

Supporting Information for
Structures, Electronic and Spectral Properties of Doped Boron
Clusters $\text{MB}_{12}^{0/-}$ (M=Li, Na, and K)

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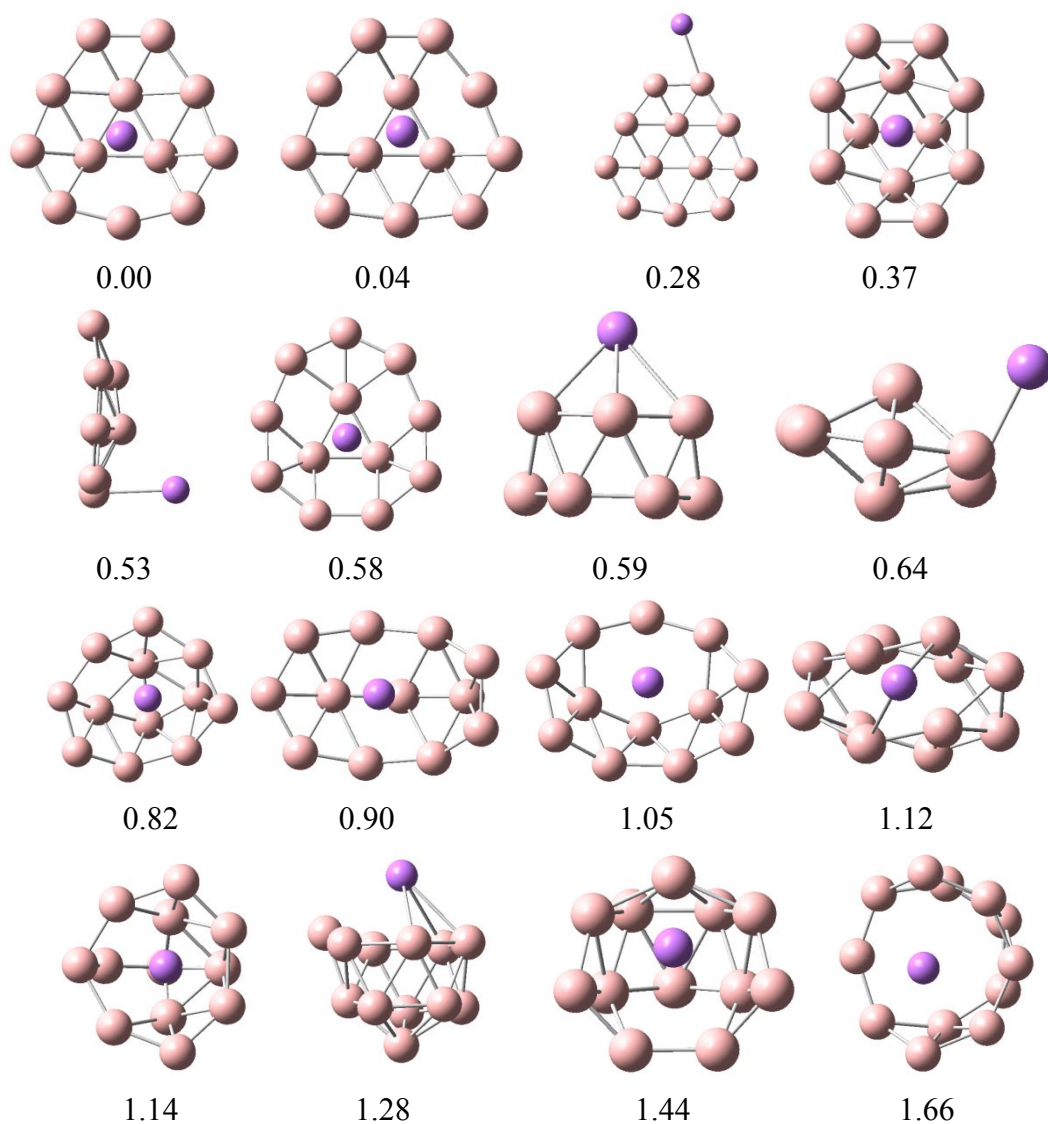


Figure S1. Low-lying isomers of LiB_{12} , with their relative energies indicated in eV at PBE0/def2-TZVP level.

