Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting information

Structural and electronic properties in MB_{22}^- (M=Na, K) clusters: Tubular boron versus quasi-planar boron forms

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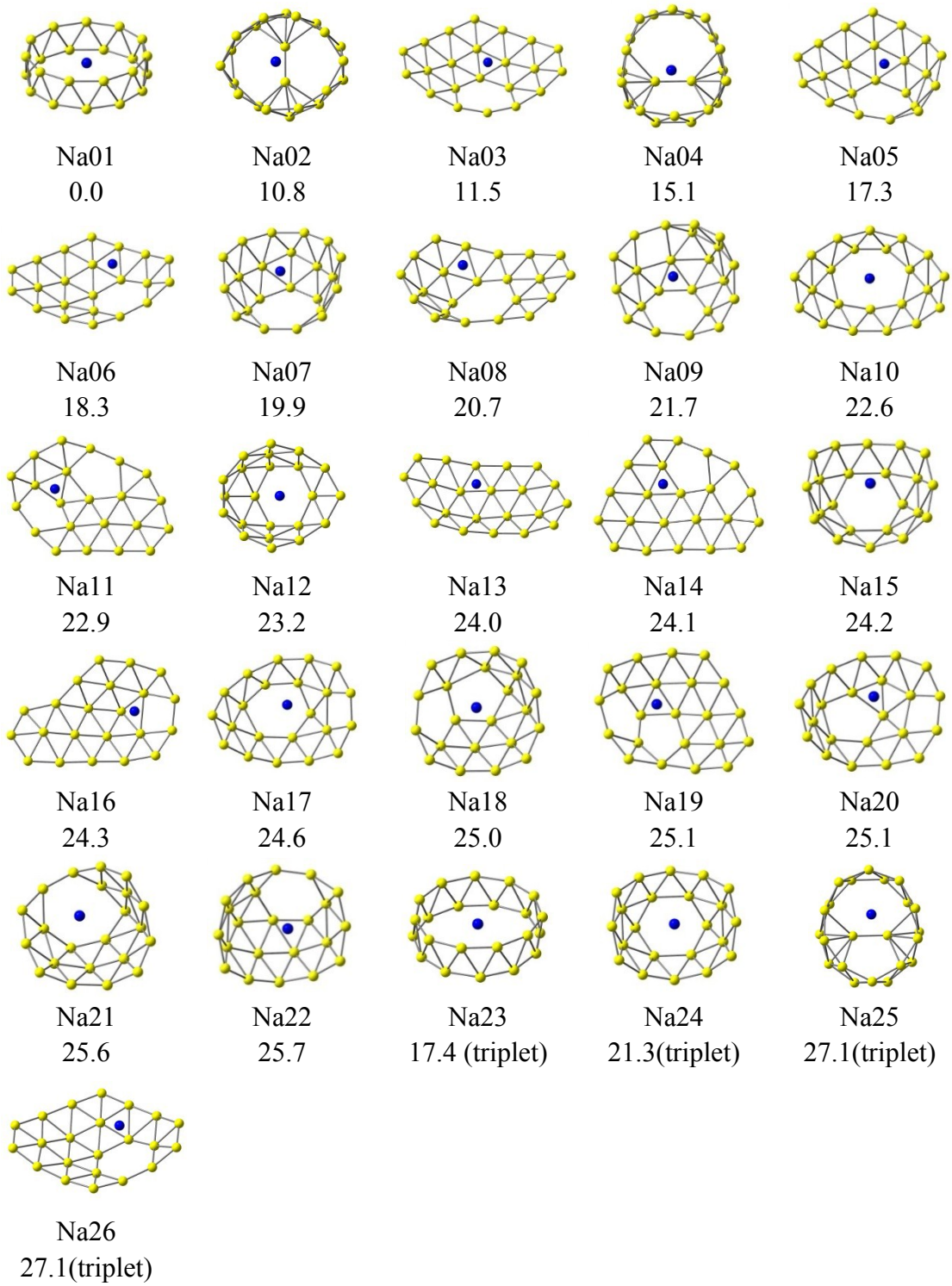
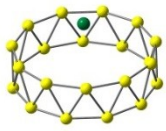


Figure S1. Structures and relative energies in kcal/mol of the low-lying isomers of NaB_{22}^- obtained at the PBE0/6-311+G(d) level. All isomers are in singlet state unless otherwise indicated. All energies are corrected for zero-point energies (ZPE).



