\ 0.000000 \\ -2.189541 \\ 0.0000000 \\ -2.189541 \\ 0.0000000 \\ -2.189541 \\ 0.0000000 \\ -2.189541 \\$	0.000000 0.000000 -1.603276 0.000000 1.603276 0.000000 0.000000 -2.432066 0.000000 2.432066 0.000000 2.432066 0.000000 2.432064 0.000000 2.189541	1.603276 0.000000 0.000000 0.000000 -1.603276 2.432066 0.000000 0.000000 0.000000 -2.432066 2.189541 0.000000 0.000000 0.000000 0.000000

${}^{1}A_{1}$	_a Mg ₆	${}^{1}A_{1g}$	Al6 ²⁻		
12	0.000000 0.000000 2.617914	13	0.000000	0.000000	1.916201
12	2.617914 0.000000 0.000000	13	1.916201	0.000000	0.000000
12	0.000000 -2.617914 0.000000	13	0.000000	-1.916201	0.000000
12	-2.617914 0.000000 0.000000	13	-1.916201	0.000000	0.000000
12	0.000000 2.617914 0.000000	13	0.000000	1.916201	0.000000
12	0.000000 0.000000 -2.617914	13	0.000000	0.000000	-1.916201
${}^{3}A_{19}$	$_{\rm g}{\rm Mg_6}^{2+}$	$^{7}A_{1g}$	Al ₆ ²⁻		
12	0.000000 0.000000 2.411867	13	0.000000	0.000000	2.025754
12	2.411867 0.000000 0.000000	13	2.025754	0.000000	0.000000
12	0.000000 -2.411867 0.000000	13	0.000000	-2.025754	0.000000
12	-2.411867 0.000000 0.000000	13	-2.025754	0.000000	0.000000
12	0.000000 2.411867 0.000000	13	0.000000	2.025754	0.000000
12	0.000000 0.000000 -2.411867	13	0.000000	0.000000	-2.025754
2.		. .			
${}^{3}A_{1g}$	_g B ₆	$^{5}A_{1g}$	Al_6^{2+}		
5	0.000000 0.000000 1.184608	13	0.000000	0.000000	2.084238
5	1.184608 0.000000 0.000000	13	2.084238	0.000000	0.000000
5	0.000000 -1.184608 0.000000	13	0.000000	-2.084238	0.000000
5	-1.184608 0.000000 0.000000	13	-2.084238	0.000000	0.000000
5	0.000000 1.184608 0.000000	13	0.000000	2.084238	0.000000
5	0.000000 0.000000 -1.184608	13	0.000000	0.000000	-2.084238
1 A .	B. ²⁺	1 A .	Si.2-		
5	g D_{6} 0 000000 0 000000 1 150851	1 <u>4</u>	0 000000	0.000000	1 75681
5		14	1 756881	0.000000	0.00000
5	0.000000 -1.150851 - 0.000000	14	0.000000	-1 756881	0.00000
5	-1 150851 0 000000 0 000000	14	-1 756881	0.00000	0.00000
5	0.000000 1.150851 0.000000	14	0.000000	1 756881	0.00000
5	0.000000 - 0.000000 - 1.150851	14	0.000000	0.000000	-1 75681
U		11	0.000000	0.000000	1.70001
${}^{2}A_{19}$	$_{\rm g}{\rm B_6}^{3+}$	${}^{4}A_{1g}S$	Si_{6}^{+}		
5	0.000000 0.000000 1.185606	14	0.000000	0.000000	1.740324
5	1.185606 0.000000 0.000000	14	1.740324	0.000000	0.000000
5	0.000000 -1.185606 0.000000	14	0.000000	-1.740324	0.000000
5	-1.185606 0.000000 0.000000	14	-1.740324	0.000000	0.000000
5	0.000000 1.185606 0.000000	14	0.000000	1.740324	0.000000
5	0.000000 0.000000 -1.185606	14	0.000000	0.000000	-1.740324
1.4					
¹ A ₁₈	$_{\rm g} {\rm B}_{6}^{\rm 4+}$				
5					
2	1.234009 0.000000 0.000000				
2	0.00000 - 1.234009 0.000000				
5	-1.234009 0.000000 0.000000				
5	0.000000 1.234009 0.000000				
5	0.000000 0.000000 -1.234009				

Table S2. Cartesian coordinates of optimized ${}^{2S+1}A_{1g}X_6^q$ clusters that are saddle-points in the potential energy surface. The number of imaginary frequencies is included.

