Photoinduced Boron Atom Insertion of Benzocyclobutene Forming Unprecedented Fused Boron Heterocyclic Radical.

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Experimental and Computational methods

The experimental setup for pulsed laser evaporation and matrix isolation infrared absorption spectroscopy has been described in detail previously,[1-2] only a short description will be provided here. The 1064 nm Nd:YAG laser fundamental wavelength (Continuum, Minilite II; 10 Hz repetition rate) was focused onto a rotating boron target to produce the boron atoms. Natural abundance boron (^{10}B, 19.8%; ^{11}B, 80.2%) and ^{10}B-enriched (97%) targets were used in different experiments. The laser evaporated boron atoms were co-deposited with benzocyclobutene reagent gas in excess neon onto a cryogenic CsI window, which was maintained at 4 K by means of a closed-cycle helium refrigerator. The samples were usually deposited for 30min at a rate of approximately 6mmol/h. The C_8H_8/Ne mixtures were prepared in a stainless steel vacuum line using standard manometric technique. The benzocyclobutene reagent was used without further purification in the experiment. The as-deposited samples were subjected to annealing and photolysis experiments to initiate diffuse and photo-induced reactions. Selected samples were also subjected to broad-band irradiation using a tungsten lamp or a high-pressure mercury arc lamp with glass filters to initiate further isomerization or dissociation reactions. The infrared absorption spectra of the products in the mid-infrared region (4000-450 cm^{-1}) were recorded on a Bruker Vertex 70V spectrometer at 0.5 cm^{-1} resolution using a liquid nitrogen cooled HgCdTe (MCT) detector.

Quantum chemical calculations were performed to determine the molecular structures and to support the assignment of vibrational frequencies of the observed reaction products. The geometry structure optimization and vibrational frequency computation were done the using the three-parameter hybrid functional according to Becke with additional correlation corrections due to Lee, Yang, and Parr (B3LYP)with Gaussian09 program package.[3-5] The dunning's correlation consistent basis set with polarized triple-zeta plus diffuse functions (aug-cc-pVTZ) has been used for the B, C, H atoms.[6-7] The zero point energy calculations were performed using the CCSD(T)/ cc-pVTZ.[8-9] Based on the various possible geometries with different spin states, energy and vibrational calculations were performed to interpret the experimental vibrational features. Transition-state optimizations were performed with the synchronous transit-

guided quasi-Newton (STQN) method and were verified through intrinsic reaction coordinate (IRC) calculations.[10]

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Table S1. Calculated vibrational frequencies (unscaled, cm^{-1}) and intensities (in parentheses in

km/mol) of **species A**. The experimentally observed values for $^{10}B(C_8H_8)$ are also listed for comparison.

^{10}B	^{11}B			
C_8H_8	C_8H_8	Δ	$^{10}B/^{11}B$	Exptl.
3176.7 (22)	3176.7 (22)	0	1.0000	
3163.0 (22)	3163.0 (22)	0	1.0000	
3142.9 (1)	3142.9 (1)	0	1.0000	
3140.6 (7)	3140.6 (7)	0	1.0000	
3103.6 (23)	3103.6 (23)	0	1.0000	
3084.4 (1)	3084.4 (1)	0	1.0000	
3048.0 (82)	3048.0 (82)	0	1.0000	
3042.0 (36)	3042.0 (36)	0	1.0000	
1639.6 (1)	1639.6 (1)	0	1.0000	
1561.3 (29)	**1561.3 (29)**	0	**1.0000**	**1544.8**
1507.5 (4)	1507.4 (4)	0.1	1.0001	
1490.6 (2)	1490.6 (2)	0	1.0000	
1440.2 (2)	1439.9 (1)	0.3	1.0002	
1393.0 (5)	1393.0 (5)	0	1.0000	
1375.9 (11)	**1359.9 (11)**	16	**1.0118**	**1323.3**
1294.0 (0)	1293.0 (1)	1	1.0008	
1241.2 (2)	1238.8 (3)	2.4	1.0019	
1239.4 (10)	1238.3 (9)	1.1	1.0009	
1214.8 (2)	1214.2 (2)	0.6	1.0005	
1199.5 (0)	1199.2 (0)	0.3	1.0003	
1169.2 (1)	1167.8 (1)	1.4	1.0012	
1151.3 (12)	**1150.0 (12)**	1.3	**1.0011**	**1138.1**
1110.0 (0)	1106.3 (0)	3.7	1.0033	
1083.9 (3)	1083.2 (3)	0.7	1.0007	
1007.5 (0)	1007.2 (0)	0.3	1.0003	
983.9 (1)	983.8 (1)	0.1	1.0001	
955.0 (6)	955.0 (6)	0	1.0000	
951.6 (3)	950.5 (3)	1.1	1.0012	
931.1 (1)	930.5 (1)	0.6	1.0006	
910.4 (17)	**906.1 (17)**	4.3	**1.0048**	**887.3**
824.8 (2)	816.1 (3)	8.7	1.0107	
796.0 (1)	795.6 (1)	0.4	1.0005	
786.3 (1)	786.0 (1)	0.3	1.0004	
754.4 (2)	744.0 (2)	10.4	1.0140	
723.7 (47)	**722.9 (46)**	0.8	**1.0011**	**704.5**
637.1 (4)	634.4 (4)	2.7	1.0043	
600.6 (18)	600.2 (18)	0.4	1.0007	
513.8 (3)	513.8 (3)	0	1.0000	
492.0 (5)	486.0 (5)	6	1.0124	
456.8 (1)	456.8 (1)	0	1.0000	
396.9 (7)	391.6 (8)	5.3	1.0135	
285.9 (10)	281.7 (10)	4.2	1.0149	
260.5 (0)	258.8 (0)	1.7	1.0066	
170.5 (4)	169.3 (4)	1.2	1.0071	
115.3 (0)	115.2 (0)	0.1	1.0009	

