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Electronic Supplementary Information

Electronic structure, stability, and aromaticity of M_2B_6 (M = Mg, Ca, Sr, and Ba). An interplay between spin pairing and electron delocalization

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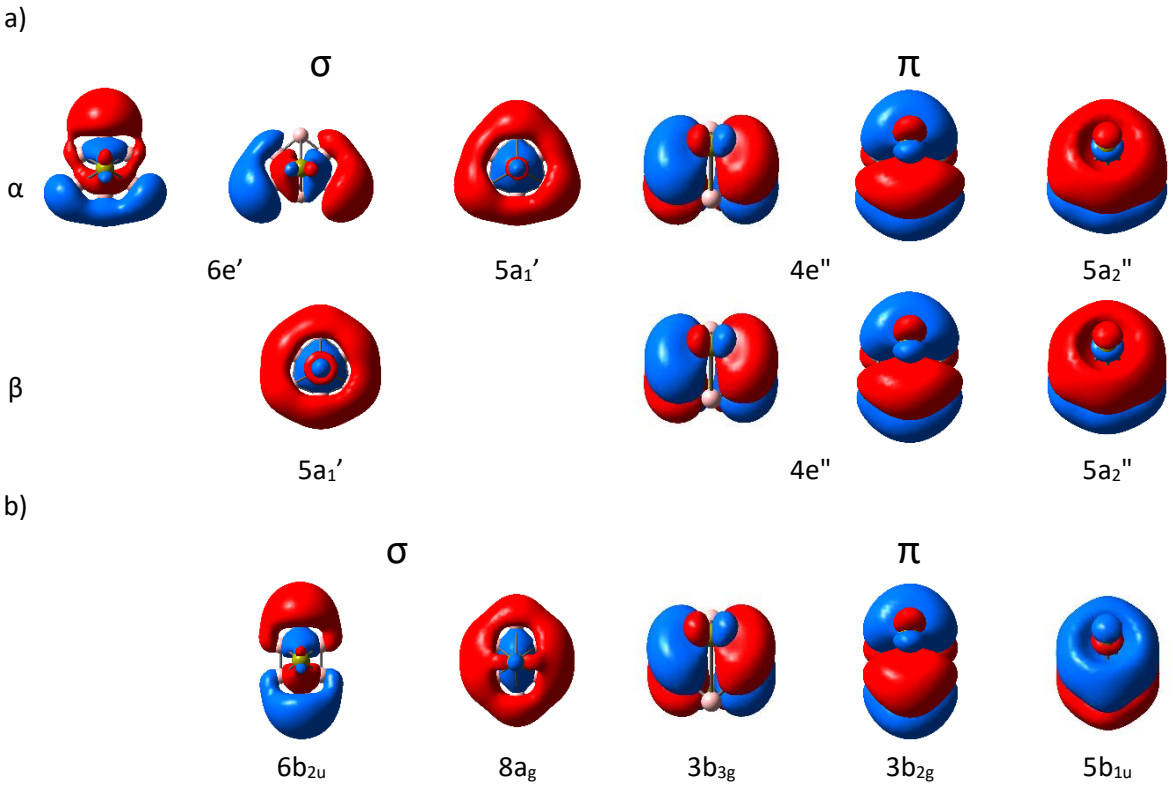

Figure S1. a) σ and π occupied canonical molecular spin (α and β) orbitals for T-Ca_2B_6 obtained at the UB3LYP/def2-TZVP level; b) σ and π occupied canonical molecular orbitals for S-Ca_2B_6 obtained at the RB3LYP/def2-TZVP.

