Supporting Information

for

Directed Gas Phase Formation of the Ethynylsulfidoboron Molecule (HCCBS)

*Tao Yang, Dorian S. N. Parker, Beni. B. Dangi, Ralf I. Kaiser**

Department of Chemistry, University of Hawaii at Manoa, Honolulu, Hawaii, USA

Domenico Stranges

Department of Chemistry, Sapienza University of Rome, Rome, Italy

*Yuan-Hsiang Su, Si-Ying Chen, Agnes H. H. Chang**

Department of Chemistry, National Dong Hwa University, Shoufeng, Hualien 974, Taiwan

*Alexander M. Mebel**

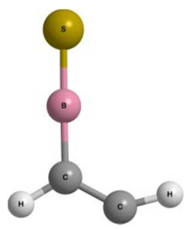
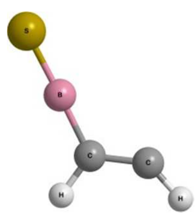
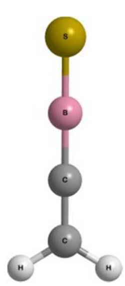
Department of Chemistry and Biochemistry, Florida International University, Miami, Florida, USA

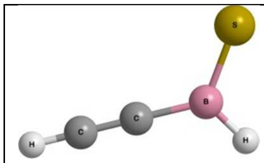
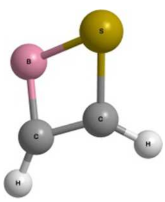
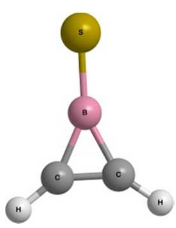
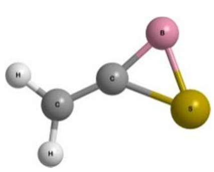
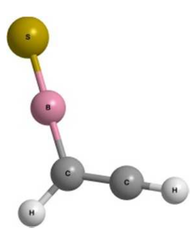
Corresponding Authors

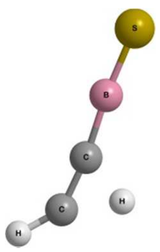
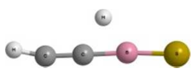
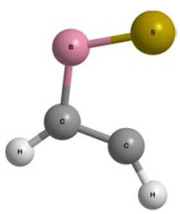
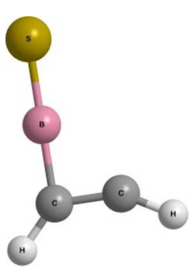
Email: ralfk@hawaii.edu (R.I.K); hhchang@mail.ndhu.edu.tw (H.H.C); mebela@fiu.edu (A.M.M)

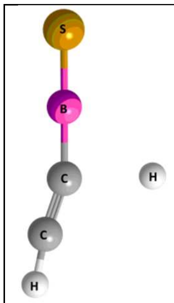
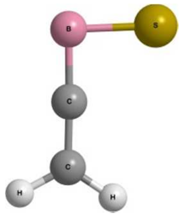
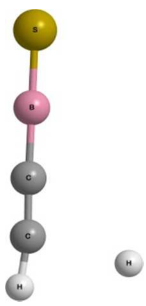
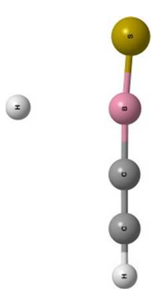
List of Contents:

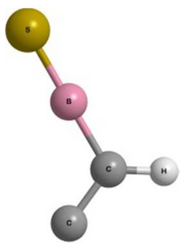
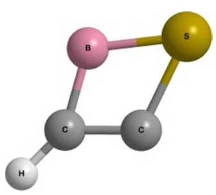
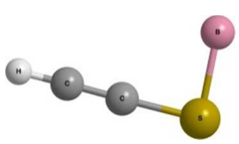
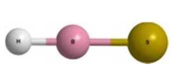
Table S1. Optimized Cartesian coordinates (Å), rotational constants (GHz), and vibrational frequencies (cm^{-1}) of intermediates, transition states, and dissociation products for the BS + C_2H_2 reaction on the adiabatic doublet ground state potential energy surface of C_2H_2BS.