Table S2. Calculated vibrational frequencies (unscaled, cm^{-1}) and intensities (in parentheses in

km/mol) of species **B**. The experimentally observed values for $^{10}B(C_8H_8)$ are also listed for comparison.

^{10}B	^{11}B			
C_8H_8	C_8H_8	Δ	$^{10}B/^{11}B$	Exptl.
3167.9 (13)	3167.9 (13)	0	1.0000	
3166.7 (48)	3166.7 (48)	0	1.0000	
3147.5 (34)	3147.5 (34)	0	1.0000	
3139.8 (17)	3139.8 (17)	0	1.0000	
3128.9 (6)	3128.9 (6)	0	1.0000	
3123.4 (23)	3123.4 (23)	0	1.0000	
3012.8 (10)	3012.8 (10)	0	1.0000	
2996.2 (25)	2996.2 (25)	0	1.0000	
1590.7 (0)	1588. 6 (1)	2.7	1.0017	
1546.8 (22)	**1546.7 (24)**	0.1	**1.0001**	**1513.8**
1529.9 (38)	**1528.1 (31)**	1.8	**1.0012**	**1498.2**
1454.2 (47)	**1445.7 (35)**	8.5	**1.0059**	**1420.2**
1444.7 (12)	1444.3 (16)	0.4	1.0003	
1395.1 (2)	1390.9 (1)	4.2	1.0030	
1376.4 (56)	**1372.6 (54)**	3.8	**1.0028**	**1352.7**
1347.8 (4)	1346.7 (5)	1.1	1.0008	
1279.9 (7)	**1272.5 (8)**	7.4	**1.0058**	**1258.6**
1223.3 (1)	1211.8 (3)	11.5	1.0095	
1198.1 (33)	**1180.2 (25)**	17.9	**1.0152**	**1176.0**
1164.6 (2)	1164.5 (2)	0.1	1.0001	
1160.4 (4)	1155.4 (6)	5	1.0043	
1136.5 (16)	**1134.9 (18)**	1.6	**1.0014**	**1116.0**
1115.6 (6)	1108.5 (13)	7.1	1.0064	
1053.2 (0)	1043.9 (1)	9.3	1.0089	
1017.2 (0)	1017.2 (0)	0	1.0000	
1015.9 (1)	1015.9 (1)	0	1.0000	
979.8 (0)	979.7 (0)	0.1	1.0001	
977.5 (0)	977.5 (0)	0	1.0000	
943.8 (12)	**942.7 (11)**	1.1	**1.0012**	**914.2**
926.2 (3)	926.1 (3)	0.1	1.0001	
846.0 (7)	845.9 (7)	0.1	1.0001	
818.8 (3)	816.6 (2)	2.2	1.0027	
785.7 (3)	783.2 (4)	2.5	1.0032	
774.8 (72)	**766.5 (78)**	8.3	**1.0108**	**751.9/750.1**
705.3 (2)	703.6 (0)	1.7	1.0024	
669.1 (1)	668.0 (1)	1.1	1.0017	
664.1 (11)	658.4 (8)	5.7	1.0087	
535.5 (0)	533.5 (0)	2	1.0038	
480.3 (2)	480.0 (2)	0.3	1.0006	
475.2 (0)	472.4 (0)	2.8	1.0059	
384.6 (5)	384.0 (5)	0.6	1.0016	
368.4 (2)	365.7 (2)	2.7	1.0074	
325.4 (0)	325.0 (0)	0.4	1.0012	
187.3 (4)	186.2 (3)	1.1	1.0059	
134.1 (0)	133.7 (0)	0.4	1.0030	

Table S3. Calculated vibrational frequencies (unscaled, cm^{-1}) and intensities (in parentheses in

km/mol) of species **A** isomer (**I1**).

