

Supplementary Information

The Structures and Bonding of Bismuth-Doped Boron Clusters: BiB₄⁻ and BiB₅⁻

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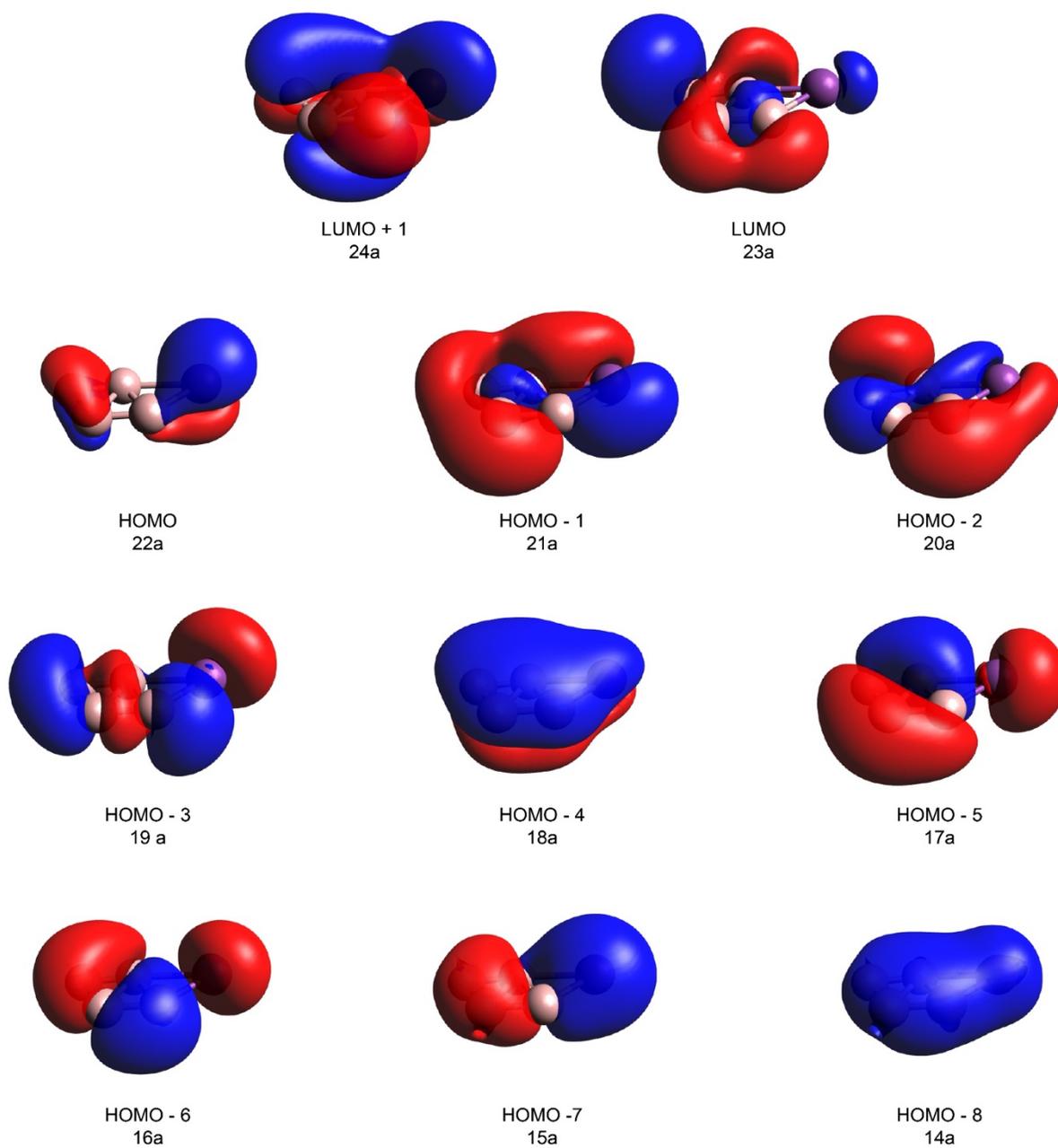


Fig. S1. The valence MOs of the global minimum of BiB_4^- (C_1 , 1A).

