Supporting Information

Transforming Benzylideneamine N,C-Chelate Boron Compounds to BN-cycloocta- / cyclohepta-trienes Bearing a Tetrasubstituted B=N Unit via Photoisomerization

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S1. Experimental

General

All reactions were carried out under an nitrogen atmosphere. Solvents were dried by standard methods and freshly distilled over sodium prior to use. ^{1}H, ^{13}C, and ^{11}B NMR spectra were recorded on a Bruker Avance 300, 400, 600 and 700 MHz spectrometers and deuterated solvents were purchased from Cambridge Isotopes and Sigma-Aldrich, further dried over 4 Å molecular sieves and C_6D_6 degassed prior to use. High resolution mass spectra (HRMS) were obtained using a Micromass GC-TOF spectrometer. Starting materials were purchased from Sigma-Aldrich without further purification. $BMes_2F$ were prepared according to literature procedures.[1S]

Syntheses and characterization

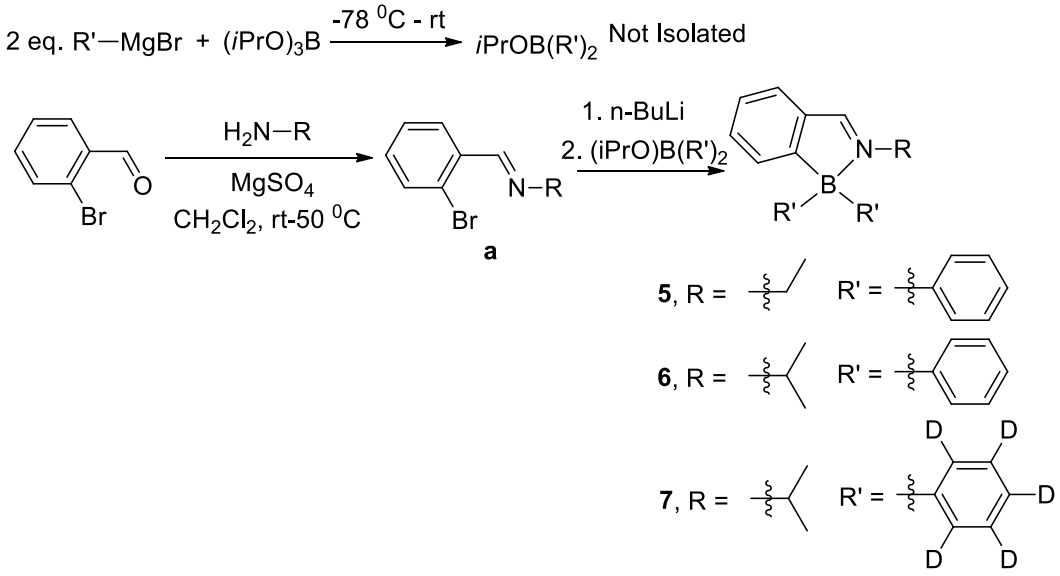
2-(dimesitylboryl)benzylideneethylamine (1). The synthesis of compound **1** was carried out using ethylamine as the starting material in THF, and a procedure similar to that reported previously[2S] to afford pale solid in a crude yield of 98%. Further purification can be achieved by washing with dry hexanes.[2S] ^{1}H NMR (400 MHz, C_6D_6): δ (ppm) 0.43 (t, J = 7.2 Hz, 3H), 1.67 (s, 3H), 1.79 (s, 3H), 2.23 (s, 6H), 2.29 (s, 3H), 2.50 (s, 3H), 3.46 (d, J = 20.8 Hz, 2H), 6.66 (s, 1H), 6.75 (s, 1H), 6.94 (s, 2H), 6.99 (t, J = 7.4 Hz, 1H), 7.09 (t, J = 7.4 Hz, 1H), 7.26 (d, J = 7.5 Hz, 1H), 7.39 (s, 1H), 7.88 (d, J = 7.5 Hz, 1H); ^{13}C NMR (101 MHz, C_6D_6): δ (ppm) 14.5, 20.7, 22.7, 25.8, 26.8, 46.0, 124.7, 125.2, 129.7, 130.5, 130.8, 131.1, 131.9, 136.9, 165.9; ^{11}B NMR (128 MHz, C_6D_6): δ (ppm) 4.7; HRMS (EI), calcd for $C_{27}H_{32}BN$ $[M]^+$: 381.2633, found: 381.2622.

2-(dimesitylboryl)benzylideneisopropylamine (2). The synthesis of compound **2** is similar as compound **1**, use isopropylamine instead of ethyl amine as the reagent to give compound **2** as pale solid in a crude yield of 98%. Further purification can be achieved by recrystallization with dry hexanes. ^{1}H NMR (400 MHz, C_6D_6): δ (ppm) 0.35 (d, J = 6.0 Hz, 3H), 0.99 (d, J = 6.4 Hz, 3H), 1.67 (s, 3H), 1.90 (s, 3H), 2.22 (s, 6H), 2.31 (s, 3H), 2.47 (s, 3H), 4.19 (hept, J = 6.4 Hz, 1H), 6.66 (s, 1H), 6.75 (s, 1H), 6.92 (s, 1H), 6.96 (s, 1H), 6.99 (t, J = 7.1 Hz, 1H), 7.09 (t, J = 7.1 Hz, 1H), 7.26 (d, J = 7.5 Hz, 1H), 7.86 (d, J = 7.5 Hz, 1H), 7.86 (s, 1H); ^{13}C NMR (101 MHz, C_6D_6): δ (ppm) 20.7, 20.8, 22.9, 24.2, 25.9, 26.0, 26.3, 26.7, 52.2, 124.8, 125.2, 129.4, 129.7, 130.4, 131.0, 131.3, 132.0, 132.8, 134.7, 136.2, 136.8, 140.5, 141.6, 143.5, 165.2; ^{11}B NMR (128

MHz, C_6D_6): δ (ppm) 6.3; HRMS (ESI), calcd for $C_{28}H_{35}BN$ $[M+H]^+$: 396.28571, found: 396.28541.

2-(dimesitylboryl)benzylidenetertbutylamine (3). The synthesis of compound **3** is similar as compound **1**, use tert-butylamine instead of ethyl amine as the reagent to give compound **3** as pale solid in a crude yield of 98%. Further purification can be achieved by recrystallization with dry hexanes. ^{1}H NMR (400 MHz, C_6D_6): δ (ppm) 1.07 (s, 9H), 1.64 (s, 3H), 1.94 (s, 3H), 2.20 (s, 6H), 2.44 (s, 6H), 6.72 (s, 2H), 6.90 (s, 2H), 7.00 (t, *J* = 7.3 Hz, 1H), 7.07 (t, *J* = 7.4 Hz, 1H), 7.40 (d, *J* = 7.5 Hz, 1H), 7.78 (d, *J* = 7.5 Hz, 1H), 8.18 (s, 1H); ^{13}C NMR (101 MHz, C_6D_6): δ (ppm) 20.7, 25.7, 30.7, 60.5, 125.4, 125.9, 129.9, 130.5, 130.7, 131.9, 137.0; ^{11}B NMR (128 MHz, C_6D_6): δ (ppm) 17.1; HRMS (EI), calcd for $C_{29}H_{36}BN$ $[M]^+$: 409.2946, found: 409.2939.

2-(dimesitylboryl)benzylidenecyclohexylamine (4). The synthesis of compound **4** is similar as compound **1**, use cyclohexylamine instead of ethylamine as the reagent to give compound **4** as pale solid in a crude yield of 98%. Further purification can be achieved by recrystallization with dry hexanes. ^{1}H NMR (400 MHz, C_6D_6): δ (ppm) 0.48 (dd, *J* = 21.4, 10.0 Hz, 1H), 0.74 – 0.82 (m, 2H), 0.93 – 0.85 (m, 1H), 1.04 (dd, J = 24.4, 11.9 Hz, 1H), 1.22 – 1.14 (m , 2H), 1.32 (d, J = 6.3 Hz, 1H), 1.56 (d, *J* = 12.1 Hz, 1H), 1.71 (s, 3H), 1.93 (s, 3H), 2.03 (d, *J* = 11.3 Hz, 1H), 2.20 (s, 3H), 2.23 (s, 3H), 2.33 (s, 3H), 2.46 (s, 3H), 3.87 (t, *J* = 11.5 Hz, 1H), 6.67 (s, 1H), 6.73 (s, 1H), 6.90 (s, 1H), 6.97 (s, 1H), 7.02 (t, *J* = 7.3 Hz, 1H), 7.11 (t, *J* = 7.4 Hz, 1H), 7.32 (d, *J* = 7.5 Hz, 1H), 7.85 (d, *J* = 7.5 Hz, 1H), 7.90 (s, 1H); ^{13}C NMR (101 MHz, C_6D_6): δ (ppm) 20.7, 20.8, 24.1, 25.6, 25.8, 26.0, 26.2, 26.3, 26.8, 33.5, 37.7, 60.9, 124.8, 125.1, 129.4, 129.7, 130.2, 130.9, 131.4, 131.9, 132.8, 134.6, 136.4, 137.0, 140.4, 141.5, 143.5, 165.6; ^{11}B NMR (128 MHz, C_6D_6): δ (ppm) 6.46; HRMS (ESI), calcd for $C_{31}H_{39}BN$ $[M+H]^+$: 436.31701, found: 436.31718.



Scheme S1. Syntheses of compounds **5-7**

The synthesis of compound **a** is similar as compound **1** to give compound **a** as pale yellow liquid.

2-(diphenylboryl)benzylideneethylamine (5). 1 M of phenylmagnesium bromide was prepared in advance by adding bromobenzene (10.9 g, 70 mmol), maganesium turnings (1.68 g, 70 mmol) and two small iodine crystals to a 250 mL oven dried Schlenk flask and the mixture was refluxed in 70 ml THF until all of the maganesium had appeared. The phenylmagnesium bromide (5 ml, 1 M in THF, 5 mmol) was added to a 50 mL oven dried Schlenk flask with 10 ml of THF and the mixture was cooled down to -78 ^{o}C under N_2, $B(O^iPr)_3$ (0.58 mL, 2.5 mmol) was added quickly to the flask. The mixture was stirred for 1 hour at the same temperature, then it allowed to warm to room temperature slowly and stirred for another two hours. The solution was cooled down to -78 ^{o}C and prepared for cannula transfer.

In another 100 ml Schlenk flask *n*-BuLi (1.2 mL, 2.5 M in hexane, 3 mmol) was added slowly to a solution of compound **d** (0.53 g, 2.5 mmol) in THF (40 mL) at -78 ^{o}C under N_2. After stirring at this temperature for 1 h, the former solution was cannula transferred to the latter flask at the same temperature. The mixture was stirred for another 1 hour at the same temperature, then allowed to warm to room temperature slowly and stirred overnight. The mixture was extracted with diethyl ether (50 ml × 3). The organic extract was purified by column chromatography on basic activated aluminum oxide (CH_2Cl_2 : hexanes = 1:4) to afford product (0.18 g, 24 % yield)

as a white solid. ^{1}H NMR (400 MHz, C_6D_6): δ (ppm) 0.47 (t, *J* = 7.2 Hz, 3H), 3.21 (q, *J* = 7.2 Hz, 2H), 7.06 (t, *J* = 7.5 Hz, 1H), 7.26 – 7.17 (m, 3H), 7.34 – 7.27 (m, 6H), 7.45 (d, J = 7.0 Hz, 4H), 7.68 (d, J = 7.3 Hz, 1H); ^{13}C NMR (101 MHz, C_6D_6): δ (ppm) 13.4, 44.3, 125.3, 125.7, 126.0, 127.7, 130.5, 132.0, 133.8, 137.7, 165.2; ^{11}B NMR (128 MHz, C_6D_6): δ (ppm) 4.20; HRMS (EI), calcd for $C_{21}H_{20}BN$ $[M]^+$: 297.1693, found: 297.1699.

2-(diphenyboryl)benzylideneisopropylamine (6). The synthesis procedure of compound **6** issimilar as compound **5** to give compound **6** as white solid, 30 % yield. ^{1}H NMR (400 MHz, C_6D_6): δ (ppm) 0.61 (d, *J* = 6.7 Hz, 1H), 4.00 – 3.87 (m, 1H), 7.07 (t, *J* = 7.4 Hz, 1H), 7.34 – 7.16 (m, 8H), 7.49 (d, *J* = 6.8 Hz, 1H), 7.68 (d, *J* = 7.3 Hz, 1H), 7.71 (s, 1H); ^{13}C NMR (101 MHz, C_6D_6): δ (ppm) 23.3, 50.2, 125.3, 125.7, 126.0, 127.7, 130.5, 132.1, 133.9, 137.9, 164.3; ^{11}B NMR (128 MHz, C_6D_6): δ (ppm) 4.73; HRMS (EI), calcd for $C_{22}H_{22}BN$ $[M]^+$: 311.1849, found: 311.1847.

2-(diphenyl-*d*$_5$ boryl)benzylideneisopropylamine (7). The synthesis procedure of compound **6** is similar as compound **5**, using C_6D_5MgBr as the reagent for the preparation of $B(O^iPr)(C_6D_5)_2$, to give compound **7** as white solid, 28 % yield. ^{1}H NMR (400 MHz, CD_2Cl_2): δ (ppm) 1.17 (d, *J* = 6.7 Hz, 6H), 4.31 – 4.18 (m, 1H), 7.31 (t, *J* = 7.4 Hz, 1H), 7.45 (t, *J* = 7.3 Hz, 1H), 7.55 (d, *J* = 7.2 Hz, 1H), 7.76 (d, *J* = 7.6 Hz, 1H), 8.70 (s, 1H); ^{2}H NMR (92 MHz, CH_2Cl_2): δ (ppm) 7.23 (d, *J* = 3.7 Hz, 10H); ^{13}C NMR (101 MHz, CD_2Cl_2): δ (ppm) ; 23.7, 50.7, 125.2 (t, *J* = 23.6), 125.6, 126.0, 126.8 (t, *J* = 23.6), 129.6, 131.9, 133.0 (t, *J* = 23.6), 137.9, 165.1; ^{11}B NMR (128 MHz, CD_2Cl_2): δ (ppm) 4.28; HRMS (EI), calcd for $C_{22}H_{12}D_{10}BN$ $[M]^+$: 321.2477, found: 321.2468.

S2. NMR Data of 1-7

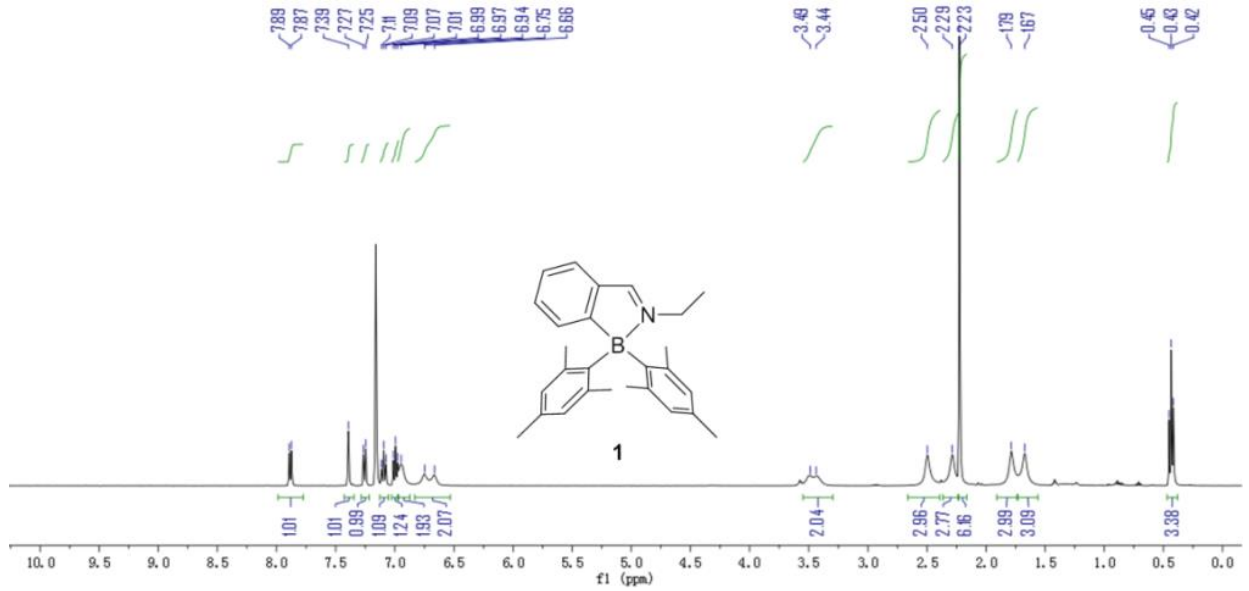


Figure S1. ^{1}H NMR spectrum of **1** in C_6D_6.

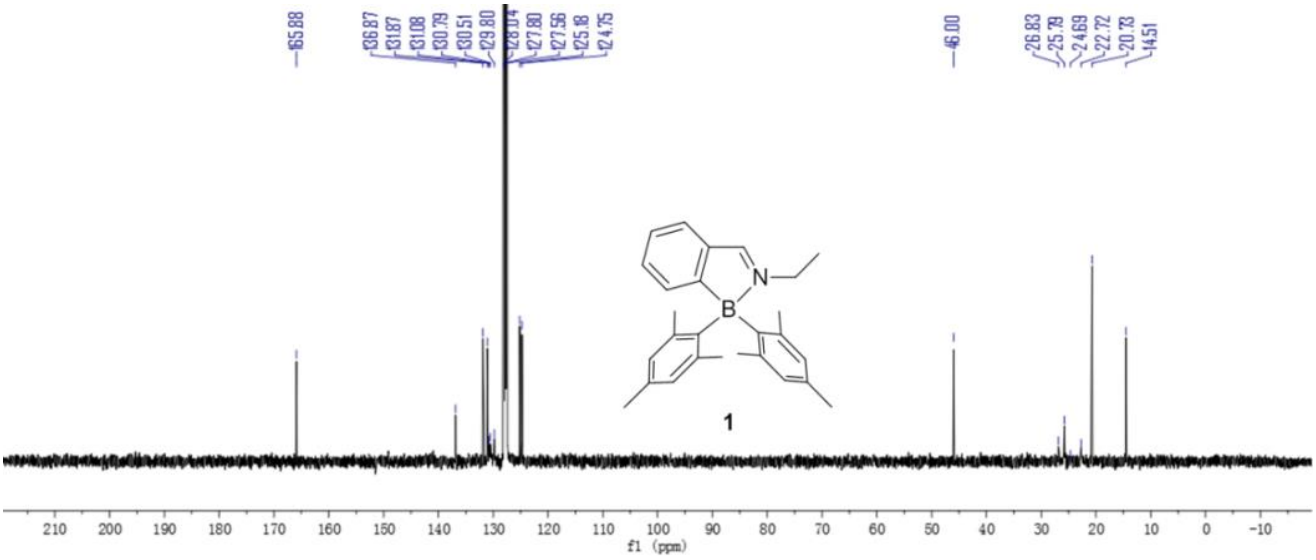


Figure S2. ^{13}C NMR spectrum of **1** in C_6D_6.

