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SUPPLEMENTARY INFORMATION

A plier-shaped binary molecular wheel $B_7Mg_4^+$ cluster: hybrid in-plane heptacoordination, double π/σ aromaticity, and electronic transmutation

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Table S1. Cartesian coordinates for the top 5 lowest-energy structures of $B_7Mg_4^+$ cluster at the PBE0/6-311+G* level.

Figure S1. Alternative optimized low-lying structures of $B_7Mg_4^+$ cluster. Relative energies at the PBE0/6-311+G* level are shown without brackets, including corrections for the zero-point energies (ZPEs). Also shown are relative energies for top low-lying isomers at the single-point CCSD(T)/6-311+G* (in brackets) and B3LYP/6-311+G* (in square brackets) levels. All energies are in eV.

Figure S2. Calculated $NICS_{zz}$ data for $B_7Mg_4^+$cluster at the PBE0/6-311+G*level. These values are calculated at the center of a B_3 triangle, as well as of a rhombic unit between a B_3 triangle and the midpoint of two vertical Mg atoms, which are associated to σ aromaticity. Other values are calculated at a distance of 1.0, 1.5, and 2.0 Å above or below the plane, which probe π aromaticity.

Figure S3. The iso-chemical shielding surfaces (ICSSs) of B_7Mg^+ cluster, calculated at the boron plane, as well as at a distance of 0.5, 1.0, and 1.5 Å above the plane, respectively. A positive ICSS value indicates π or σ aromaticity; and vice versa.

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(a) GM, $B_7Mg_4^+$ (C_s, $^1A'$)

B	-1.44375200	1.60305300	0.76907200
B	-0.30314300	1.09670100	1.71952700
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B	-0.30314300	1.09670100	-1.71952700
B	-0.03066600	0.83612600	0.00000000
B	0.87583200	0.12057100	1.43694200
B	0.87583200	0.12057100	-1.43694200
Mg	-1.44375200	-0.96698000	1.41234400
Mg	2.50150800	0.86356200	0.00000000
Mg	-1.44375200	-0.96698000	-1.41234400
Mg	1.12466000	-1.62825800	0.00000000

(b) LM, $B_7Mg_4^+$ (D_2, ^1A)

B	0.04142600	1.40399000	0.80764300
B	-0.04142600	1.40399000	-0.80764300
B	0.00000000	0.00000000	-1.62073900
B	0.04142600	-1.40399000	-0.80764300
B	-0.04142600	-1.40399000	0.80764300
B	0.00000000	0.00000000	1.62073900
B	0.00000000	0.00000000	0.00000000
Mg	2.37745600	-0.93313500	1.01522900
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Mg	-2.37745600	0.93313500	1.01522900
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(c) Structure 3, $B_7Mg_4^+$ (C_s, $^1A'$)

B	-0.92077800	0.14198300	0.00000000
B	-0.51193400	1.17170600	-1.46980800
B	-0.51193400	1.17170600	1.46980800
B	-1.63918800	-1.34563600	0.76843200
B	-1.63918800	-1.34563600	-0.76843200
B	-1.09322000	-0.23975000	1.73253300
B	-1.09322000	-0.23975000	-1.73253300
Mg	-0.14950500	2.74878100	0.00000000
Mg	1.40400200	-0.01798700	-1.49136400
Mg	0.42877700	-2.42723400	0.00000000
Mg	1.40400200	-0.01798700	1.49136400

(d) Structure 4, $B_7Mg_4^+$ (C_s, $^1A'$)

B	-0.09103100	-1.44154900	0.79867300
B	1.34033600	-1.11430000	1.57929700
B	1.34033600	-1.11430000	-1.57929700
B	0.03724300	-0.58980800	-2.21680700
B	1.50464300	-1.36716200	0.00000000
B	-0.09103100	-1.44154900	-0.79867300
B	0.03724300	-0.58980800	2.21680700
Mg	-1.95640200	0.24832600	1.41245500
Mg	1.10687300	1.34719000	-1.41119100

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Mg	1.10687300	1.34719000	1.41119100

(e) Structure 5, $B_7Mg_4^+$ (C_1, ^{1}A)