${}^{1}A_{1g} Li_{6}^{2}$	^{1}A
3 0.000000 0.000000) 2.109438 4
3 2.109438 0.000000) 0.000000 4
3 0.000000 -2.109438	8 0.000000 4
3 -2.109438 0.00000	0 0.000000 4
3 0.000000 2.109438	3 0.000000 4
3 0.000000 0.000000) -2.109438 4
Number of imaginary frequ	uencies = 3 Nu
${}^{5}\mathrm{A}_{1\mathrm{g}}\mathrm{Li}_{6}$	⁷ A
3 0.000000 0.000000) 2.028595 4
3 2.028595 0.000000) 0.000000 4
3 0.000000 -2.028595	5 0.000000 4
3 -2.028595 0.00000	0 0.000000 4
3 0.000000 2.028595	5 0.000000 4
3 0.000000 0.000000) -2.028595 4
Number of imaginary frequ	uencies = 3 Nu
${}^{5}A_{1a}Lie^{2+}$	² A
3 0 000000 0 000000) 2 505651 12
3 0,000000 2,505651	12 0 000000 12
3 0,000000 0,000000	12 -2505651 12
3 0.000000 -2.50565	1 = 0.000000 = 12
3 -2 505651 0 00000	1 0.000000 12
2.505051 0.000000	12
Number of imaginary frequ	12 sencies = 3 Nu
$^{6}A_{1g}$ Na $^{-}$	⁴ A
11 0.000000 0.00000	0 2.794959 12
11 2.794959 0.00000	0 0.000000 12
11 0.000000 -2.79493	59 0.000000 12
11 -2.794959 0.0000	00 0.000000 12
11 0.000000 2.79495	59 0.000000 12
11 0.000000 0.00000	00 -2.794959 12
Number of imaginary frequ	uencies = 2 Nu
${}^{5}A_{1g}Na_{6}{}^{2+}$	¹ A
11 0.000000 0.00000	0 3.024430 12
11 3.024430 0.00000	0 0.000000 12
11 0.000000 -3.02443	30 0.000000 12
11 -3.024430 0.00000	00 0.000000 12
11 0.000000 3.02443	30 0.000000 12
11 0.000000 0.00000	00 -3.024430 12
Number of imaginary frequ	uencies = 3 Nu
${}^{4}A_{1a}Be_{6}{}^{1+}$	¹ A
4 0,000000 0,000000) 1 473887 5
4 1 473887 0 000000) 0,000000 5
4 0,000,000 -1,47388'	7 0 000000 5
) 0.000000 5
	7 0 000000 5
	3 1 472887 5
4 0.00000 0.000000	y = 1.4/300/ 3
number of imaginary frequ	tencies = 3 NU