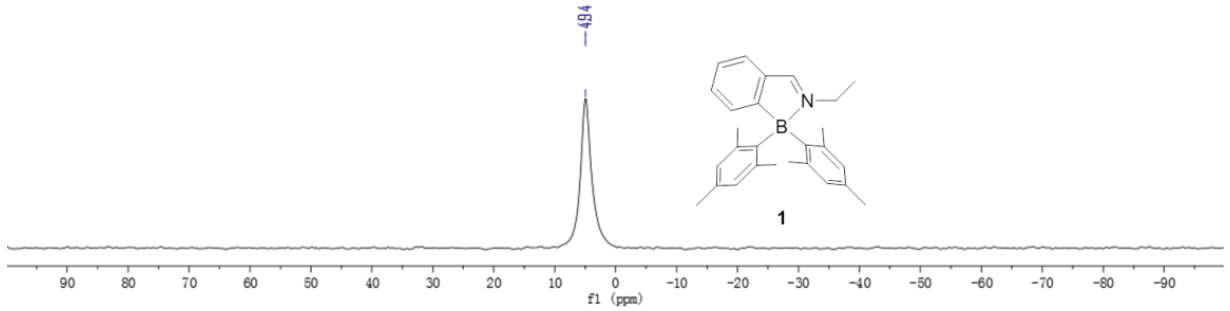


Figure S3. ^{11}B NMR spectrum of **1** in C_6D_6.

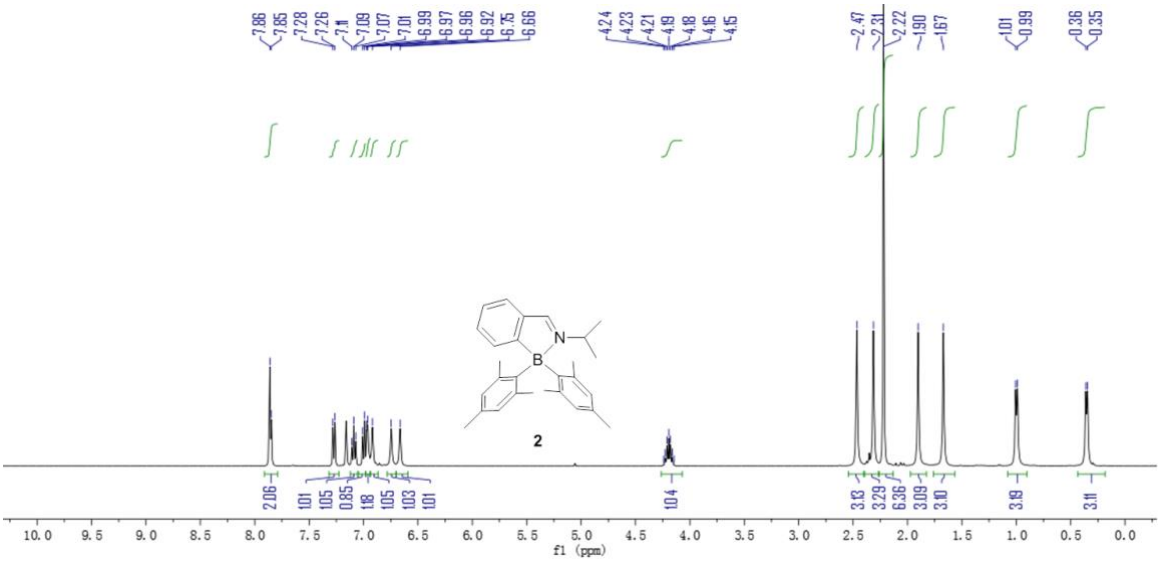


Figure S4. ^{1}H NMR spectrum of **2** in C_6D_6.

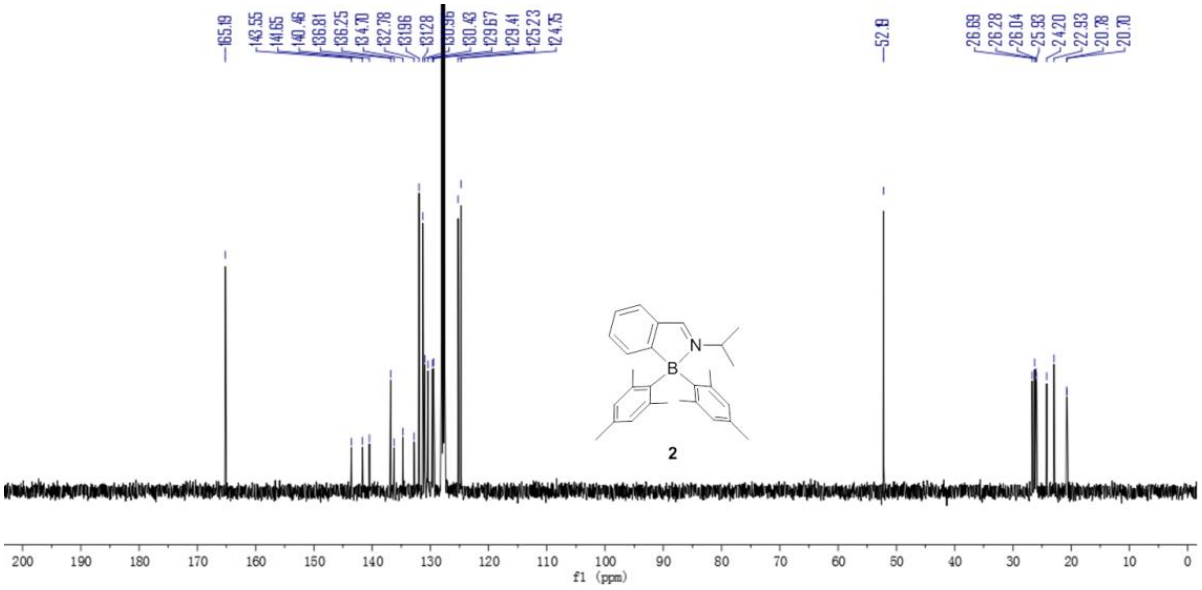


Figure S5. ^{13}C NMR spectrum of **2** in C_6D_6.

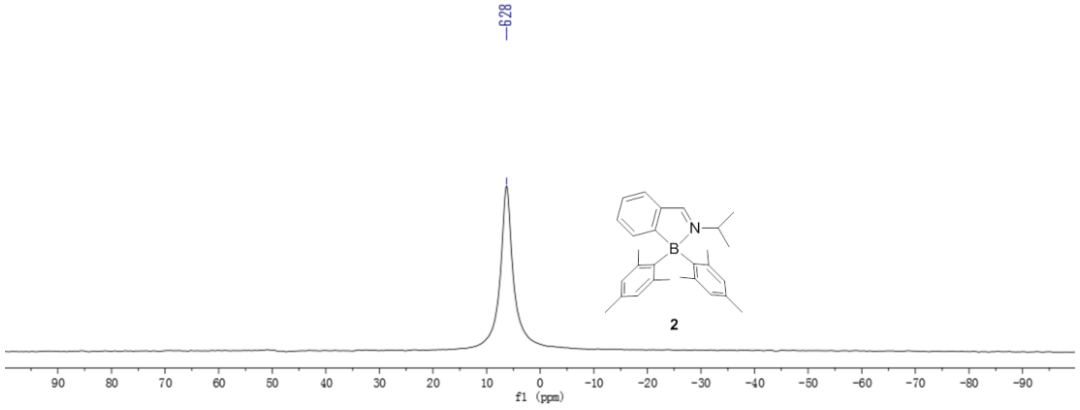


Figure S6. ^{11}B NMR spectrum of **2** in C_6D_6.

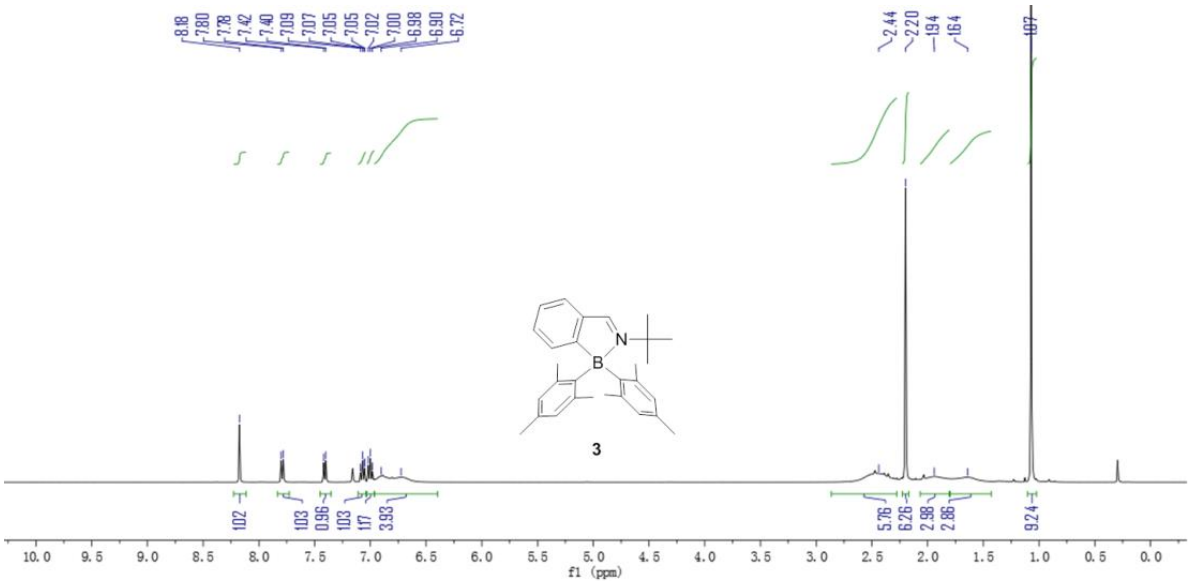


Figure S7. ^{1}H NMR spectrum of **3** in C_6D_6.

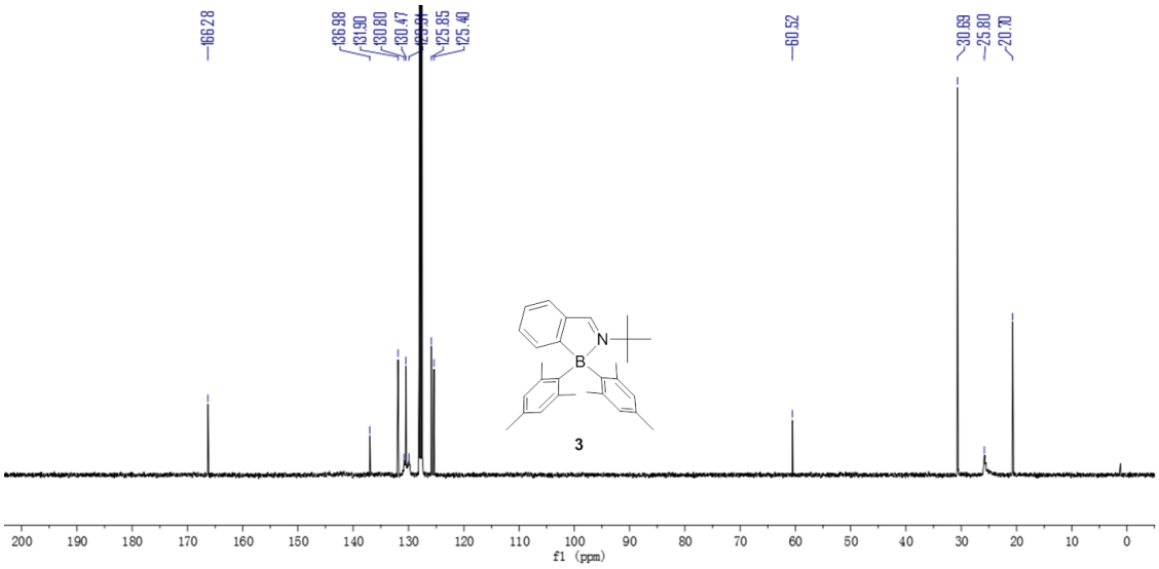


Figure S8. ^{13}C NMR spectrum of **3** in C_6D_6.

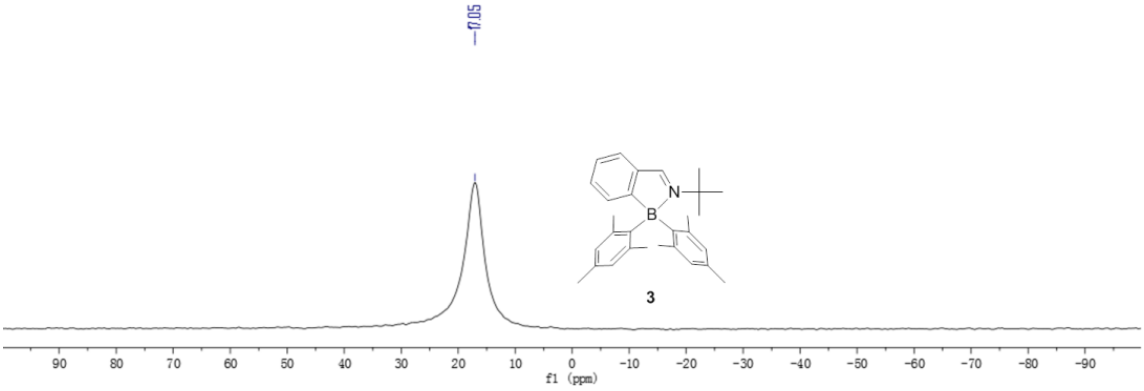


Figure S9. ^{11}B NMR spectrum of **3** in C_6D_6.

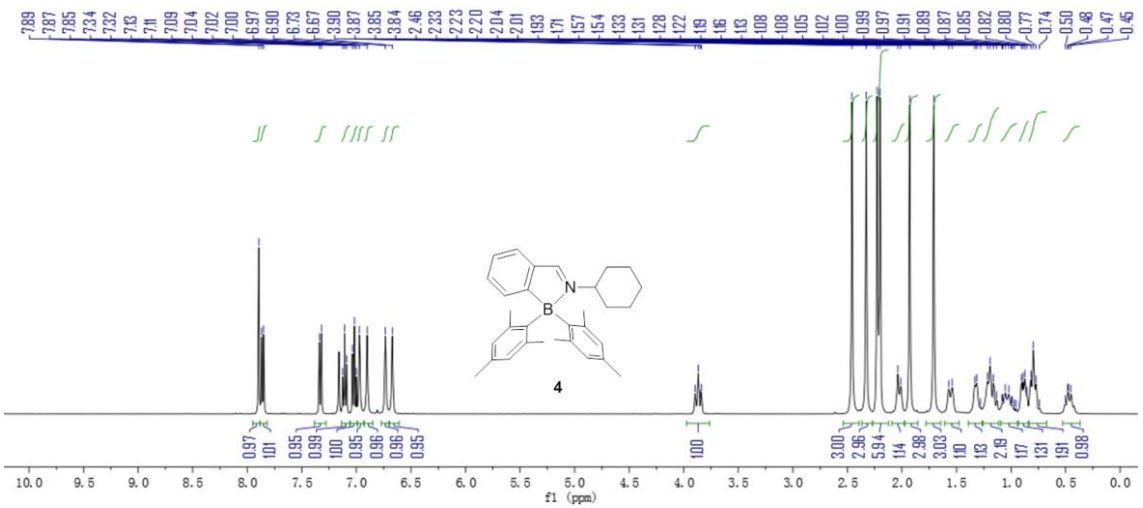


Figure S10. ^{1}H NMR spectrum of **4** in C_6D_6.

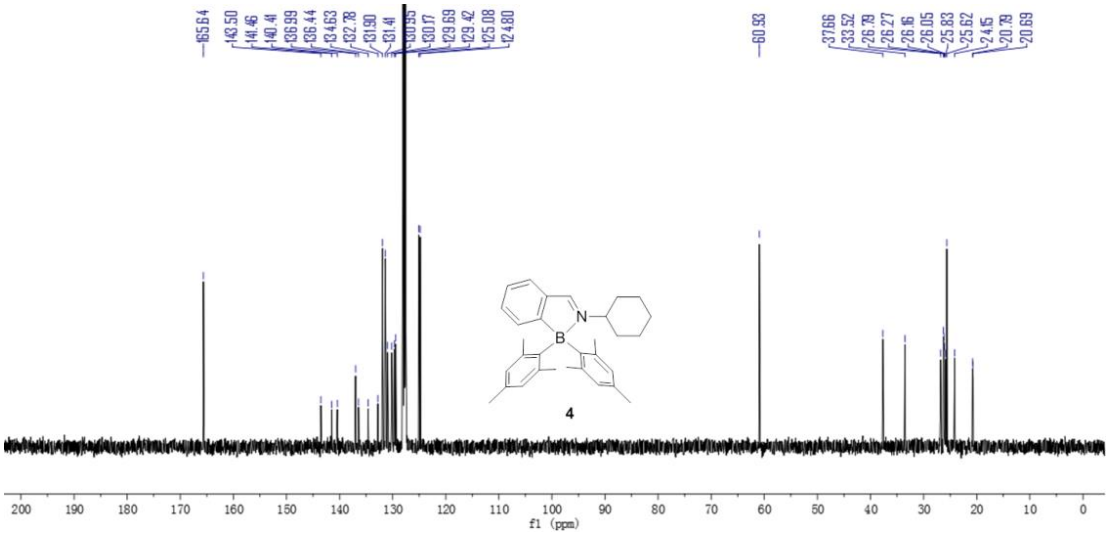


Figure S11. ^{13}C NMR spectrum of **4** in C_6D_6.