B	-0.33216500	0.87665700	-1.24808800
B	-1.11766300	1.59121900	-0.06736100
B	-1.22035200	1.06244700	1.37799400
B	0.52150300	-1.16002900	1.47871200
B	0.07034700	0.24166800	0.46958200
B	-0.57892200	-0.21409500	2.02298000
B	1.02877200	0.07678000	-1.12942700
Mg	-0.28095700	-1.89170000	-0.86610500
Mg	2.32241400	-1.07980900	0.23800900
Mg	-2.52916400	-0.34537700	-0.27503000
Mg	1.16624100	2.28578400	-0.30703800

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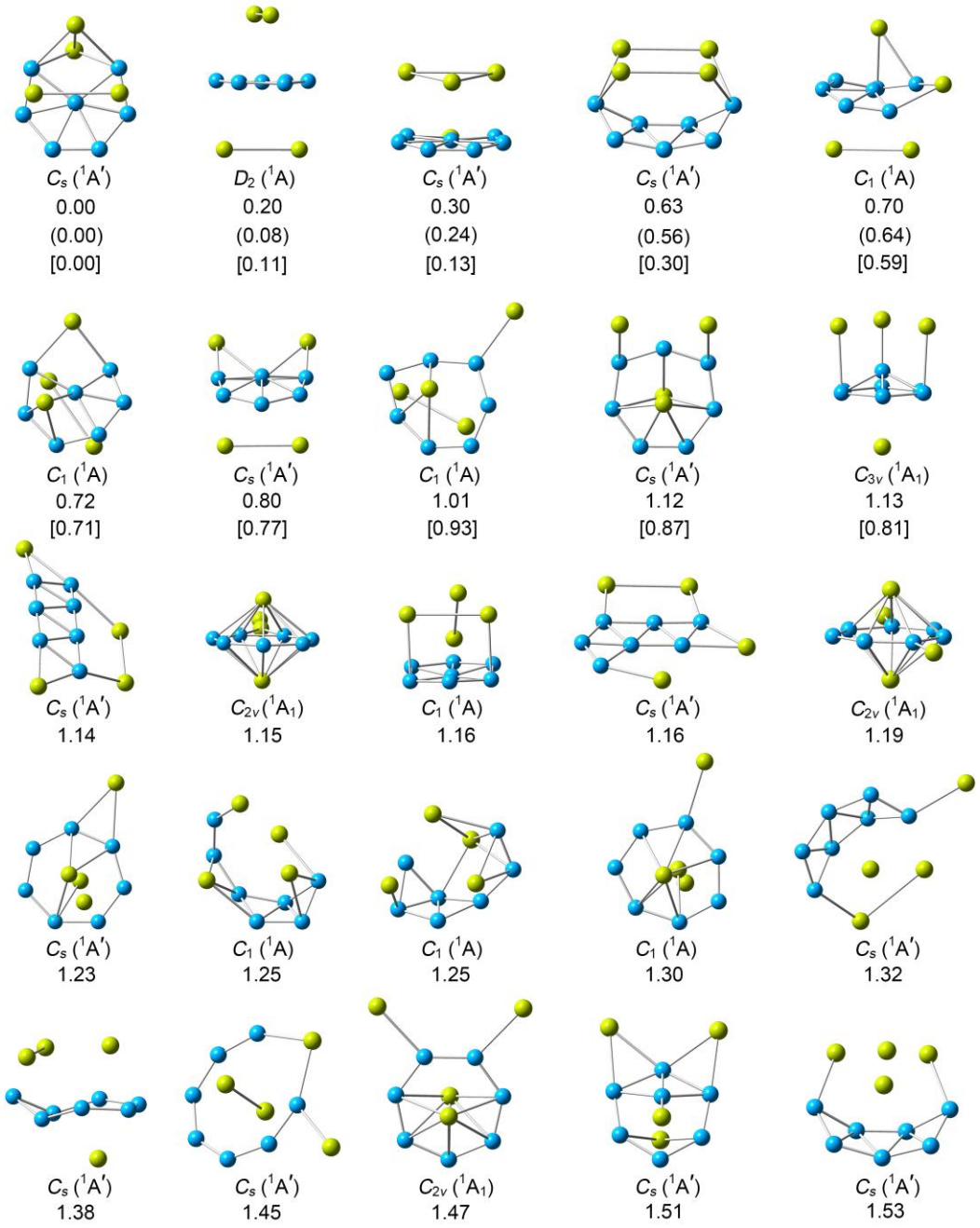

