

# Supplementary Information

## **The Structures and Bonding of Bismuth-Doped Boron Clusters: $\text{BiB}_4^-$ and $\text{BiB}_5^-$**

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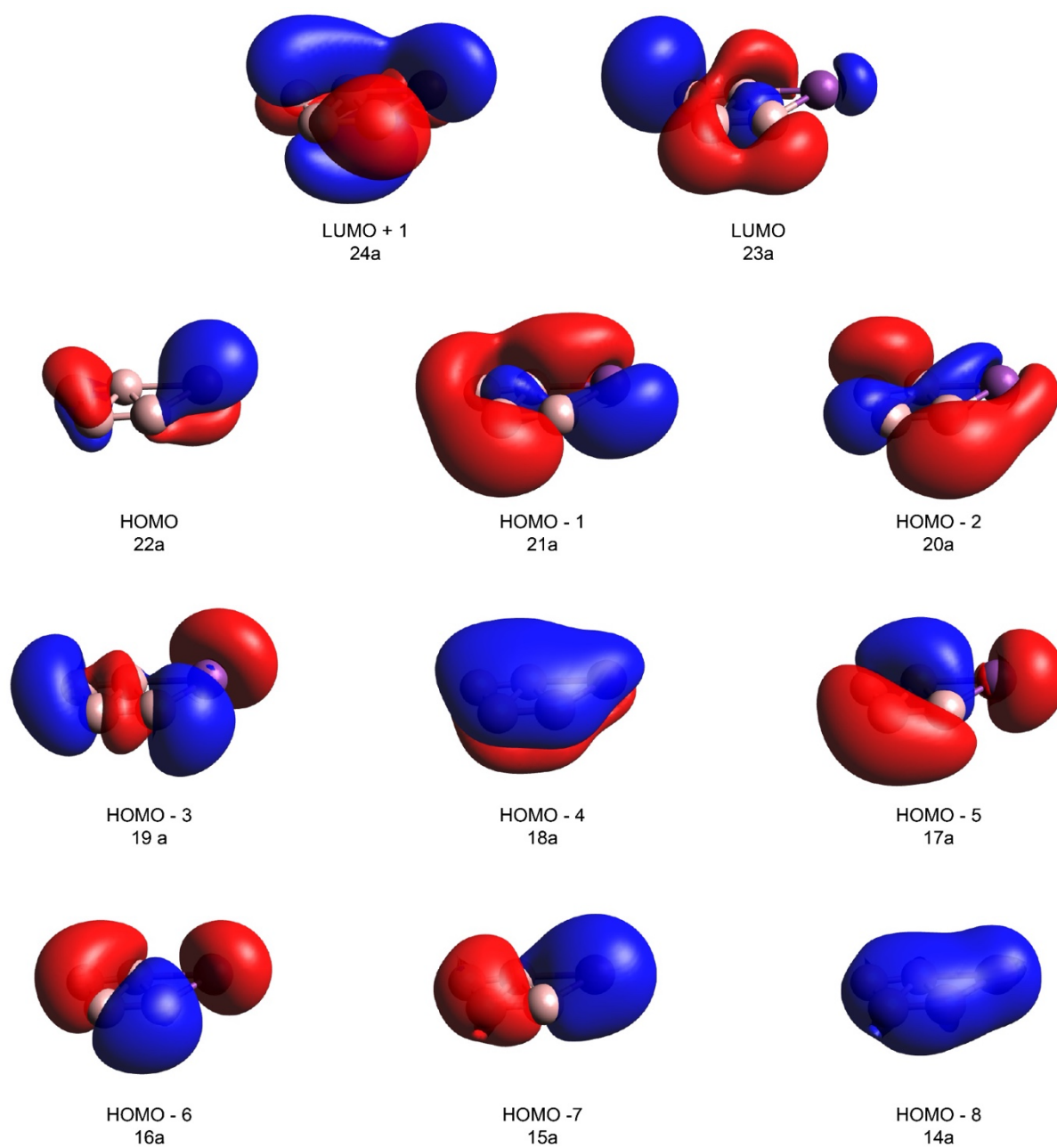


Fig. S1. The valence MOs of the global minimum of  $\text{BiB}_4^-$  ( $C_{1v}$ ,  $^1A_1$ ).