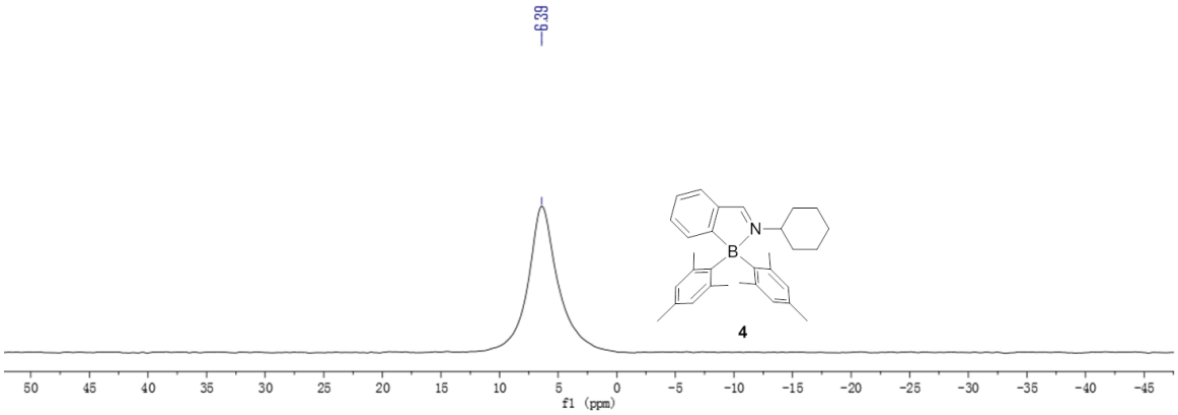


Figure S12. ^{11}B NMR spectrum of **4** in C_6D_6.

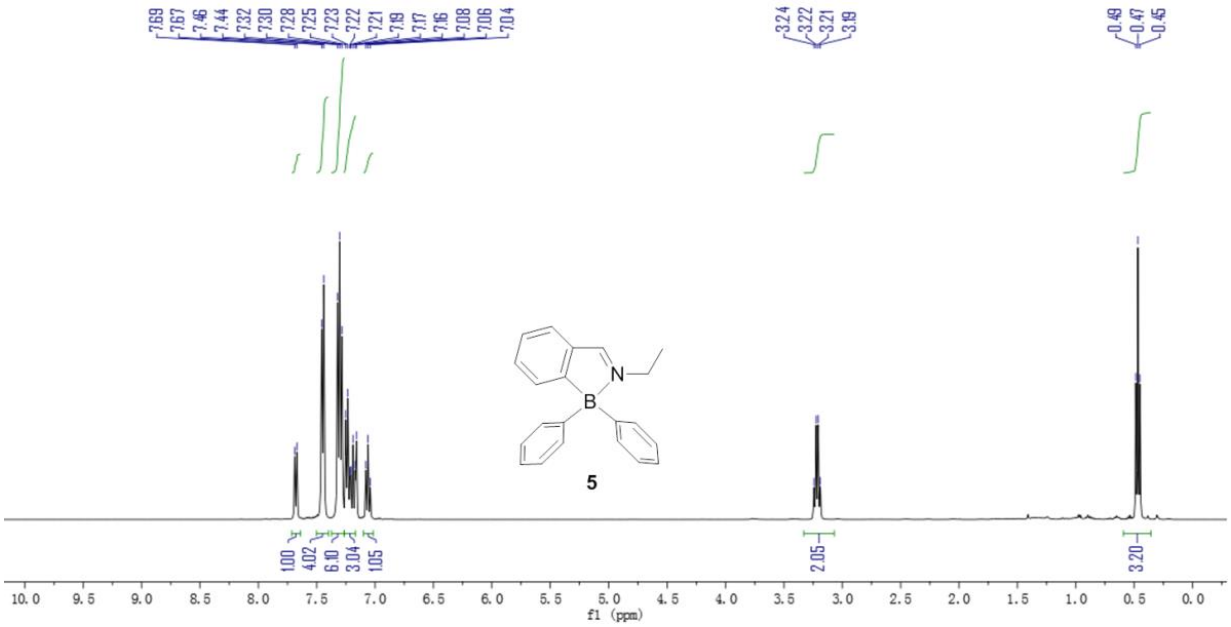


Figure S13. ^{1}H NMR spectrum of **5** in C_6D_6.

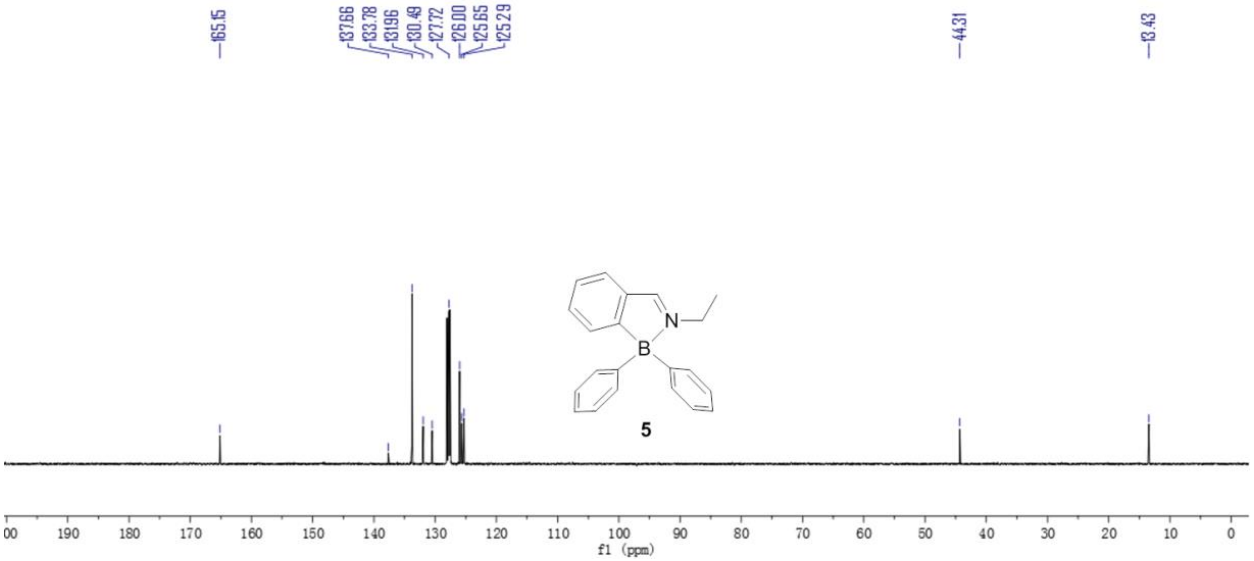


Figure S14. ^{13}C NMR spectrum of **5** in C_6D_6.

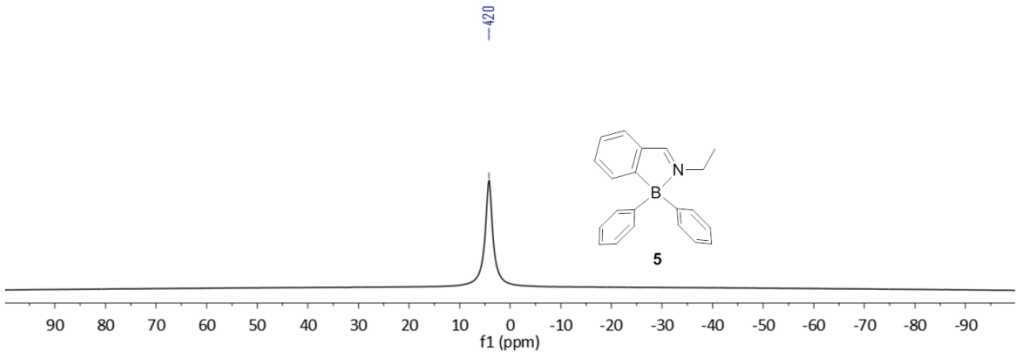


Figure S15. ^{11}B NMR spectrum of **5** in C_6D_6.

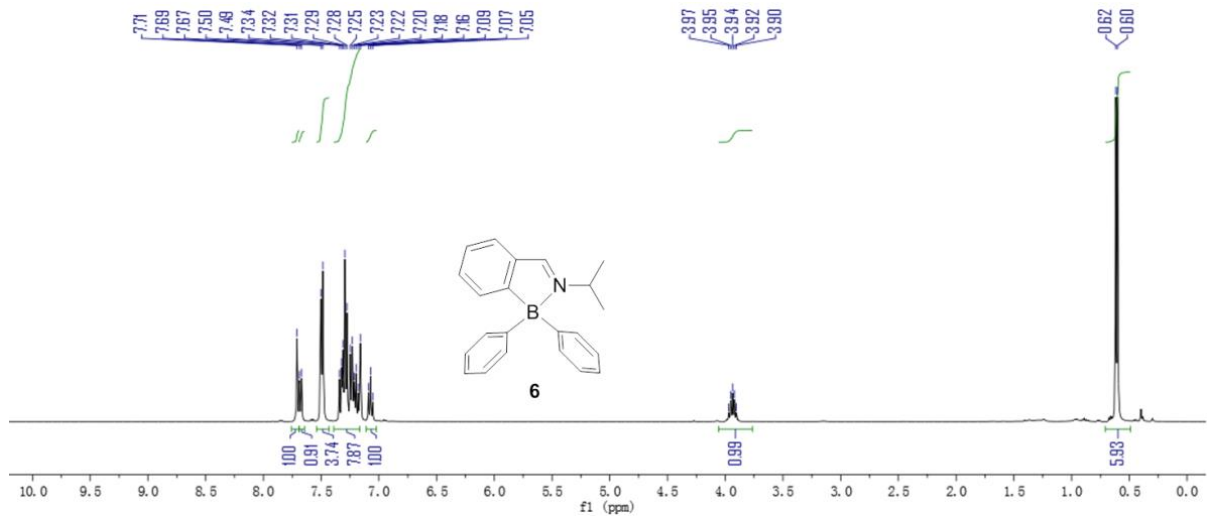


Figure S16. ^{1}H NMR spectrum of **6** in C_6D_6.

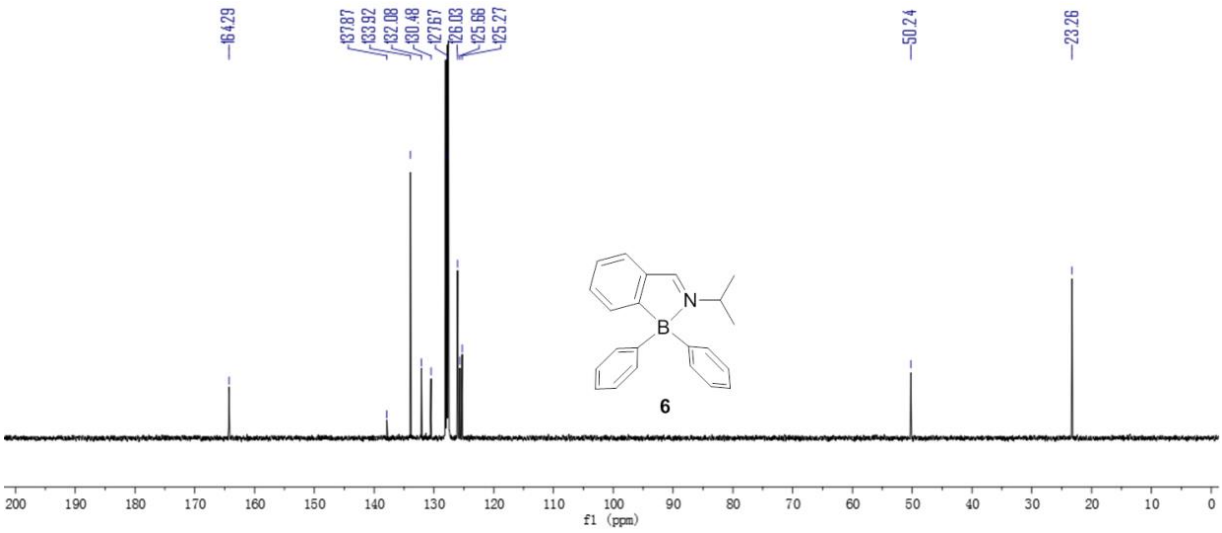


Figure S17. ^{13}C NMR spectrum of **6** in C_6D_6.

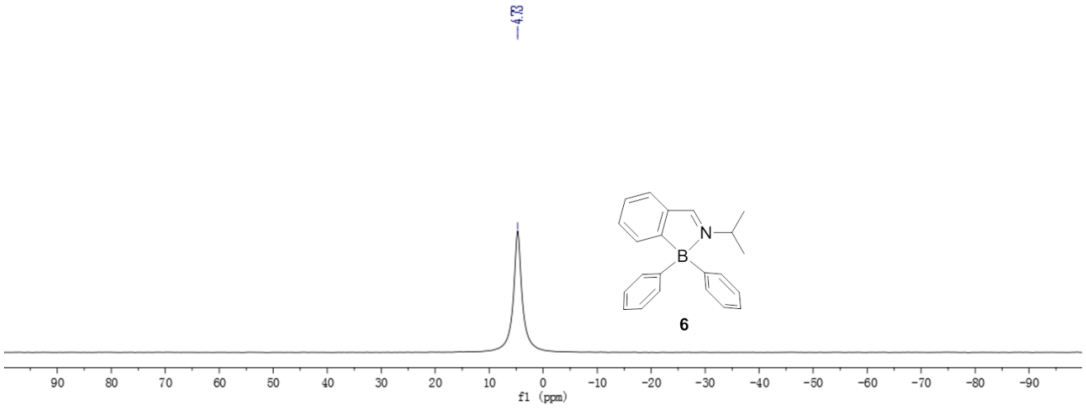


Figure S18. ^{11}B NMR spectrum of **6** in C_6D_6.

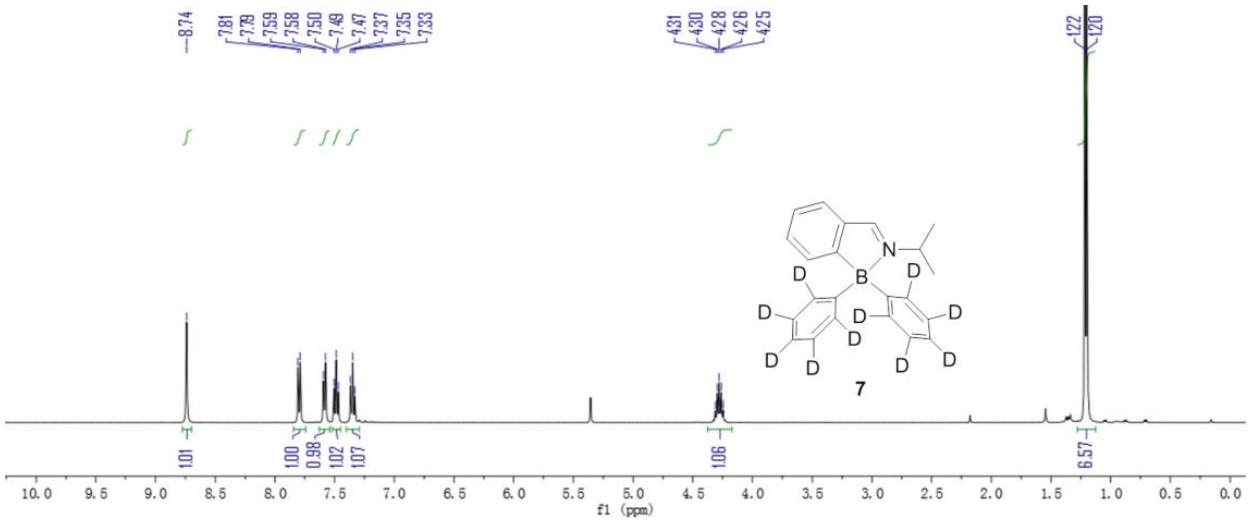


Figure S19. ^{1}H NMR spectrum of **7** in CD_2Cl_2.

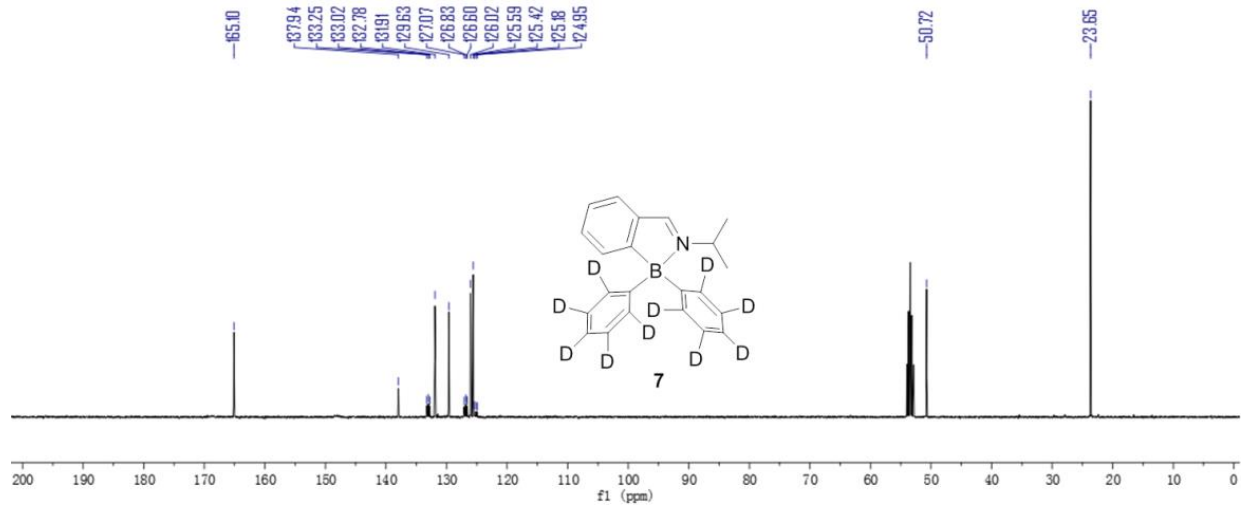


Figure S20. ^{13}C NMR spectrum of **7** in CD_2Cl_2.