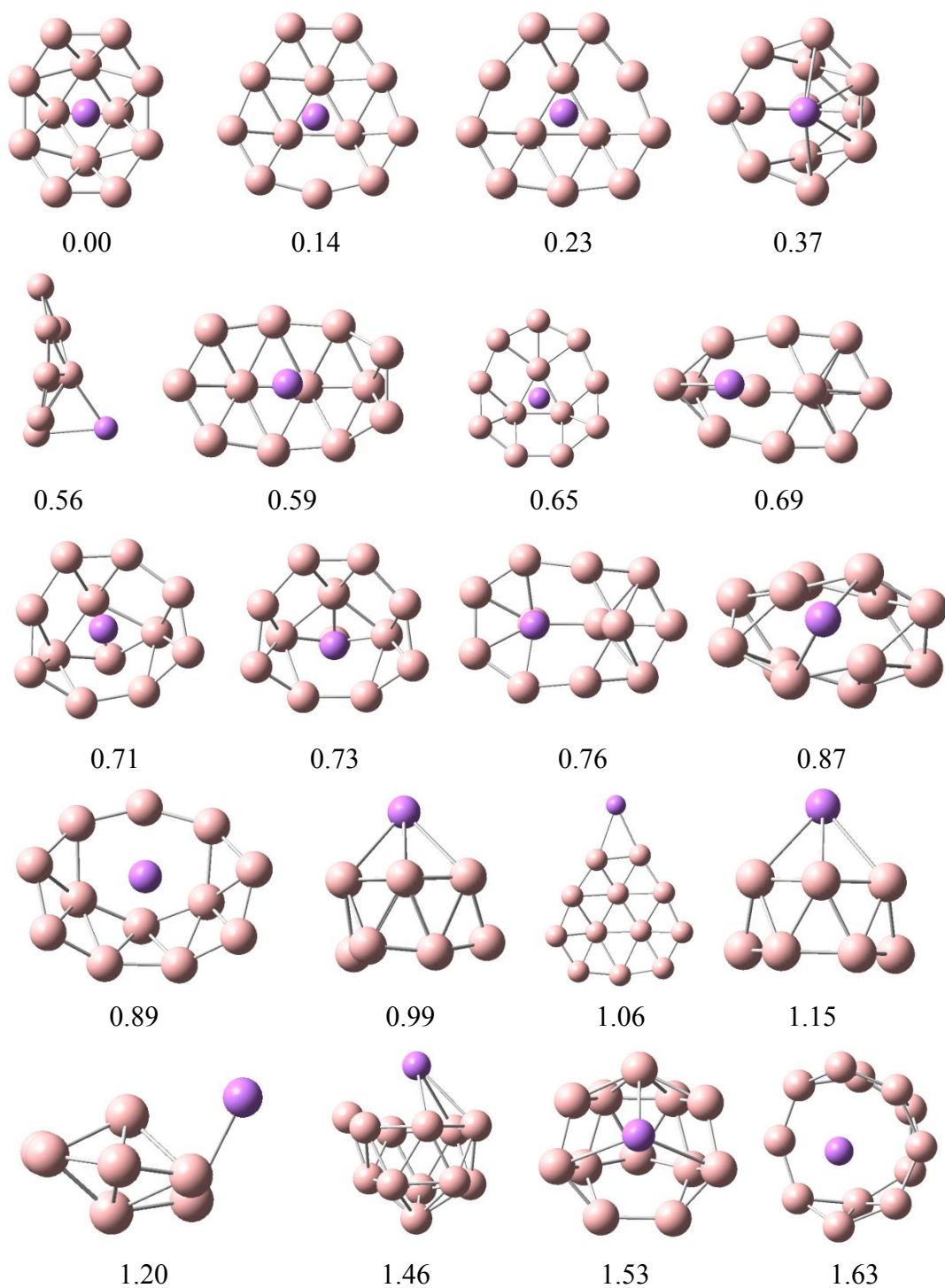


Figure S2. Low-lying isomers of LiB_{12}^- , with their relative energies indicated in eV at PBE0/def2-TZVP level.

