

Supporting Information

for

A Combined Crossed Molecular Beams and *ab Initio* Investigation on the Formation of Vinylsulfidoboron ($C_2H_3^{11}B^{32}S$)

by

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Table S1. The calculated energies for the B3LYP/cc-pVTZ optimized geometries of collision complexes, intermediates, transition states, and dissociation products for the BS + C₂H₄ reaction on the adiabatic doublet ground state potential energy surface of C₂H₄BS has been demonstrated.

	B3LYP/ cc-pVTZ + E _{zpc} ^a	E _{zpc} ^b	CCSD(T)/ cc-pVTZ	E ^c (kJ/mol)	E ^d (kJ/mol)
BS + ethylene	-501.582274	0.053608	-500.892256	0.0	0.0
i1	-501.650433	0.055193	-500.960618	-178.9	-175.1
i2	-501.668800	0.056540	-500.976136	-226.9	-212.3
p1+H	-501.597208	0.047060	-500.900561	-39.3	-38.9
p2+H	-501.468298	0.043565	-500.784834	236.1	255.4
p3+H	-501.492187	0.044859	-500.778552	298.9	275.4
tsi1p1	-500.767424 ^e	0.049603 ^f	-500.894638 ^g	-12.5 ^h	-18.4
tsi1i2	-501.604443	0.052196	-500.907124	-58.1	-42.6
tsi2p1	-501.596048	0.047821	-500.898366	-35.9	-31.4

^a B3LYP/cc-pVTZ energy with zero-point energy correction in hartree.

^b zero-point energy by B3LYP/cc-pVTZ.

^c relative energy by B3LYP/cc-pVTZ with zero-point energy correction.

^d relative energy by CCSD(T)/cc-pVTZ with B3LYP/cc-pVTZ zero-point energy correction.


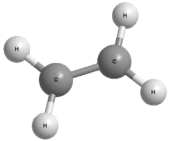
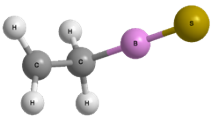
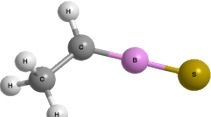
^e mp2/cc-pVTZ energy with zero-point energy correction in hartree.

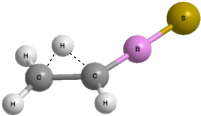
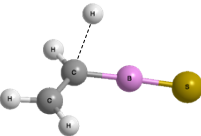
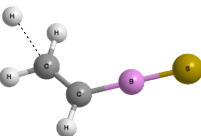
^f zero-point energy by mp2/cc-pVTZ.

^g relative energy by CCSD(T)/cc-pVTZ with mp2/cc-pVTZ zero-point energy correction.

^h relative energy by MP2/cc-pVTZ with zero-point energy correction.

Table S2. Optimized Cartesian coordinates (Å), rotational constants (GHz), and vibrational frequencies (cm⁻¹) of reactants, intermediates, transition states, and dissociation products computed at the cc-pVTZ basis set for the BS + C₂H₄ reaction on the adiabatic doublet ground state potential energy surface of C₂H₄BS.

Species	Rotational Constants (GHz)	Vibrational Frequencies (cm ⁻¹)	Cartesian Coordinates (Å)			
			Atom	X	Y	Z
BS (C _{∞v} , ² Σ ⁺) 	23.718417	1181	B	0.000000	0.000000	-1.228970
			S	0.000000	0.000000	0.384053
C ₂ H ₄ (D _{2h} , ¹ A _g) 	147.87034, 30.38348, 25.20459	837, 979, 984, 1067, 1247, 1382, 1479, 1693, 3125, 3139, 3194, 3222	C	0.000000	0.000000	0.662029
			C	0.000000	0.000000	-0.662029
			H	0.000000	0.920758	1.231574
			H	0.000000	-0.920758	1.231574
			H	0.000000	0.920758	-1.231574
			H	0.000000	-0.920758	-1.231574
i1(C _s , ² A) 	25.19982, 2.66255, 2.48618	132, 166, 305, 428, 536, 671, 736, 972, 1047, 1195, 1245, 1426, 1431, 1465, 3007, 3048, 3154, 3261	C	-1.475418	-0.103358	0.000000
			C	-1.537115	-1.596012	0.000000
			H	-1.969664	0.319140	0.880492
			H	-1.969664	0.319140	-0.880492
			H	-1.462731	-2.143917	0.926978
			H	-1.462731	-2.143917	-0.926978
			B	0.000000	0.341599	0.000000
			S	1.558749	0.758611	0.000000
i2(C ₁ , ² A) 	37.15961, 2.38026, 2.26792	117, 150, 313, 484, 636, 672, 984, 987, 1097, 1274, 1392, 1463, 1473, 1508, 2996, 3029, 3109, 3133	C	-1.192212	0.581766	0.000026
			C	-2.313478	-0.403091	0.000042
			H	-1.478596	1.629530	0.000808
			H	-2.955442	-0.255856	0.875141