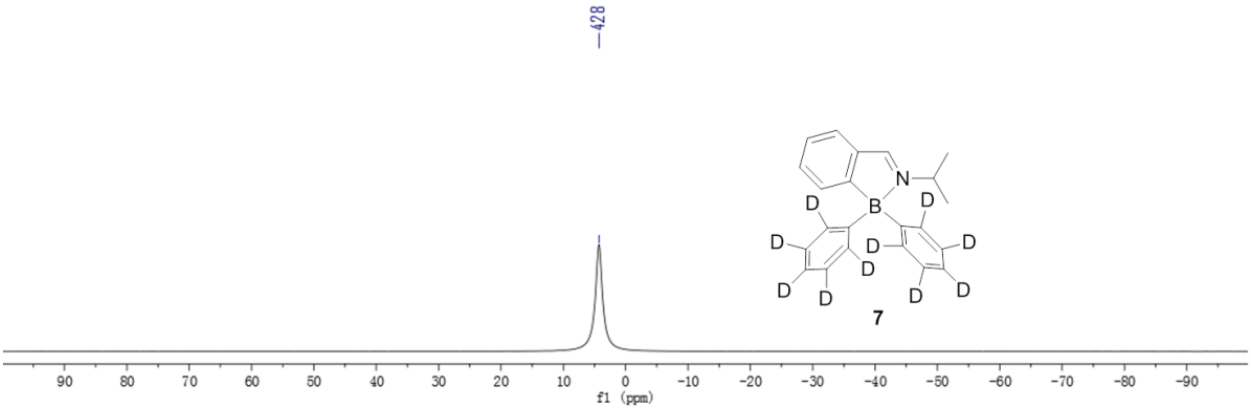


Figure S21. ^{11}B NMR spectrum of **7** in CD_2Cl_2.

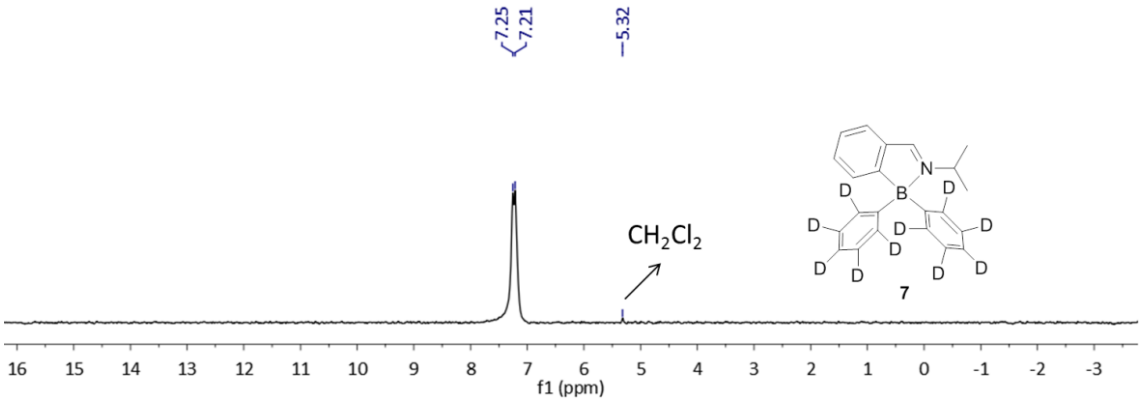


Figure S22. ^{2}H NMR spectrum of **7** in CH_2Cl_2.

S3. NMR Photoreactivity Study of 1-7

General Procedures:

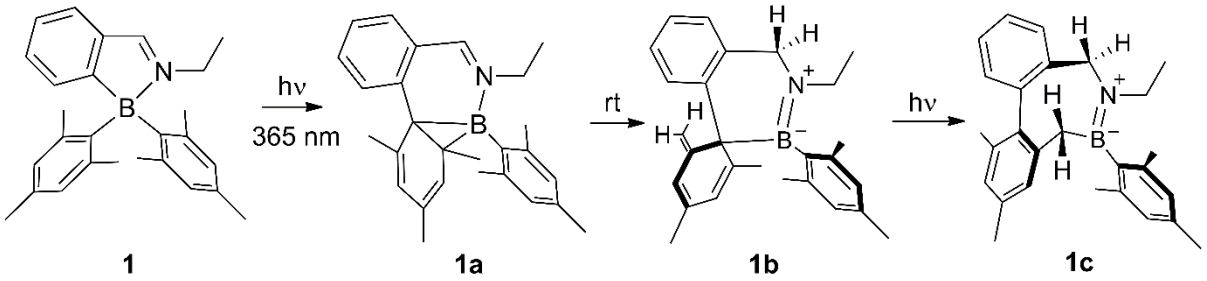
For NMR study: All the sample used for photoisomerization studies were dissolved in C_6D_6 and the C_6D_6 solvent was dried with molecular sieves and stored in N_2 filled glove box. Compound **1-7** were dissolved in 0.5 ml of C_6D_6 in J-Young NMR tubes and sealed with teflon caps, then removed from the glove box and irradiated in an Rayonet Photochemical Reactor (350 nm). ^{1}H, ^{11}B NMR spectra were monitored periodically until no additional spectra change.

The conversion of intermediate **a** to respective isomer **b** can be driven by room temperature and the intermediate **a** can not be monitored by room temperature NMR spectra. While the conversion of **a→b** can be prevented under low temperature, compound **2** in toluene-d_8 was irradiate with 365 nm hand UV light in dry ice/acetone bath (-78 ^{0}C) and low temperature (-70 ^{0}C) NMR spectra observed the presence of intermediate isomer **1a**.

The thermal isomerization reaction of **4b→4c** was performed by putting the sealed NMR tube in an oil bath. The temperature of the oil bath is same as the thermal isomerization reaction temperature.

3.1. NMR spectra of the sequential isomerization

3.1.1. **1 → 1c**



Scheme S2. The structures of **1** - **1c**

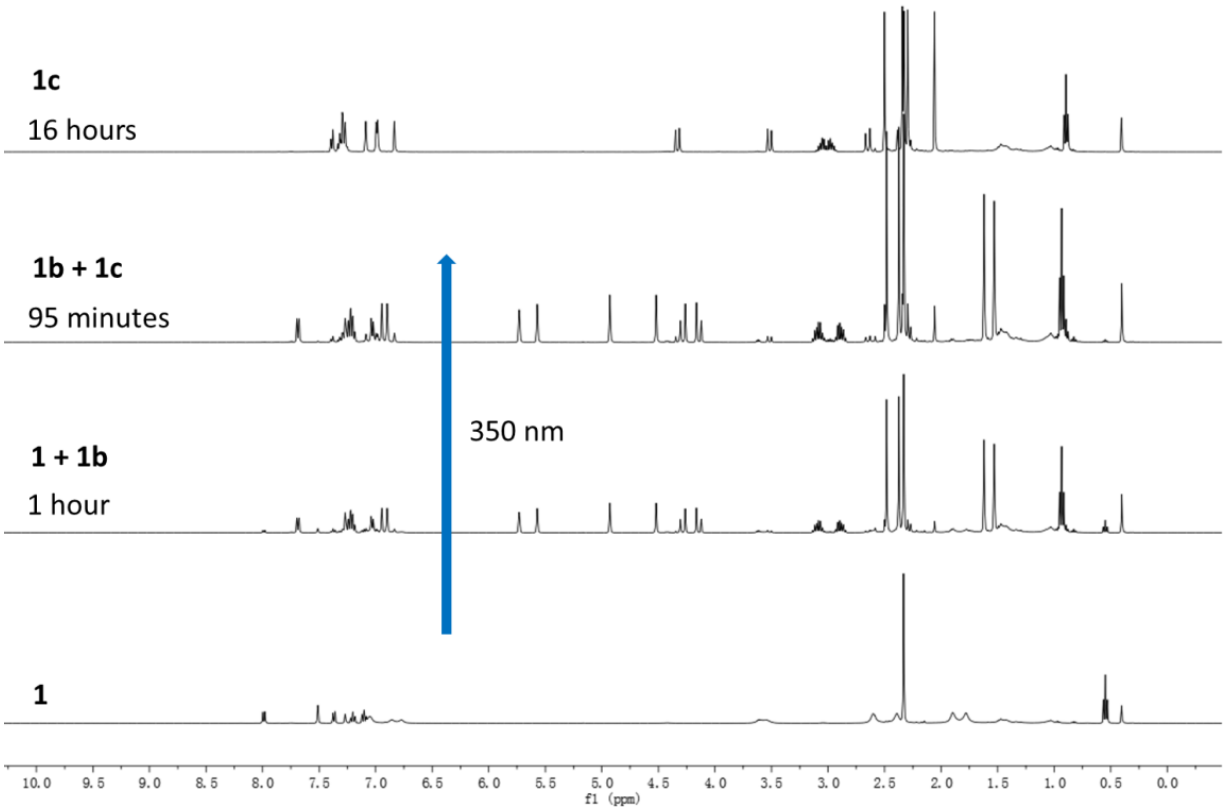


Figure S23. ^{1}H NMR spectra showing the sequential conversion of **1** → **1c** (0.1M in C_6D_6).

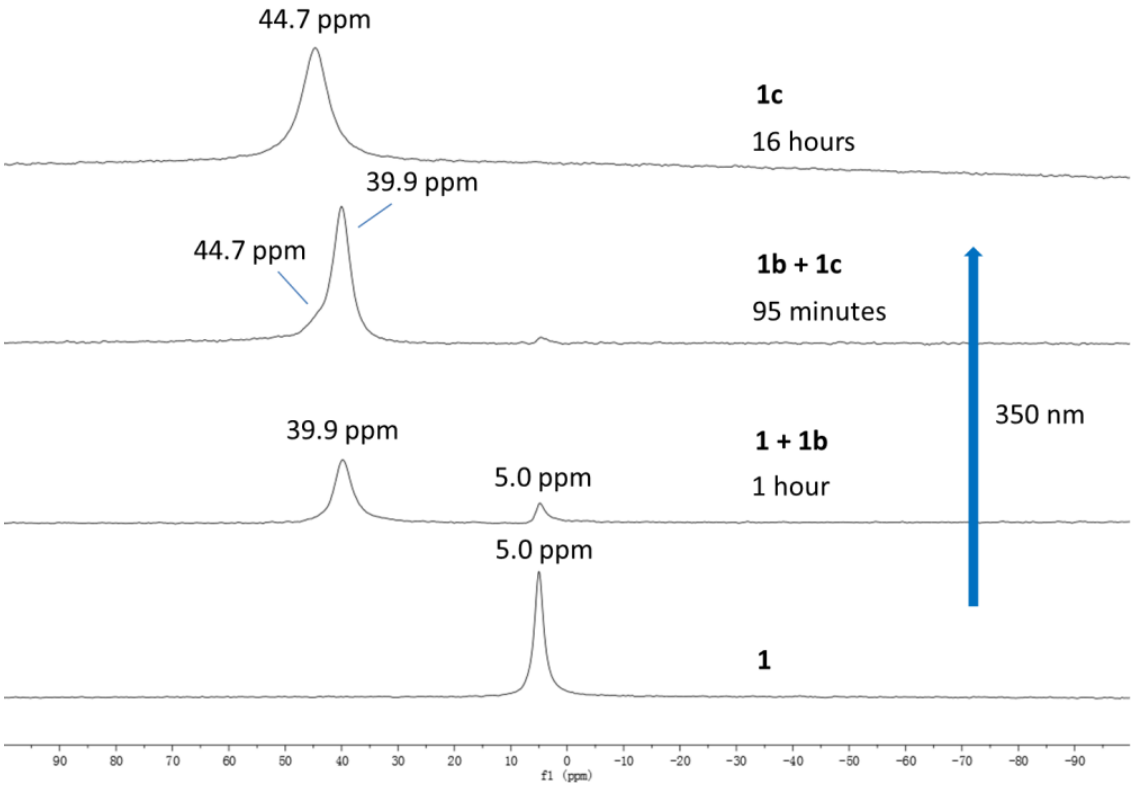


Figure S24. ^{11}B NMR spectra showing the sequential conversion of **1** → **1c** (0.1M in C_6D_6).

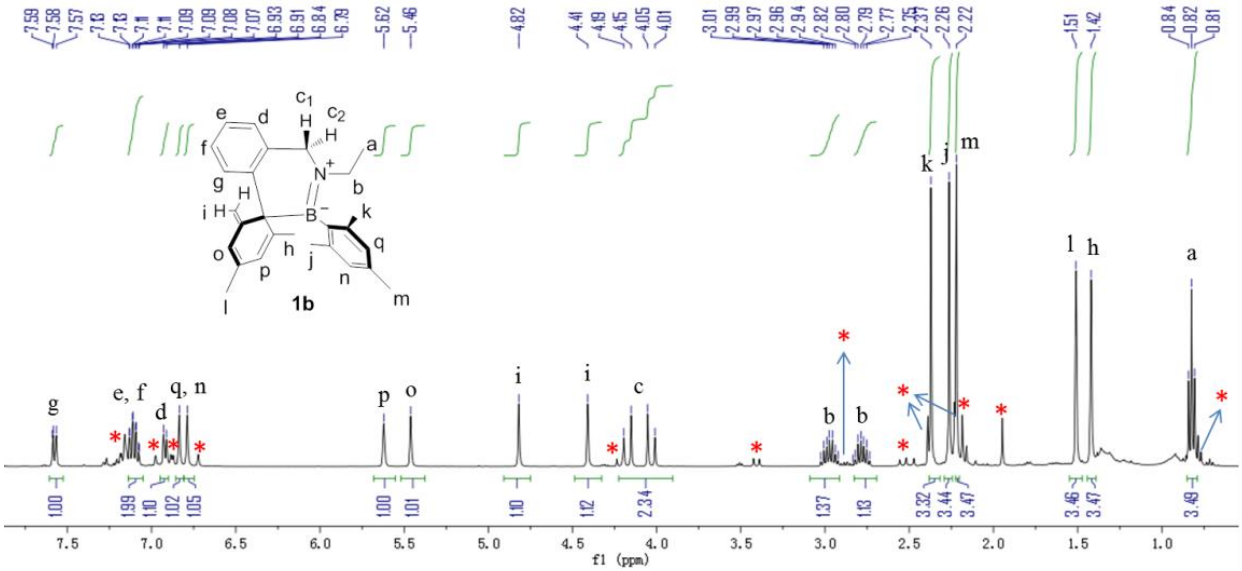


Figure S25. ^{1}H NMR spectrum of **1b** (mixed with some **1c** labeled with *) in C_6D_6 with the assignment of all peaks.

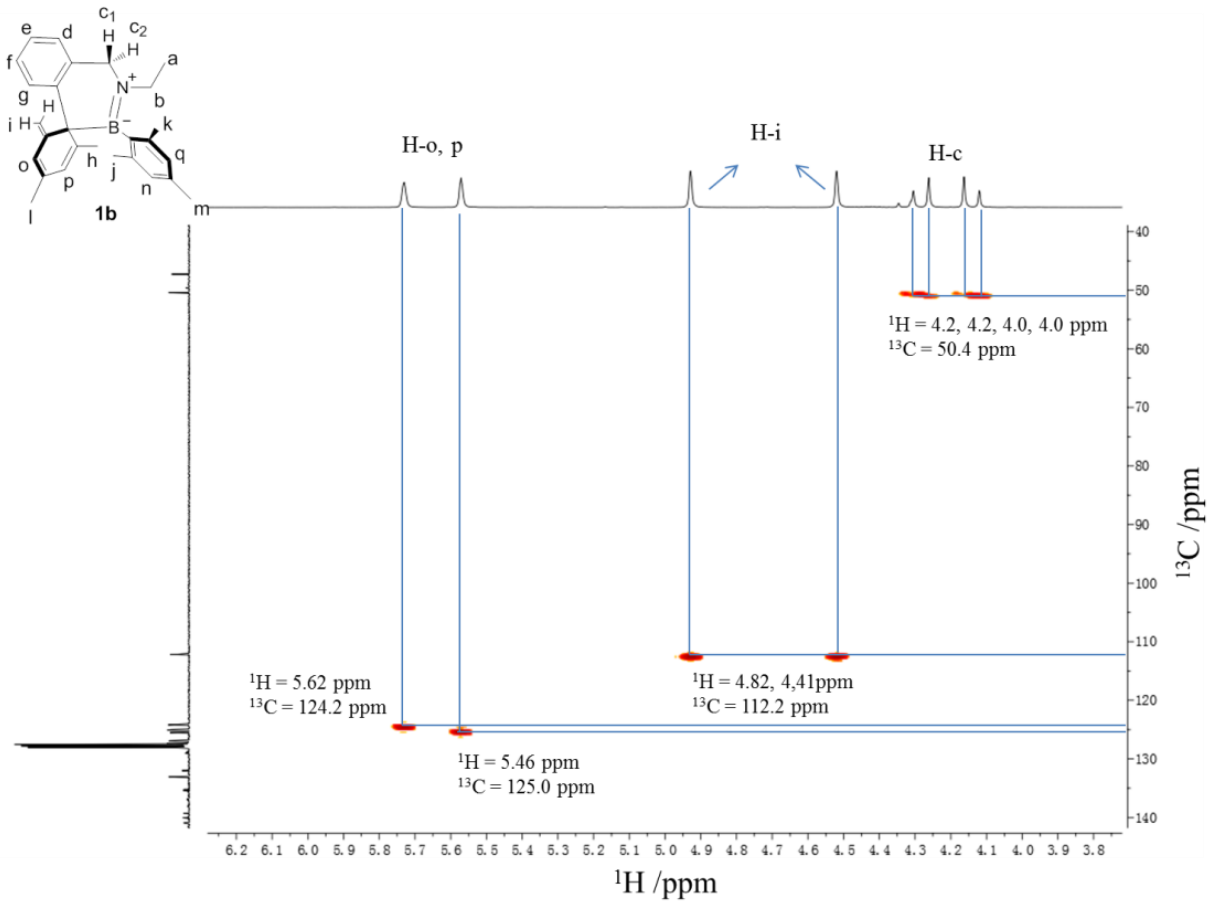


Figure S26. ^{1}H-^{13}C HSQC NMR spectrum of **1b** in C_6D_6 showing the key correlations.

