Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPLEMENTARY INFORMATION

Planar $B_3S_2H_3^-$ and $B_3S_2H_3$ clusters with a five-membered B_3S_2 ring: boron-sulfur hydride analogues of cyclopentadiene†

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Figure S1. Alternative optimized low-lying structures of $B_3S_2H_3^-$ monoanion. Relative energies are indicated in eV at the B3LYP/aug-cc-pVTZ level with zero-point energy (ZPE) corrections, as well as at the CCSD(T)//B3LYP/aug-cc-pVTZ level (in the parentheses) for top 8 isomers. The B, S, and H atoms are in pink, yellow, and gray, respectively.

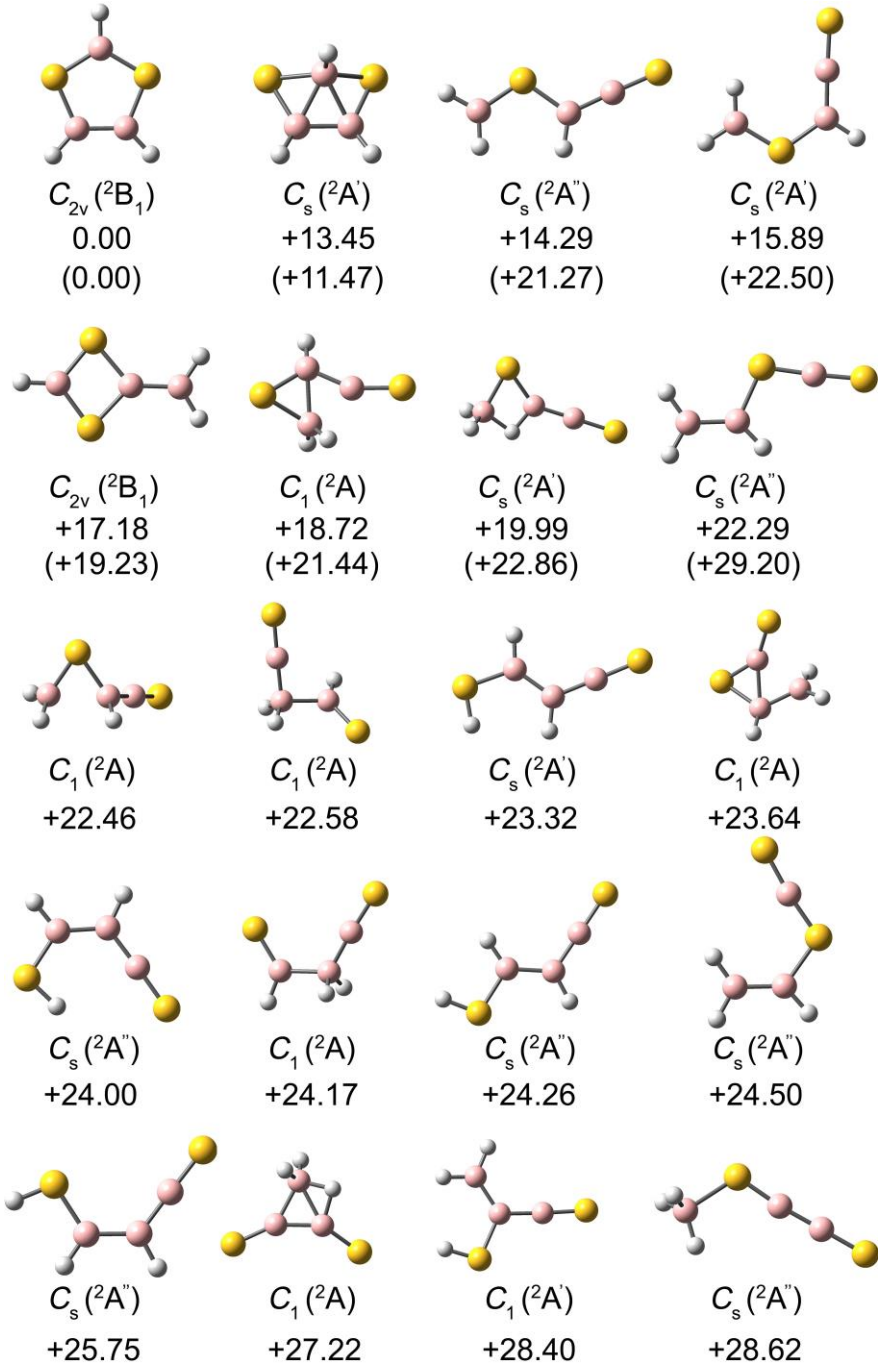

Figure S2. Alternative optimized low-lying structures of $B_3S_2H_3$ neutral cluster. Relative energies are indicated in eV at the B3LYP/aug-cc-pVTZ level with zero-point energy (ZPE) corrections, as well as at the CCSD(T)//B3LYP/aug-cc-pVTZ level (in the parentheses) for top 8 isomers. The B, S, and H atoms are in pink, yellow, and gray, respectively.