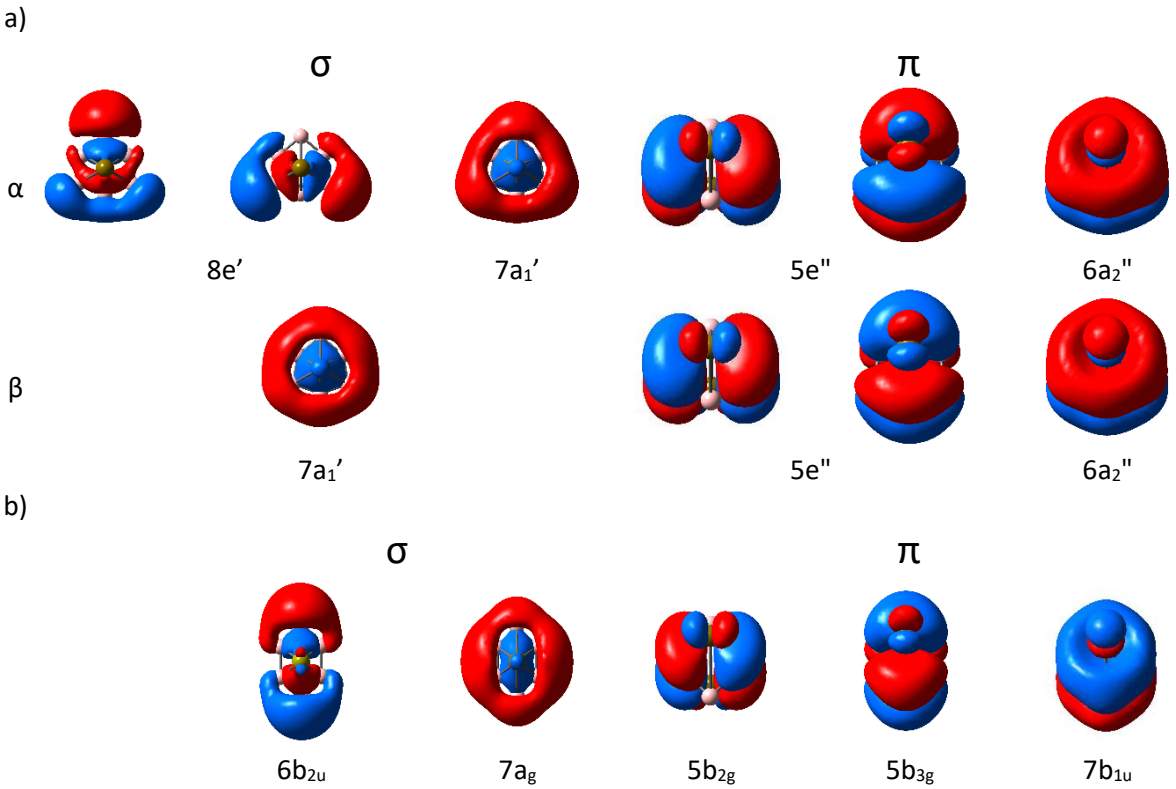

Figure S2. a) σ and π occupied canonical molecular spin (α and β) orbitals for T-Sr_2B_6 obtained at the UB3LYP/def2-TZVP level; b) σ and π occupied canonical molecular orbitals for S-Sr_2B_6 obtained at the RB3LYP/def2-TZVP.

