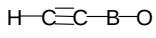
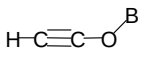
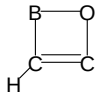
Electronic Supplementary Information

Table 2: The branching ratio with RRKM rate constants computed with UB3LYP/cc-pVTZ zero-point energy corrected CCSD(T)/cc-pVTZ energies, and UB3LYP/cc-pVTZ harmonic frequencies at collision energies of 0.0, 0.13, 0.63, 8.36, 13, 20.9, and 41.8 kJ/mol.

	0	**0.13**	**0.63**	**8.36**	**13**	**20.9**	**41.8**
k_1 *(i2→p1)*	3.21×10^{9}	3.25×10^{9}	3.43×10^{9}	7.40×10^{9}	1.11×10^{10}	2.04×10^{10}	7.39×10^{10}
k_2*(i1→i3)*	3.60×10^{7}	3.70×10^{7}	4.12×10^{7}	1.68×10^{8}	3.26×10^{8}	8.34×10^{8}	5.06×10^{9}
$\frac{k_1\,(i2 \rightarrow\ p1)}{k_1 + k_2}\times 100\%$	98.90%	98.90%	98.80%	97.80%	97.10%	96.10%	93.60%
$\frac{k_2\,(i1 \rightarrow\ i3)}{k_1 + k_2}\times 100\%$	1.10%	1.10%	1.20%	2.20%	2.90%	3.90%	6.40%

Table 3: List of OBCCH isomers investigated at the CCSD(T) and B3LYP level

OBCCH isomers	
	p1
	p4
	p5

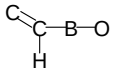
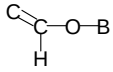
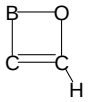
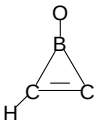
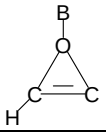
	p6
	480 kJ/mol
	not found
	not found
	not found

Table 4. The b3lyp/cc-pVTZ vibrational frequencies (cm^{-1}) and zero-point energy (Hartree) for the species in C_2H_2+BO reaction.

	Vibrational Frequencies (cm^{-1})	**Zero-Point Energy (Hartree)**
C_2H_2	650.0, 650.0, 764.6, 764.6, 2073.2, 3420.0, 3523.4	0.026987
BO	1918.2	0.004370
HBO	778.3, 778.3, 1867.5, 2896.9	0.014400
BOH	574.8, 1429.2, 3813.2	0.013252
C_2H	285.5, 285.5, 2094.7, 3461.1	0.013958
p1	205.1, 205.1, 519.7, 519.7, 744.2, 744.2, 767.9, 1994.3, 2235.0, 3454.1	0.025947

p4	84.4, 399.2, 404.6, 636.0, 637.0, 905.8, 1504.8, 2300.9, 3481.6	0.023589
p5 [a]	479.0, 489.1, 691.0, 840.7, 69.0, 1021.9, 253.4, 1562.1, 3397.2	0.024384
p6	118.0, 373.2, 385.0, 604.9, 831.5, 901.5, 1712.6, 2038.9, 3119.1	0.022975
i1	185.7, 366.6, 521.5, 682.5, 796.1, 883.9, 909.6, 1210.8, 1629.9, 2016.9, 3094.5, 3228.4	0.035372
i2	196.9, 350.5, 524.6, 654.9, 746.3, 863.3, 909.9, 1209.8, 1639.9, 2027.0, 3019.6, 3231.1	0.035024
i3	96.4, 201.9, 408.5, 529.1, 747.0, 941.0, 956.2, 1415.9, 1760.6, 2030.8, 3047.6, 3103.9	0.034717
i4	286.8, 405.7, 569.3, 682.4, 715.3, 844.3, 891.4, 935.6, 1516.0, 1740.1, 3181.4, 3222.3	0.034151
i5	286.8, 706.5, 741.7, 810.6, 880.3, 927.5, 1061.7, 1153.5, 1256.6, 1534.3, 3137.8, 3292.0	0.035971
i6	366.1, 370.0, 589.1, 690.4, 864.2, 871.4, 1017.9, 1351.4, 1436.1, 1805.9, 3143.6, 3230.1	0.035850
i7	97.4, 150.1, 472.2, 674.2, 709.4, 814.4, 980.9, 1289.2, 1499.1, 1666.9, 3131.4, 3303.8	0.033692
i8	86.9, 144.1, 424.8, 693.9, 770.7, 867.3, 900.8, 1299.0, 1485.5,1657.5,3195.1,3299.3	0.033773
i9	82.7, 135.1, 432.7, 595.9, 863.4, 864.0, 1069.5, 1387.7, 1471.7, 1719.4, 3108.0, 3231.2	0.034085
tsi1i2	-726.9, 186.6, 373.5, 536.1, 730.5, 744.5, 826.1, 1204.5, 1632.3, 2015.7, 2981.9, 3421.6	0.033382
tsi1i3	-1985.9, 193.2, 200.7, 383.6, 466.0, 570.3, 729.5, 862.3, 1799.2, 2057.6, 2366.5, 3087.4	0.028970
tsi1p1	-668.2, 189.6, 225.0, 340.9, 494.4, 520.4, 657.5, 747.0, 778.2, 1965.2, 2168.1, 3446.5	0.026274
tsi2i4	-434.6, 323.3, , 402.6, 630.2, 757.7, 822.5, 822.8, 1014.6, 1656.7, 1832.8, 3131.3, 3246.4	0.033354
tsi2i5	-777.8, 319.0, 576.7, 644.8, 681.5, 759.6, 900.3, 954.1, 1410.8, 1707.7, 3294.2, 3340.2	0.033236
tsi3i6	-818.1, 301.1, 334.1, 517.0, 769.9, 866.5, 904.9, 1331.6, 1466.2, 1796.7, 3127.2, 3206.5	0.033311