- - Ig	Be ₆		
4 [°]	0.000000	0.000000	1.761753
4	1.761753	0.000000	0.000000
4	0.000000	-1.761753	0.000000
4	-1.761753	0.000000	0.000000
4	0.000000	1 761753	0.000000
1	0.000000	0.000000	-1 761753
л	ber of imagi	0.000000	-1.701733
Inull	iber of imagi	nary nequei	leles = 3
7Δ.	\mathbf{Re}^{4+}		
Λ Ig		0.000000	1 750750
4	0.000000	0.000000	0.000000
4	1.750759	1.750750	0.000000
4	0.000000	-1./30/39	0.000000
4	-1./50/59	0.000000	0.000000
4	0.000000	1.750759	0.000000
4	0.000000	0.000000	-1.750759
Num	ber of imagi	nary frequer	ncies = 3
2.4			
$^{2}A_{1g}$	Mg ₆ -		
12	0.000000	0.000000	2.468836
12	2.468836	0.000000	0.000000
12	0.000000	-2.468836	0.000000
12	-2.468836	0.000000	0.000000
12	0.000000	2.468836	0.000000
12	0.000000	0.000000	-2.468836
Num	ber of imagi	narv frequer	ncies = 3
${}^{4}A_{1\sigma}$	Mg_6^+		
⁴ A _{1g} 12	Mg ₆ ⁺ 0.000000	0.000000	2.261198
⁴ A _{1g} 12 12	Mg ₆ ⁺ 0.000000 2.261198	0.000000 0.000000	2.261198 0.000000
⁴ A _{1g} 12 12 12	Mg6 ⁺ 0.000000 2.261198 0.000000	0.000000 0.000000 -2.261198	2.261198 0.000000 0.000000
⁴ A _{1g} 12 12 12 12	Mg ₆ ⁺ 0.000000 2.261198 0.000000 -2.261198	0.000000 0.000000 -2.261198 0.000000	2.261198 0.000000 0.000000 0.000000
⁴ A _{1g} 12 12 12 12 12 12	$\begin{array}{c} Mg_6^+ \\ 0.000000 \\ 2.261198 \\ 0.000000 \\ -2.261198 \\ 0.000000 \end{array}$	0.000000 0.000000 -2.261198 0.000000 2.261198	2.261198 0.000000 0.000000 0.000000 0.000000
${}^{4}A_{1g}$ 12 12 12 12 12 12 12 12	$Mg_{6}^{+} \\ 0.000000 \\ 2.261198 \\ 0.000000 \\ -2.261198 \\ 0.0000000 \\ 0.0000000 \\ 0.000000 \\ 0.0000000 \\ 0.0000000 \\ 0.00000000$	0.000000 0.000000 -2.261198 0.000000 2.261198 0.000000	2.261198 0.000000 0.000000 0.000000 0.000000 -2.261198
⁴ A _{1g} 12 12 12 12 12 12 12 12	Mg ₆ ⁺ 0.000000 2.261198 0.000000 -2.261198 0.000000 0.000000	0.000000 0.000000 -2.261198 0.000000 2.261198 0.000000	2.261198 0.000000 0.000000 0.000000 -2.261198
⁴ A _{1g} 12 12 12 12 12 12 12 12 Num	Mg_6^+ 0.000000 2.261198 0.000000 -2.261198 0.000000 0.000000 ber of imagi	0.000000 0.000000 -2.261198 0.000000 2.261198 0.000000 nary frequer	2.261198 0.000000 0.000000 0.000000 0.000000 -2.261198 ncies = 3
⁴ A _{1g} 12 12 12 12 12 12 12 12 Num	Mg_6^+ 0.000000 2.261198 0.000000 -2.261198 0.000000 0.000000 uber of imagi	0.000000 0.000000 -2.261198 0.000000 2.261198 0.000000 nary frequer	2.261198 0.000000 0.000000 0.000000 -2.261198 ncies = 3
⁴ A _{1g} 12 12 12 12 12 12 12 12 Num	$Mg_{6}^{+} \\ 0.00000 \\ 2.261198 \\ 0.00000 \\ -2.261198 \\ 0.00000 $	0.000000 0.000000 -2.261198 0.000000 2.261198 0.000000 nary frequer	2.261198 0.000000 0.000000 0.000000 0.000000 -2.261198 ncies = 3 2.491603
⁴ A _{1g} 12 12 12 12 12 12 12 12 Num ¹ A _{1g} 12	$Mg_{6}^{+} \\ 0.00000 \\ 2.261198 \\ 0.00000 \\ -2.261198 \\ 0.00000 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ 2.491603 \\ 0.000000 \\ 0.00000 \\ 0.00000 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ 0.00000 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ 0.0$	0.000000 0.000000 -2.261198 0.000000 2.261198 0.000000 nary frequer 0.000000	2.261198 0.000000 0.000000 0.000000 -2.261198 ncies = 3 2.491603 0.000000
⁴ A _{1g} 12 12 12 12 12 12 12 12 Num ¹ A _{1g} 12 12	$\begin{array}{c} Mg_6^+ \\ 0.00000 \\ 2.261198 \\ 0.00000 \\ -2.261198 \\ 0.00000 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ 2.491603 \\ 0.000000 \\ 0.00000 \\ 0.000$	0.000000 0.000000 -2.261198 0.000000 2.261198 0.000000 nary frequer 0.000000 0.000000 2.401602	2.261198 0.000000 0.000000 0.000000 -2.261198 ncies = 3 2.491603 0.000000
⁴ A _{1g} 12 12 12 12 12 12 12 12 12 12 12 12	Mg_6^+ 0.000000 2.261198 0.000000 -2.261198 0.000000 0.000000 lber of imagi Mg_6^{4+} 0.000000 2.491603 0.000000 2.401602	0.000000 0.000000 -2.261198 0.000000 2.261198 0.000000 nary frequer 0.000000 0.000000 -2.491603	2.261198 0.000000 0.000000 0.000000 -2.261198 ncies = 3 2.491603 0.000000 0.000000
⁴ A _{1g} 12 12 12 12 12 12 12 12 12 12 12 12 12	Mg_6^+ 0.000000 2.261198 0.000000 -2.261198 0.000000 0.000000 uber of imagi Mg_6^{4+} 0.000000 2.491603 0.000000 -2.491603	0.000000 0.000000 -2.261198 0.000000 2.261198 0.000000 nary frequer 0.000000 0.000000 -2.491603 0.000000	2.261198 0.000000 0.000000 0.000000 -2.261198 ncies = 3 2.491603 0.000000 0.000000
${}^{4}A_{1g}$ 12 12 12 12 12 12 12 12 12 12	Mg_6^+ 0.000000 2.261198 0.000000 -2.261198 0.000000 0.000000 uber of imagi Mg_6^{4+} 0.000000 2.491603 0.000000 -2.491603 0.000000	0.000000 0.000000 -2.261198 0.000000 2.261198 0.000000 nary frequer 0.000000 0.000000 -2.491603 0.000000 2.491603	$2.261198 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ -2.261198 \\ ncies = 3$ $2.491603 \\ 0.000000 \\ 0.00000 \\ 0.00000 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ 0.00000 \\ 0.0000000 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ 0.0000000 $
${}^{4}A_{1g}$ 12 12 12 12 12 12 12 12 12 12	Mg_6^+ 0.000000 2.261198 0.000000 -2.261198 0.000000 0.000000 uber of imagi Mg_6^{4+} 0.000000 2.491603 0.000000 -2.491603 0.000000 0.000000 0.000000	0.000000 0.000000 -2.261198 0.000000 2.261198 0.000000 nary frequer 0.000000 -2.491603 0.000000 2.491603 0.000000	2.261198 0.000000 0.000000 0.000000 -2.261198 ncies = 3 2.491603 0.000000 0.000000 0.000000 0.000000 -2.491603
