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 $\text{B}_3\text{S}_2\text{H}_3^-$ 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 B₃S₂H₃ 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 $\text{B}_3\text{S}_2\text{H}_3^{2-}$ 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 $C_1$ ($^1A$) of the $\text{B}_3\text{S}_2\text{H}_3^{2-}$ dianion cluster, based on the adaptive natural density partitioning (AdNDP) analysis. Occupation numbers (ONs) are shown.