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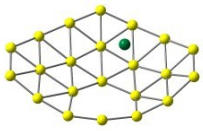

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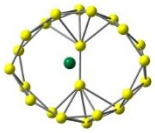

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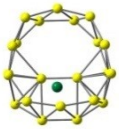

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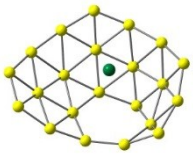

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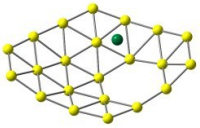

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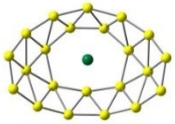

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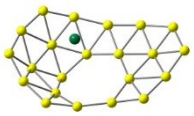

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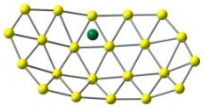

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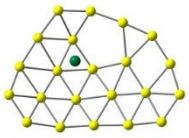

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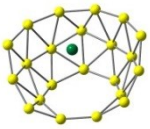

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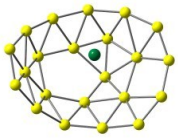

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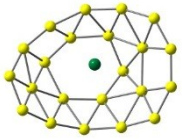

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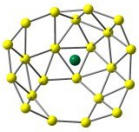

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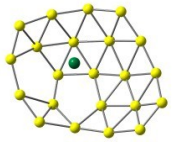

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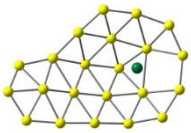

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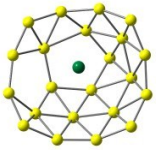

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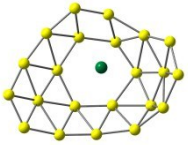

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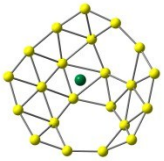

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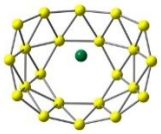

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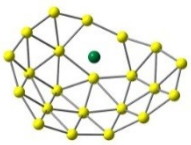

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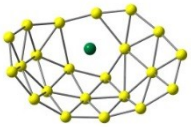

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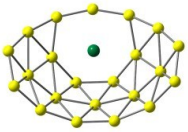

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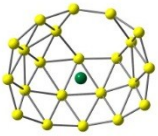

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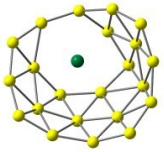

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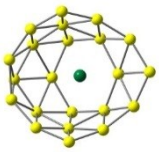

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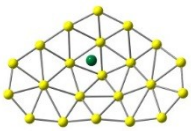

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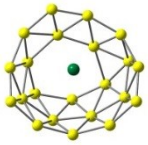

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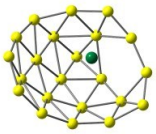

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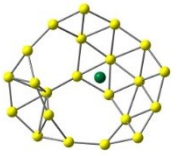

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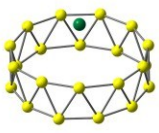

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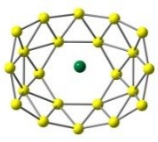

K32(triplet)
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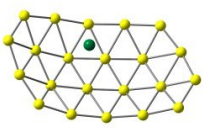

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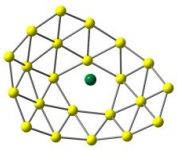

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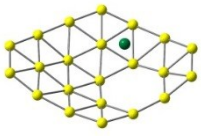

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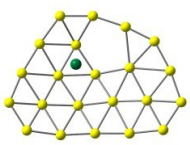

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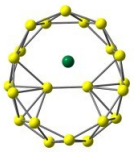


K37 (triplet)
26.2

Figure S2. Structures and relative energies in kcal/mol of the low-lying isomers of KB_{22}^- obtained at the PBE0/6-311+G(d) level. All isomers are in singlet state unless otherwise indicated. All energies are corrected for zero-point energies (ZPE).