Species	Rotational Constants (GHz)	Vibrational Frequencies (cm^{-1})	Cartesian Coordinates (Å)			
			Atom	X	Y	Z
	43.13109, 2.79523, 2.62511	151.4313, 304.8443, 452.5202, 661.4431, 676.6734, 878.3100, 881.8421, 1200.5137, 1439.0372, 1619.6493, 3084.3867, 3224.0502	C C H H B S	1.512785 2.131583 2.082515 1.860937 0.000000 -1.6131	0.199229 -0.95884 1.127655 -2.00391 0.242549 0.263824	0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
	58.29189, 2.64394, 2.52922	160.4078, 290.6536, 455.6455, 624.9876, 644.8735, 858.3686, 864.5850, 1196.1116, 1440.5580, 1640.6956, 3001.9344, 3224.9372	C C H H B S	1.451115 1.817651 2.218058 2.729428 0.000000 -1.53501	-0.23581 -1.49487 0.546984 -2.0724 0.192751 0.684108	0.000000 0.000000 0.000000 0.000000 0.000000 0.000000
	294.25582, 2.29010, 2.27241	146.5694, 172.6738, 348.0766, 478.4760, 599.4594, 945.8092, 950.6145, 1320.0187, 1448.9433, 1848.6776, 3058.2004, 3117.4347	C C H B S H	0.000000 0.000000 0.000000 0.000000 0.000000 0.000000	0.000000 0.000000 0.923078 0.000000 0.000000 -0.923078	-1.273408 -2.573159 -3.151209 0.159041 1.786663 -3.151209
	37.53188, 2.83178, 2.63311	137.8684, 273.1992, 394.8347, 668.2475, 692.1230, 746.0716, 754.7900, 906.2240,1100.7783,	C C H	1.301554 2.348411 3.271859	-0.02031 -0.61955 -1.14509	0.000000 0.000000 0.000000

		2160.6696, 2570.3316, 3457.7002	B 0.000000 0.741269 0.000000 S -1.57159 -0.04112 0.000000 H -0.02623 1.935795 0.000000
	20.24288, 6.46796, 5.02818	343.1678, 527.7299, 565.7582, 665.0405, 822.6565, 895.4317, 984.6489, 1063.1984, 1232.9519, 1437.8170, 3114.4799, 3242.8166	C -1.49609 -0.16258 -0.17625 C -0.55096 0.781424 0.05186 B -0.38049 -1.08427 0.236605 S 1.08685 0.000434 -0.05161 H -0.63886 1.774224 0.485282 H -2.56605 -0.07288 -0.09625
	33.54049, 3.57593, 3.23141	229.8128, 339.5234, 571.4073, 730.0246, 837.2445, 884.8443, 928.6767, 1034.5627, 1106.9624, 1640.4721, 3198.2828, 3230.2032	C 0.000000 0.657272 -1.56119 C 0.000000 -0.65727 -1.56119 B 0.000000 0.000000 -0.20419 S 0.000000 0.000000 1.509659 H 0.000000 1.52694 -2.19968 H 0.000000 -1.52694 -2.19968
	19.16284, 5.19935, 4.08971	316.4517, 361.7538, 548.7372, 630.2353, 790.8362, 846.3699, 1020.4764, 1043.8991, 1450.2498, 1965.3740, 3183.0020, 3279.7247	C 0.000000 0.709199 0.000000 C 1.024837 1.563569 0.000000 H 0.810999 2.623561 0.000000 B -1.36692 0.136089 0.000000 H 2.055008 1.239316 0.000000 S -0.13628 -1.13625 0.000000
	46.63243, 2.73554, 2.58396	-729.1787, 146.5701, 310.6330, 454.1106, 685.0097, 713.0115, 738.6594, 1192.6507, 1436.6525, 1622.8581, 2970.3423, 3421.9770	C 1.506399 0.048908 0.000000 C 2.005795 -1.15442 0.000000 H 2.153699 0.934574 0.000000 H 2.423243 -2.13346 0.000000 B 0.000000 0.234188 0.000000