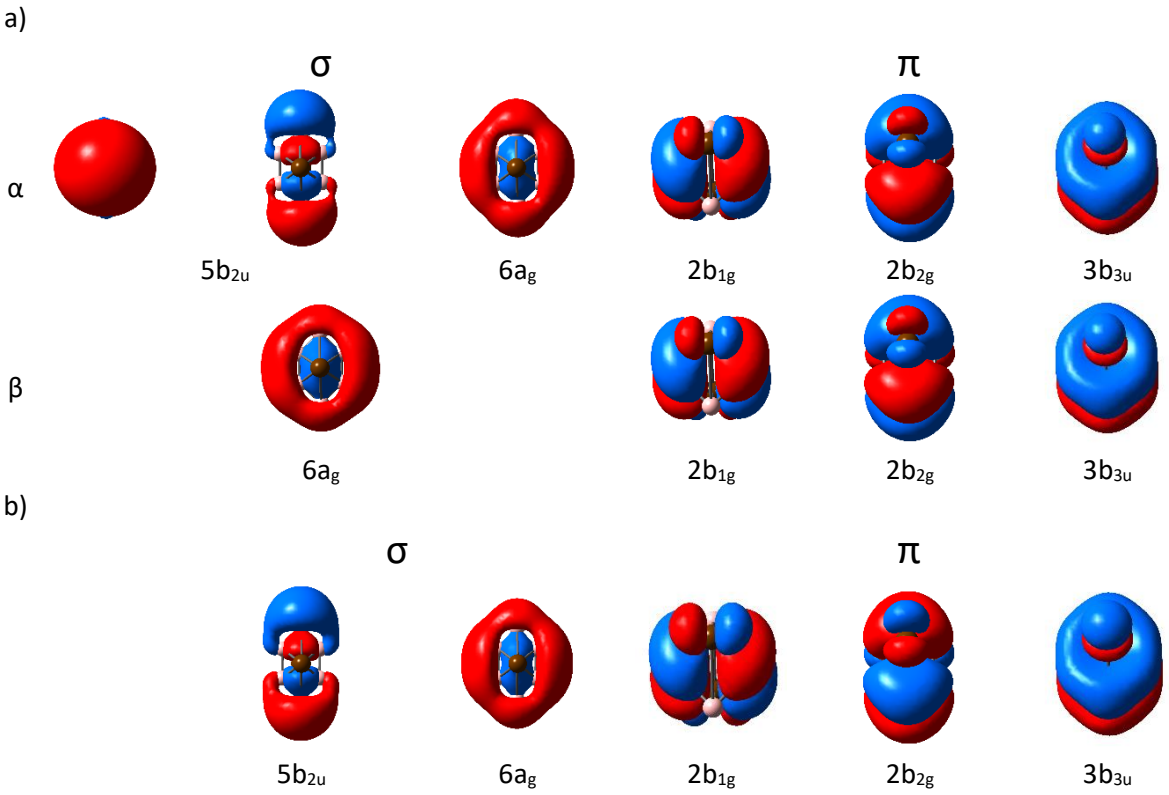

Figure S3. a) σ and π occupied canonical molecular spin (α and β) orbitals for T-Ba_2B_6 obtained at the UB3LYP/def2-TZVP level; b) σ and π occupied canonical molecular orbitals for S-Ba_2B_6 obtained at the RB3LYP/def2-TZVP.

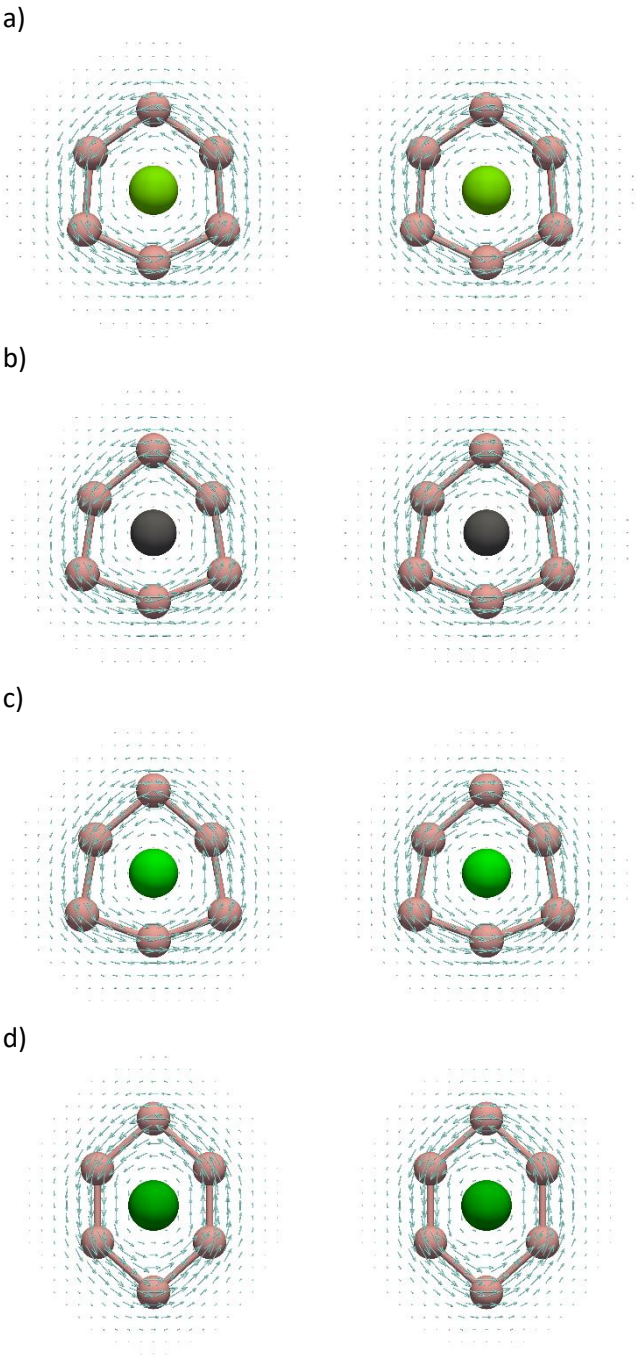

Figure S4. α (left) and β (right) π electron current density maps of the Mg_2B_6 (a), Ca_2B_6 (b), Sr_2B_6 (c) and Ba_2B_6 (d) calculated 1 bohr above the boron ring planes.