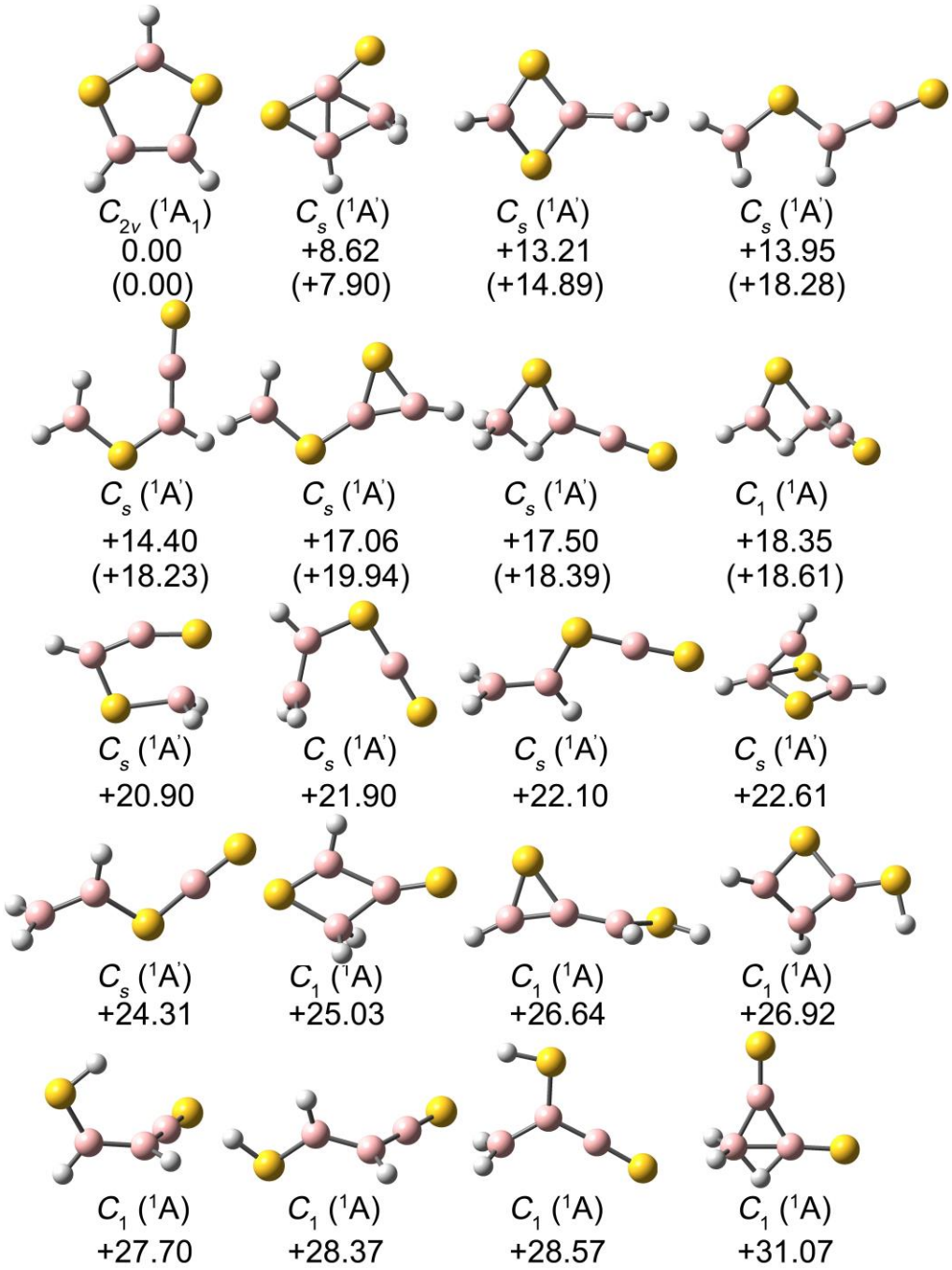

Figure S3. Alternative optimized low-lying structures of $B_3S_2H_3^{2-}$ dianion. Relative energies are indicated in eV at the B3LYP/aug-cc-pVTZ level with zero-point energy (ZPE) corrections, as well as at the CCSD(T)//B3LYP/ aug-cc-pVTZ level (in the parentheses). The