			S -1.60313 0.416313 0.000000
	276.68969, 2.33287, 2.31337	-1877.5249, 175.1319, 178.8287, 327.2455, 412.4987, 497.6058, 589.9771, 814.8118, 1381.1775, 1901.3526, 2357.9750, 3111.2358	C 0.410414 -1.25064 0.000000 C 0.917259 -2.43338 0.000000 H 1.842091 -3.0018 0.000000 B 0.000000 0.14958 0.000000 S -0.58861 1.659895 0.000000 H -0.39035 -2.20029 0.000000
	317.00971, 2.36986, 2.35227	-1094.5136, 180.7017, 224.3919, 362.2304, 463.8082, 570.6772, 603.5881, 750.2688, 1375.8286, 1576.8149, 1943.4265, 3423.8163	C 0.20639 -1.349 0.000000 C 0.395818 -2.57567 0.000000 H 0.799617 -3.56026 0.000000 B 0.000000 0.090896 0.000000 S -0.35712 1.6945 0.000000 H 1.300996 -0.45819 0.000000
	18.00483, 5.50476, 4.21582	-821.0694, 278.9892, 509.5811, 577.8806, 741.4212, 906.6567, 910.7248, 1079.8611, 1206.1022, 1513.9385, 3071.8852, 3143.0218	C 1.400862 0.451871 0.000000 C 1.097878 -0.84794 0.000000 H 2.414006 0.840207 0.000000 H 1.656591 -1.78454 0.000000 B 0.000000 1.070509 0.000000 S -1.19144 -0.12699 0.000000
	33.44474, 3.28406, 2.99042	-424.0756, 252.2963, 334.7437, 605.7653, 634.1784, 720.4701, 836.7982, 1074.5938, 1416.4378, 1630.7400, 3102.6470, 3255.9960	C 1.885342 -0.3749 0.000000 C 1.401561 0.830184 0.000000 B 0.000000 0.288099 0.000000 S -1.51883 -0.30904 0.000000 H 2.727233 -1.04624 0.000000 H 1.852557 1.818621 0.000000
	105.91344, 2.397660,	-1013.3020, 177.3928, 201.6311, 405.9148,	C 1.368464 0.108408 0.000000

	2.344584	462.0846, 462.1500, 609.5067, 673.2465, 749.8696, 1466.0797, 2074.7914, 3464.5419	C 2.551295 -0.226858 0.000000 B -0.124507 0.030405 0.000000 S -1.730430 -0.064485 0.000000 H 1.220173 1.932078 0.000000 H 3.608150 -0.381975 0.000000
	23.34197, 4.04571, 3.44807	-326.8755, 319.5562, 358.2176, 539.4770, 887.9245, 891.4818, 950.6682, 982.4535, 1392.9839, 1799.3031, 3126.9513, 3211.3204	C 0.88918 0.352539 0.000001 C 2.001666 -0.32402 0.000002 H 2.945495 0.21107 0.000004 B -0.31728 1.138183 0.000002 H 2.030957 -1.40544 0.000001 S -1.29595 -0.29173 -0.000002
	119.69620, 2.31042, 2.26667	-494.2426, 150.7457, 179.8252, 309.7119, 470.3112, 476.4700, 611.1903, 715.0057, 769.5854, 1450.4396, 2133.7567, 3445.9494	C 0.507542 1.190597 0.000000 C 0.888692 2.341143 0.000000 H -0.89195 3.549904 0.000000 B 0.000000 -0.1822 0.000000 S -0.5533 -1.69499 0.000000 H 1.367357 3.290568 0.000000
	80.29662, 2.42130, 2.35042	-293.0161, 178.1215, 181.7894, 199.6682, 458.0074, 468.7030, 607.6773, 728.2473, 733.0890, 1440.1841, 2179.9604, 3453.2604	C -0.23993 -1.36684 0.000000 C -0.45047 -2.55465 0.000000 H -0.63514 -3.60174 0.000000 B 0.000000 0.080691 0.000000 S 0.147508 1.688901 0.000000 H 2.417428 -0.29517 0.000000
	2.425169	178.8808, 178.8808, 468.8034, 468.8034, 609.6339, 730.9264, 730.9264, 1455.3233,	C 0.000000 0.000000 -1.383527 C 0.000000 0.000000 -2.589912