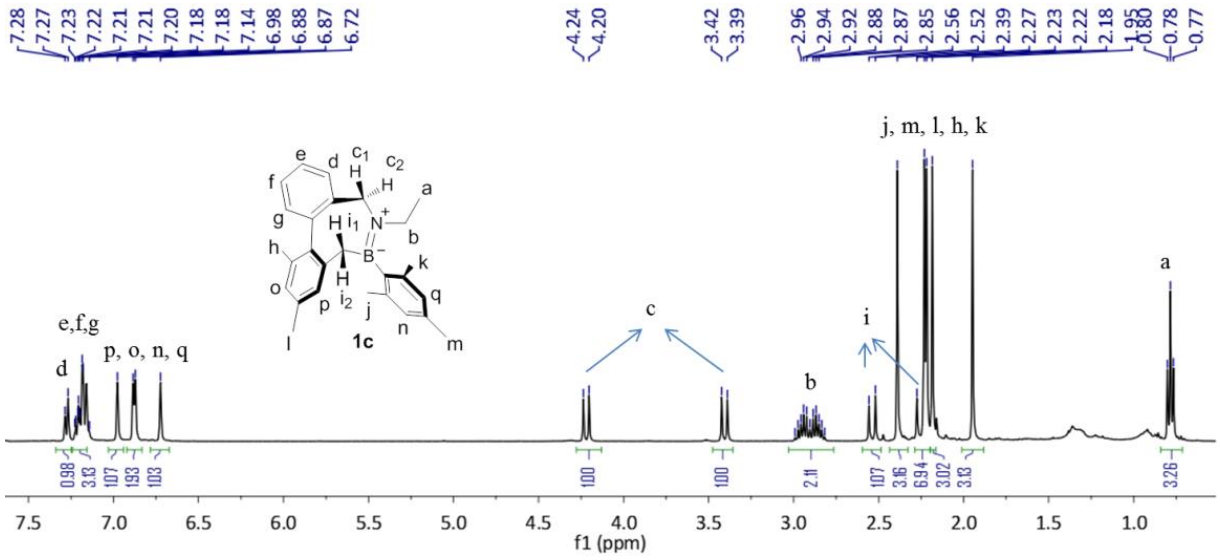


Figure S27. ^{1}H NMR spectrum of **1c** in C_6D_6 with the assignment of all peaks.

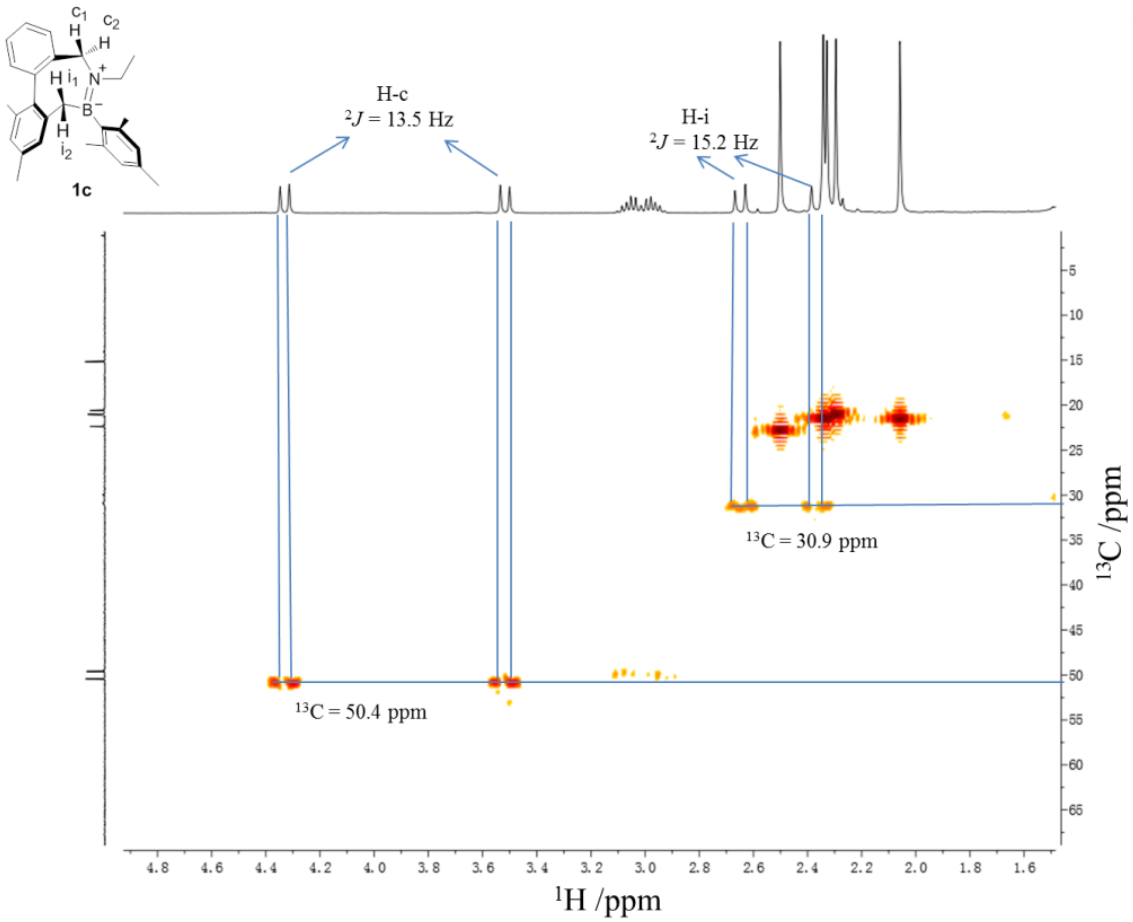


Figure S28. ^{1}H-^{13}C HSQC NMR spectrum in C_6D_6 showing the key correlations of **1c**.

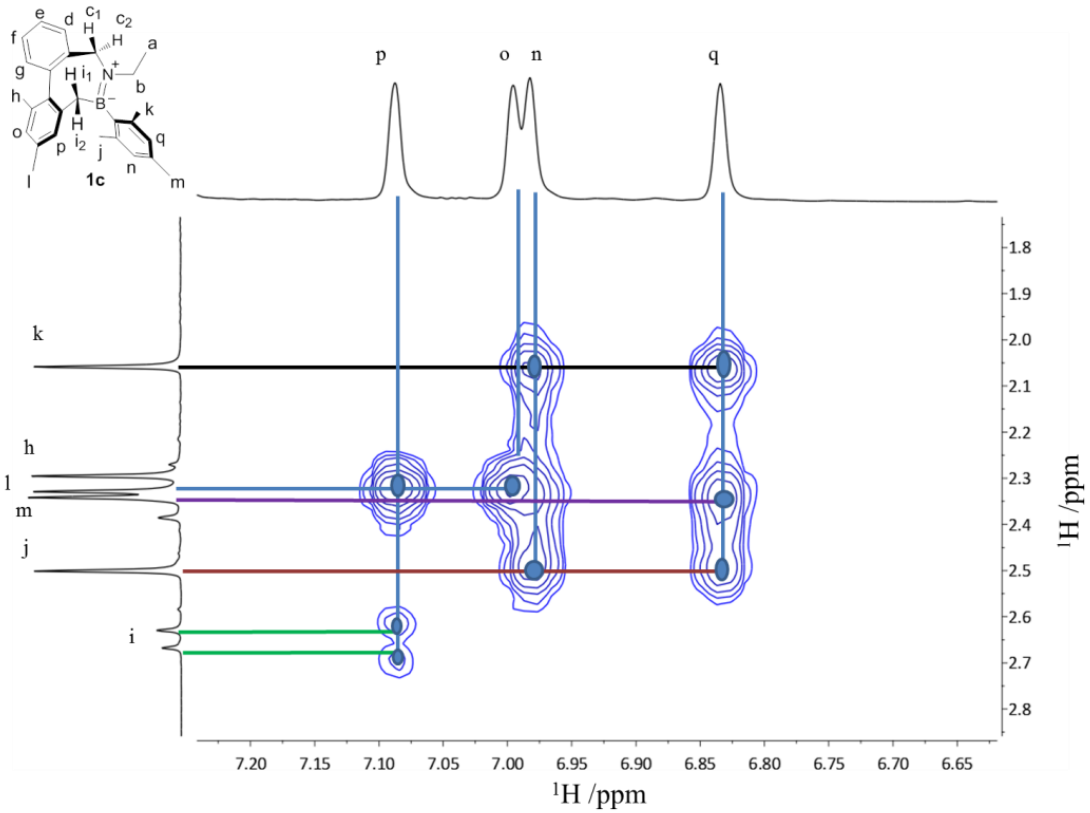


Figure S29. ^{1}H-^{1}H COSY NMR spectrum of **1c** in C_6D_6 with the assignment of part of the peaks.

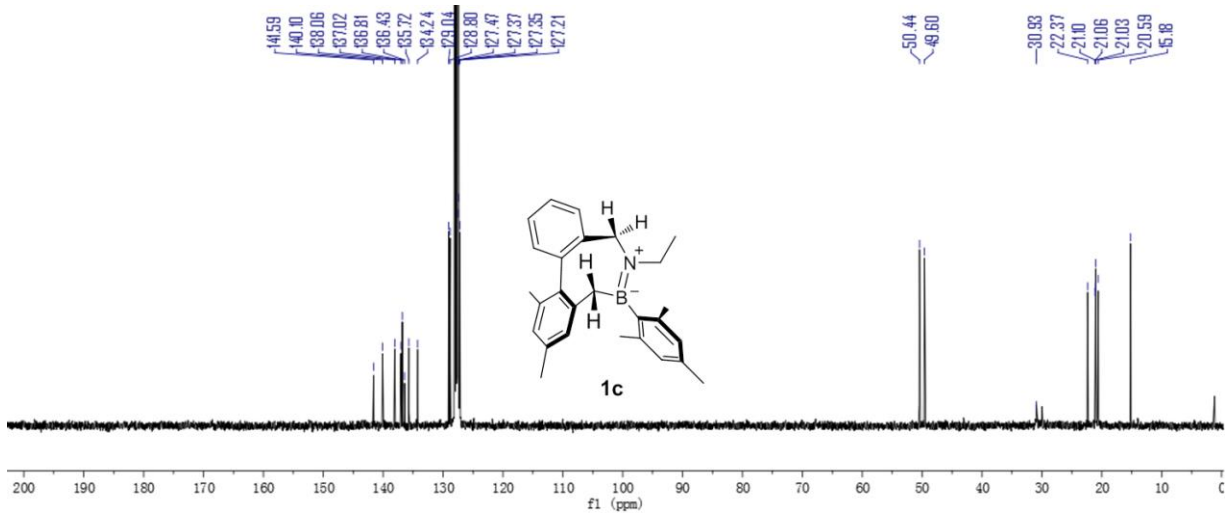


Figure S30. ^{13}C NMR spectrum of **1c** in C_6D_6.

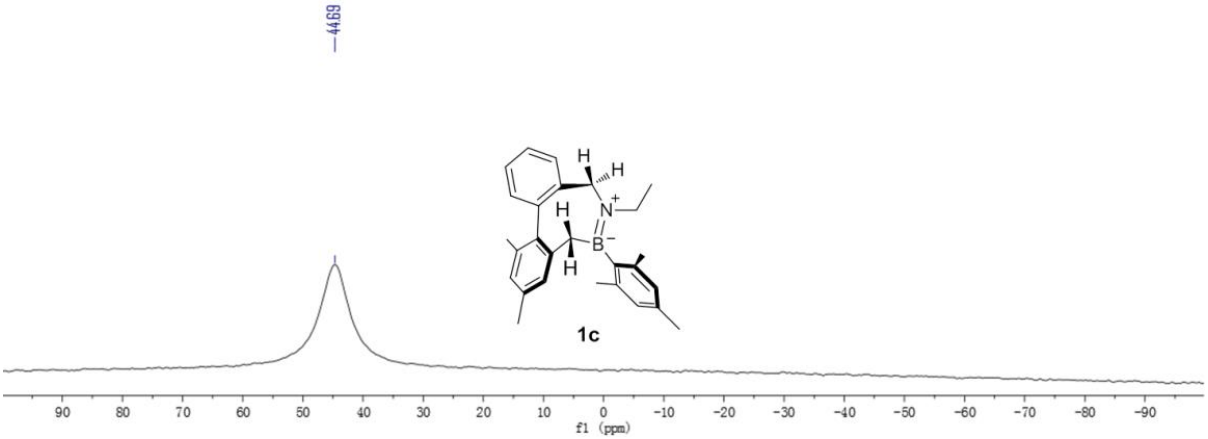
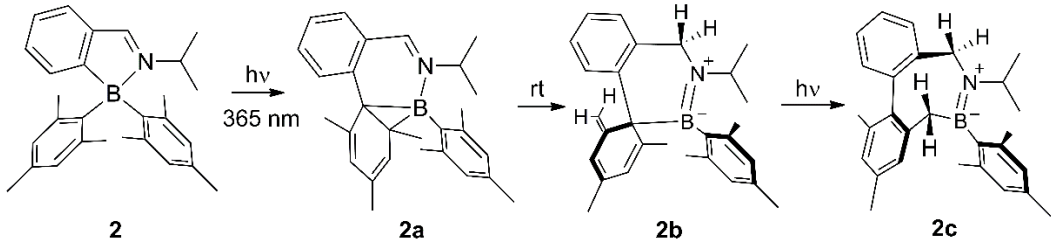


Figure S31. ^{11}B NMR spectra of **1c** in C_6D_6.

3.1.2. **2 → 2c**



Scheme S3. The structures of **2 - 2c**

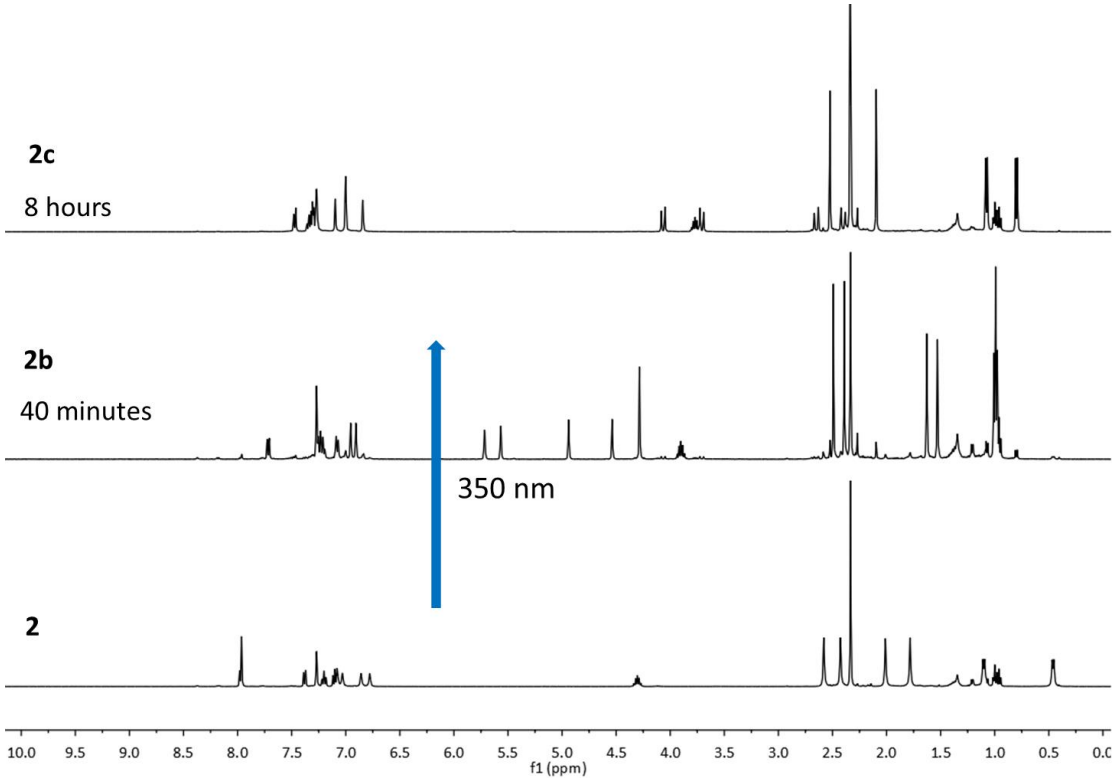


Figure S32. ^{1}H NMR spectra showing the sequential conversion of **2 → 2c** (0.02M in C_6D_6).

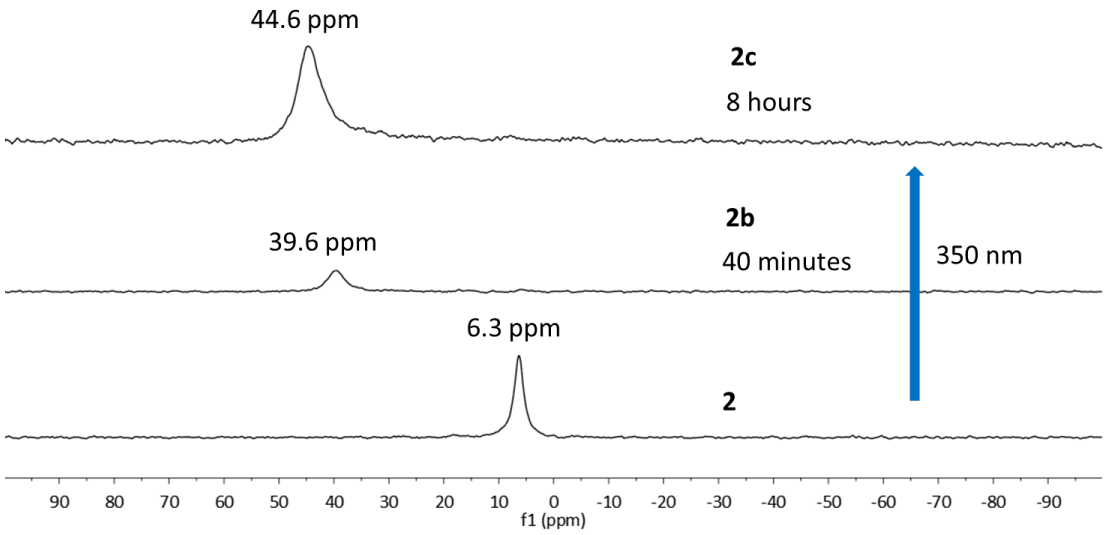


Figure S33. ^{11}B NMR spectra showing the sequential conversion of **2** → **2c** (0.02M in C_6D_6).