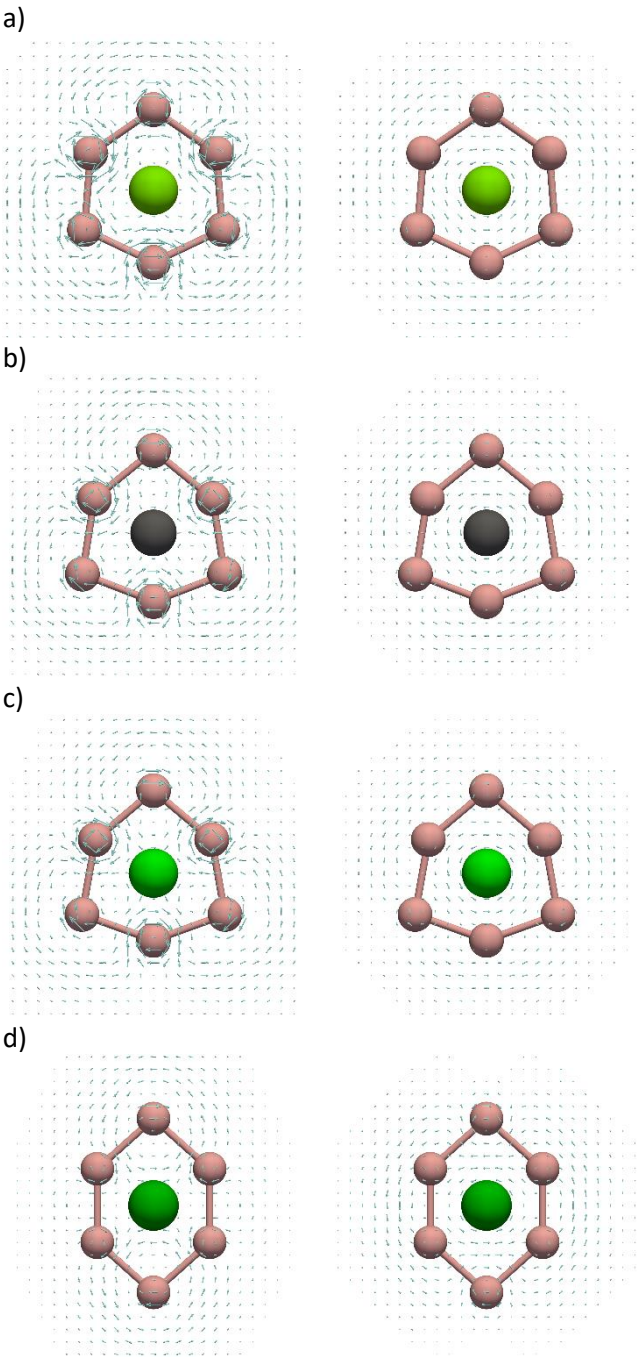

Figure S5. α (left) and β (right) σ electron current density maps of the Mg_2B_6 (a), Ca_2B_6 (b), Sr_2B_6 (c) and Ba_2B_6 (d) calculated 1 bohr above the boron ring planes.