tsi3p1	-561.7, 171.0, 207.2, 354.4, 520.0, 520.7, 727.6, 767.7, 798.3, 1980.1, 2189.8, 3442.3	0.026607
tsi5i7	-292.2, 122.9, 562.7, 680.9, 746.1, 805.9, 929.4, 1191.6, 1397.1, 1652.4, 3161.5, 3284.8	0.033114
tsi5p5 [a]	-938.7, 245.7, 280.9, 321.5, 596.7, 681.6, 876.7, 967.7, 1418.6, 1451.4, 2219.9, 3387.7	0.028360
tsi6i9	-410.1, 85.0, 361.8, 550.7, 852.6, 882.1, 972.2, 1338.6, 1388.1, 1705.3, 3101.6, 3223.1	0.032945
tsi7i8	-571.1, 85.4, 152.0, 508.0, 627.5, 822.7, 851.4, 1292.3, 1479.3, 1674.4, 3143.2, 3434.8	0.032056
tsi8	-727.1, 31.5, 109.5, 358.4, 525.8, 683.6, 781.0, 1054.0, 1476.4, 1791.4, 3335.4, 3418.1	0.030904
tsi8i9	-2036.4, 80.5, 154.0, 168.7, 487.1, 632.9, 682.2, 803.0, 1425.1, 1822.5, 2351.3, 3244.3	0.027000
tsp2	-155.3, 4.8, 125.0, 126.5, 515.0, 515.1, 790.4, 790.4, 1688.3, 2079.9, 2272.5, 3452.4	0.028159

Table 5. The calculated energies for the B3LYP/cc-pVTZ optimized geometries of collision complexes, intermediates, transition states, and dissociation products for the C_2H_2+BO reaction on the adiabatic doublet ground state potential energy surface of C_2H_2BO.

	[a] UB3LYP / cc-pVTZ + E_{zpc}	**E_{zpc} [b]**	**CCSD(T)/ cc-pVTZ**	**E(kJ/mol)[c]**	**E(kJ/mol)[d]**
C_2H_2+BO	-177.397894	0.031357	-177.0572581	0	0
H	-0.502156	0.000000	-0.4998098	-	-
C_2H	-76.62366	0.013958	-76.4671305	-	-
C_2H_2	-77.336565	0.026987	-77.1872726	-	-
BO	-100.061329	0.004370	-99.8699855	-	-
HBO	-100.740063	0.014400	-100.5529372	-	-
BOH	-100.665321	0.013252	-100.4822945	-	-
CHCBO	-176.919651	0.025947	-176.5740286	-	-
CHCOB	-176.785375	0.023589	-176.4397079	-	-
i1	-177.473898	0.035372	-177.1316292	-199.5	-184.7
i2	-177.473400	0.035024	-177.1306336	-198.2	-183.0
i3	-177.489373	0.034717	-177.1413695	-240.2	-212.0
i4	-177.459011	0.034151	-177.1096279	-160.5	-130.2
i5	-177.399752	0.035971	-177.0628840	-4.9	-2.7