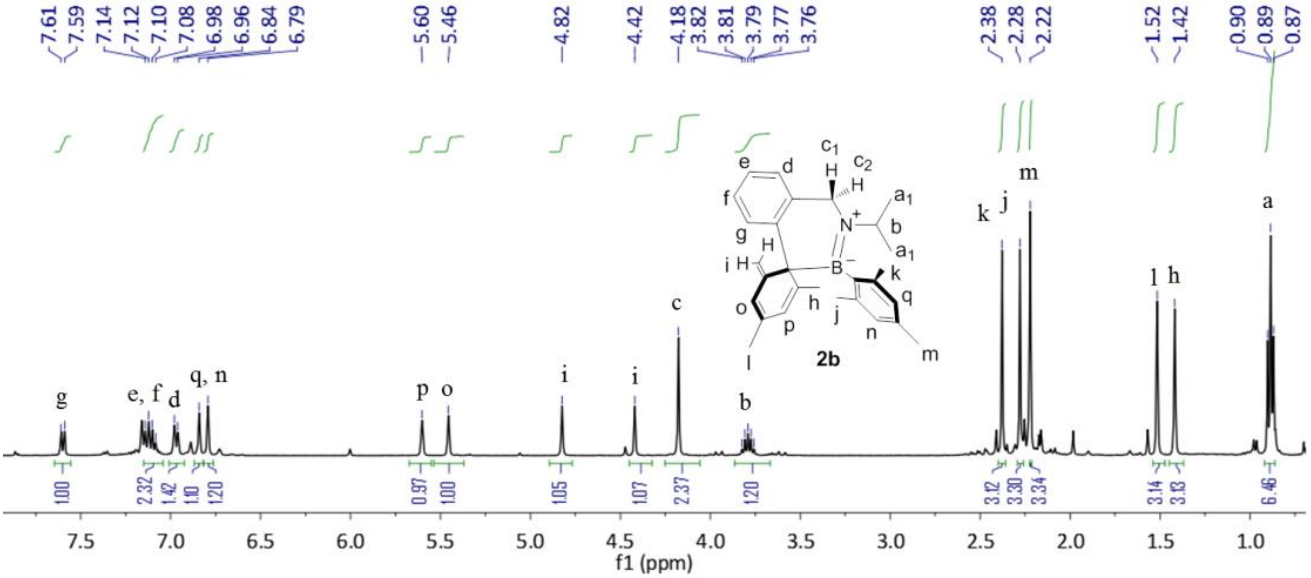


Figure S34. ^{1}H NMR spectrum of **2b** (mixed with some unknown impurities) in C_6D_6 with the assignment of all peaks.

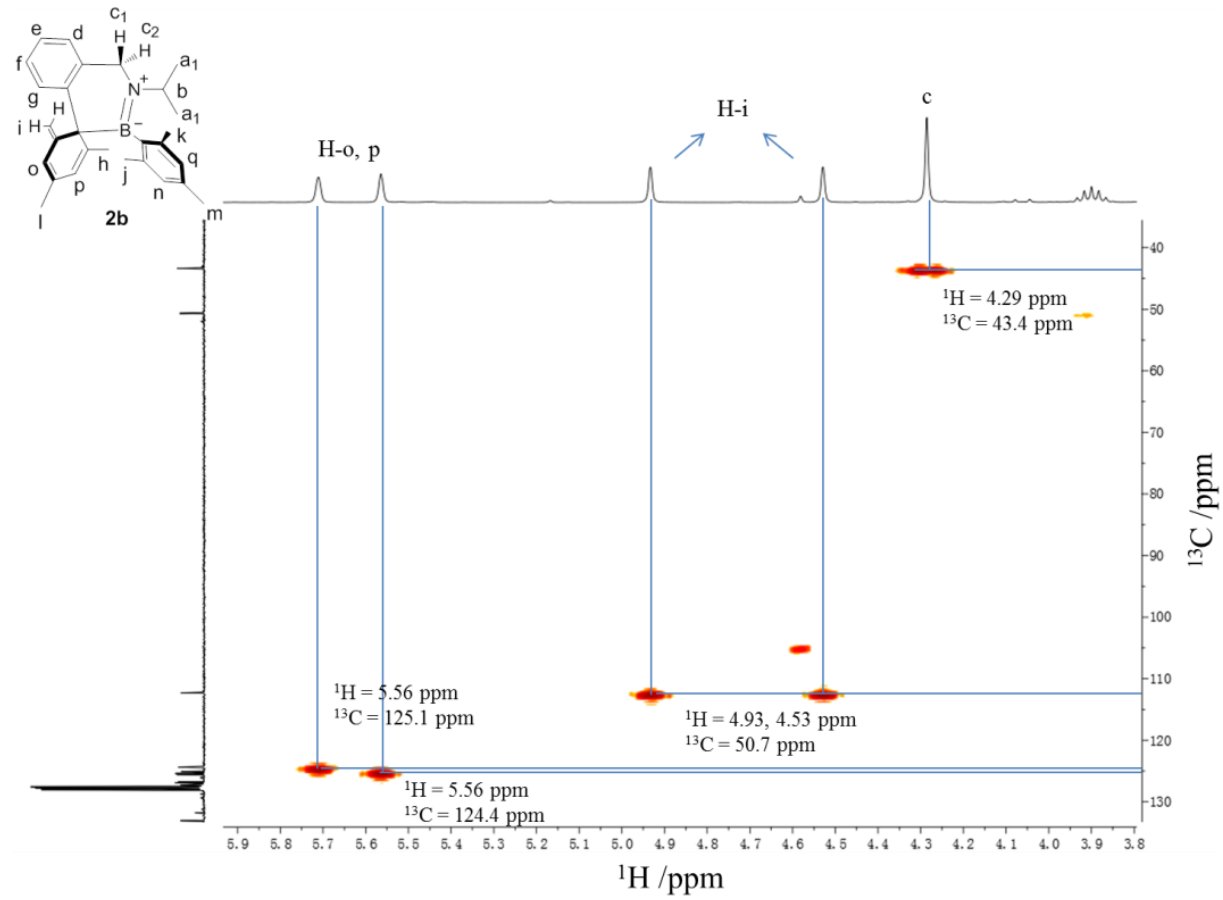


Figure S35. ^{1}H-^{13}C HSQC NMR spectrum of **2b** in C_6D_6 showing the key correlations.

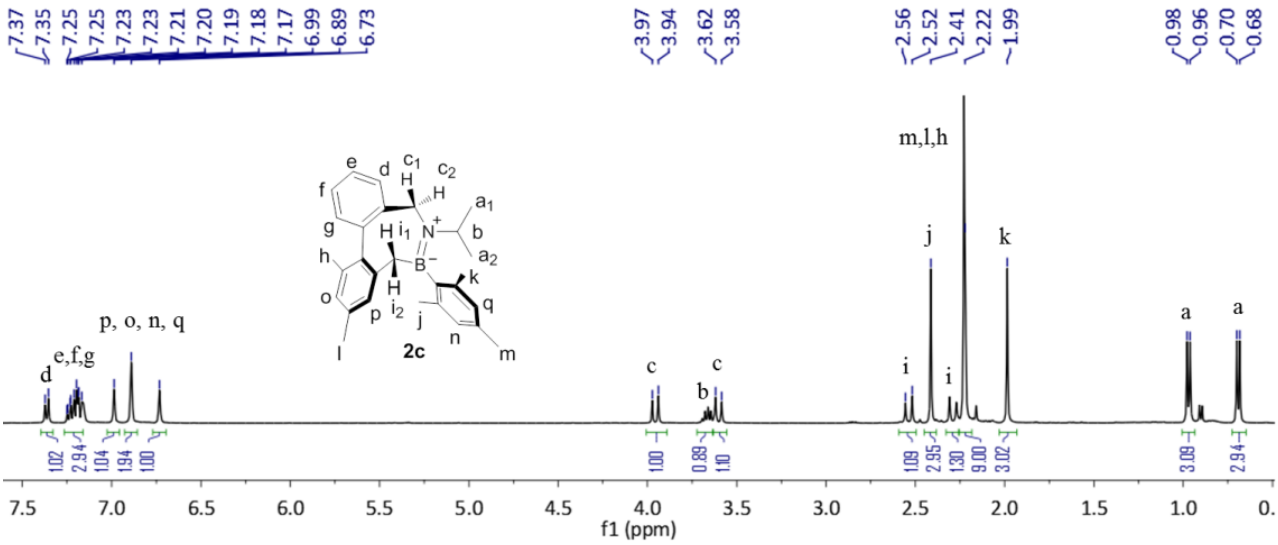


Figure S36. ^{1}H NMR spectrum of **2c** in C_6D_6 with the assignment of all peaks.

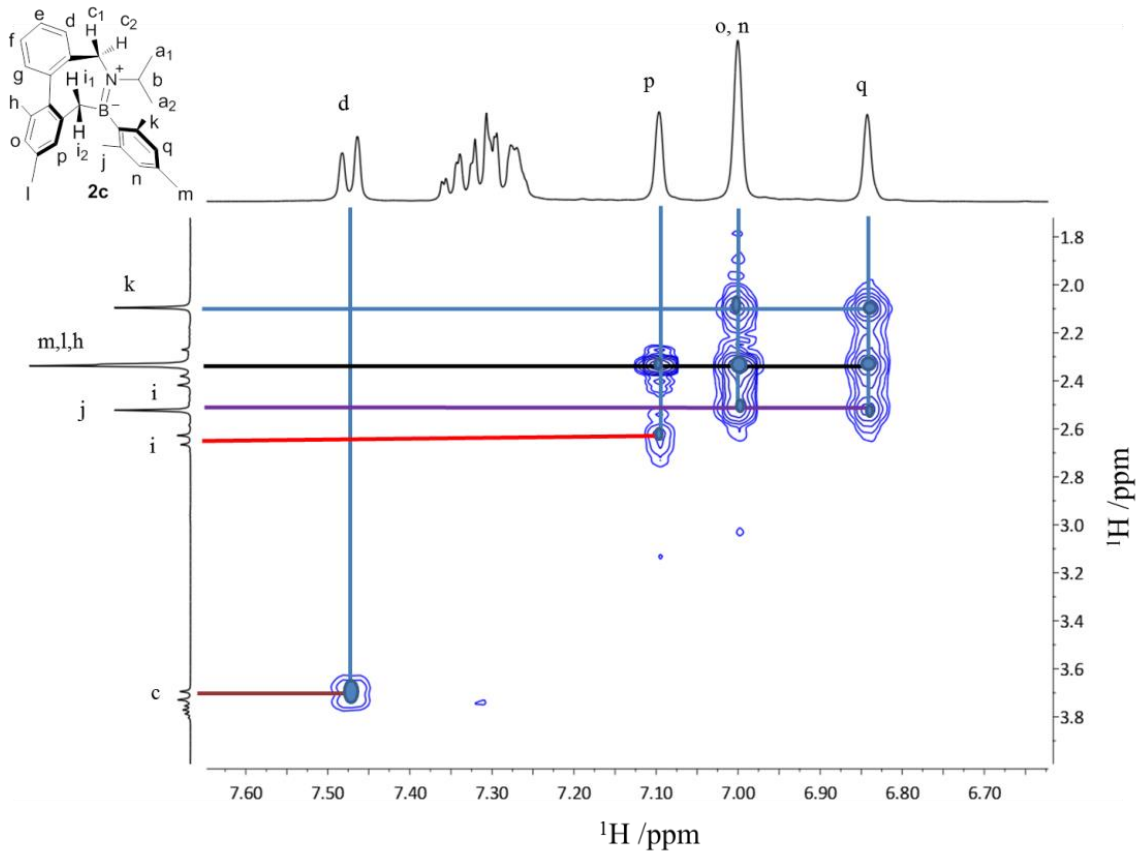


Figure S37. ^{1}H-^{1}H COSY NMR spectrum of **2c** in C_6D_6 with the assignment part of the peaks.

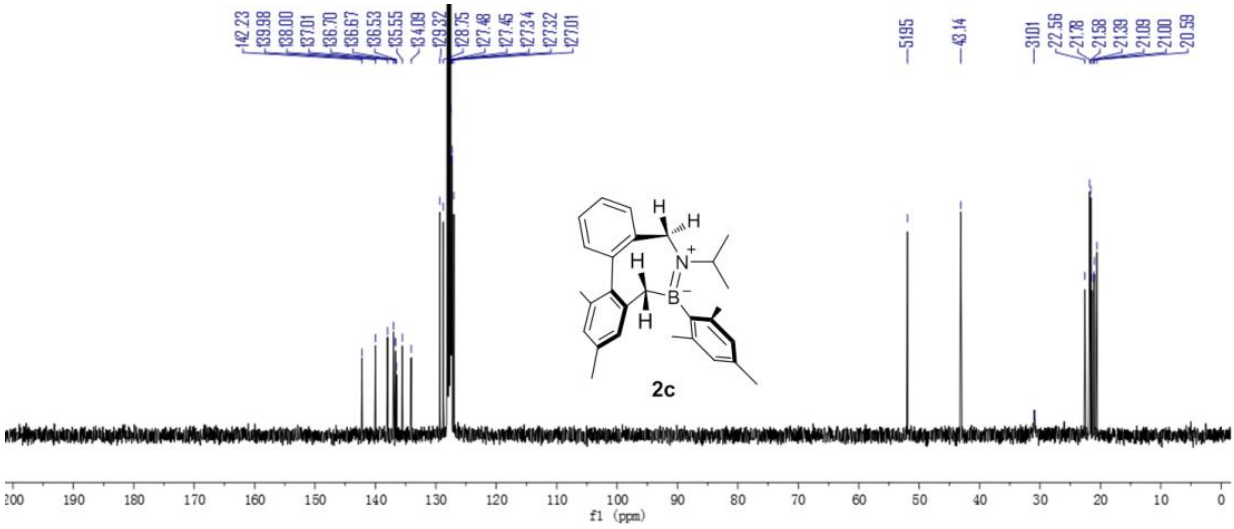


Figure S38. ^{13}C NMR spectrum of **2c** in C_6D_6.

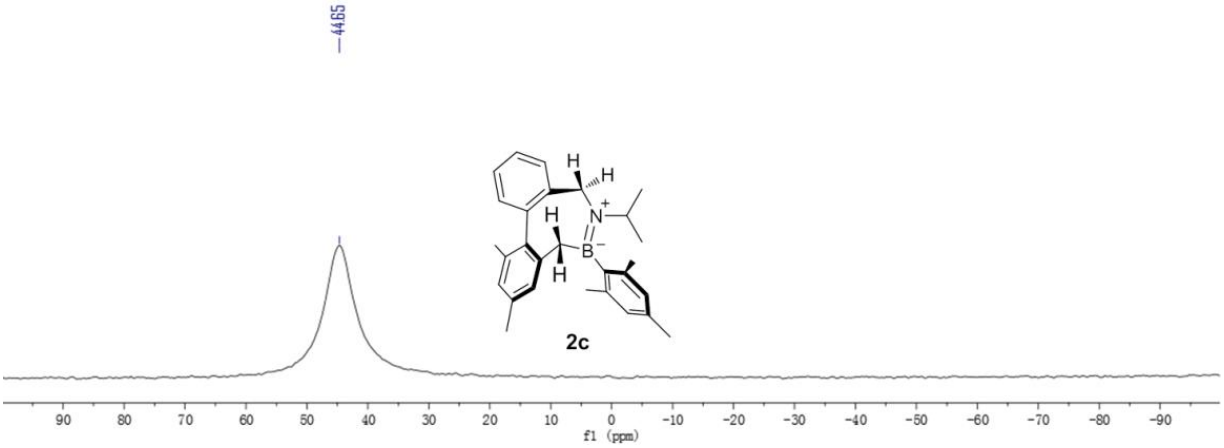


Figure S39. ^{11}B NMR spectra of **2c** in C_6D_6.

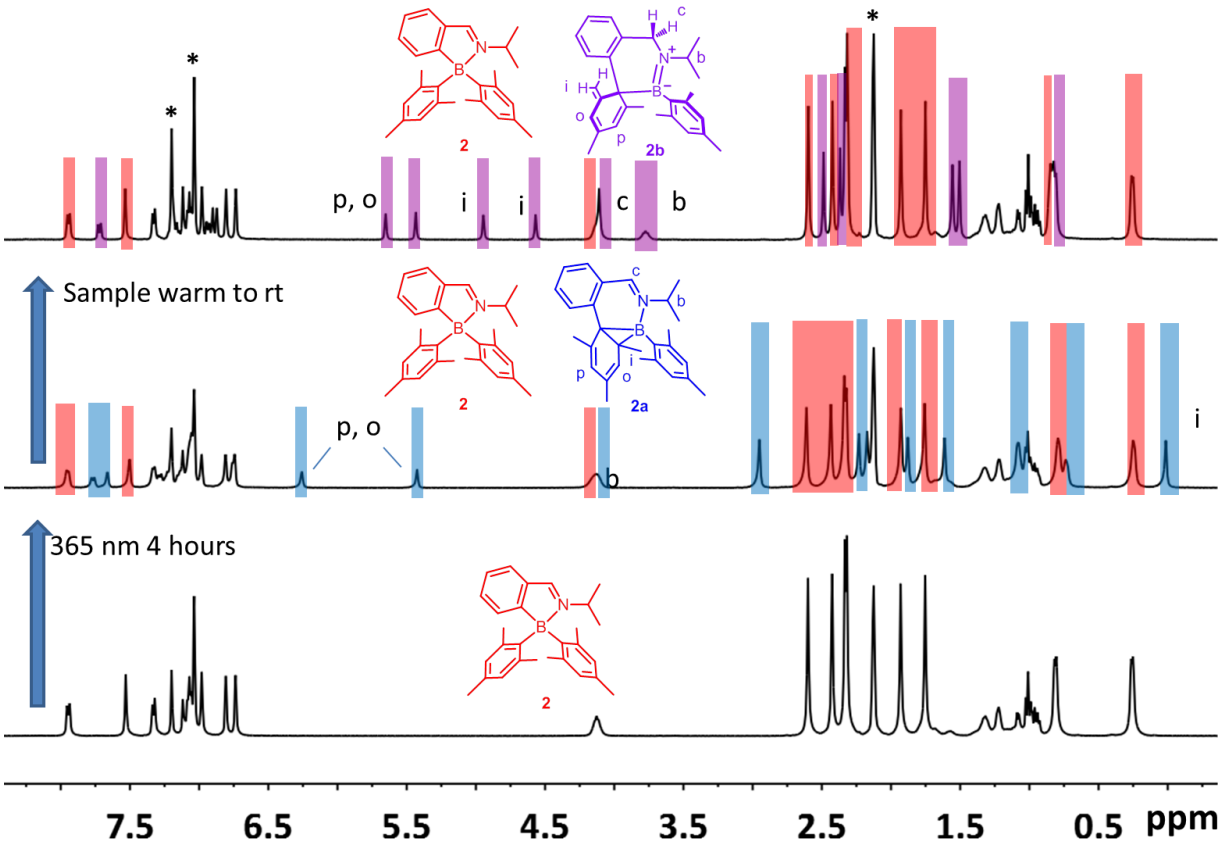


Figure S40. (a) ^{1}H NMR (203K) of **2** (0.02M in C_6D_6); (b) ^{1}H NMR (203k) of a mixture of **2** and **2a** after 4 hours irradiation of **2** at 365 nm in dry ice/acetone bath; (c) ^{1}H NMR (203k) of a mixture of **2** and **2b** after the sample warm to room temperature (the solvent peaks were labeled with ***)**.