		2179.9949	H 0.000000 0.000000 -3.65318 B 0.000000 0.000000 0.082342 S 0.000000 0.000000 1.692631
	50.39727, 2.97816, 2.81199	93.4289, 311.9075, 320.0110, 612.7250, 689.0944, 916.3587, 1472.6356, 1690.3419, 3203.3779	C 1.428659 0.723966 0.000000 C 2.325452 -0.22187 0.000000 H 1.659441 1.783015 0.000000 B 0.000000 0.188809 0.000000 S -1.51151 -0.35873 0.000000
	30.87975, 6.30288, 5.23447	422.0247, 423.5217, 633.8322, 701.0333, 868.8612, 1014.2477, 1064.2084, 1519.3785, 3302.5023	C 0.000000 0.94242 0.000000 C 1.34132 0.848322 0.000000 B 0.84771 -0.52019 0.000000 S -0.90252 -0.60566 0.000000 H 2.153897 1.547131 0.000000
	18.09312, 4.91069, 3.86241	120.7842, 336.9696, 350.1133, 621.6426, 700.6138, 703.9758, 730.4181, 2157.3709, 3487.7094	C -0.80147 -0.13069 0.004906 C -1.98361 0.112933 -0.000825 H -3.02733 0.308443 -0.009021 S 0.877232 -0.44634 -0.000977 B 1.140424 1.387924 0.000031
	19.073800	726.4789, 726.4789, 1186.9297, 2839.7902	B 0.000000 0.000000 -1.111827 S 0.000000 0.000000 0.489962 H 0.000000 0.000000 -2.280261
	282.05193, 18.58375,	573.1479, 760.1420, 2622.5626	B 0.061514 1.401006 0.000000 S 0.061514 -0.41535 0.000000

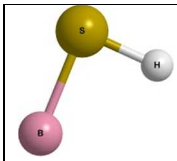
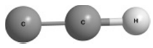
	17.43500		H -1.2918 -0.3594 0.000000
	44.704369	285.5315, 285.5315, 2094.7224, 3461.0533	C 0.000000 0.000000 0.727606 C 0.000000 0.000000 -0.471887 H 0.000000 0.000000 -1.534313

Table S2. The calculated energies refined with the coupled cluster CCSD(T)/cc-pVTZ method with B3LYP/cc-pVTZ zero-point energy corrections of collision complexes, intermediates, transition states, and dissociation products for the BS + C_2H_2 reaction on the adiabatic doublet ground state potential energy surface of C_2H_2BS.

	B3LYP / CC-pVTZ + E_{zpc}[a]	**E_{zpc}[b]**	**[c]CCSD(T)/ cc-pVTZ**	**E(kJ/mol)[d]**	**E(kJ/mol)[e]**
BS + C_2H_2	-500.346576	0.029676	-499.640917	0.0	0.0
i1	-500.423020	0.033204	-499.715436	-201	-186
i2	-500.422081	0.032814	-499.713934	-198	-183
i3	-500.447244	0.032885	-499.732230	-264	-231
i4	-500.426796	0.031582	-499.717049	-210	-195
i5	-500.376248	0.033935	-499.674764	-78	-78
i6	-500.434055	0.033562	-499.722982	-230	-205
[f]i7	—	0.035168	-499.675770	—	-77
tsi1i2	-500.416935	0.031194	-499.705774	-185	-166
tsi1i3	-500.367337	0.026764	-499.647965	-54	-26
tsi2i4	-500.380800	0.026143	-499.657733	-90	-54
tsi2i5	-500.338204	0.031758	-499.629142	22	36
tsi2i6	-500.414676	0.031586	-499.703303	-179	-159
[g]tsi2p1	—	0.024484	-499.650453	—	
tsi3i7	-500.376944	0.032951	-499.663582	-80	-51
tsi3p1	-500.371689	0.024406	-499.655066	-66	-51
tsi4p1	-500.372901	0.024214	-499.658166	-69	-60
p1	-499.871851	0.023819	-499.160113	-72	-65
[h]p2	—	0.021209	-499.084214	—	127
p3	-499.776514	0.022668	-499.070640	178	167

[i]**p4**	—	0.020981	-499.022532	—	289
p5	-500.309523	0.026442	-499.600918	97	97
p6	-500.206103	0.022970	-499.500579	369	351
cch	-76.623660	0.013958	-76.467131	—	—

[a] B3LYP/ cc-pVTZ energy with zero-point energy correction in hartree

[b] zero-point energy by B3LYP/cc-pVTZ in hartree

[c] CCSD(T)/cc-pVTZ energy

[d] relative energy by B3LYP/ cc-pVTZ with zero-point energy correction

[e] relative energy by CCSD(T)/cc-pVTZ with B3LYP/ cc-pVTZ zero-point energy correction