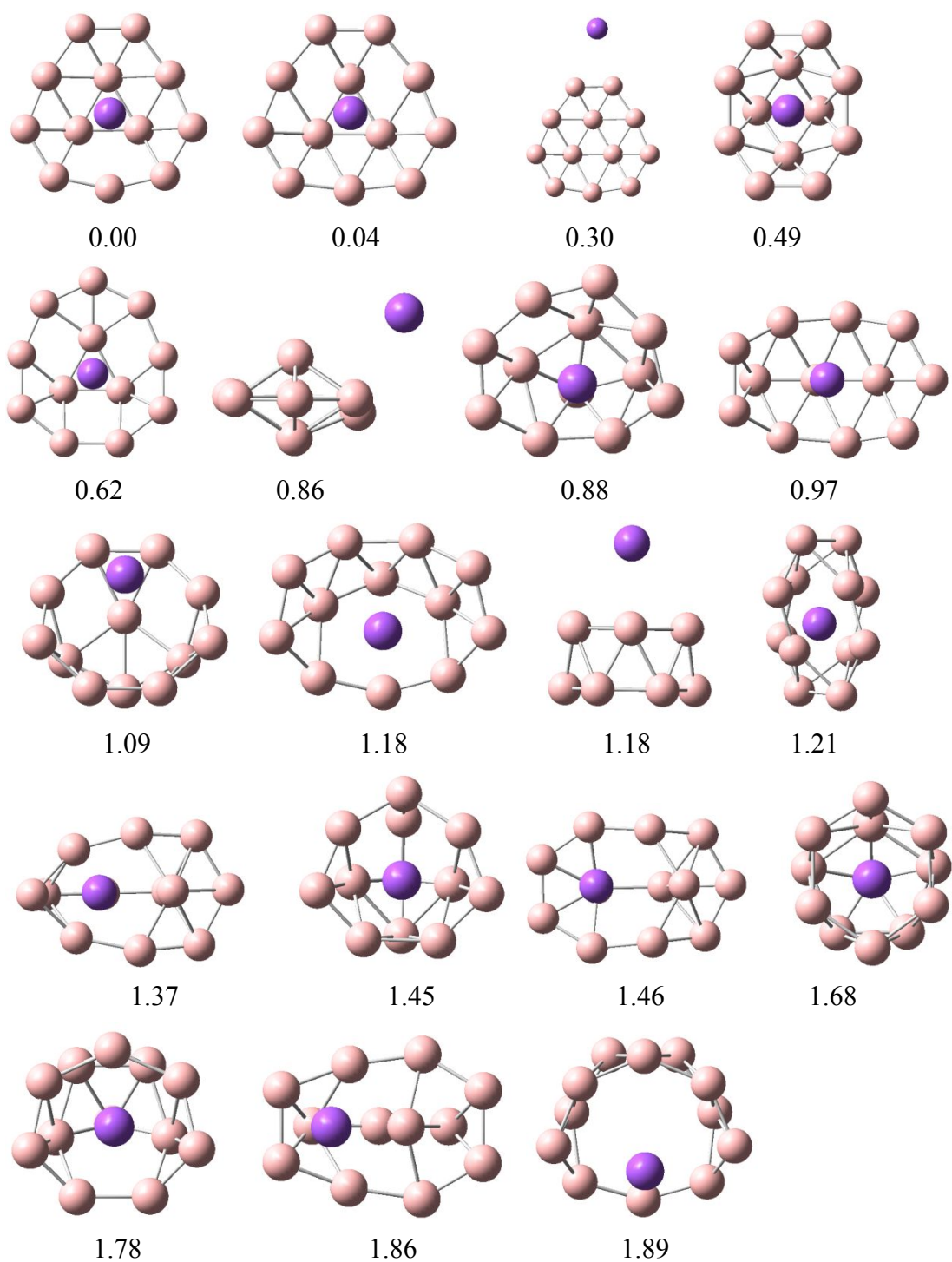


Figure S3. Low-lying isomers of NaB_{12} , with their relative energies indicated in eV at PBE0/def2-TZVP level.

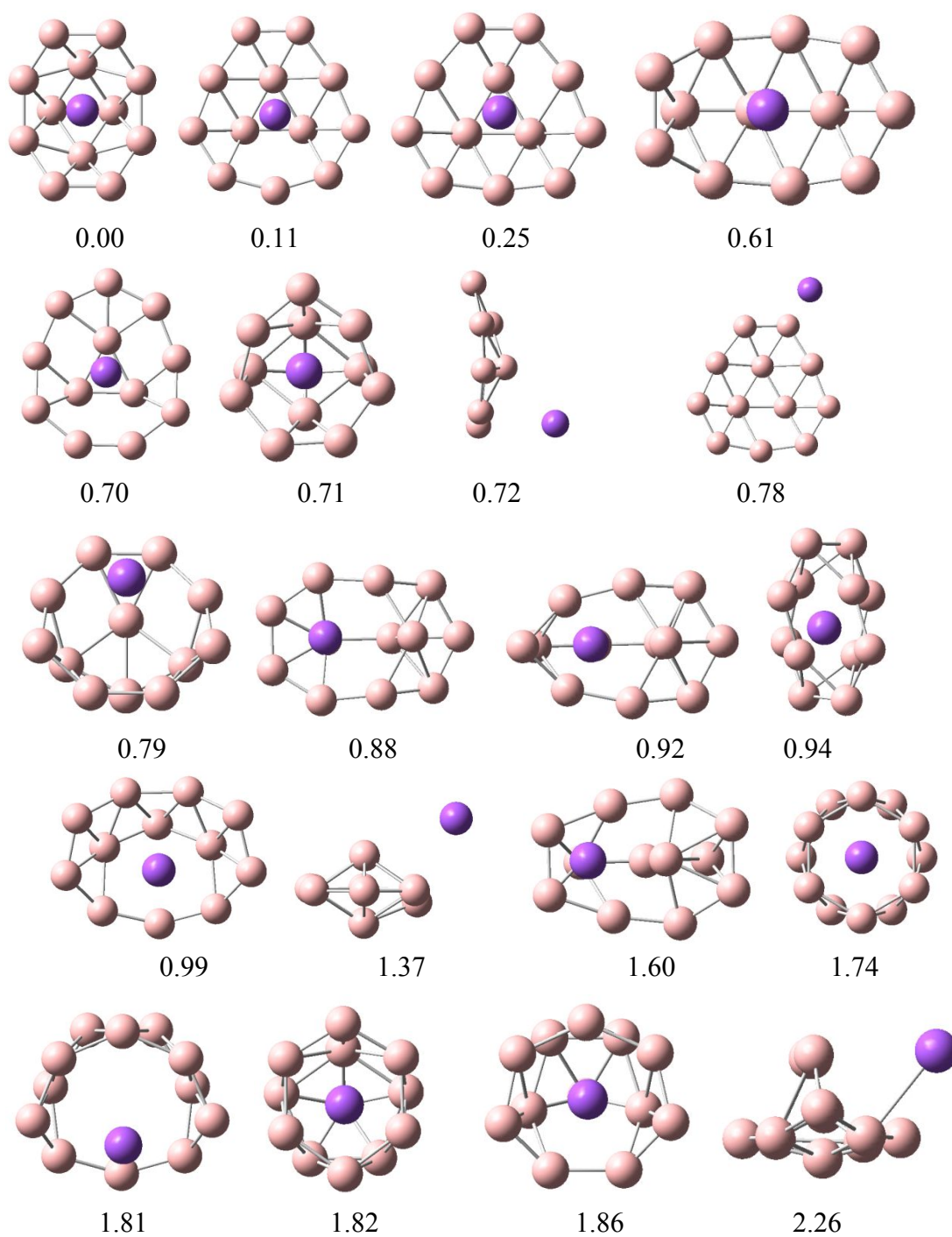


Figure S4. Low-lying isomers of NaB_{12}^- , with their relative energies indicated in eV at PBE0/def2-TZVP level.