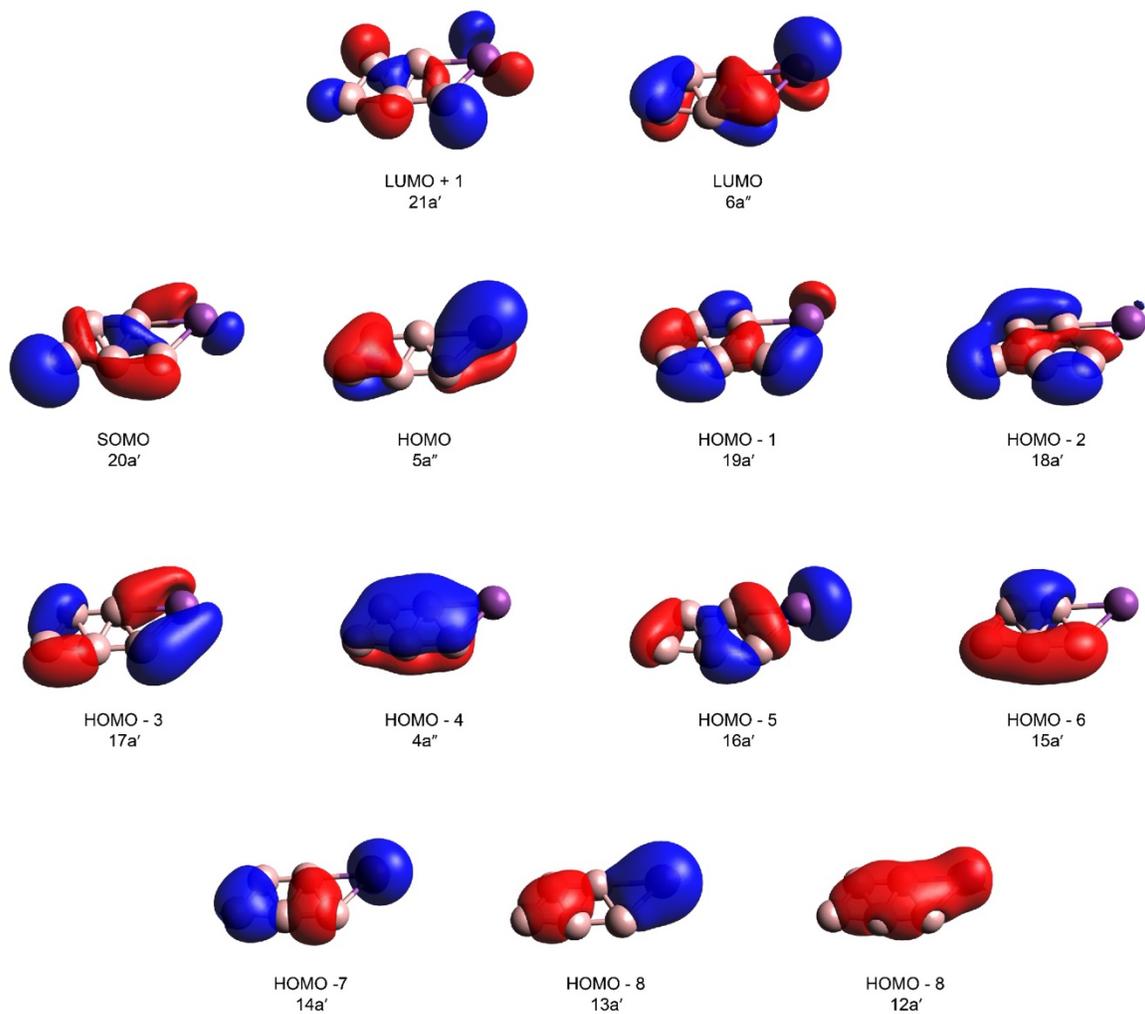


Fig. S2. The valence MOs of the global minimum of BiB_5^- ($C_s, ^2A'$).

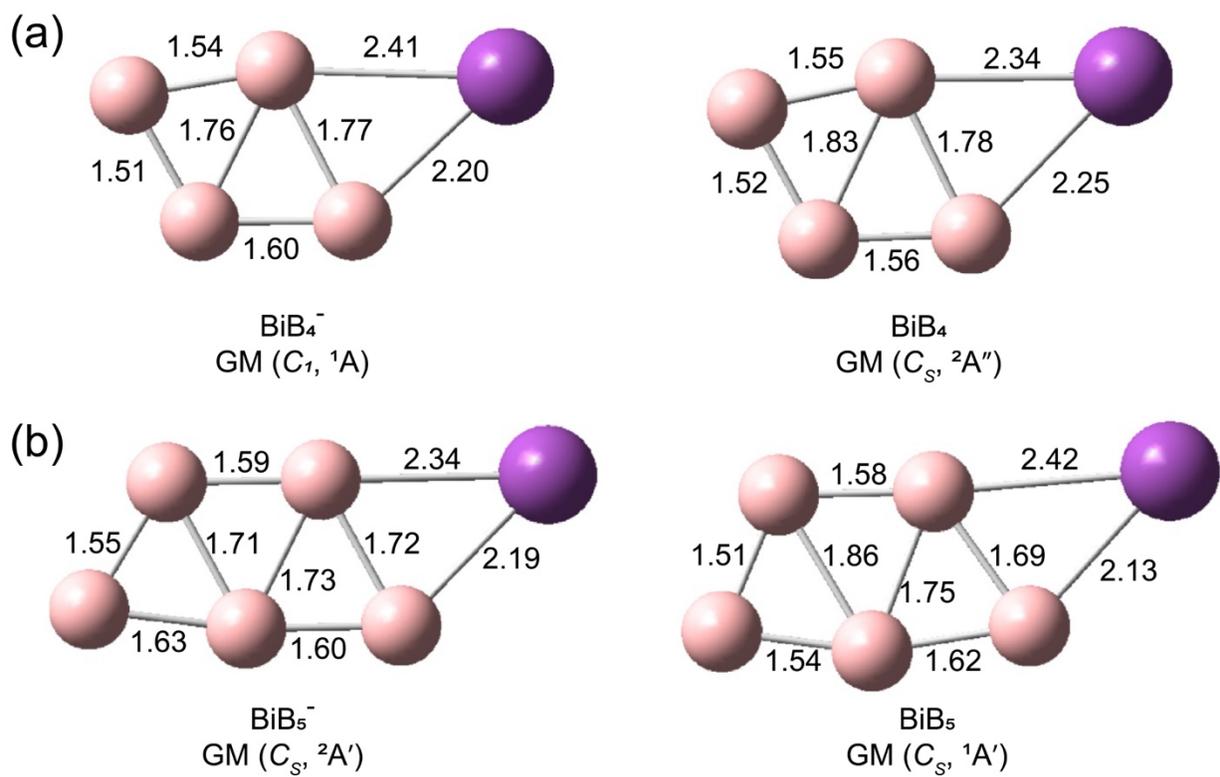


Fig. S3. The bond lengths (in Å) for (a) the ground state of BiB₄⁻ (C_1 , 1A) and BiB₄ (C_s , $^2A''$) and (b) the ground state of BiB₅⁻ (C_s , $^2A'$) and BiB₅ (C_s , $^1A'$).