⁴ A _{1g} 12 12 12 12 12 12 12 12 12 12 12 12 12	Mg_6^+ 0.000000 2.261198 0.000000 -2.261198 0.000000 0.000000 iber of imagi Mg_6^{4+} 0.000000 2.491603 0.000000 -2.491603 0.000000 iber of imagi	0.000000 0.000000 -2.261198 0.000000 2.261198 0.000000 nary frequer 0.000000 -2.491603 0.000000 2.491603 0.000000 nary frequer	2.261198 0.000000 0.000000 0.000000 -2.261198 heies = 3 2.491603 0.000000 0.000000 0.000000 0.000000 -2.491603 heies = 6
⁴ A _{1g} 12 12 12 12 12 12 12 12 12 12 12 12 12	Mg_6^+ 0.00000 2.261198 0.00000 -2.261198 0.000000 0.000000 iber of imagi Mg_6^{4+} 0.000000 2.491603 0.000000 -2.491603 0.0000000 0.000000 0.0000000 0.0000000 0.000000 0.0000000 0.00000000	0.000000 0.000000 -2.261198 0.000000 2.261198 0.000000 nary frequer 0.000000 -2.491603 0.000000 2.491603 0.000000 nary frequer	2.261198 0.000000 0.000000 0.000000 -2.261198 ncies = 3 2.491603 0.000000 0.000000 0.000000 0.000000 -2.491603 ncies = 6
⁴ A _{1g} 12 12 12 12 12 12 12 12 12 12 12 12 12	Mg_6^+ 0.000000 2.261198 0.000000 -2.261198 0.000000 0.000000 uber of imagi Mg_6^{4+} 0.000000 2.491603 0.000000 -2.491603 0.000000 0.000000 uber of imagi B_6^{2-}	0.000000 0.000000 -2.261198 0.000000 2.261198 0.000000 nary frequer 0.000000 -2.491603 0.000000 2.491603 0.000000 nary frequer	2.261198 0.000000 0.000000 0.000000 -2.261198 ncies = 3 2.491603 0.000000 0.000000 0.000000 0.000000 -2.491603 ncies = 6 1.225567
⁴ A _{1g} 12 12 12 12 12 12 12 12 12 12 12 12 12	Mg_6^+ 0.000000 2.261198 0.000000 -2.261198 0.000000 0.000000 uber of imagi Mg_6^{4+} 0.000000 2.491603 0.000000 -2.491603 0.000000 uber of imagi B_6^{2-} 0.000000 1.225567	0.000000 0.000000 -2.261198 0.000000 2.261198 0.000000 nary frequer 0.000000 -2.491603 0.000000 2.491603 0.000000 nary frequer	$2.261198 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ -2.261198 \\ ncies = 3$ $2.491603 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ -2.491603 \\ ncies = 6$ $1.235567 \\ 0.000000$
⁴ A _{1g} 12 12 12 12 12 12 12 12 12 12 12 12 12	Mg_6^+ 0.000000 2.261198 0.000000 -2.261198 0.000000 0.000000 uber of imagi Mg_6^{4+} 0.000000 2.491603 0.000000 -2.491603 0.000000 uber of imagi B_6^{2-} 0.000000 1.235567 0.000000	0.000000 0.000000 -2.261198 0.000000 2.261198 0.000000 nary frequer 0.000000 -2.491603 0.000000 2.491603 0.000000 nary frequer 0.000000 0.000000	$\begin{array}{c} 2.261198\\ 0.000000\\ 0.000000\\ 0.000000\\ -2.261198\\ \text{ncies}=3\\ \end{array}$ $\begin{array}{c} 2.491603\\ 0.000000\\ 0.000000\\ 0.000000\\ -2.491603\\ \text{ncies}=6\\ \end{array}$ $\begin{array}{c} 1.235567\\ 0.000000\\ 0.00000\\ 0.00000\\ 0.00000\\ 0.00000\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.000\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.0000\\ 0.000\\ 0.000\\ 0.0000\\ 0.000\\ $
⁴ A _{1g} 12 12 12 12 12 12 12 12 12 12 12 12 12	Mg_6^+ 0.000000 2.261198 0.000000 -2.261198 0.000000 0.000000 iber of imagi Mg_6^{4+} 0.000000 -2.491603 0.000000 0.000000 iber of imagi B_6^{2-} 0.000000 1.235567 0.000000	0.000000 0.000000 -2.261198 0.000000 2.261198 0.000000 nary frequer 0.000000 -2.491603 0.000000 2.491603 0.000000 nary frequer 0.000000 nary frequer	$\begin{array}{c} 2.261198\\ 0.000000\\ 0.000000\\ 0.000000\\ -2.261198\\ \text{ncies} = 3\\ \end{array}$ $\begin{array}{c} 2.491603\\ 0.000000\\ 0.000000\\ 0.000000\\ 0.000000\\ -2.491603\\ \text{ncies} = 6\\ \end{array}$ $\begin{array}{c} 1.235567\\ 0.000000\\ 0.00000\\ 0.00000\\ 0.00000\\ 0.00000\\ 0.00000\\ 0.00000\\ 0.000\\ 0.0$
⁴ A _{1g} 12 12 12 12 12 12 12 12 12 12 12 12 12	$\begin{tabular}{lllllllllllllllllllllllllllllllllll$	0.000000 0.000000 -2.261198 0.000000 2.261198 0.000000 nary frequer 0.000000 -2.491603 0.000000 2.491603 0.000000 nary frequer 0.000000 nary frequer 0.000000 -1.235567 0.000000	$2.261198 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ -2.261198 \\ hcies = 3$ $2.491603 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ -2.491603 \\ hcies = 6$ $1.235567 \\ 0.0000000 \\ 0.0000000 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ 0.000$
${}^{4}A_{1g}$ 12 12 12 12 12 12 12 12 12 12	$\begin{tabular}{lllllllllllllllllllllllllllllllllll$	0.000000 0.000000 -2.261198 0.000000 2.261198 0.000000 nary frequer 0.000000 -2.491603 0.000000 2.491603 0.000000 nary frequer 0.000000 nary frequer 0.000000 -1.235567 0.000000 1.235567	$\begin{array}{c} 2.261198\\ 0.000000\\ 0.000000\\ 0.000000\\ 0.000000\\ -2.261198\\ \text{ncies} = 3\\ \end{array}$ $\begin{array}{c} 2.491603\\ 0.000000\\ 0.000000\\ 0.000000\\ -2.491603\\ \text{ncies} = 6\\ \end{array}$ $\begin{array}{c} 1.235567\\ 0.000000\\ 0.000000\\ 0.000000\\ 0.000000\\ 0.000000\\ 0.000000\\ \end{array}$
${}^{4}A_{1g}$ 12 12 12 12 12 12 12 12 12 12	Mg_6^+ 0.000000 2.261198 0.000000 -2.261198 0.000000 0.000000 iber of imagi Mg_6^{4+} 0.000000 -2.491603 0.000000 0.000000 iber of imagi B_6^{2-} 0.000000 1.235567 0.000000 -1.235567 0.000000 0.000000	0.000000 0.000000 -2.261198 0.000000 2.261198 0.000000 nary frequer 0.000000 -2.491603 0.000000 2.491603 0.000000 nary frequer 0.000000 -1.235567 0.000000 1.235567 0.000000	$\begin{array}{c} 2.261198\\ 0.000000\\ 0.000000\\ 0.000000\\ 0.000000\\ -2.261198\\ \text{ncies} = 3\\ \end{array}$ $\begin{array}{c} 2.491603\\ 0.000000\\ 0.000000\\ 0.000000\\ -2.491603\\ \text{ncies} = 6\\ \end{array}$ $\begin{array}{c} 1.235567\\ 0.000000\\ 0.000000\\ 0.000000\\ 0.000000\\ 0.000000\\ -1.235567\end{array}$