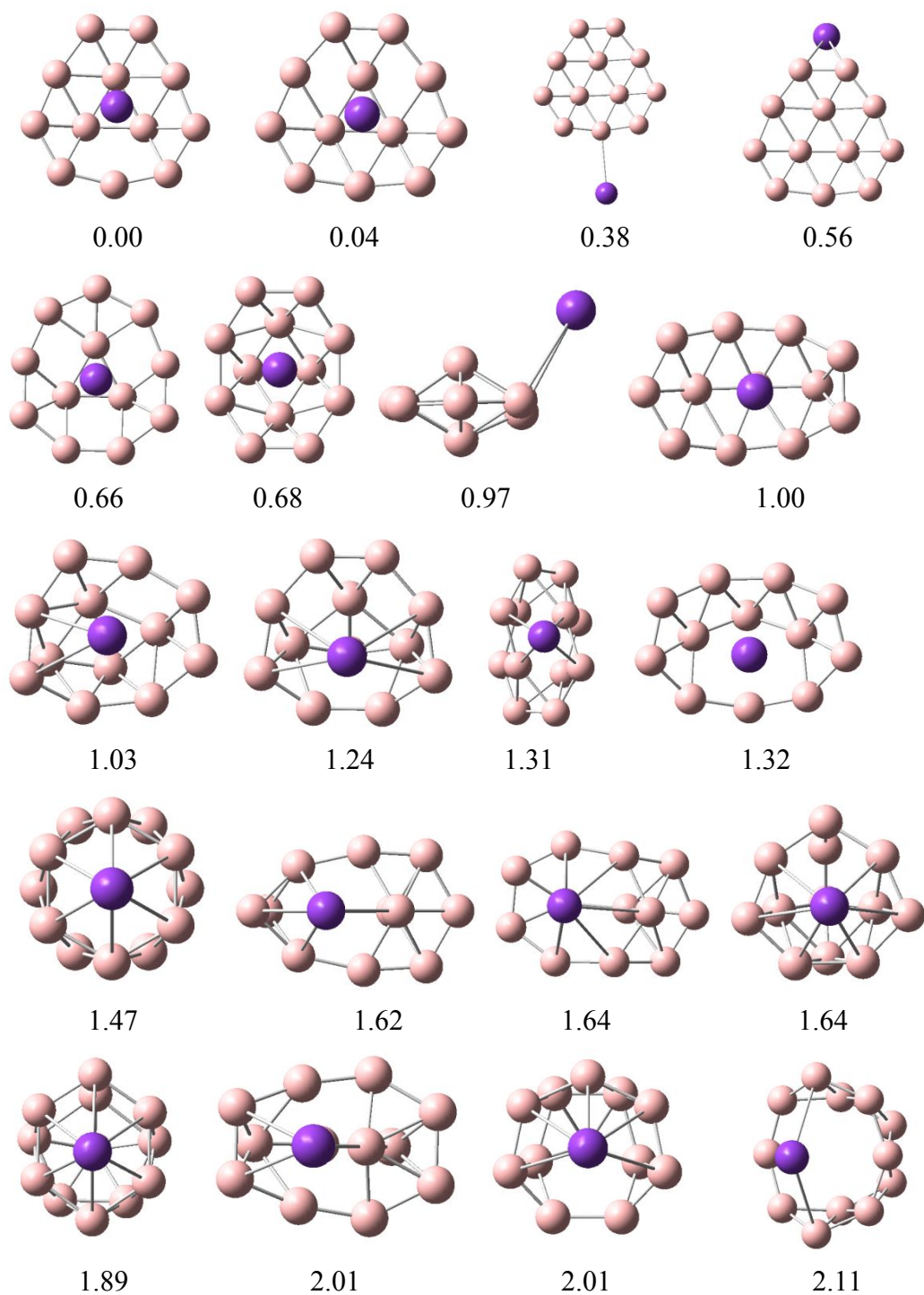


Figure S5. Low-lying isomers of KB_{12} , with their relative energies indicated in eV at PBE0/def2-TZVP level.