^{10}B	^{11}B		
C_8H_8	C_8H_8	Δ	$^{10}B/^{11}B$
3198.5 (16)	3198.5 (16)	0	1.0000
3195.2 (9)	3195.2 (9)	0	1.0000
3177.1 (11)	3177.1 (11)	0	1.0000
3169.9 (2)	3169.9 (2)	0	1.0000
3114.7 (22)	3114.7 (22)	0	1.0000
3097.6 (0)	3097.6 (0)	0	1.0000
3064.1 (54)	3064.1 (54)	0	1.0000
3054.7 (30)	3054.7 (30)	0	1.0000
1614.5 (7)	1614.5 (7)	0	1.0000
1567.1 (8)	1566.9 (8)	0.2	1.0001
1493.4 (0)	1493.4 (0)	0	1.0000
1466.6 (3)	1466.6 (3)	0	1.0000
1360.0 (6)	1360.0 (6)	0	1.0000
1309.1 (3)	1308.4 (3)	0.7	1.0005
1292.4 (6)	1291.6 (6)	0.8	1.0006
1267.3 (6)	1267.1 (6)	0.2	1.0002
1216.3 (1)	1216.1 (1)	0.2	1.0002
1207.8 (0)	1207.8 (0)	0	1.0000
1189.9 (4)	1189.3 (3)	0.6	1.0005
1188.2 (2)	1186.3 (3)	1.9	1.0016
1117.3 (2)	1117.0 (2)	0.3	1.0003
1094.4 (4)	1092.9 (4)	1.5	1.0014
1079.9 (3)	1078.9 (3)	1.0	1.0009
1039.8 (0)	1038.4 (0)	1.4	1.0014
1024.0 (2)	1022.6 (2)	1.4	1.0014
966.6 (7)	964.0 (7)	2.6	1.0027
937.9 (2)	937.3 (1)	0.6	1.0006
913.1 (21)	**910.1 (20)**	**3.0**	**1.0033**
911.8 (6)	911.7 (4)	0.1	1.0001
907.6 (8)	904.7 (14)	2.9	1.0032
838.5 (3)	834.1 (4)	4.4	1.0053
818.1 (6)	813.4 (3)	4.7	1.0058
776.9 (8)	774.6 (5)	2.3	1.0030
766.7 (11)	**764.1 (14)**	**2.6**	**1.0034**
717.0 (18)	**710.6 (16)**	**6.4**	**1.0090**
696.8 (7)	684.8 (5)	12	1.0175
668.1 (8)	666.3 (9)	1.8	1.0027
612.7 (2)	611.5 (2)	1.2	1.0020
553.9 (6)	548.1 (6)	5.8	1.0106
524.9 (8)	519.6 (7)	5.3	1.0102
461.8 (2)	455.8 (3)	6.0	1.0132
412.7 (2)	409.6 (2)	3.1	1.0076
397.8 (0)	396.2 (0)	1.6	1.0040
270.9 (3)	269.7 (3)	1.2	1.0045
194.0 (1)	193.6 (1)	0.4	1.0021

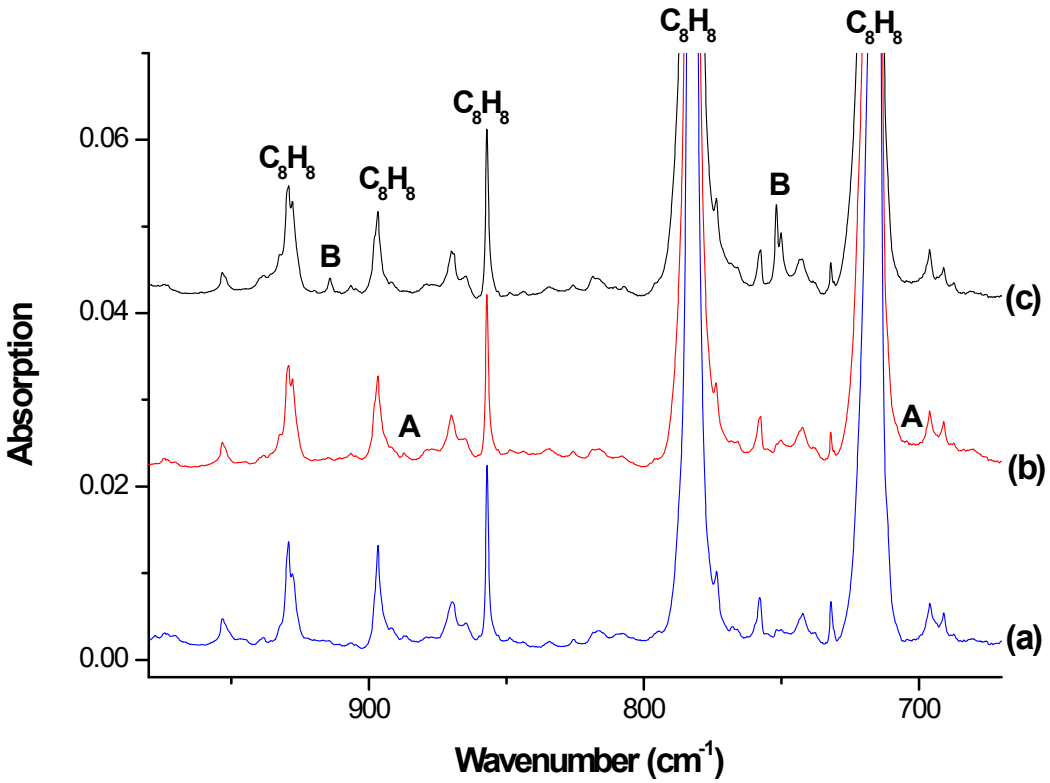


Figure S1. Infrared spectra in the 970-670 cm^{-1} region from co-deposition of boron atoms (^{10}B-enriched,97%) with 0.05 % benzocyclobutene in solid neon. (a) after 30 min deposition at 4K, (b) afterward annealing to 12 K, (c) after 15 min of UV−visible light (280 <λ< 580 nm) irradiation.