			H -2.956774 -0.254636 -0.873861 B 0.241375 0.249743 -0.000732 S 1.824108 -0.125323 0.000128 H -1.967647 -1.434633 -0.000879
tsi1i2(C ₁ , ² A) 	39.00509, 2.40294, 2.28797	1675 i, 156, 255, 479, 493, 663, 705, 778, 997, 1110, 1205, 1282, 1447, 1526, 2215, 3150, 3165, 3284	C 1.228344 0.544982 -0.018101 C 2.332535 -0.446842 -0.050764 H 1.529858 1.573964 -0.178028 H 1.779968 0.158130 1.032210 H 3.340960 -0.111029 -0.227420 H 2.111764 -1.501544 -0.029351 B -0.227448 0.227970 -0.029421 S -1.811912 -0.115513 -0.002320
tsi1p1(C ₁ , ² A) 	31.81362, 2.53283, 2.41037	1168 i, 159, 244, 344, 451, 491, 629, 684, 1046, 1057, 1100, 1304, 1405, 1521, 1641, 3194, 3206, 3296	C -1.320139 0.472143 -0.167264 C -2.212953 -0.503855 0.034105 H -1.044902 1.418985 1.418564 H -1.656781 1.412744 -0.585414 H -3.269518 -0.343763 -0.123880 H -1.912114 -1.477031 0.393042 B 0.180249 0.206159 -0.065923 S 1.761289 -0.115716 0.001641
tsi2p1(C ₁ , ² A) 	30.54037, 2.40473, 2.31939	275 i, 129, 170, 197, 307, 491, 637, 674, 1005, 1024, 1045, 1300, 1387, 1499, 1638, 3128, 3138, 3222	C -1.226810 -0.581131 0.089377 C -2.201733 0.257706 -0.294348 H -1.506401 -1.564017 0.457710 H -3.243244 -0.035768 -0.274124 H -2.870536 1.470338 1.626017 B 0.238757 -0.233905 0.042092

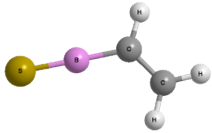
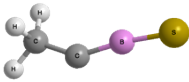
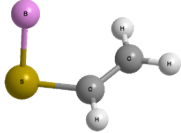
			S 1.811446 0.124881 -0.006285 H -1.985486 1.241422 -0.689673
<p>p1(C_s,¹A')</p> 	46.31678, 2.56772, 2.43284	165, 273, 491, 620, 673, 1014, 1033, 1044, 1302, 1396, 1501, 1662, 3126, 3134, 3217	C 1.380472 -0.344007 0.000000 C 1.603936 -1.662236 0.000000 H 2.234667 0.327127 0.000000 H 2.607425 -2.069033 0.000000 H 0.793015 -2.379257 0.000000 B 0.000000 0.264307 0.000000 S -1.471347 0.927318 0.000000
<p>p2(C₁,¹A)</p> 	93.44812, 2.22349, 2.19996	108, 158, 354, 369, 582, 670, 1038, 1180, 1306, 1340, 1504, 1587, 2894, 2988, 3044	C -1.179583 -0.387281 -0.024438 C -2.503236 0.151444 -0.021832 H -2.646184 1.133386 -0.487173 H -2.627826 0.327437 1.069224 B 0.213366 -0.082095 -0.009372 S 1.850323 0.056837 0.002177 H -3.301070 -0.544713 -0.292407
<p>p3(C₁,¹A)</p> 	13.45857, 5.15273, 4.11598	131, 203, 394, 610, 680, 749, 971, 994, 1043, 1300, 1416, 1632, 3144, 3184, 3238	C 0.743138 -0.481376 0.323448 C 1.724599 0.231116 -0.220783 H 1.559572 0.902047 -1.051028 H 0.911311 -1.150460 1.155698 H 2.735806 0.136098 0.153953 B -0.888406 1.403001 0.367905 S -0.973193 -0.337570 -0.169634

Table S3. The calculated energies for the B3LYP/aug-cc-pVTZ optimized geometries of collision complexes, intermediates, transition states, and dissociation products for the BS + C₂H₄ reaction on the adiabatic doublet ground state potential energy surface of C₂H₄BS has been demonstrated.