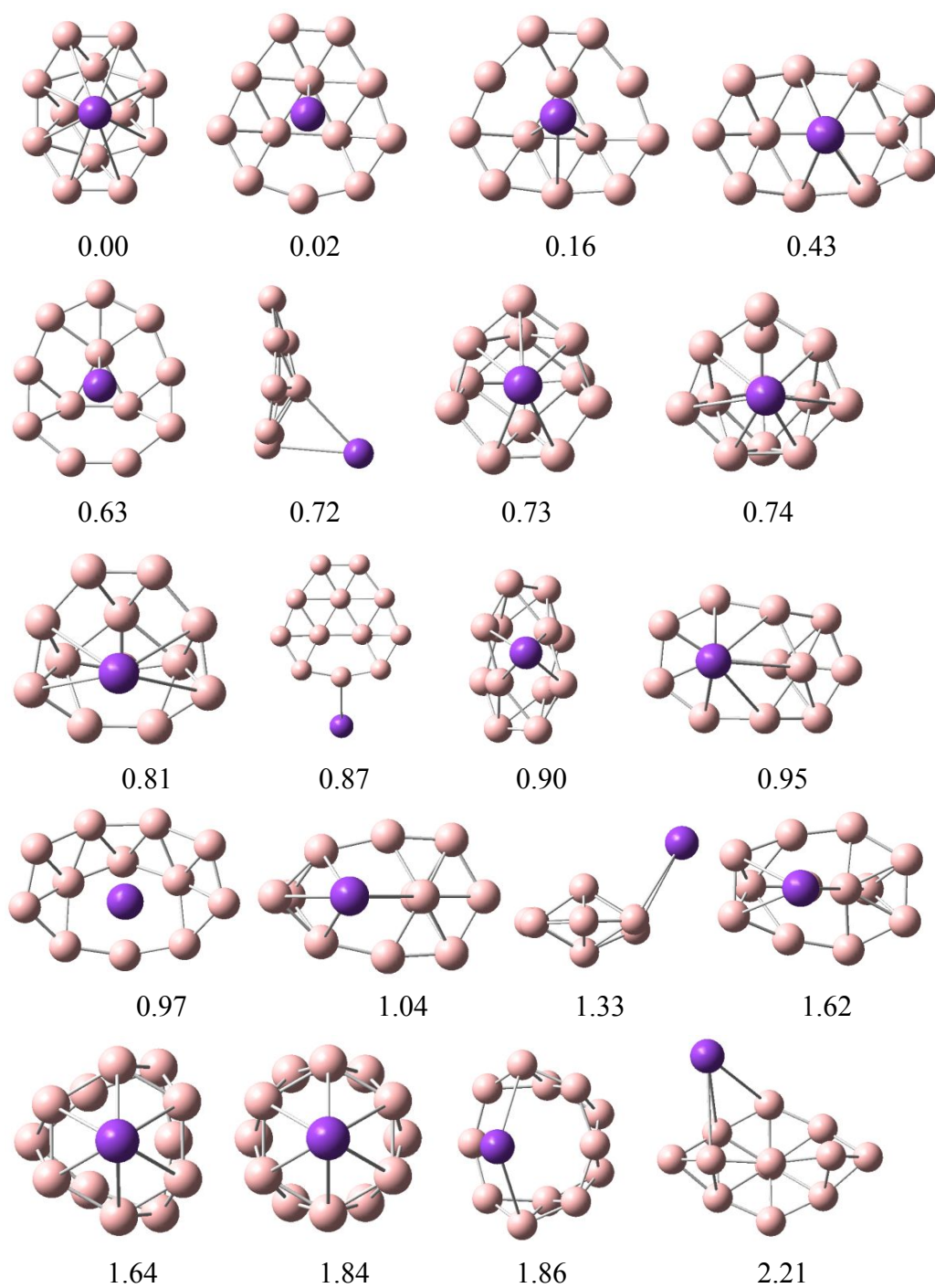


Figure S6. Low-lying isomers of KB_{12}^- , with their relative energies indicated in eV at PBE0/def2-TZVP level.