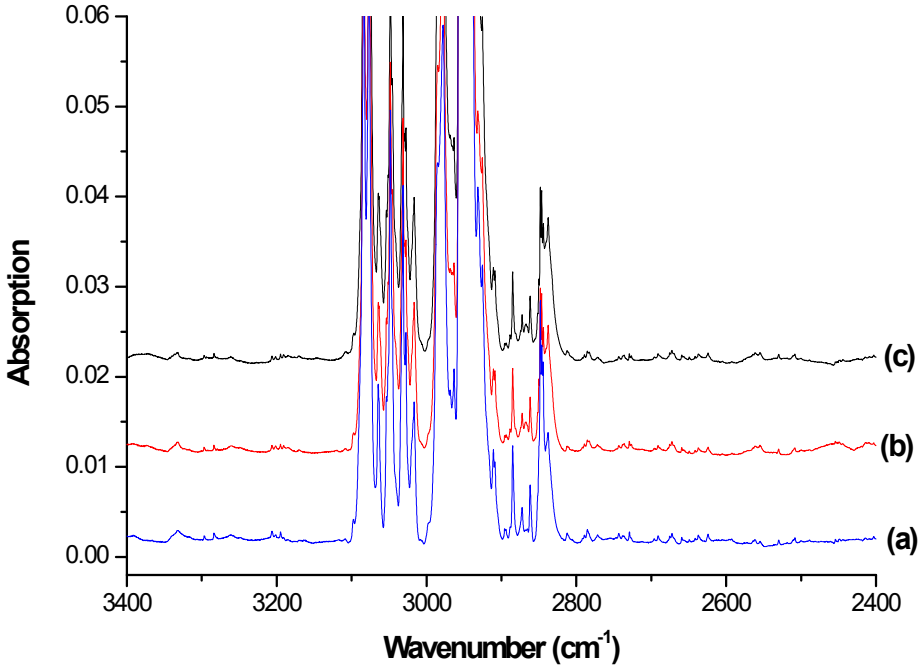


Figure S2. Infrared spectra in the 3400-2400 cm^{-1} region from co-deposition of boron atoms (^{10}B-enriched,97%) with 0.05 % benzocyclobutene in solid neon. (a) after 30 min deposition at 4K, (b) afterward annealing to 12 K, (c) after 15 min of UV−visible light (280 <λ< 580 nm) irradiation.

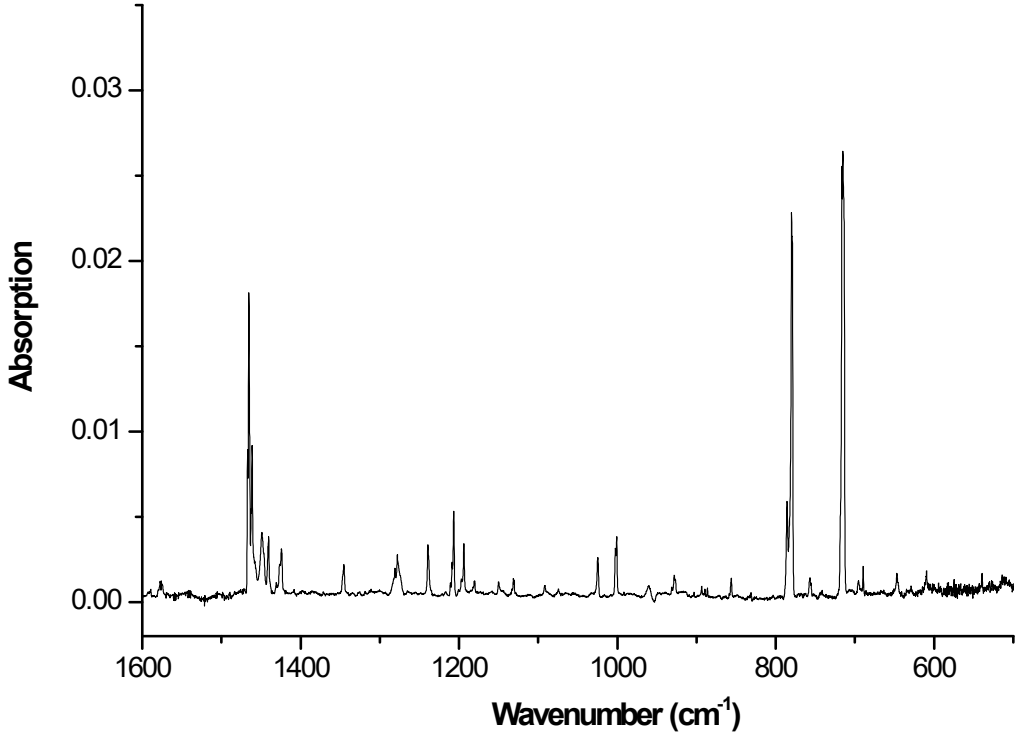


Figure S3. Infrared spectra in the 1600-500 cm^{-1} region from 10 minutes deposition of net 0.05 % benzocyclobutene in solid argon.