	B3LYP/ cc-pVTZ + E _{zpc} ^a	B3LYP/ aug-cc-pVTZ + E _{zpc}	E ^b (kJ/mol)	E ^c (kJ/mol)
BS + ethylene	-501.582274	(-501.583695)	0.0	
i1	-501.650433	(-501.651728)	-178.9	(-178.5)
i2	-501.668800	(-501.669932)	-226.9	(-226.2)
p1+H	-501.597208	(-501.598511)	-39.3	(-38.9)
p2+H	-501.468298	(-501.492291)	236.1	(239.8)
p3+H	-501.492187	(-501.469833)	298.9	(298.7)
tsi1p1	-500.767424 ^d	(-500.777908) ^e	-12.5 ^f	(-15.2) ^g
tsi1i2	-501.604443	(-501.60607)	-58.1	(-58.7)
tsi2p1	-501.596048	(-501.597293)	-35.9	(-35.7)

^a B3LYP/cc-pVTZ energy with zero-point energy correction in hartree.

^b relative energy by B3LYP/cc-pVTZ with zero-point energy correction.

^c relative energy by B3LYP/aug-cc-pVTZ with zero-point energy correction.


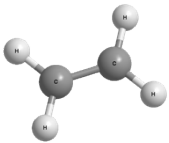
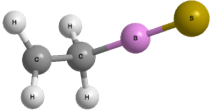
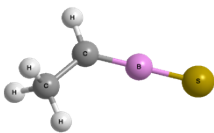
^d mp2/cc-pVTZ energy with zero-point energy correction in hartree.

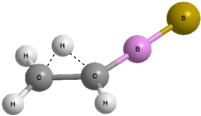
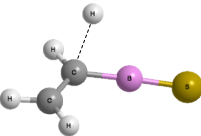
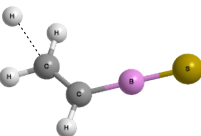
^e mp2/aug-cc-pVTZ energy with zero-point energy correction in hartree.

^f relative energy by MP2/cc-pVTZ with zero-point energy correction.

^g relative energy by MP2/aug-cc-pVTZ with zero-point energy correction.

Table S4. Optimized Cartesian coordinates (Å), rotational constants (GHz), and vibrational frequencies (cm⁻¹) of reactants, intermediates, transition states, and dissociation products computed at the aug-cc-pVTZ basis set for the BS + C₂H₄ reaction on the adiabatic doublet ground state potential energy surface of C₂H₄BS.

Species	Rotational Constants (GHz)	Vibrational Frequencies (cm ⁻¹)	Cartesian Coordinates (Å)			
			Atom	X	Y	Z
BS (C _{∞v} , ² Σ ⁺) 	23.724916	1179	B	0.000000	0.000000	-1.228970
			S	0.000000	0.000000	0.384053
C ₂ H ₄ (D _{2h} , ¹ A _g) 	147.91079, 30.35661, 25.18727	835, 979, 985, 1060, 1245, 1381, 1480, 1689, 3126, 3140, 3195, 3223	C	0.000000	0.000000	0.662414
			C	0.000000	0.000000	-0.662414
			H	0.000000	0.920632	1.231825
			H	0.000000	-0.920632	1.231825
			H	0.000000	0.920632	-1.231825
			H	0.000000	-0.920632	-1.231825
i1(C _s , ² A') 	25.22074, 2.66199, 2.48589	131, 166, 305, 428, 540, 671, 735, 971, 1046, 1194, 1245, 1423, 1429, 1465, 3006, 3047, 3154, 3259	C	-1.474996	-0.104508	0.000000
			C	-1.536251	-1.597003	0.000000
			H	-1.969354	0.317577	0.880470
			H	-1.969354	0.317577	-0.880470
			H	-1.463814	-2.145089	0.926956
			H	-1.463814	-2.145089	-0.926956
			B	0.000000	0.341446	0.000000
			S	1.558364	0.759803	0.000000
i2(C ₁ , ² A) 	37.16581, 2.38014, 2.26782	116, 150, 313, 483, 636, 671, 984, 986, 1096, 1273, 1390, 1462, 1472, 1507, 2996, 3028, 3108, 3132	C	-1.192261	0.581613	0.000032
			C	-2.313527	-0.403130	0.000050
			H	-1.478566	1.629322	0.000774
			H	-2.955471	-0.255271	0.874895