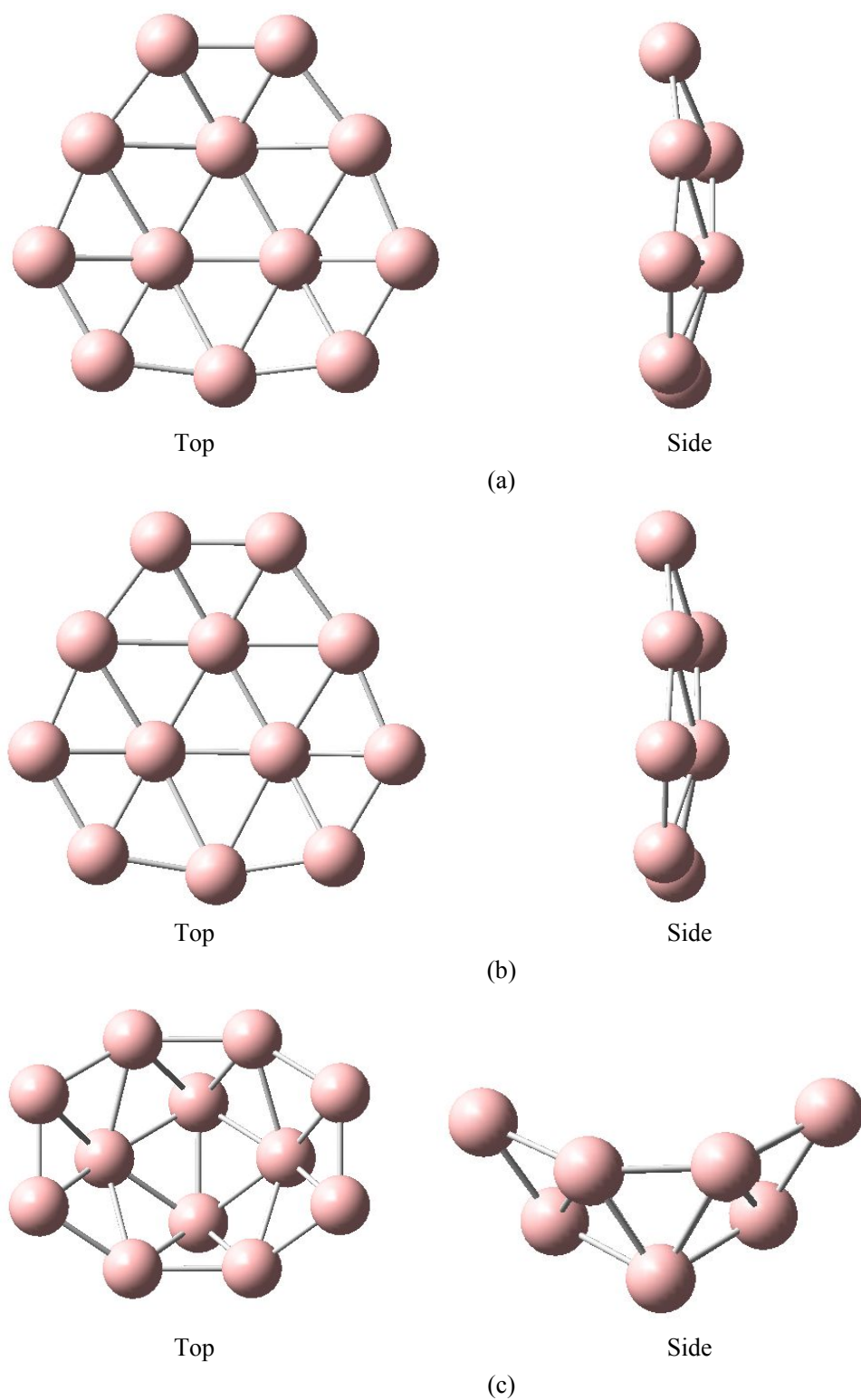
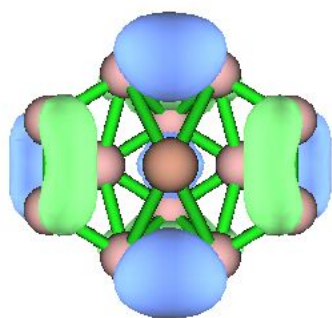
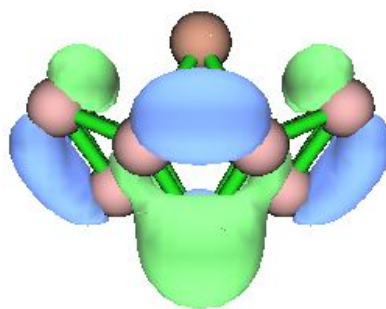


Figure S7. Structures of boron clusters $B_{12}^{0/-}$. (a) $C_{3v} B_{12}$, (b) $C_s B_{12}^-$, (c) $C_{2v} B_{12}^{0/-}$.

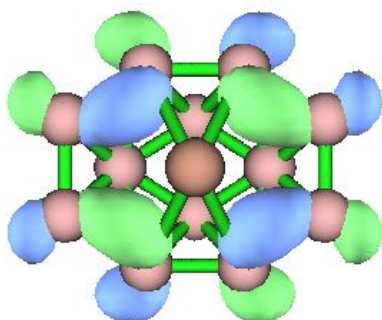


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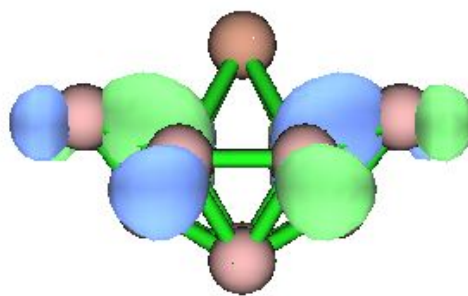


Side

(a) C_{2v} LiB_{12}^- HOMO (-1.39 eV)

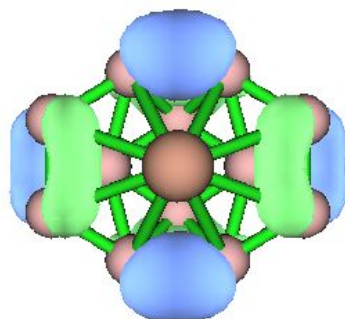


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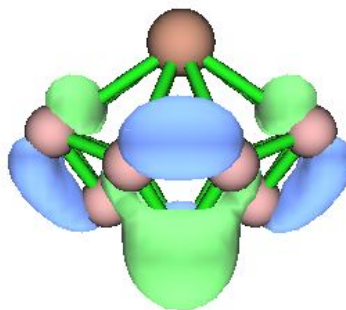


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(b) C_{2v} LiB_{12}^- LUMO (2.02 eV)

