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Supporting Information

Structural and Bonding Properties of $BS^{-/0}$ and $BS_3^{-/0}$

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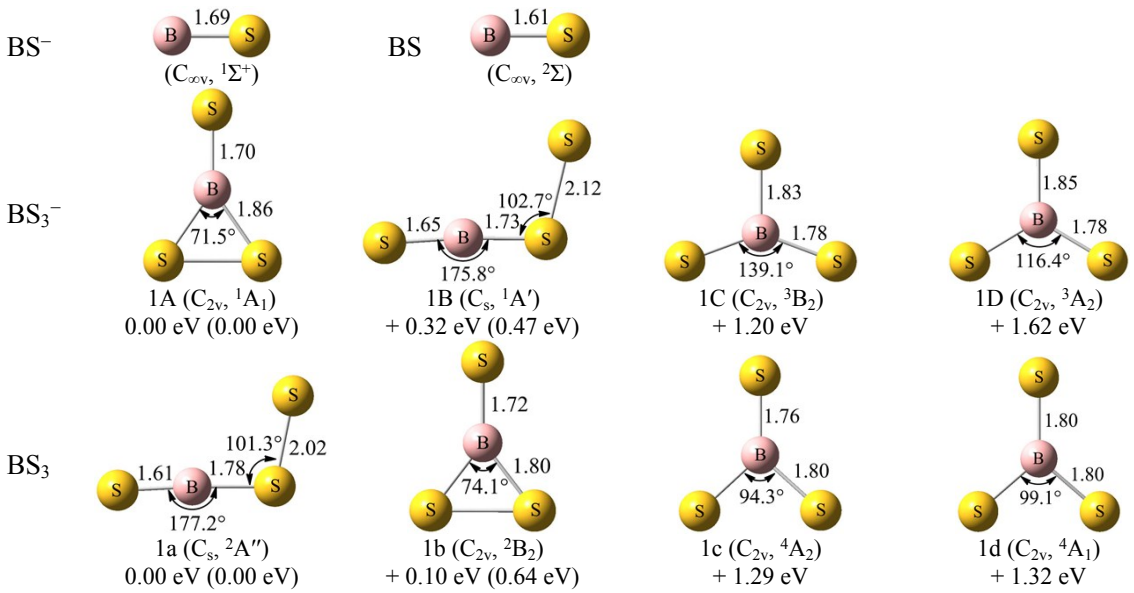

Fig. S1 Typical low-lying isomers of BS^- and BS_3^- as well as their corresponding neutrals. The electronic state, bond lengths (in Å) and bond angles are labeled. The relative energies to their most stable isomers obtained at the B3LYP and single-point CCSD(T) levels are given with the ones at the CCSD(T) level in the parentheses.

Table S1 Relative energies, ADEs and VDEs of the low-lying isomers of BS^- and BS_3^- obtained by theoretical calculations and the comparison with experimental ADEs and VDEs.

Isomer			ADE (eV)				VDE (eV)		
			Theo.			Expt.	Theo.		Expt.
			MP2[b]	CCSD(T)[c]	CCSD(T)[d]		MP2[b]	CCSD(T)[c]	
BS^-		$C_{\infty v}$, $^1\Sigma^+$	2.21	2.29	2.30	2.32(5)[a]	2.31	2.36	2.47(5)[a]
BS_3^-	1A	C_{2v}, $^1A_1$		3.34	3.44	3.34(5)[a]		3.44	3.42(5)[a]
	1B	C_s, $^1A'$		2.87				3.01	

[a]The numbers in the parentheses indicate the uncertainties of the experimental values in the last digits.

[b]obtained at the MP2(full) level/aug-cc-pVTZ level.

[c]obtained at the single-point CCSD(T) level/aug-cc-pVTZ level.

[d]obtained at the single-point CCSD(T) level/CBS level.