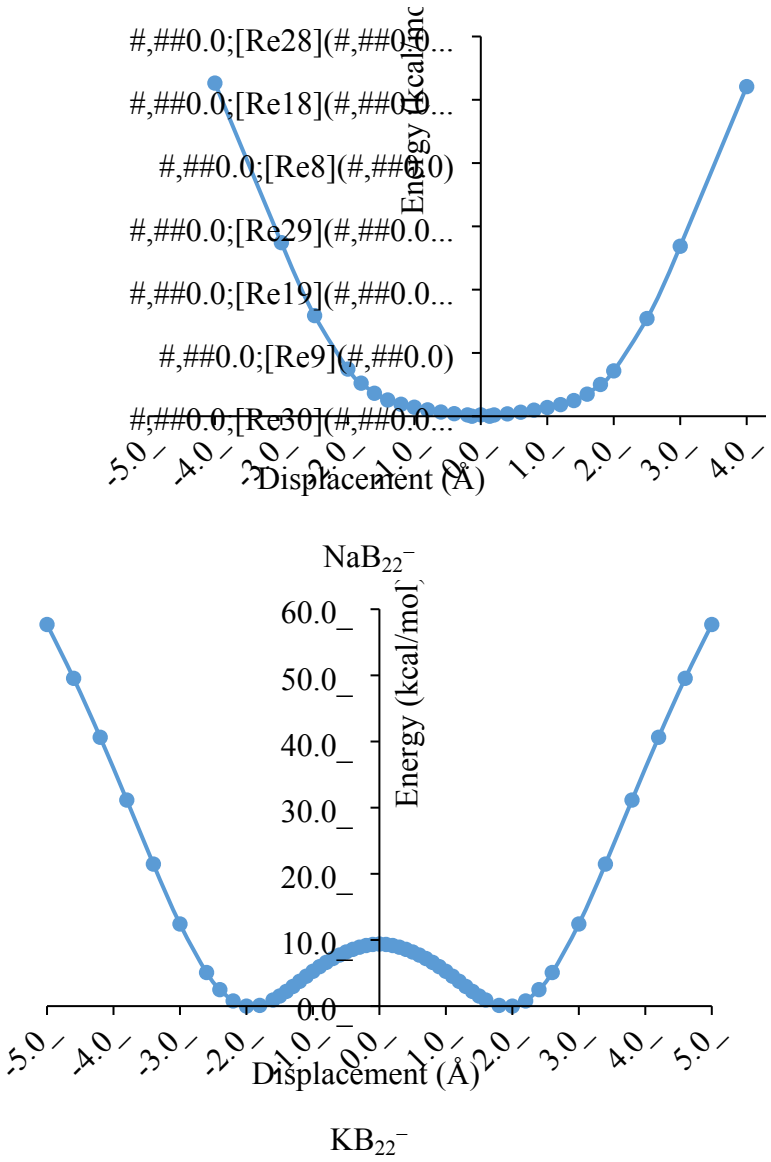
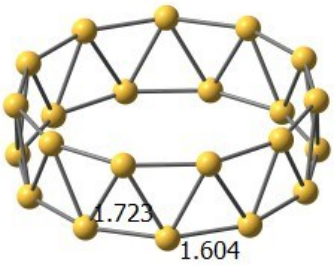
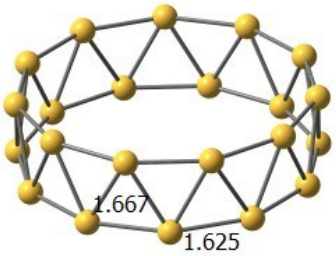


Figure S3. Relative energy in kcal/mol as a function of the displacement of M (M=Na, K) along the C_{11} axis.



B_{22}^{2+}



B_{22}^{2-}

Figure S4. Structure and selected bond distances of B_{22}^{2+} and B_{22}^{2-} clusters computed at the PBE0/6-311+G(d) level.

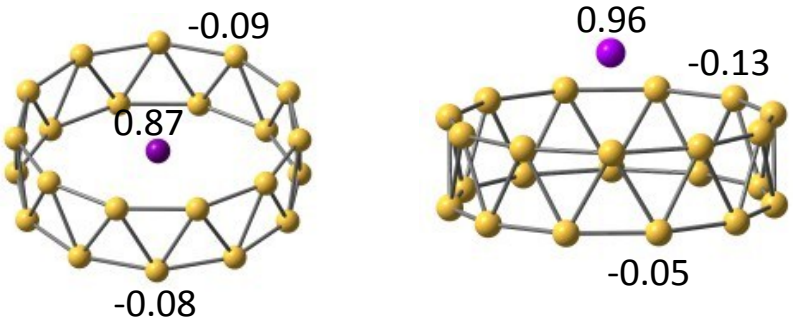


Figure S5. NPA charges of NaB_{22}^- (left) and KB_{22}^- (right) species computed at the PBE0/6-311+G(d) level.