[f] geometry optimize by mp2/ cc-pVTZ

[g] geometry optimize by ccsd/cc-pVTZ

[h] geometry optimize by ccsd/cc-pVTZ

[i] geometry optimize by ccsd/cc-pVTZ

Table S3. The RRKM rate constants (s^{-1}) computed with B3LYP/cc-pVTZ zero-point energy corrected CCSD(T)/cc-pVTZ energies, and B3LYP/ cc-pVTZ harmonic frequencies at collision energies of 0.0, 0.1, 0.6, 8.4, 19.0, 20.9, and 41.8 kJ mol^{-1}.

	0.0	**0.1**	**0.6**	**8.4**	**19.0**	**20.9**	**41.8**
k_1 (i1 → ts-i1i2)	9.31×10^{12}	9.31×10^{12}	9.33×10^{12}	9.67×10^{12}	1.01×10^{13}	1.02×10^{13}	1.10×10^{13}
k_{-1} (i2 → ts-i1i2)	9.44×10^{12}	9.45×10^{12}	9.47×10^{12}	9.76×10^{12}	1.01×10^{13}	1.02×10^{13}	1.09×10^{13}
k_2 (i1 → ts-i1i3)	5.30×10^{8}	5.38×10^{8}	5.75×10^{8}	1.41×10^{9}	3.75×10^{9}	4.46×10^{9}	1.84×10^{10}
k_{-2} (i3 → ts-i1i3)	3.64×10^{7}	3.70×10^{7}	3.96×10^{7}	1.02×10^{8}	2.88×10^{8}	3.46×10^{8}	1.59×10^{9}
k_3 (i2 → ts-i2i4)	1.49×10^{10}	1.50×10^{10}	1.55×10^{10}	2.52×10^{10}	4.46×10^{10}	4.95×10^{10}	1.22×10^{11}
k_{-3} (i4 → ts-i2i4)	4.47×10^{9}	4.50×10^{9}	4.66×10^{9}	7.67×10^{9}	1.38×10^{10}	1.53×10^{10}	3.86×10^{10}
k_4 (i2 → ts-i2i6)	2.99×10^{12}	2.99×10^{12}	3.00×10^{12}	3.13×10^{12}	3.29×10^{12}	3.32×10^{12}	3.63×10^{12}
k_{-4} (i6 → ts-i2i6)	2.85×10^{12}	2.85×10^{12}	2.87×10^{12}	3.07×10^{12}	3.35×10^{12}	3.40×10^{12}	3.96×10^{12}
k_5 (i3 → ts-i3p1)	3.62×10^{9}	3.66×10^{9}	3.81×10^{9}	6.93×10^{9}	1.40×10^{10}	1.59×10^{10}	4.82×10^{10}
k_6 (i3 → ts-i3i7)	7.30×10^{7}	7.36×10^{7}	7.60×10^{7}	1.21×10^{8}	2.12×10^{8}	2.34×10^{8}	5.72×10^{8}
k_{-6} (i7 → ts-i3i7)	1.46×10^{12}	1.47×10^{12}	1.49×10^{12}	1.78×10^{12}	2.17×10^{12}	2.25×10^{12}	3.05×10^{12}
k_7 (i4 → ts-i4p1)	2.78×10^{10}	2.80×10^{10}	2.89×10^{10}	4.67×10^{10}	8.22×10^{10}	9.11×10^{10}	2.24×10^{11}
k_8 (i2 → ts-i2p1)	2.36×10^{9}	2.39×10^{9}	2.51×10^{9}	5.04×10^{9}	1.13×10^{10}	1.29×10^{10}	4.37×10^{10}

Table S4. Calculated relative yields (%) of the product **p1** ethynylsulfidoboron (HCCBS) formed from intermediates **i2**, **i3**, and **i4** at collision energies of 0.0, 0.1, 0.6, 8.4, 19.0, 20.9, and 41.8 kJ mol^{-1}.

	0.0	**0.1**	**0.6**	**8.4**	**19.0**	**20.9**	**41.8**
from **i2**	15.0	15.1	15.3	17.9	21.2	21.6	26.4
from **i3**	3.4	3.4	3.5	5.0	7.0	7.4	10.8
from **i4**	81.6	81.5	81.2	77.1	71.8	71.0	62.8