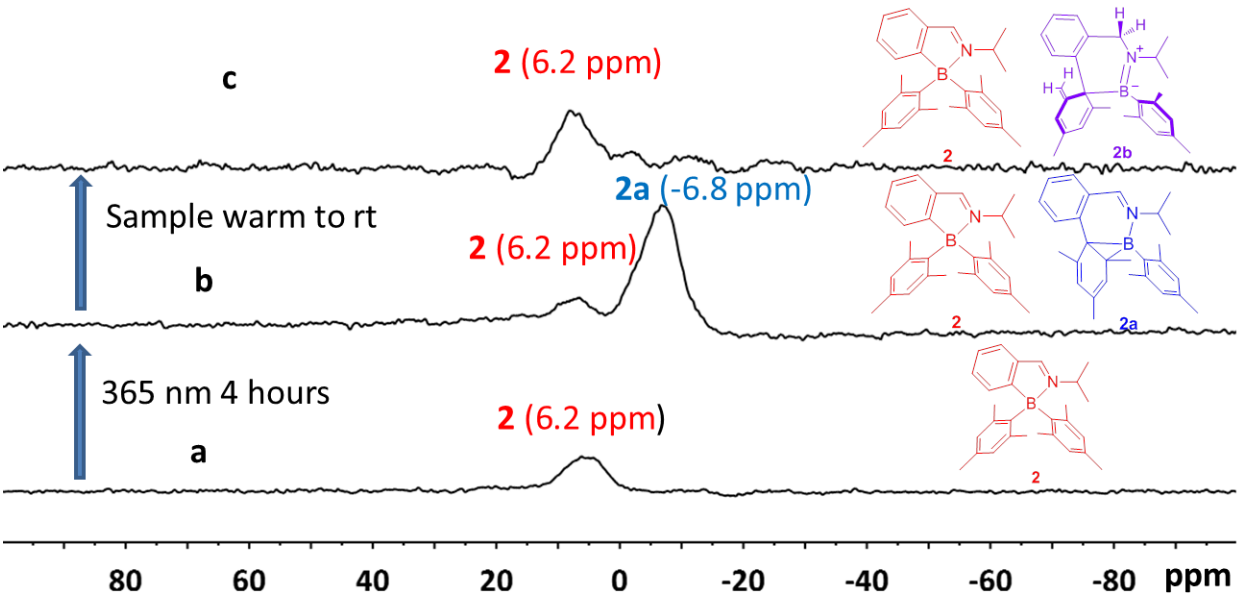


Figure S41. (a) ^{11}B NMR (203K) of **2** (0.02M in C_6D_6); (b) ^{11}B NMR (203k) of a mixture of **2** and **2a** after **4** hours irradiation of **2** at 365 nm in dry ice/acetone bath; (c) ^{11}B NMR (203k) of a mixture of **2** and **2b** after the sample warm to room temperature (the ^{11}B signal of **2b** is not show up 203k).

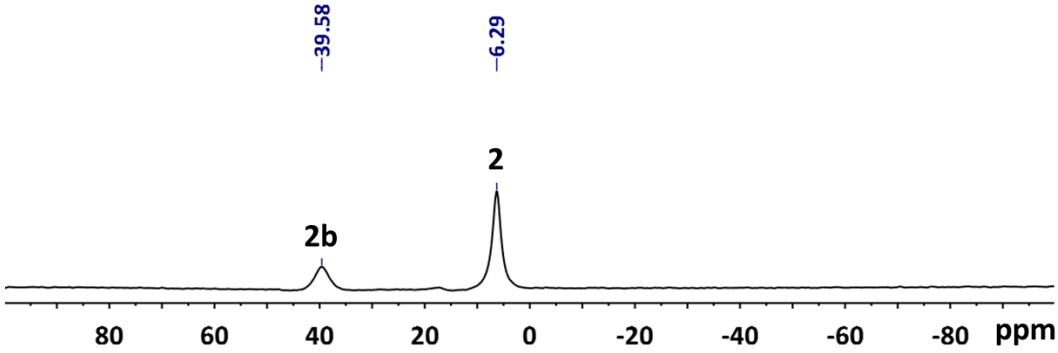


Figure S42. ^{11}B NMR (298k) of a mixture of **2** and **2b** after **2** irradiate for 4 hours at 365nm in dry ice bath and then warm to room temperature.

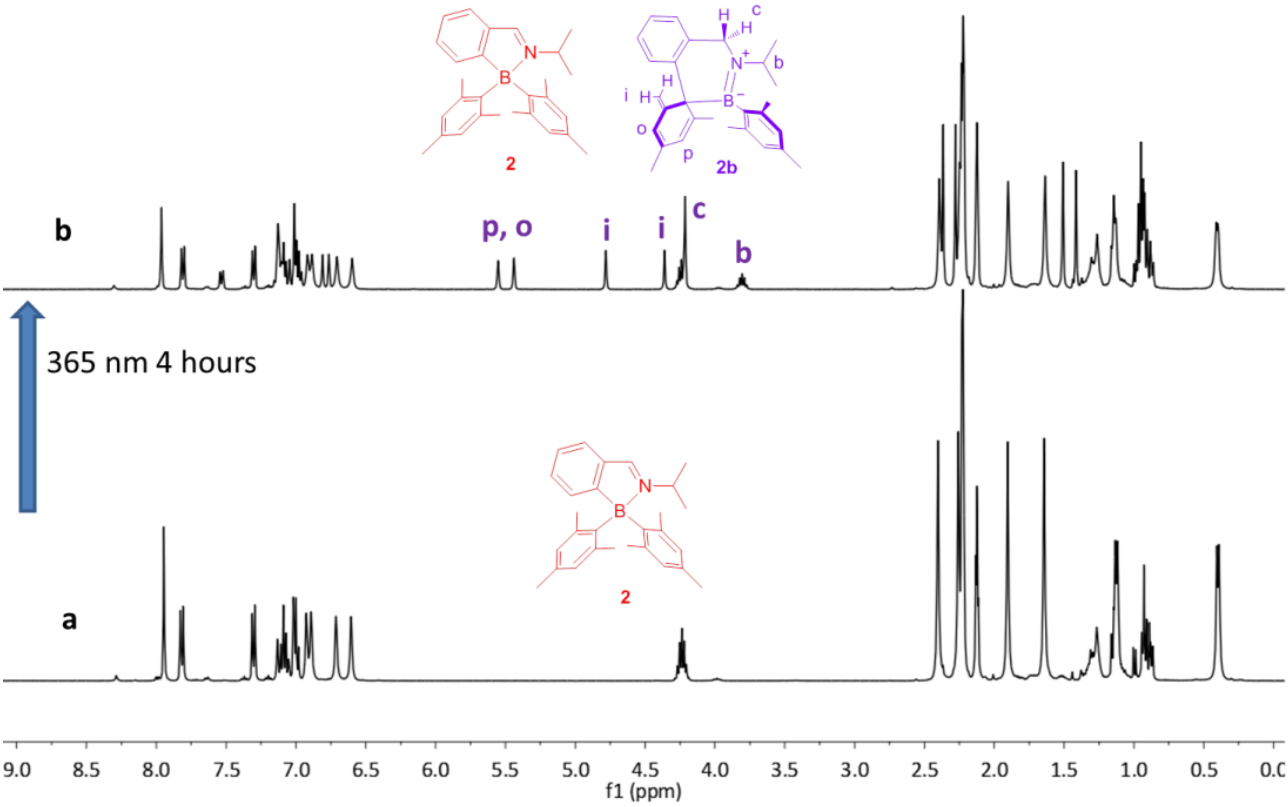
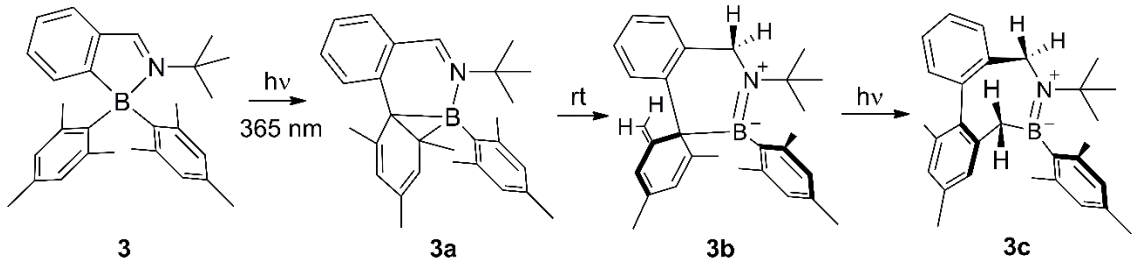


Figure S43. (a) ^{1}H NMR (298k) of **2** (0.02M in C_6D_6); (b) ^{1}H NMR (298k) of a mixture of **2** and **2b** after irradiation of **2** for 4 hours at 365nm in dry ice/acetone bath and then warm to room temperature.

3.1.3. **3 → 3c**



Scheme S4. The structures of **3 - 3c**

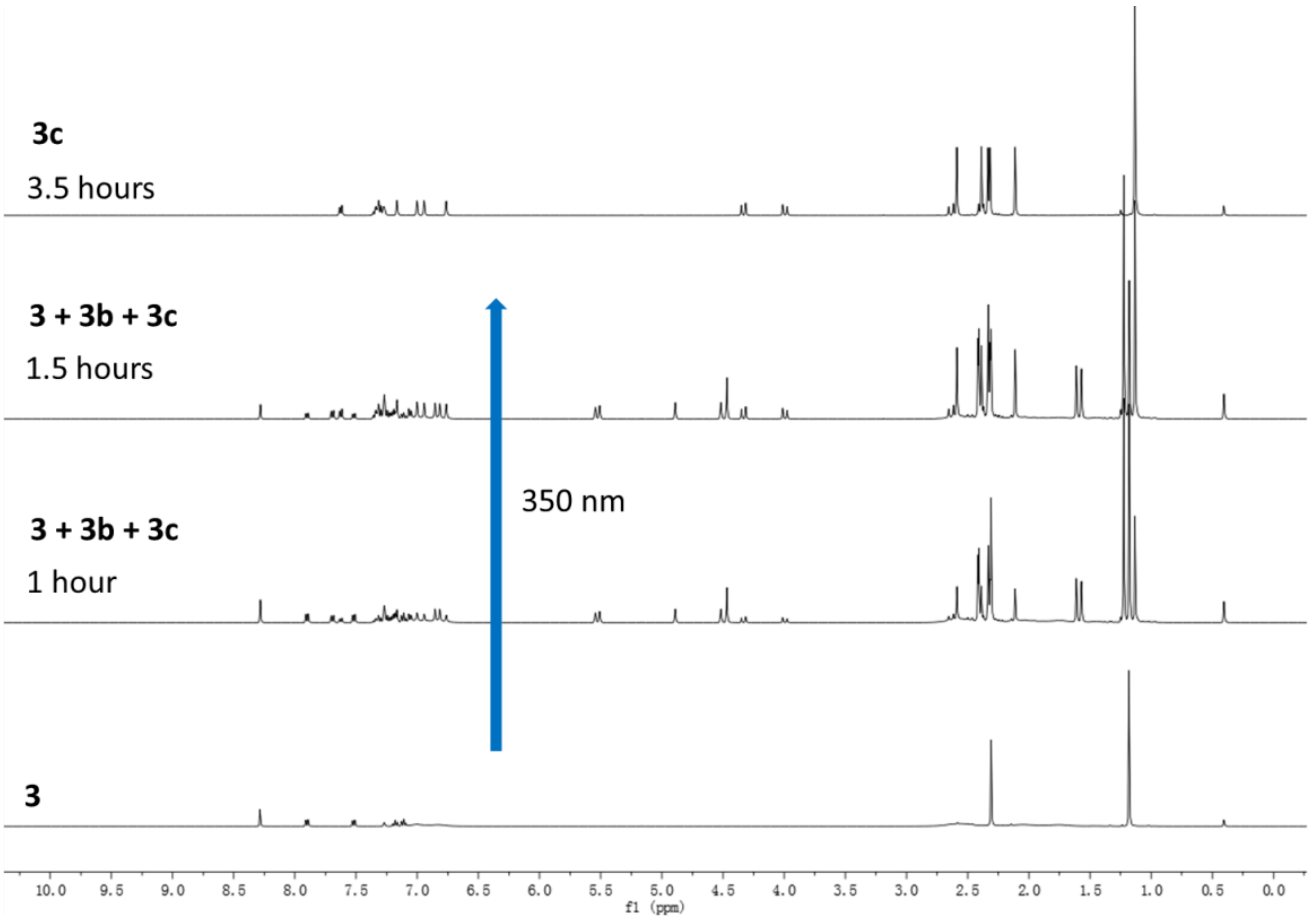


Figure S44. ^{1}H NMR spectra showing the sequential conversion of **3 → 3c** (0.1M in C_6D_6).

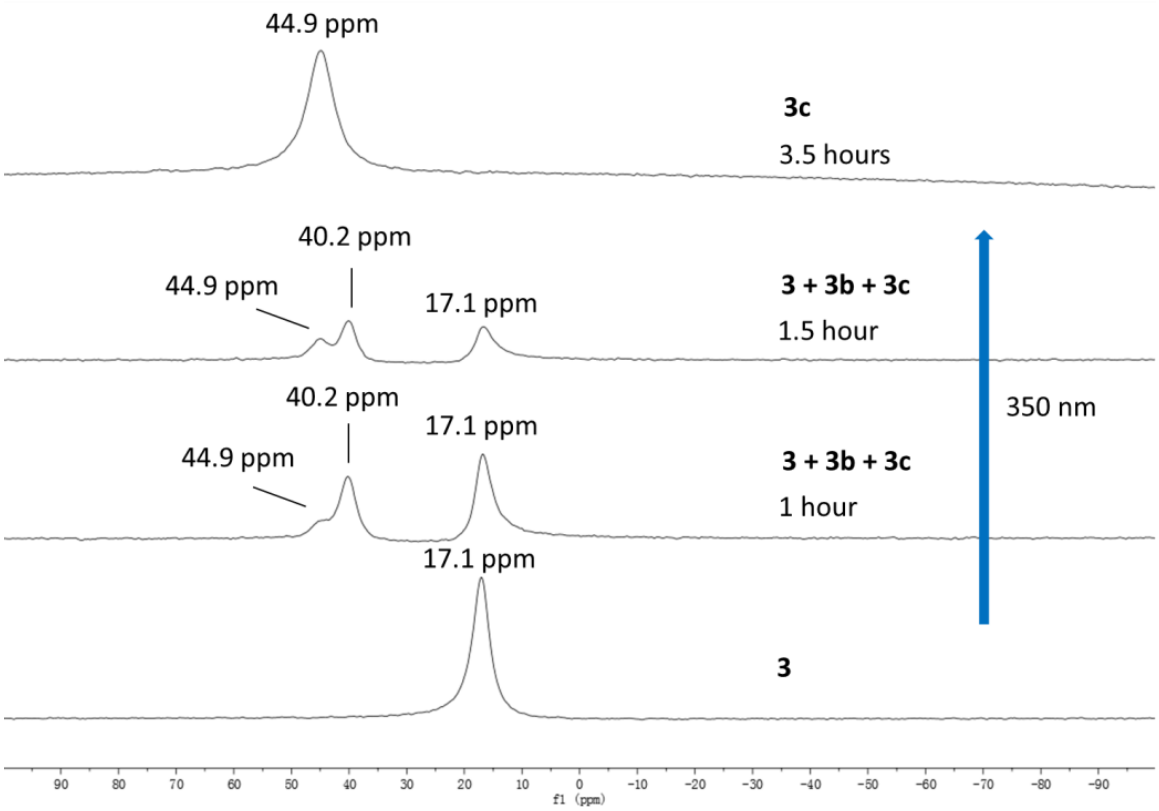


Figure S45. ^{11}B NMR spectra showing the sequential conversion of **3** → **3c** (0.1M in C_6D_6).