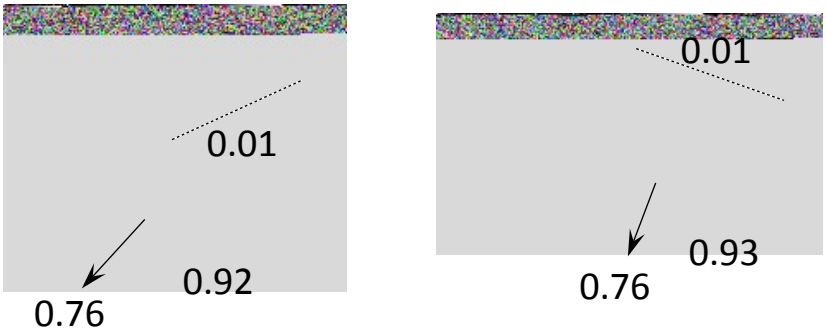
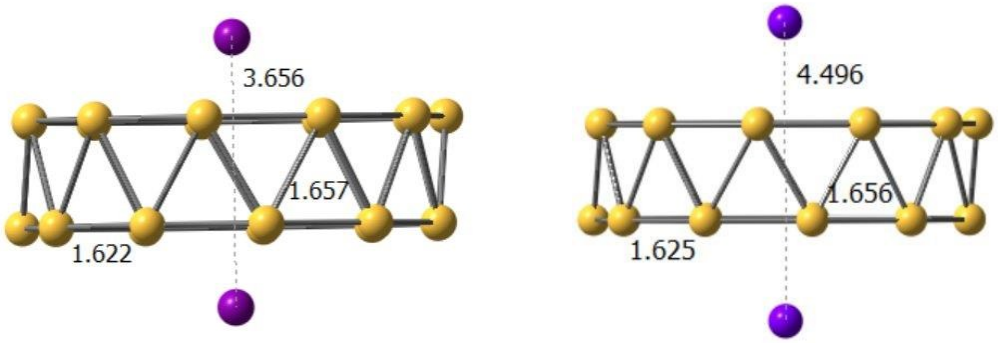
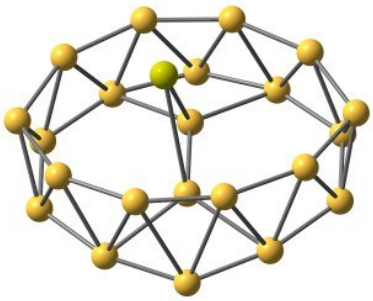


Figure S6. Wiberg bond index values of NaB_{22}^- (left) and KB_{22}^- (right) species computed at the PBE0/6-311+G(d) level.



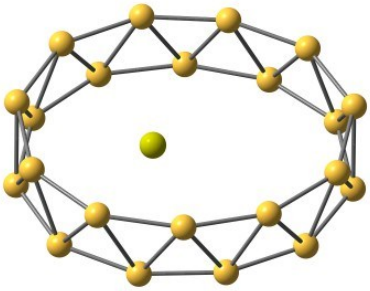
Na_2B_{22} K_2B_{22}

Figure S7. Structure and selected bond distances of Na_2B_{22} and K_2B_{22} clusters computed at the PBE0/6-311+G(d) level.



0.0 kcal/mol

Mg01



12.2 kcal/mol

Mg02

MgB_{22}

Figure S8. The structures and relative energy of MgB_{22} at the PBE0/6-311+G(d) level.

Table S1. Coordinates of tubular structures

NaB_{22}^-

B	1.890173000	-2.181376000	-0.711900000
B	2.886686000	0.000000000	0.735038000
B	-2.886374000	0.000000000	-0.711900000
B	-1.890377000	2.181611000	0.735038000
B	2.428434000	-1.560660000	0.735038000
B	2.769456000	-0.813186000	-0.711900000
B	-2.769755000	0.813273000	0.735038000
B	-2.428172000	1.560492000	-0.711900000
B	-1.199043000	-2.625538000	-0.711900000
B	1.199173000	2.625822000	0.735038000
B	0.410774000	-2.856995000	-0.711900000
B	2.428434000	1.560660000	0.735038000
B	-2.428172000	-1.560492000	-0.711900000
B	-0.410818000	2.857303000	0.735038000
B	1.890173000	2.181376000	-0.711900000
B	-0.410818000	-2.857303000	0.735038000
B	0.410774000	2.856995000	-0.711900000
B	-1.890377000	-2.181611000	0.735038000
B	2.769456000	0.813186000	-0.711900000
B	1.199173000	-2.625822000	0.735038000
B	-1.199043000	2.625538000	-0.711900000
B	-2.769755000	-0.813273000	0.735038000
Na	0.000000000	0.000000000	-0.121880000

KB_{22}^-

B	-2.767904000	0.812730000	-0.453474000
B	-1.889114000	2.180154000	-0.453474000
B	-0.410544000	2.855394000	-0.453474000
B	1.198371000	2.624067000	-0.453474000
B	2.426812000	1.559617000	-0.453474000
B	2.884757000	0.000000000	-0.453474000
B	2.426812000	-1.559617000	-0.453474000
B	1.198371000	-2.624067000	-0.453474000
B	-0.410544000	-2.855394000	-0.453474000
B	-1.889114000	-2.180154000	-0.453474000
B	-2.767904000	-0.812730000	-0.453474000
B	-2.888285000	0.000000000	0.989918000
B	-2.429780000	-1.561525000	0.989918000
B	-1.199837000	-2.627276000	0.989918000

B	0.411046000	-2.858886000	0.989918000
B	1.891424000	-2.182820000	0.989918000
B	2.771289000	-0.813724000	0.989918000
B	2.771289000	0.813724000	0.989918000
B	1.891424000	2.182820000	0.989918000
B	0.411046000	2.858886000	0.989918000
B	-1.199837000	2.627276000	0.989918000
B	-2.429780000	1.561525000	0.989918000
K	0.000000000	0.000000000	-1.667313000