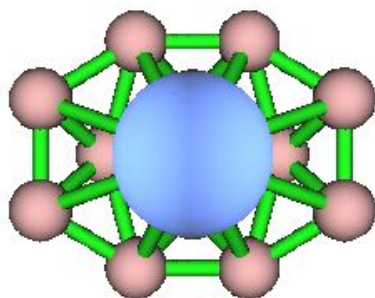


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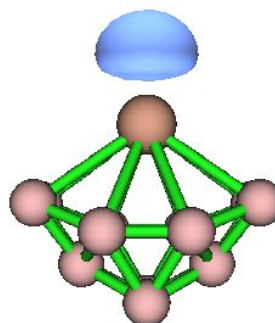


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(c) C_{2v} NaB_{12}^- HOMO (-1.23eV)



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Side

(d) C_{2v} NaB_{12}^- LUMO (2.00eV)

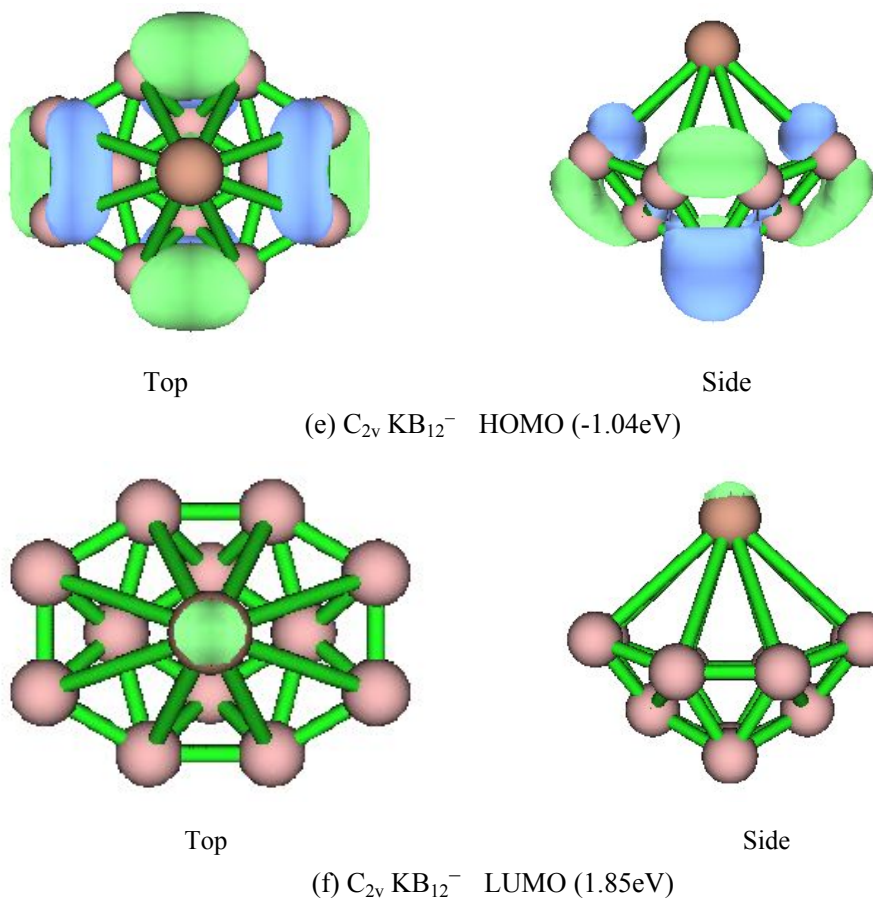
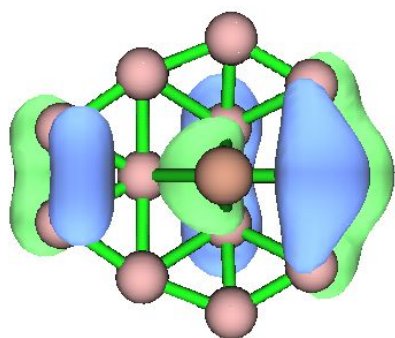
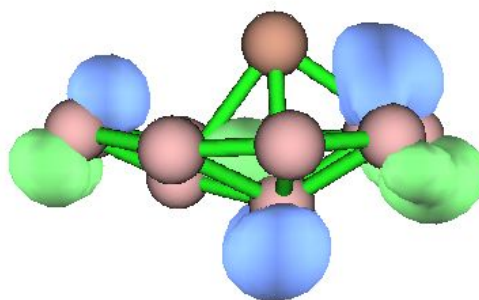


Figure S8. Frontline molecular orbital diagrams and energy levels of $C_{2v} MB_{12}^-$ (M=Li, Na, and K) calculated by the PBE0/def2-TZVP level.