B, S, and H atoms are in pink, yellow, and gray, respectively.

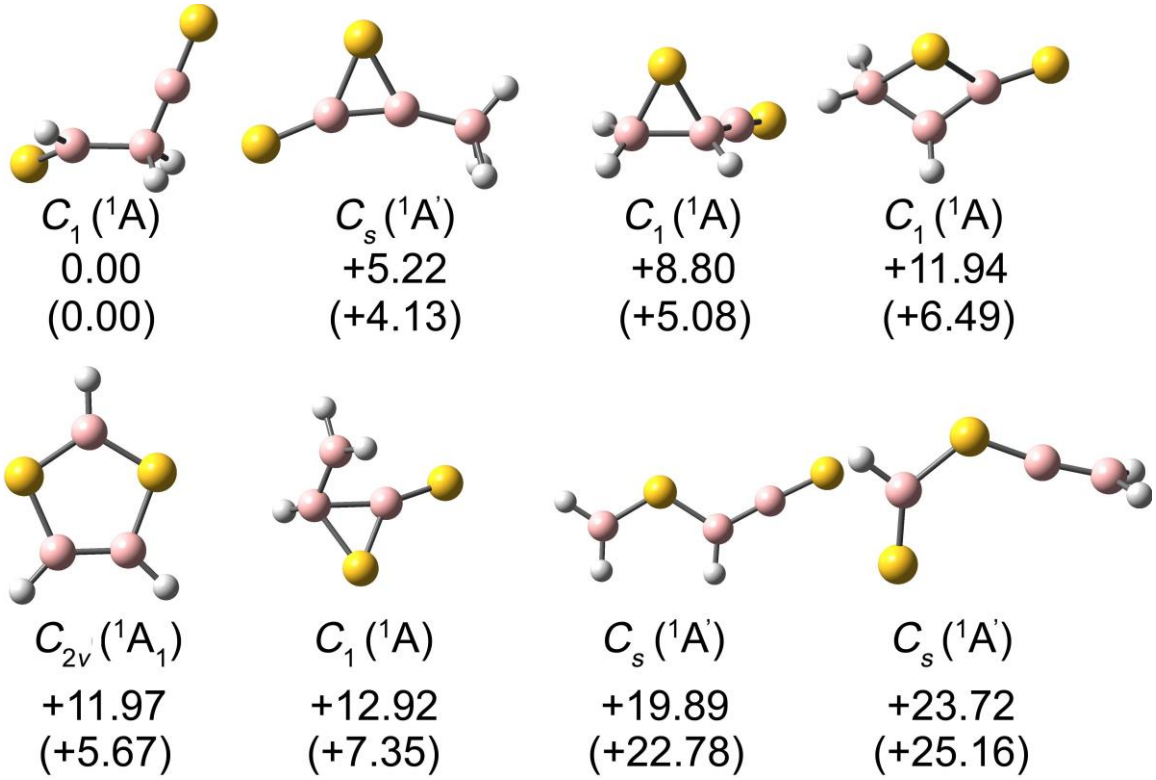

Figure S4. Bonding pattern of chain-like open structure C_1 (^{1}A) of the $B_3S_2H_3^{2-}$ dianion cluster, based on the adaptive natural density partitioning (AdNDP) analysis. Occupation numbers (ONs) are shown.