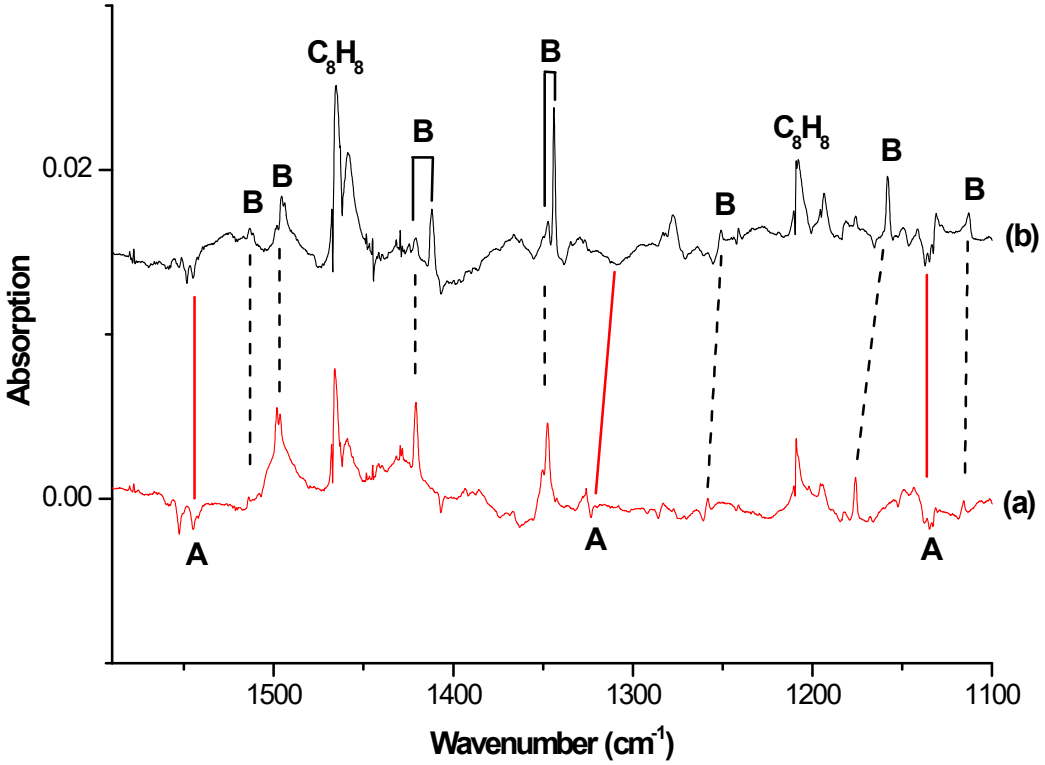


Figure S4. Infrared difference spectra in the 1590-1100 cm^{-1} regions from co-deposition of boron with benzocyclobutene in solid neon (spectra taken after 15 min λ>280 nm UV light irradiation minus spectrum after annealing to 12 K): (a) ^{10}B+0.05% C_8H_8, (b) ^{n}B+0.05% C_8H_8.

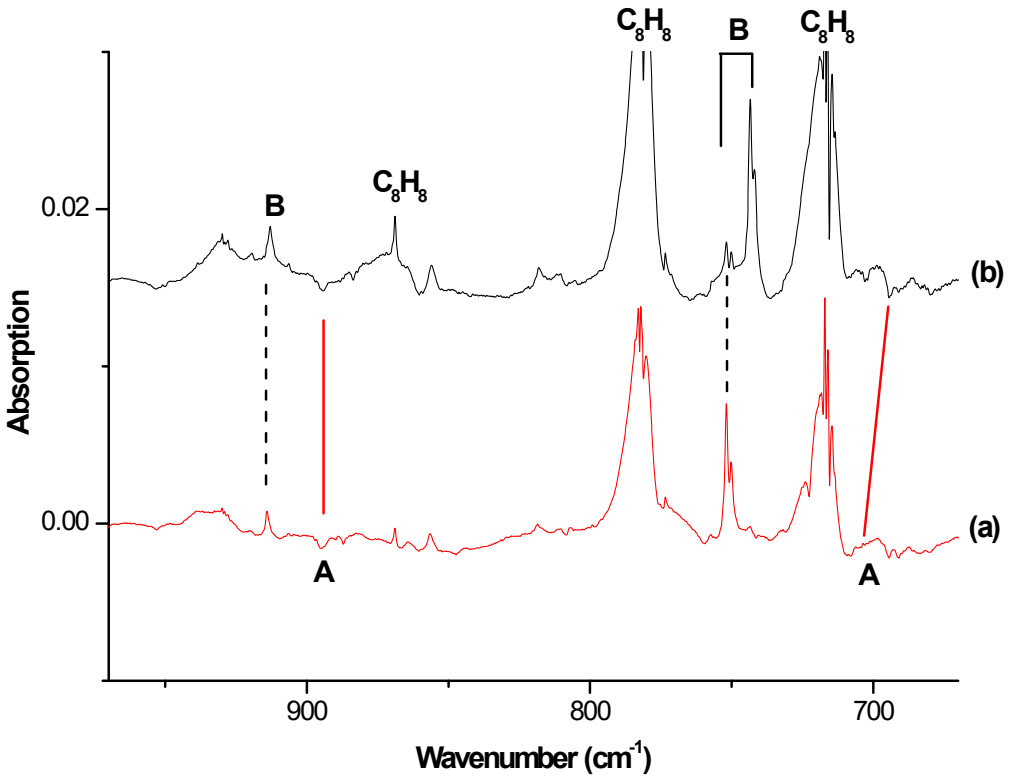
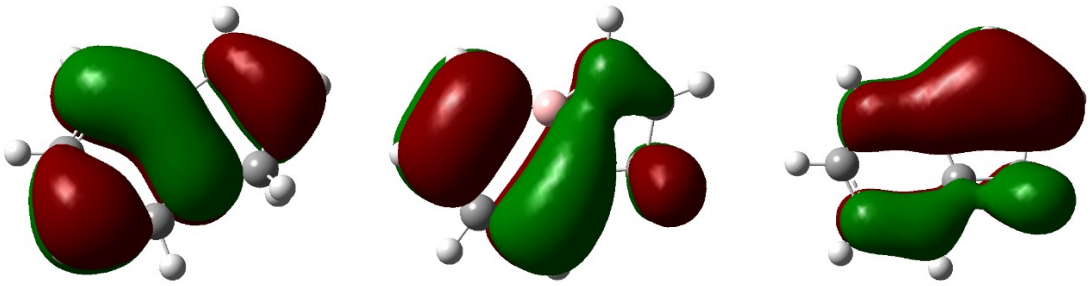


