

## Supporting Information

Title: Is Bi<sup>2+</sup> Responsible for the Red-orange Emission of Bismuth-doped SrB<sub>4</sub>O<sub>7</sub>?

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1) AIM<sup>®</sup> embedding potential of SrB<sub>4</sub>O<sub>7</sub>, consisting of total-ion embedding Sr<sup>2+</sup>, B<sup>3+</sup>, and O<sup>2-</sup> AIMPs, and additional point charges, in MOLCAS format.

2) a'(6s), a''(6p<sub>x</sub>), a'(6p<sub>y</sub>), a'(6p<sub>z</sub>), 2<sub>a</sub>a', and 3<sub>a</sub>a' natural orbitals, and 1<sup>2</sup>A'', 1-3<sup>2</sup>A' electron densities, in cube format.

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