 $^{7}A_{1g} B_{6}^{4+}$ 5 0.000000 0.000000 1.40017 5 0.000000 0.00000 1.400117 5 0.000000 -1.400117 0.00000 5 0.00000 -1.400117 0.000000 5 0.000000 1.400117 0.00000 5 0.000000 0.000000 -1.40017 Number of imaginary frequencies = 6 $^{7}A_{1g}Al_{6}^{4+}$ 13 0.000000 0.000000 2.084372 2.084372 0.000000 0.000000 13 13 0.000000 -2.084372 0.000000 13 0.000000 -2.084372 0.000000 13 0.000000 2.084372 0.000000 13 0.000000 0.000000 -2.084372 Number of imaginary frequencies = 3 ${}^{1}A_{1g} C_{6}{}^{2-}$ 6 0.0000000.000000 1.135696 6 0.000000 0.000000 1.135696 6 0.000000 -1.135696 0.000000 6 -1.135696 0.000000 0.000000 1.135696 6 0.000000 0.000000 0.000000 0.000000 -1.135696 6 Number of imaginary frequencies = 3 ${}^{4}A_{1g} C_{6}^{+}$ 6 0.000000 0.000000 1.136705 6 1.136705 0.000000 0.000000 6 0.000000 -1.136705 0.000000 6 -1.136705 0.000000 0.000000 6 0.000000 1.136705 0.000000 0.000000 0.000000 -1.136705 6 Number of imaginary frequencies = 3 $^6A_{1g} \, C_6{}^{3+}$ 6 0.000000 0.000000 1.109483 6 1.109483 0.000000 0.000000 6 0.000000 -1.109483 0.000000 6 -1.109483 0.000000 0.000000 6 0.000000 1.109483 0.000000 6 0.000000 0.000000 -1.109483