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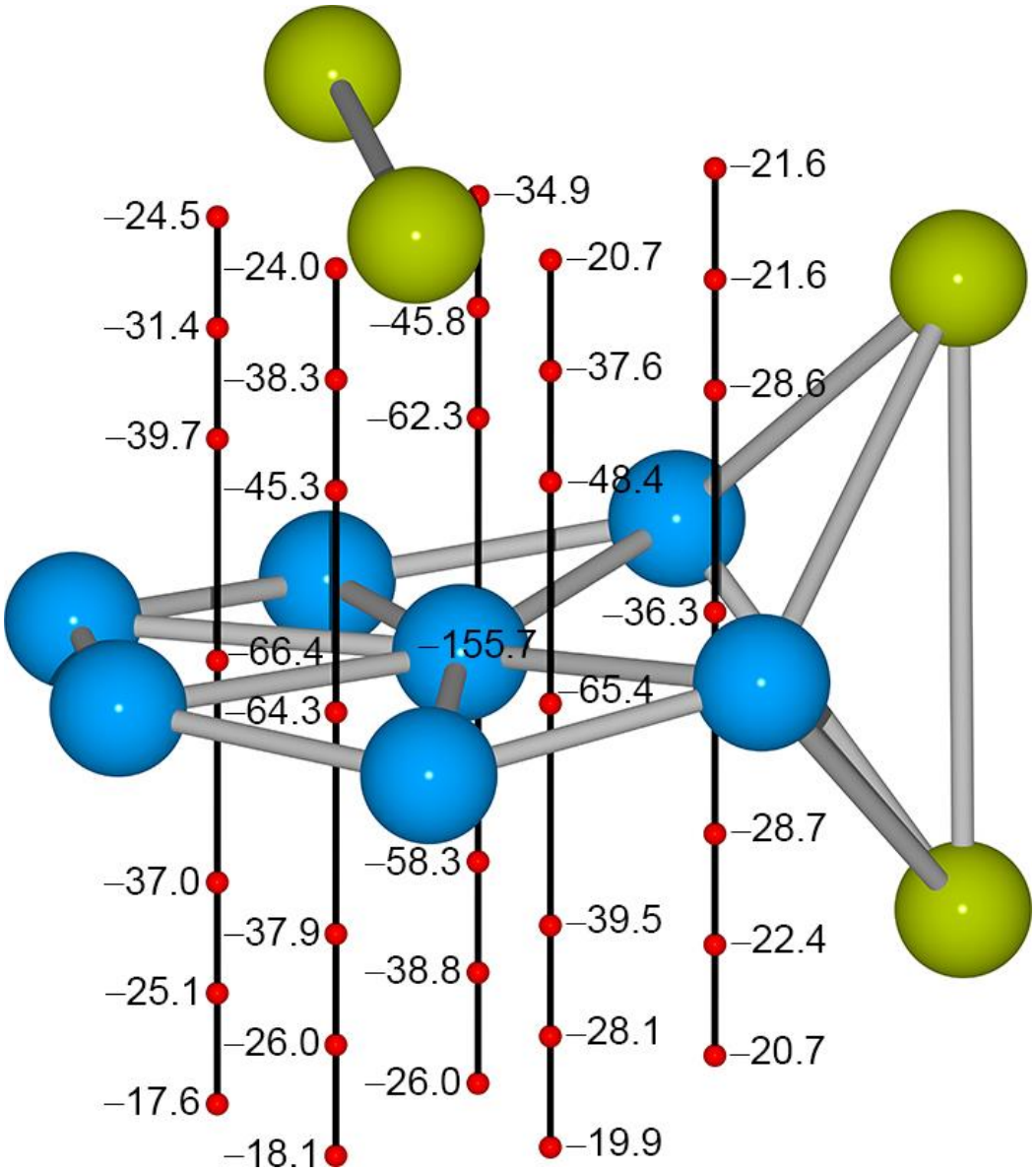

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