Figure S5. Infrared difference spectra in the 970-670 cm^{-1} regions from co-deposition of boron with benzocyclobutene in solid neon (spectra taken after 15 min λ>280 nm UV light irradiation minus spectrum after annealing to 12 K): (a) ^{10}B+0.05% C_8H_8, (b) ^{n}B+0.05% C_8H_8.



(B) SOMO **(B)** HOMO **(B)** HOMO-1

Figure S6. Shapes of the SOMO, HOMO and HOMO-1 of species **B** plotted with isosurfaces = 0.03 a.u.

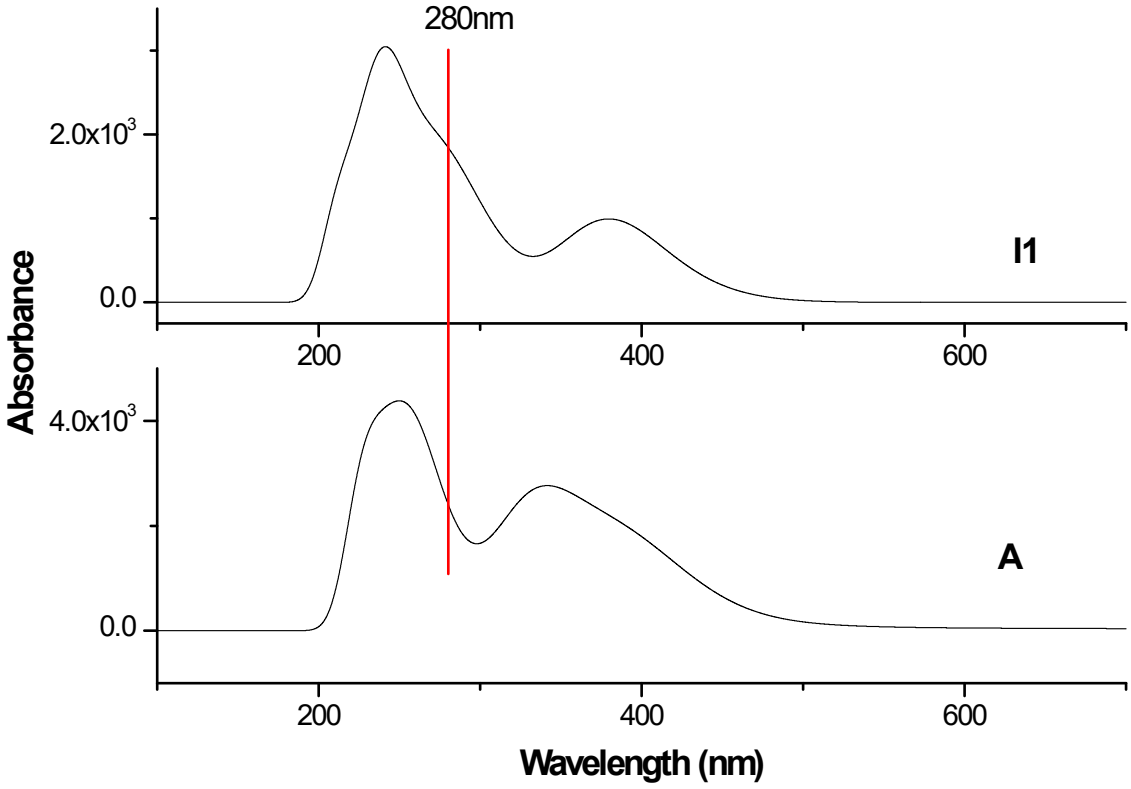


Figure S7. The calculated electronic absorptions spectrum of species **A** and intermediate **I1** at the B3LYP-TD/aug-cc-pVTZ level of theory.