Number of imaginary frequencies = 3

$^{1}A_{19}$	$_{\rm g} C_6^{-1}$		
6	0.000000	0.000000	1.209339
6	1.209339	0.000000	0.000000
6	0.000000	-1.209339	0.000000
6	-1.209339	0.000000	0.000000
6	0.000000	1.209339	0.000000
6	0.000000	0.000000	-1.209339
Nur	nber of imag	inary freque	encies $= 6$
	e	- 1	

$^{7}A_{1g}$	C_6^{4+}
- 5	0

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6	0.000000	0.000000	1.168386
6	1.168386	0.000000	0.000000
6	0.000000	-1.168386	0.000000
6	-1.168386	0.000000	0.000000
6	0.000000	1.168386	0.000000
6	0.000000	0.000000	-1.168386
Nu	mber of imag	inary freque	ncies = 6

$^{7}A_{1g}S$	Si ₆ ²⁻		
14	0.000000	0.000000	1.786330
14	1.786330	0.000000	0.000000
14	0.000000	-1.786330	0.000000
14	-1.786330	0.000000	0.000000
14	0.000000	1.786330	0.000000
14	0.000000	0.000000	-1.786330
Numb	per of imagir	nary frequen	cies = 6

${}^{1}A_{1g}$	Si_{6}^{4+}		
14	0.000000	0.000000	1.813384
14	1.813384	0.000000	0.000000
14	0.000000	-1.813384	0.000000
14	-1.813384	0.000000	0.000000
14	0.000000	1.813384	0.000000
14	0.000000	0.000000	-1.813384
Nun	nber of imagir	nary frequen	cies = 3