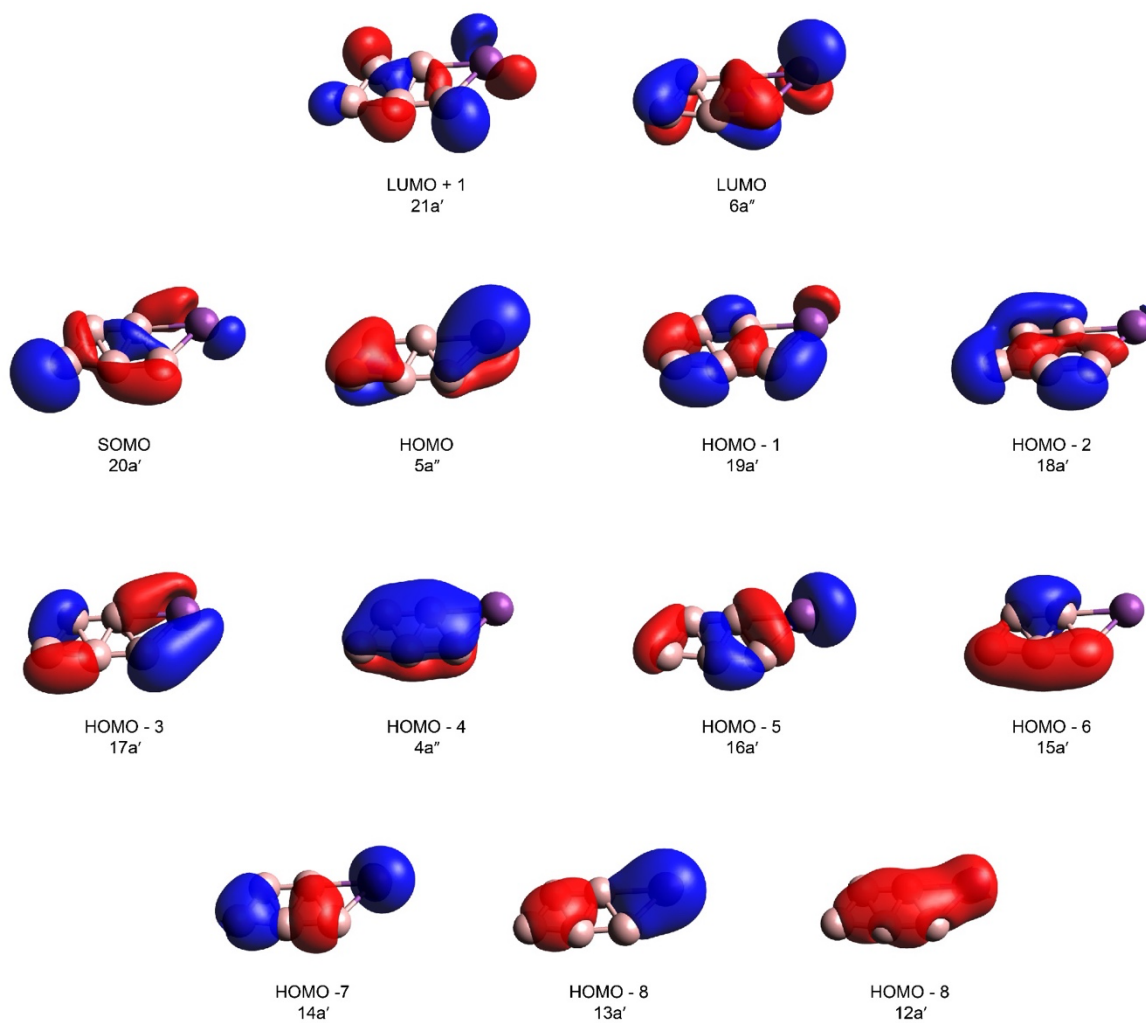


Fig. S2. The valence MOs of the global minimum of  $\text{BiB}_5^-$  ( $C_s$ ,  $^2A'$ ).