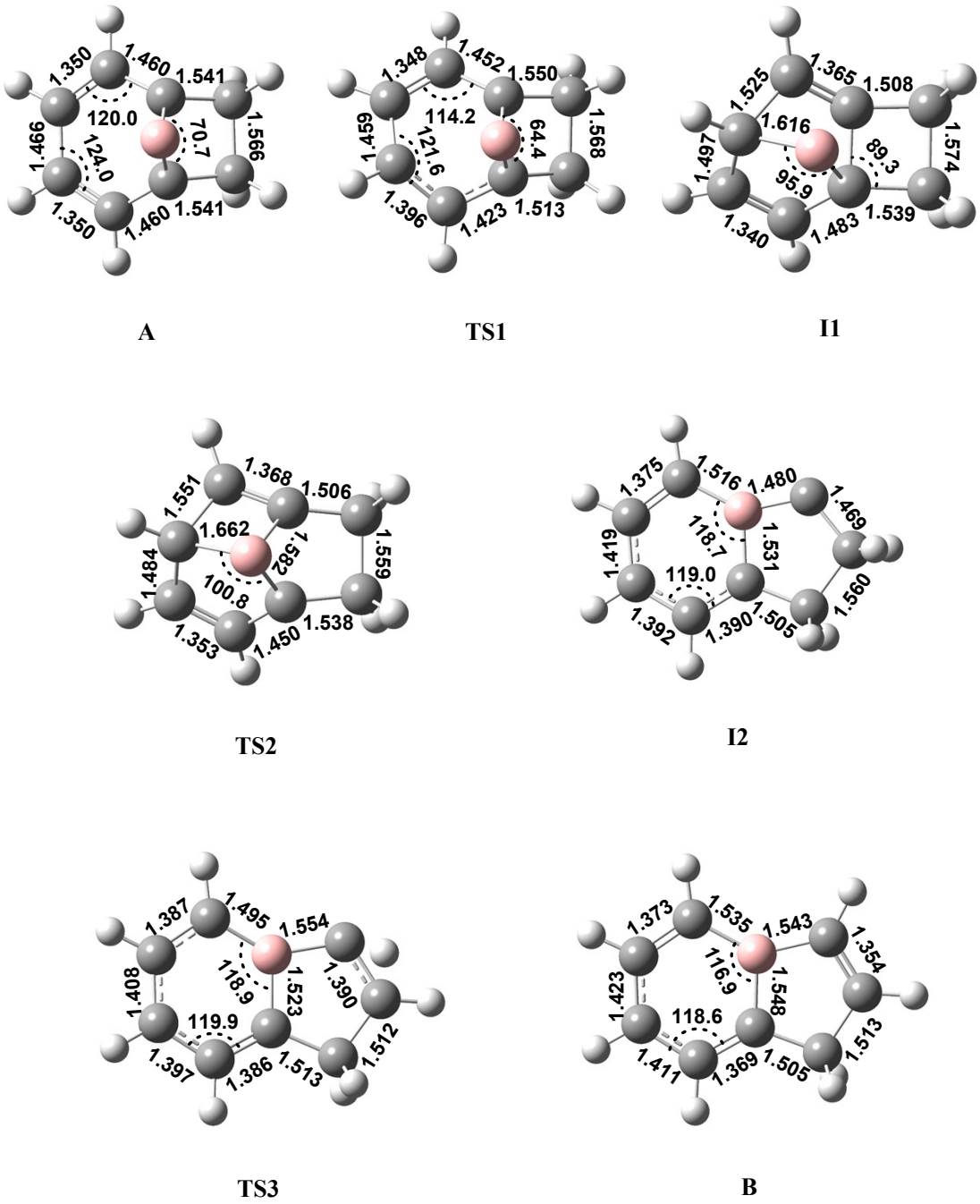


Figure S8. Optimized structures of the intermediates and transition states involved in the reaction pathways as shown in figure 3 at the B3LYP/aug-ccpVTZ level. Bond lengths in angstroms and bond angles in degrees.

Table S6. Calculated atomic coordinates (in Angstroms) of species **A**, **B**, and the intermediates and transition states at the B3LYP/aug-cc-pVTZ level.

(a) **A**, (C_s, $^2A'$)

C	-0.20665800	0.59518500	0.87121600
C	-0.20665800	0.59518500	-0.87121600
B	-1.34781700	1.05127100	0.00000000
C	-0.43677600	-1.82355100	0.73304800
H	-0.46927000	-2.79246800	1.21465500
C	-0.43677600	-1.82355100	-0.73304800
H	-0.46927000	-2.79246800	-1.21465500
C	-0.20665800	-0.72843000	1.48768500
C	-0.20665800	-0.72843000	-1.48768500
H	0.02898900	-0.82349800	2.54167800
H	0.02898900	-0.82349800	-2.54167800
C	1.01748000	1.52662200	-0.78278600
H	1.91344500	1.06398100	-1.19275600
H	0.89205000	2.50484900	-1.24753100
C	1.01748000	1.52662200	0.78278600
H	0.89205000	2.50484900	1.24753100
H	1.91344500	1.06398100	1.19275600

(b) **B**, (C_s, $^2A''$)