i6	-177.398892	0.035850	-177.0576332	-2.6	10.8
i7	-177.361798	0.033692	-177.0211114	94.8	101.0
i8	-177.36165	0.033773	-177.0207407	95.2	102.2
i9	-177.367805	0.034085	-177.0261125	79.0	88.9
p1	-177.421807	0.025947	-177.0738384	-62.8	-57.7
p2	-177.363723	0.028358	-177.0200677	89.7	89.8
p3	-177.288981	0.027210	-176.9494250	286.0	272.2
p4	-177.287531	0.023589	-176.9395177	289.8	288.7
p5[e]	-176.886255	0.024384	-176.9488011	253.9	266.4
p6	-177.348069	0.022975	-176.9982335	130.8	133.0
ts-i1i2	-177.468197	0.033382	-177.1223522	-184.6	-165.6
ts-i1i3	-177.411686	0.028970	-177.0590682	-36.2	-11.0
ts-i2p1	-177.416641	0.026274	-177.0647836	-49.2	-33.1
ts-i2i4	-177.45666	0.033354	-177.1093836	-154.3	-131.6
ts-i2i5	-177.375172	0.033236	-177.0305575	59.7	75.0
ts-i3i6	-177.380875	0.033311	-177.0295637	44.7	77.8
ts-i3p1	-177.418764	0.026607	-177.0681049	-54.8	-40.9
ts-i5i7	-177.357685	0.033114	-177.0163265	105.6	112.1
ts-i5p5	-176.871287	0.028360	-176.9482392	293.2	281.0
ts-i6i9	-177.358999	0.032945	-177.0182140	102.1	106.7
ts-i7i8	-177.359124	0.032056	-177.0151278	101.8	112.4
ts-i8i9	-177.289125	0.027000	-176.9396818	285.6	297.3
ts-i8	-177.350622	0.030904	-176.9957453	124.1	160.3
ts-p2	-177.361511	0.028159	-177.0138253	95.5	105.6

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

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

[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] by MP2/cc-pVTZ methode.

Table 6. The calculated energies for the CCSD/cc-pVTZ optimized geometries of collision complexes, intermediates, transition states, and dissociation products for the C_2H_2 + BO reaction on the adiabatic doublet ground state potential energy surface of C_2H_2BO.

	[a] CCSD/ cc-pVTZ + E_{zpc}	**E_{zpc} [b]**	**CCSD(T) / cc-pVTZ**	**E(kJ/mol)[c]**	**E(kJ/mol)[d]**
C_2H_2+BO	-176.995524	0.031260	-177.0576394	0	0
H	-0.499810	0.000000	-0.4998098	-	-
C_2H	-76.437759	0.014886	-76.4673842	-	-
C_2H_2	-77.144320	0.026864	-77.1875668	-	-

BO	-99.851204	0.004396	-99.8700726	-	-
HBO	-100.523967	0.014402	-100.5530248	-	-
BOH	-100.456455	0.013550	-100.4825126	-	-
CHCBO	-176.515486	0.025925	-176.5743531	-	-
CHCOB	-176.387249	0.023680	-176.4410904	-	-
i1	-177.066171	0.035940	-177.1318842	-185.5	-182.6
i2	-177.065655	0.035593	-177.1308821	-184.1	-180.9
i3	-177.076498	0.034983	-177.1416381	-212.6	-210.8
i4	-177.044063	0.034095	-177.1100481	-127.4	-130.2
i5	-176.995238	0.036651	-177.0628435	0.8	0.5
i6	-176.988774	0.036958	-177.0576852	17.7	14.8
i7	-176.95947	0.034445	-177.0216203	94.7	102.9
i8	-176.958908	0.034574	-177.0212838	96.1	104.2
i9	-176.964096	0.034643	-177.0267748	82.5	89.9
p1	-177.015296	0.025925	-177.0741629	-51.9	-57.4
p2	-176.961726	0.029288	-177.020409	88.7	92.6
p3	-176.894214	0.028436	-176.9498968	266.0	275.5
p4	-176.887059	0.023680	-176.9409002	284.8	286.6
p5	-176.886109	0.024070	-176.9493168	287.3	265.5
p6	-176.944506	0.023316	-176.9986050	133.9	134.1
ts-i1i2	-177.058949	0.033769	-177.1225612	-166.5	-163.9
ts-i1i3	-176.99687	0.029319	-177.0593538	-3.5	-9.6
ts-i2p1	-177.004725	0.026678	-177.0644196	-24.2	-29.8
ts-i2i4	-177.043437	0.033570	-177.1093307	-125.8	-129.7
ts-i2i5	-176.962031	0.033580	-177.0306355	87.9	77.0
ts-i3i6	-176.960437	0.034019	-177.0285622	92.1	83.6
ts-i3p1	-177.006980	0.026960	-177.0670423	-30.1	-36.0
ts-i5i7	-176.953203	0.033716	-177.0167189	111.1	113.9
ts-i5p5	-176.883130	0.025248	-176.9471627	293.2	281.0
ts-i6i9	-176.954819	0.033588	-177.0180082	106.9	110.2
ts-i7i8	-176.954899	0.032631	-177.0155629	106.7	114.1
ts-i8i9	-176.8814	0.027330	-176.9402498	299.6	297.9
ts-i8	-177.350622	0.030904	-176.9957453	-932.3	161.6
ts-p2	-176.954219	0.026844	-177.0131382	108.4	105.2

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

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

[c] relative energy by CCSD/ cc-pVTZ with zero-point energy correction.

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