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

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 S3. The calculated energies for the B3LYP/aug-cc-pVTZ optimized geometries of collision complexes, intermediates, transition states, and dissociation products for the BS + C_2H_4 reaction on the adiabatic doublet ground state potential energy surface of C_2H_4BS has been demonstrated……...……...…….…….7

Table S4. Optimized Cartesian coordinates (Å), rotational constants (GHz), and vibrational frequencies (cm^{-1}) of reactants, intermediates, transition states, and dissociation products computed with the B3LYP/au-gcc-pVTZ for the BS + C_2H_4 reaction on the adiabatic doublet ground state potential energy surface of C_2H_4BS…….……...8

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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 + C_2H_4 reaction on the adiabatic doublet ground state potential energy surface of C_2H_4BS 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.

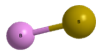
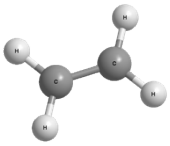
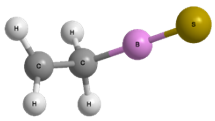
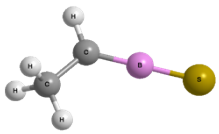
[e] mp2/cc-pVTZ energy with zero-point energy correction in hartree.

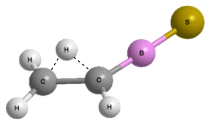
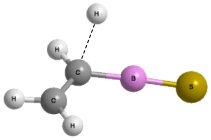
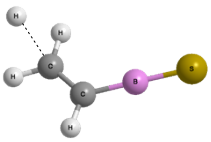
[f] zero-point energy by mp2/cc-pVTZ.

[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 + C_2H_4 reaction on the adiabatic doublet ground state potential energy surface of C_2H_4BS.

Species	Rotational Constants (GHz)	Vibrational Frequencies (cm^{-1})	Cartesian Coordinates (Å)			
			Atom	X	Y	Z
BS ($C_{\infty v}$, $^2\Sigma^+$) 	23.718417	1181	B	0.000000	0.000000	-1.228970
			S	0.000000	0.000000	0.384053
C_2H_4 (D_{2h}, ^1A_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, $^2A'$) 	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, ^2A) 	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

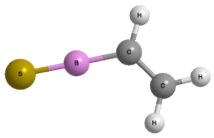
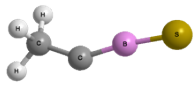
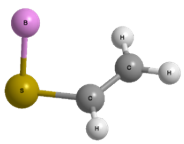
			S	1.811446	0.124881	-0.006285
			H	-1.985486	1.241422	-0.689673
p1(C_S,^{1}A') 	46.31678, 2.56772, 2.43284	165, 273, 491, 620, 673, 1014, 1033, 1044, 1302, 1396, 1501, 1662, 3126, 3134, 3217	C	1.380472	-0.344007	0.000000
			C	1.603936	-1.662236	0.000000
			H	2.234667	0.327127	0.000000
			H	2.607425	-2.069033	0.000000
			H	0.793015	-2.379257	0.000000
			B	0.000000	0.264307	0.000000
			S	-1.471347	0.927318	0.000000
p2(C_1,^{1}A) 	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
p3(C_1,^{1}A) 	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 + C_2H_4 reaction on the adiabatic doublet ground state potential energy surface of C_2H_4BS 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.

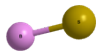
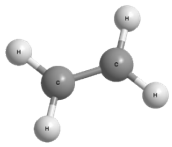
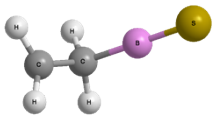
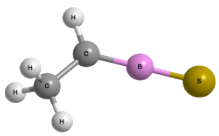
[d] mp2/cc-pVTZ energy with zero-point energy correction in hartree.

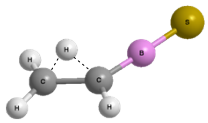
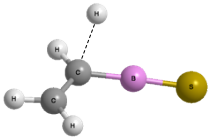
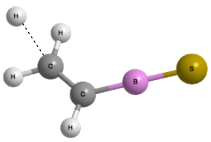
[e] mp2/aug-cc-pVTZ energy with zero-point energy correction in hartree.

[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 + C_2H_4 reaction on the adiabatic doublet ground state potential energy surface of C_2H_4BS.

Species	Rotational Constants (GHz)	Vibrational Frequencies (cm^{-1})	Cartesian Coordinates (Å)			
			Atom	X	Y	Z
BS ($C_{\infty v}$,$^2\Sigma^+$) 	23.724916	1179	B	0.000000	0.000000	-1.228970
			S	0.000000	0.000000	0.384053
C_2H_4 (D_{2h},^1A_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,$^2A'$) 	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,^2A) 	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

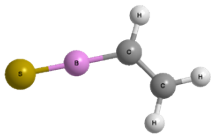
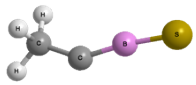
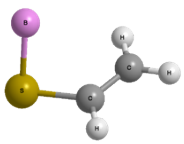
			S	1.811481	0.125054	-0.006434
			H	-1.986088	1.240056	-0.691310
p1(C_S,^{1}A') 	46.31679, 2.56772, 2.43284	165, 276, 491, 621, 673, 1015, 1034, 1043, 1302, 1394, 1500, 1661, 3125, 3134, 3215	C	1.380472	-0.344007	0.000000
			C	1.603936	-1.662236	0.000000
			H	2.234667	0.327127	0.000000
			H	2.607425	-2.069033	0.000000
			H	0.793015	-2.379257	0.000000
			B	0.000000	0.264307	0.000000
			S	-1.471347	0.927318	0.000000
p2(C_1,^{1}A) 	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
p3(C_1,^{1}A) 	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}