C	1.33675700	1.04630900	0.00000000
C	2.26377600	-0.01708400	0.00000000
C	1.89489600	-1.39169700	0.00000000
C	0.58778700	-1.81078200	0.00000000
C	-2.02912200	-0.61218000	0.00000000
C	-2.36596300	0.69971300	0.00000000
H	1.71572500	2.06386400	0.00000000
H	3.32074400	0.22020400	0.00000000
H	2.70578000	-2.11224400	0.00000000
H	0.39779300	-2.87867800	0.00000000
H	-2.79006600	-1.38307800	0.00000000
H	-3.38412200	1.07475100	0.00000000
C	-1.19815800	1.66184500	0.00000000
H	-1.22736900	2.32364500	0.87345100
H	-1.22736900	2.32364500	-0.87345100
B	-0.49018900	-0.71821200	0.00000000
C	0.00000000	0.75036900	0.00000000

(c) **TS1**

B	0.05244500	-0.47786600	1.38081100
C	0.40423200	0.70170600	0.45090400
C	0.49261100	-0.86193100	-0.04431200
C	-0.79920500	-1.42421500	-0.24438400
C	-1.87778500	-0.58251700	0.03162000
C	-1.83048100	0.84512200	-0.26744800
C	-0.64796500	1.48488300	-0.17070600
C	1.91124100	0.77592400	0.09456800
C	1.90940500	-0.66052400	-0.53493800
H	-0.94501300	-2.49259700	-0.35003500
H	-2.84308200	-1.04186700	0.19916400
H	-2.72577400	1.31814100	-0.64764100
H	-0.47365700	2.47979000	-0.56055700
H	2.13117800	1.56065300	-0.62616100
H	2.57768500	0.89124500	0.94810300
H	1.99705000	-0.63785600	-1.62047600
H	2.64706800	-1.35887100	-0.13827100

(d) **I1**

C	-0.34858400	0.64747100	0.30434300
C	0.75354100	1.46736600	-0.25334200
H	0.60891800	2.45380800	-0.67226300
B	0.35905000	-0.54426300	1.17163000
C	-0.52668400	-0.69169400	-0.35367900
C	-1.87684300	0.82940400	0.30757600
H	-2.33584800	0.92610400	1.28943400
H	-2.22542700	1.64072300	-0.32913600
C	-2.03131500	-0.58481100	-0.36580300
H	-2.44681000	-0.53430500	-1.37111600
H	-2.56530800	-1.34736200	0.20077100
C	1.88888100	0.75652200	-0.29217300
H	2.81643300	1.08246000	-0.74165300
C	0.60958200	-1.44808000	-0.35158500
H	0.68639200	-2.51273900	-0.51680800
C	1.71123900	-0.61123600	0.28963300
H	2.58749800	-1.17701900	0.57281100

(e) **TS2**

C	-0.33544300	0.80462900	0.42397000
C	-0.54730500	-0.97537500	-0.03873800
C	0.66224300	-1.47404100	-0.43820700
C	1.67598300	-0.59104600	0.33572400
C	1.85920500	0.73499900	-0.30461400
C	0.72466400	1.47283900	-0.30626400
C	-1.84316600	0.85650300	0.12699700
C	-1.98159900	-0.62553300	-0.33763100
B	0.26063200	-0.36687300	1.17731600
H	0.91611300	-2.44087200	-0.85580400
H	2.56960000	-1.11823500	0.64630000
H	2.78926300	1.03454100	-0.76891300
H	0.59440800	2.40795000	-0.83720200
H	-2.45025800	1.11062600	0.99503100
H	-2.08223100	1.55632800	-0.67161000
H	-2.69750000	-1.21707100	0.23254000
H	-2.23004500	-0.71675600	-1.39433700

(f) **I2**

C	-1.52057800	-1.35419900	-0.00006400
C	1.30459300	-1.46528400	0.00002000
C	0.81432400	1.43286600	-0.00002600
C	-0.30368600	0.60620600	0.00009500
C	2.32415300	-0.54200400	-0.00008200
H	3.36073500	-0.86052300	-0.00016400
C	2.08102100	0.85580200	-0.00010300
H	2.94280500	1.51312500	-0.00022300
H	1.56552800	-2.51753000	0.00003600
H	0.73286000	2.51584900	-0.00008500
B	-0.10756000	-0.91261000	0.00010200
C	-1.74960700	1.02210600	0.00008200
H	-1.99809700	1.62909800	0.87543000
H	-1.99806900	1.62916700	-0.87522400
C	-2.55681600	-0.31297400	0.00001200
H	-3.21425900	-0.40053800	-0.87245700
H	-3.21412500	-0.40071300	0.87257900

(g) **TS3**

C	-1.62491900	-1.32244600	-0.03306200
C	1.24077100	-1.47038100	-0.02972500
C	0.84332700	1.41920000	0.00675000
C	-0.28965700	0.62964400	-0.10915400
C	2.29507700	-0.57133700	0.02354500
H	3.31720600	-0.93378900	0.05474600
C	2.10630600	0.82377600	0.04270000
H	2.97954600	1.46125000	0.10128700
H	1.47572400	-2.52870400	-0.05499500
H	0.77487000	2.50157000	0.08237500
B	-0.13433200	-0.88573200	-0.09018500
C	-1.73529300	1.06685400	-0.01164800
H	-1.95934400	1.65628900	0.88303200
H	-2.09429500	1.66504300	-0.85972700
C	-2.49659500	-0.23965400	-0.00069800
H	-3.57211800	-0.31214400	-0.12845300
H	-2.28403400	-1.09479700	1.04041400