$^{7}A_{1g}$	Si_{6}^{4+}		
14	0.000000	0.000000	2.171685
14	2.171685	0.000000	0.000000
14	0.000000	-2.171685	0.000000
14	-2.171685	0.000000	0.000000
14	0.000000	2.171685	0.000000
14	0.000000	0.000000	-2.171685
Num	ber of imagir	nary frequen	cies = 6

r ²	MCI ₆	MCI ₄	MCI ₃	NICS(0) ₆	NICS(0) ₃	PDI
MCI ₆	1.00					
MCI ₄	0.58	1.00				
MCI ₃	0.33	0.31	1.00			
NICS(0) ₆	0.37	0.71	0.30	1.00		
NICS(0) ₃	0.20	0.66	0.26	0.88	1.00	
PDI	0.09	0.22	0.82	0.25	0.26	1.00

Table S3. Linear correlation coefficients between the different computed indices including all the possible combinations.

Table S4. Relative energies of Li_6^+ , Na_6^{2-} , Mg_6^{2-} and Al_6^{2-} between two electronic states. Values in kcal/mol.

Electronic state	Li ₆ +
$^{4}A_{1g}$	0.00
$^{6}A_{1g}$	62.3

Electronic state	Na ₆ ²⁻	Mg62-	Al ₆ ²⁻
${}^{1}A_{1g}$	0.00	0.00	0.00
$^{7}A_{1g}$	40.5	35.2	44.7

System	q	Spin	Electronic state	d(X–X)	MCI ₆	MCI ₄	MCI ₃	NICS(0) ₆	NICS(0) ₃	PDI
Li ₆	-2	S=0	${}^{1}A_{1g}$	2.983	0.038	0.0466	0.0999	-13.18	-13.29	0.374
	0	S=2	⁵ A _{1g}	2.869	0.112	0.0538	0.0944	-24.00	-16.94	0.312
	2	S=2	${}^{5}A_{1g}$	3.544	0.0245	0.0169	0.0240	-13.56	-10.84	0.197
	1	S=3/2	${}^{4}A_{1g}$	2.084	0.043	0.0269	0.1396	126.80	112.94	0.548
Be ₆	4	S=0	${}^{1}A_{1g}$	2.491	0.049	0.0373	0.1090	-36.72	-29.11	0.391
	4	S=3	$^{7}A_{1g}$	2.476	0.055	0.0297	0.0908	-6.88	-2.50	0.391
B ₆	-2	S=0	${}^{1}A_{1g}$	1.747	0.059	0.057	0.153	-102.72	-85.49	0.744
	4	S=3	⁷ A _{1g}	1.980	0.059	0.051	0.120	-71.07	-57.80	0.545
C ₆	-2	S=0	${}^{1}A_{1g}$	1.606	0.032	0.034	0.159	-24.10	-48.37	0.786
	1	S=3/2	${}^{4}A_{1g}$	1.608	0.050	0.046	0.148	-63.03	-70.53	0.742
	3	S=5/2	⁶ A _{1g}	1.569	0.072	0.049	0.169	-15.49	-27.90	0.771
	4	S=0	${}^{1}A_{1g}$	1.710	0.072	0.069	0.124	-110.45	-91.27	0.688
	4	S=3	$^{7}A_{1g}$	1.652	0.033	0.028	0.144	3.29	-12.10	0.704
Na ₆	-1	S=5/2	⁶ A _{1g}	3.953	0.041	0.022	0.040	3.65	5.91	0.227
	2	S=2	$^{7}A_{1g}$	4.277	0.017	0.019	0.040	-14.28	-11.00	0.167
Mg ₆	-1	S=1/2	$^{21}A_{1g}$	3.491	0.030	0.018	0.054	16.05	17.45	0.337
	1	S=3/2	${}^{4}A_{1g}$	3.198	0.046	0.034	0.081	-2.37	2.84	0.363
	4	S=0	${}^{1}A_{1g}$	3.524	0.030	0.039	0.073	-32.40	-25.37	0.317
Al ₆	4	S=3	$^{7}A_{1g}$	2.948	0.061	0.067	0.093	-58.73	-47.15	0.484
Si ₆	-2	S=3	$^{7}A_{1g}$	2.526	0.055	0.052	0.131	65.41	65.76	0.818
	4	S=0	${}^{1}A_{1g}$	2.565	0.086	0.092	0.111	54.74	38.28	0.649
	4	S=3	$^{7}A_{1g}$	3.071	0.059	0.027	0.107	3.85	-0.98	0.508

Table S5. Molecular structures of octahedral clusters ${}^{2S+1}A_{1g}X_6^q$ that are saddle-points in the potential surface. Values of X–X bond distance in Å, MCI and PDI in electrons and NICS in ppm.