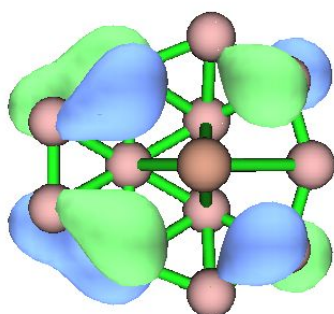


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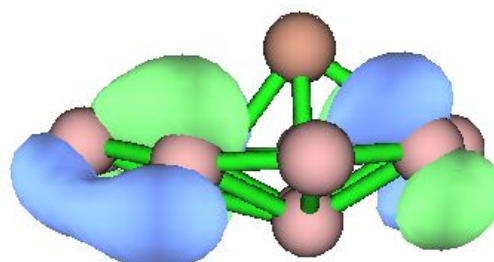


Side

(a) C_s LiB₁₂⁻ HOMO (-1.04 eV)

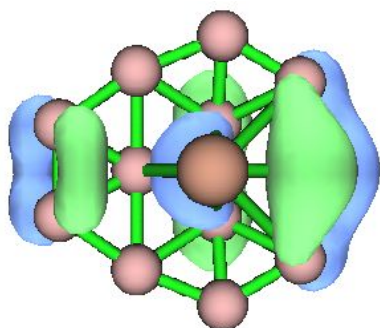


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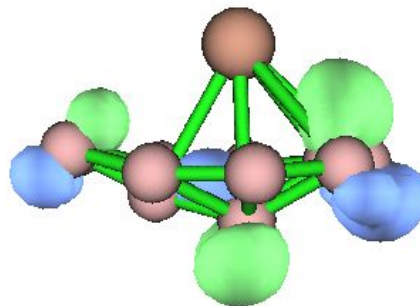


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(b) C_s LiB₁₂⁻ LUMO (1.05 eV)

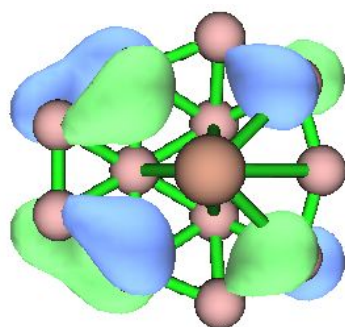


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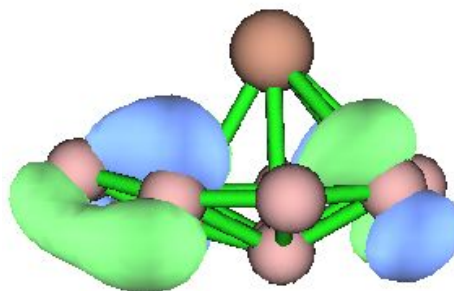


Side

(c) C_s NaB₁₂⁻ HOMO [-0.81 eV]



Top



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(d) C_s NaB₁₂⁻ LUMO [1.22eV]

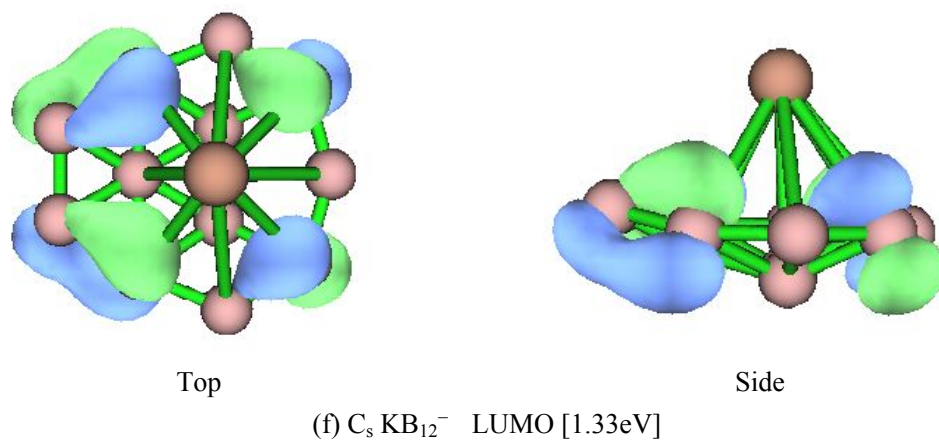
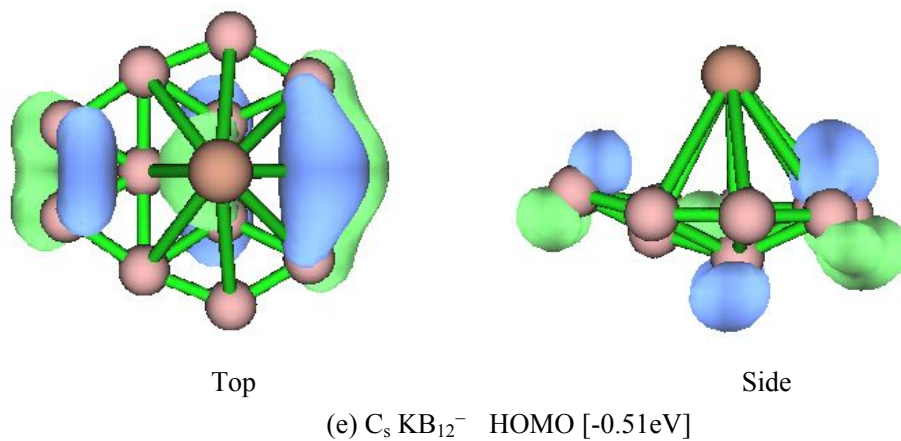


Figure S9. Frontline molecular orbital diagrams and energy levels of $C_s MB_{12}^-$ (M=Li, Na, and K) calculated by the PBE0/def2- TZVP level.