			H -2.956441 -0.254419 -0.873948 B 0.241280 0.249866 -0.000723 S 1.824176 -0.125323 0.000126 H -1.968010 -1.434686 -0.000620
tsi1i2(C ₁ , ² A) 	38.95225, 2.40429, 2.28900	1667 i, 155, 254, 480, 494, 662, 709, 781, 995, 1110, 1204, 1281, 1447, 1522, 2212, 3149, 3165, 3282	C 1.228772 0.545375 -0.018673 C 2.331160 -0.447359 -0.051142 H 1.530947 1.574225 -0.177467 H 1.780173 0.157504 1.032278 H 3.340465 -0.112823 -0.224874 H 2.109630 -1.501865 -0.029335 B -0.227255 0.228973 -0.028917 S -1.811533 -0.115625 -0.002320
tsi1p1(C ₁ , ² A) 	31.82791, 2.53075, 2.40875	1167 i, 158, 241, 342, 451, 490, 627, 682, 1043, 1054, 1098, 1302, 1402, 1517, 1640, 3188, 3199, 3291	C -1.320564 0.472102 -0.167058 C -2.214106 -0.503399 0.034087 H -1.041966 1.414966 1.421726 H -1.657362 1.413604 -0.584803 H -3.270959 -0.342261 -0.124275 H -1.913497 -1.477475 0.392381 B 0.180235 0.206068 -0.066627 S 1.761914 -0.115712 0.001621
tsi2p1(C ₁ , ² A) 	30.51581, 2.40463, 2.31907	275 i, 128, 170, 196, 307, 491, 637, 673, 1005, 1024, 1044, 1299, 1385, 1498, 1636, 3127, 3137, 3221	C -1.226711 -0.581336 0.090181 C -2.201918 0.256884 -0.294611 H -1.50626 -1.563522 0.460087 H -3.243184 -0.036917 -0.272797 H -2.870442 1.477714 1.622451 B 0.238811 -0.234296 0.042218

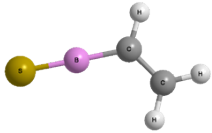
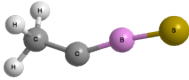
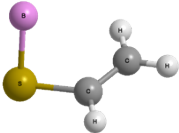
			S 1.811481 0.125054 -0.006434 H -1.986088 1.240056 -0.691310
<p>p1(C_s,¹A')</p> 	46.31679, 2.56772, 2.43284	165, 276, 491, 621, 673, 1015, 1034, 1043, 1302, 1394, 1500, 1661, 3125, 3134, 3215	C 1.380472 -0.344007 0.000000 C 1.603936 -1.662236 0.000000 H 2.234667 0.327127 0.000000 H 2.607425 -2.069033 0.000000 H 0.793015 -2.379257 0.000000 B 0.000000 0.264307 0.000000 S -1.471347 0.927318 0.000000
<p>p2(C₁,¹A)</p> 	93.44808, 2.22349, 2.19996	110, 159, 355, 369, 581, 668, 1038, 1178, 1305, 1339, 1504, 1583, 2893, 2986, 3042	C -1.179583 -0.387281 -0.024438 C -2.503236 0.151444 -0.021832 H -2.646184 1.133386 -0.487173 H -2.627826 0.327437 1.069224 B 0.213366 -0.082095 -0.009372 S 1.850323 0.056837 0.002177 H -3.301070 -0.544713 -0.292407
<p>p3(C₁,¹A)</p> 	13.47689, 5.14736, 4.11656	130, 202, 393, 609, 679, 749, 972, 993, 1042, 1300, 1416, 1632, 3144, 3185, 3237	C 0.743702 -0.479716 0.324985 C 1.725114 0.231389 -0.221297 H 1.560796 0.899568 -1.053824 H 0.911600 -1.146414 1.159021 H 2.735940 0.137480 0.154385 B -0.891830 1.401013 0.368081 S -0.972630 -0.337858 -0.170132

Table S5. The RRKM rate constants (s^{-1}) computed with B3LYP/cc-pVTZ frequencies and CCSD(T)/cc-pVTZ energies at collision energies of 0.0, 0.1, 0.6, 8.4, 18.0, 21.0, and 41.8 kJ/mol, in the reaction of boron monosulfide (BS; $X^2\Sigma^+$) with ethylene (C_2H_4 ; X^1A_g).

	0.0	0.1	0.6	8.4	18.0	21.0	41.8
$k_1(i1 \rightarrow ts-i1i2)$	1.20×10^8	1.21×10^8	1.26×10^8	2.29×10^8	4.36×10^8	5.20×10^8	1.54×10^9
$k_{-1}(i2 \rightarrow ts-i1i2)$	3.67×10^7	3.72×10^7	3.89×10^7	7.49×10^7	1.53×10^8	1.86×10^8	6.30×10^8
$k_2(i1 \rightarrow ts-i1p1)$	1.92×10^6	1.96×10^6	2.14×10^6	7.14×10^6	2.35×10^7	3.22×10^7	1.99×10^8
$k_3(i2 \rightarrow ts-i2p1)$	3.52×10^7	3.58×10^7	3.82×10^7	9.64×10^7	2.56×10^8	3.34×10^8	1.66×10^9