1t _{2u}	1t _{2u}	1t _{2u}
2t _{1u}	2t _{1u}	2t _{1u}
1e _g	 1e _g	2 a _{1g}
— 2a _{1g}	1t _{2g}	1t _{2g}
1t _{2g}	 2a _{1g}	1e _g
1t _{1u}	1t _{1u}	1t _{1u}
$1a_{1g}$ $^{4}A_{1g}Li_{6}^{+}$	$1a_{1g}$ $^{6}A_{1g}Li_{6}^{+}$	$1a_{1g}$ $^{4}A_{1g}Na_{6}^{+}$
1e _g	1t _{2g}	2t _{1u}
2a _{1g}	2t _{1u}	— 1e _g
2t _{1u}	2 a _{1g}	1t _{2g}
1t _{1u}	— 1e _g	2a _{1g}
1 a _{1g}	1t _{1u}	1t _{1u}
¹ A _{1g} Na ₆ ²⁻	$1a_{1g}$ ⁷ A _{1g} Na ₆ ²⁻	$1a_{1g}$ ⁷ A _{1g} Be ₆ ²⁻¹ A _{1g} Be ₆ ²⁺ ⁵ A _{1g} Be ₆ ² A _{1g} Be ₆ ³⁺ ⁴ A _{1g} Be ₆ ⁻
1t _{2g}	2t _{1u}	1t _{2u}
2t _{1u}	1t _{2g}	2t _{1u}
2a _{1g}	2 a _{1g}	1t _{2g}
1eg	1eg	 2a _{1g}
1t _{1u}	1t _{1u}	—— 1e _g
$1a_{1g}$ $^{1}A_{1g}Mg_{6}^{2}$	$1a_{1g}$ $^{7}A_{1g}Mg_{6}^{2}$	

Figure S1. Energetic order of molecular orbitals for studied $O_h^{2S+1}A_{1g}X_6^q$ clusters that are minima (Table S1).

2t _{1u}	1t _{2u}	2t _{1u}
1eg	2t _{1u}	1t _{2g}
1t _{2g}	— 1e _g	2a _{1g}
 2a _{1g}	2 a _{1g}	 1e _g
1t _{1u}	1t _{2g}	1t _{1u}
$- 1a_{1g}$ $^{3}A_{1g}B_{6}$	$ \begin{array}{c} 1a_{1g} \\ 1A_{1g}B_6^{2+} \\ {}^2A_{1g}B_6^{3+} \\ {}^1A_{1g}B_6^{4+} \end{array} $	$\frac{1a_{1g}}{^{1}A_{1g}Al_{6}^{2-}}$ $^{7}A_{1g}Al_{6}^{2-}$
1t _{2u}	3t _{1u}	1t _{2u}
2t _{1u}	2t _{1u}	2t _{1u}
 2a _{1g}	1t _{2g}	1t _{2g}
1t _{2g}	2a _{1g}	 2a _{1g}
 1e _g	— 1e _g	—— 1e _g
1t _{1u}	1t _{1u}	1t _{1u}
$1a_{1g}$ $^{5}A_{1g}A{l_{6}}^{2+}$	$1a_{1g}$ $1a_{1g}$ $1a_{1g}$	$^{4}A_{1g}Si_{6}^{+}$

Figure S2. CMO-NICS for Na_6^{2-} , Be_6^{2+} [a], Mg_6^{2-} , Mg_6 , B_6^{2+} , B_6^{4+} , Al_6^{2-} and Si_6^{2-} [a] in the ${}^{1}A_{1g}$ electronic state	9.
Contributions of the core molecular orbitals are not included.	



^[a] CMO-NICS for Si₆²⁻and Be₆²⁺ were computed using 6-311++G and aug-cc-pVQZ basis sets, respectively, due to technical problems experienced by the NBO 6.0 program when the 6-311++G(3df,3pd) basis set is used. Si₆²⁻ (NICS(0)₃=-10.2 and NICS(0)₆=14.6) – Be₆²⁺ (NICS(0)₃=-37.1 and NICS(0)₆=-50.3).