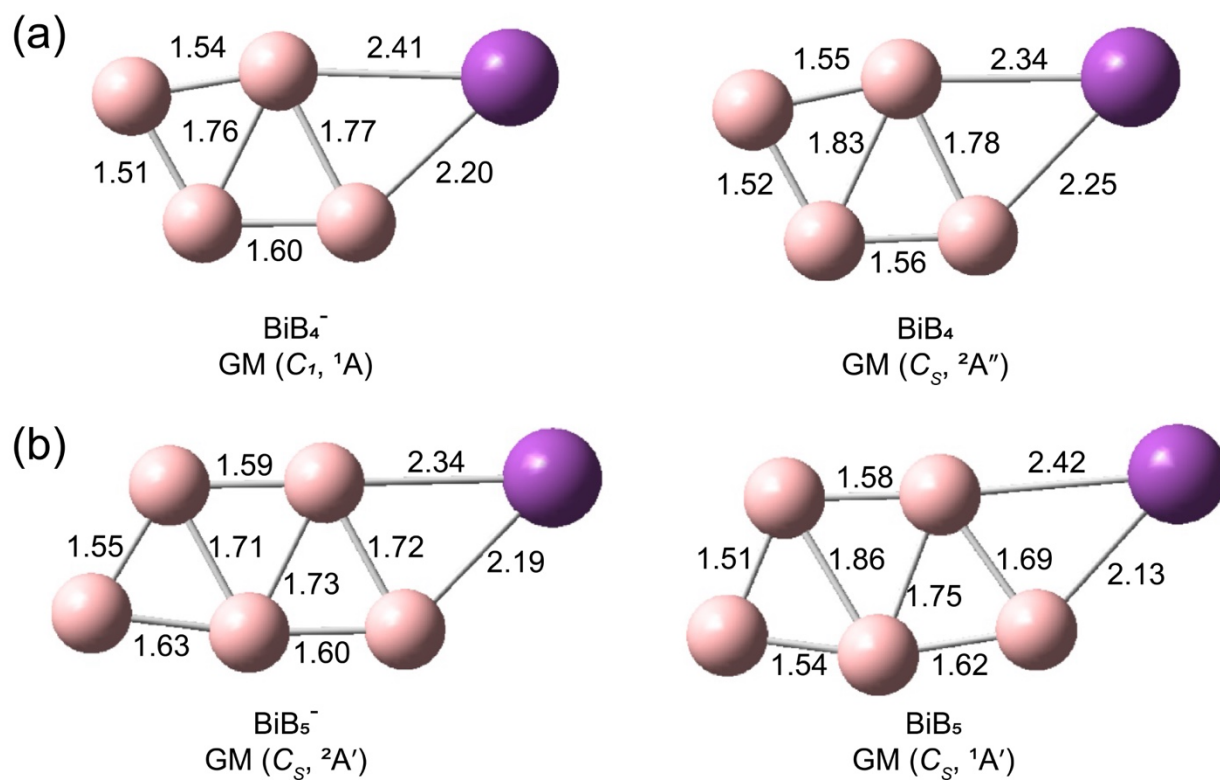


Fig. S3. The bond lengths (in Å) for (a) the ground state of BiB<sub>4</sub><sup>-</sup> ( $C_1$ ,  $^1A$ ) and BiB<sub>4</sub> ( $C_s$ ,  $^2A''$ ) and (b) the ground state of BiB<sub>5</sub><sup>-</sup> ( $C_s$ ,  $^2A'$ ) and BiB<sub>5</sub> ( $C_s$ ,  $^1A'$ ).