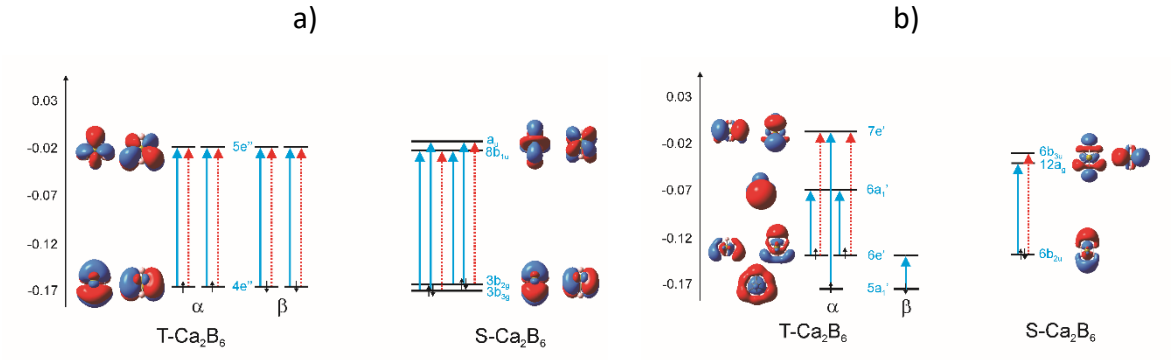

Figure S6. π (a) and σ (b) frontier orbital energy levels (in au) of Ca_2B_6 obtained at the B3LYP/def2-TZVP level of theory. Full (blue) arrows represent the main translational transitions, and dashed (red) arrows represent the main rotational transitions.

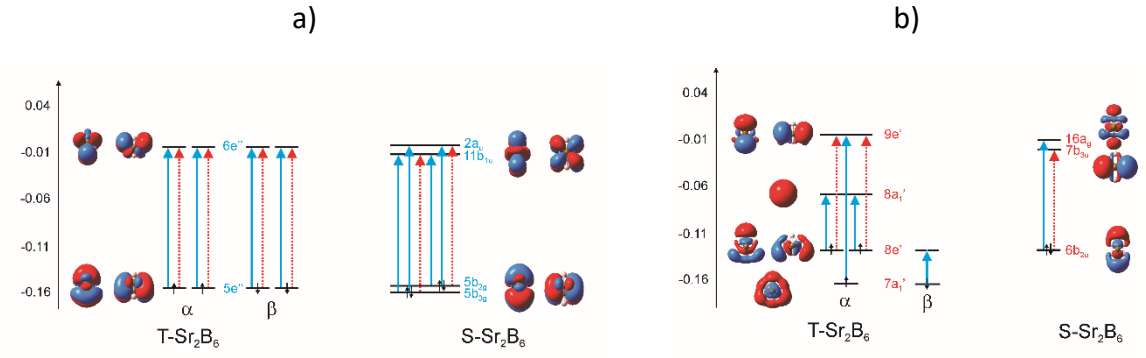

Figure S7. π (a) and σ (b) frontier orbital energy levels (in au) of Sr_2B_6 obtained at the B3LYP/def2-TZVP level of theory. Full (blue) arrows represent the main translational transitions, and dashed (red) arrows represent the main rotational transitions.

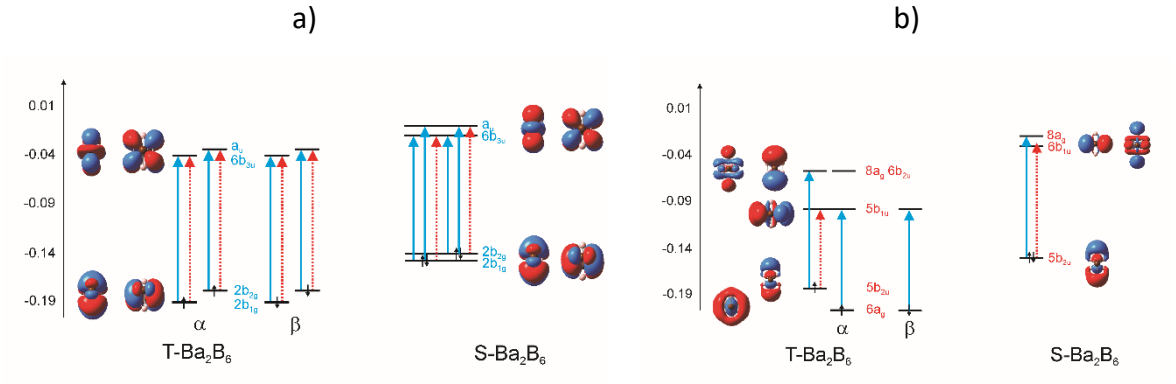

Figure S8. π (a) and σ (b) frontier orbital energy levels (in au) of Ba_2B_6 obtained at the B3LYP/def2-TZVP level of theory. Full (blue) arrows represent the main translational transitions, and dashed (red) arrows represent the main rotational transitions.