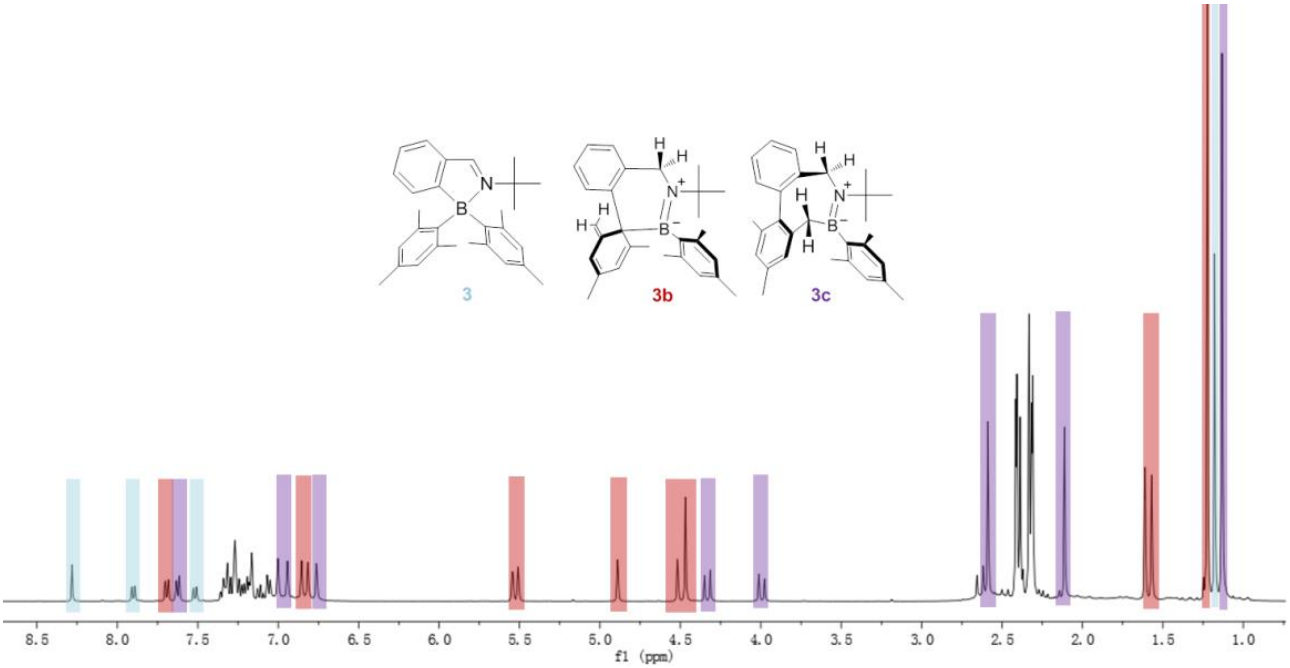


Figure S46. ^{1}H NMR spectrum of **3** (blue), **3b** (red)**, 3c** (purple) highlighted with different color in C_6D_6.

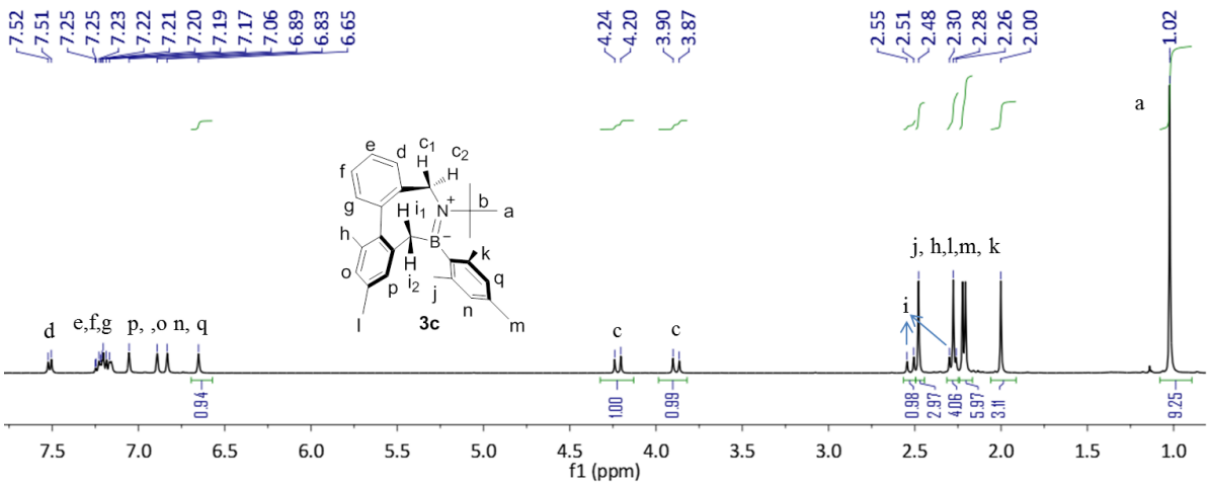


Figure S47. ^{1}H NMR spectrum of **3c** in C_6D_6 with the assignment of all peaks.

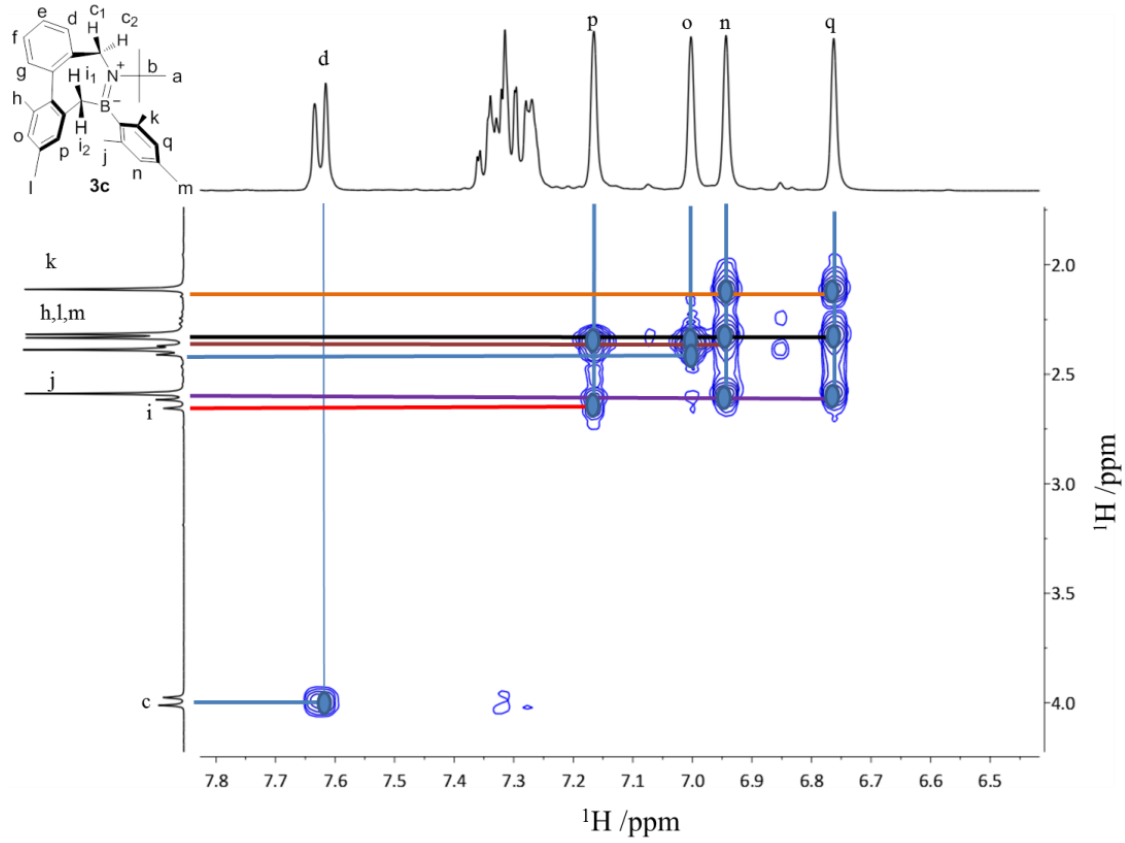


Figure S48. ^{1}H-^{1}H COSY NMR spectrum of **3c** in C_6D_6 with the assignment of part of the peaks.

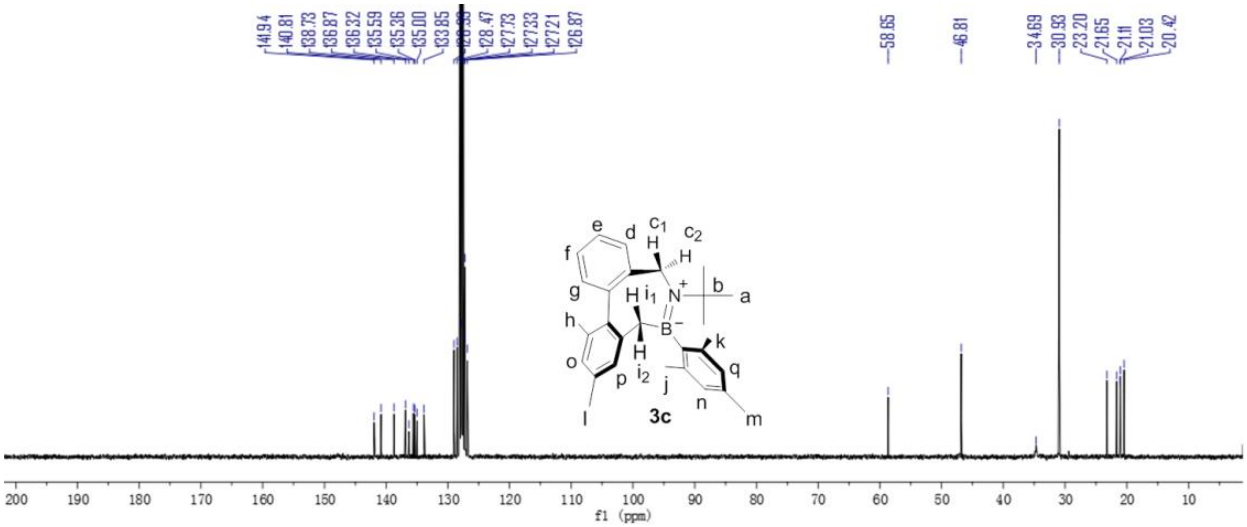


Figure S49. ^{13}C NMR spectrum of **3c** in C_6D_6.

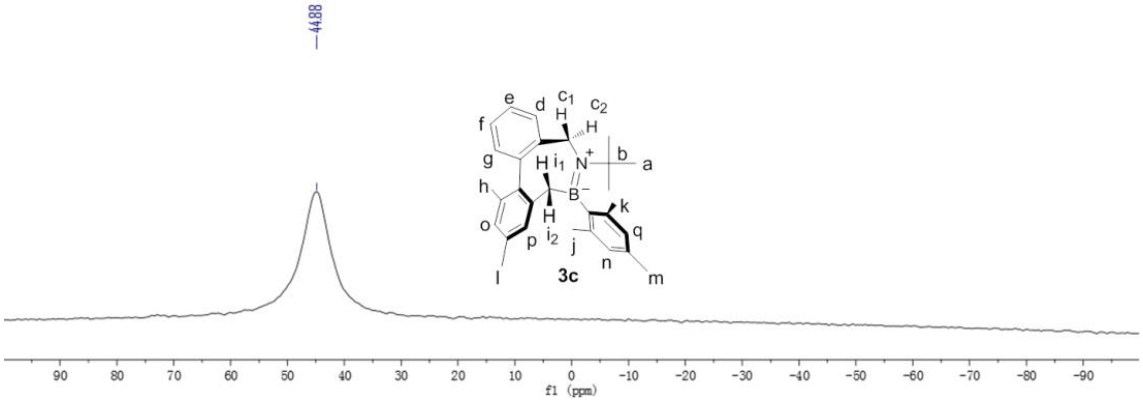
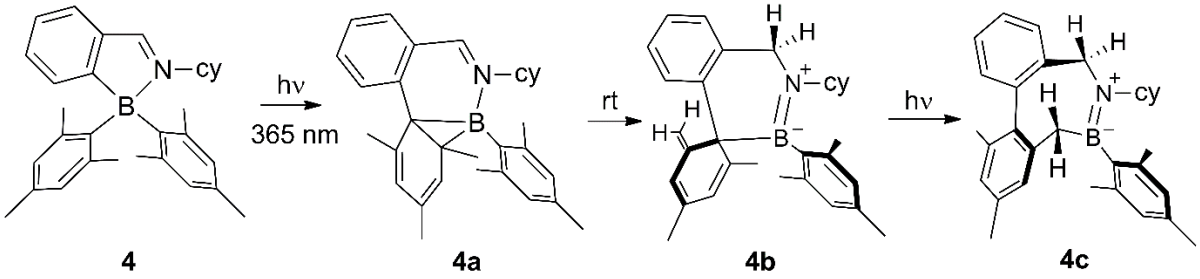


Figure S50. ^{11}B NMR spectra of **3c** in C_6D_6.

3.1.4. **4 → 4c**



Scheme S5. The structures of **4** - **4c**

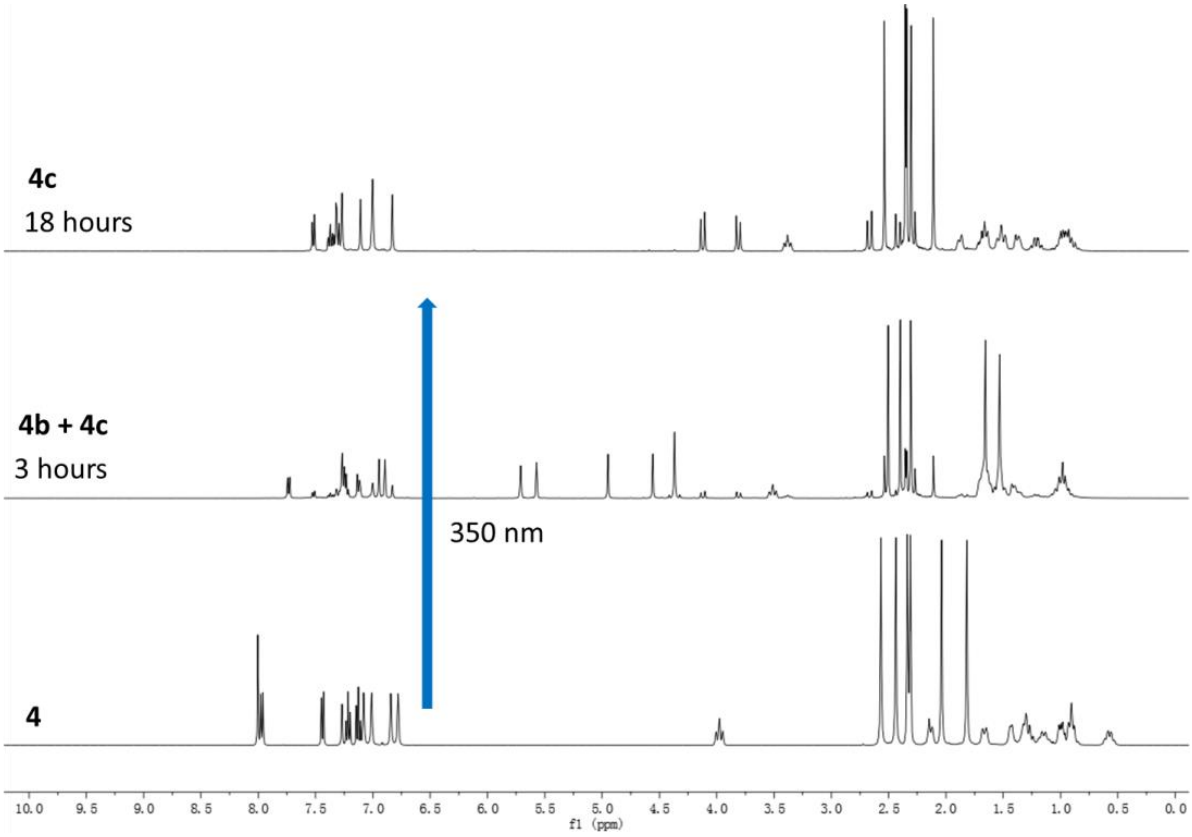


Figure S51. ^{1}H NMR spectra showing the conversion of **4 → 4c** (0.07M in C_6D_6).

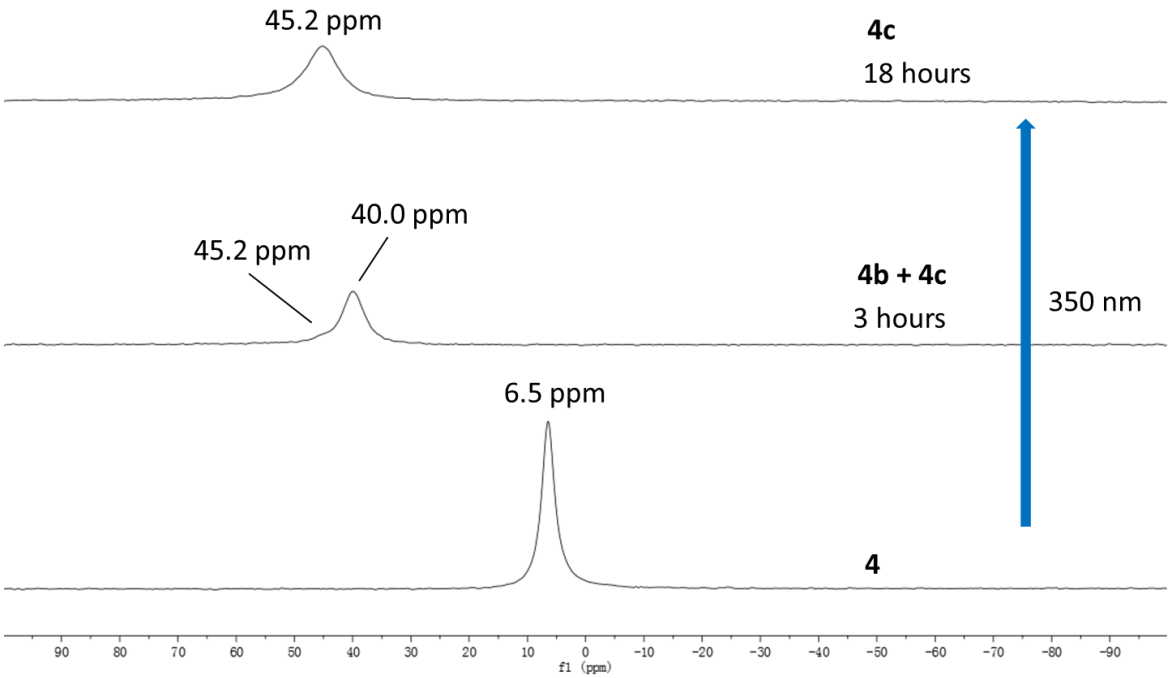


Figure S52. ^{11}B NMR spectra showing the conversion of **4** → **4c** (0.07M in C_6D_6).

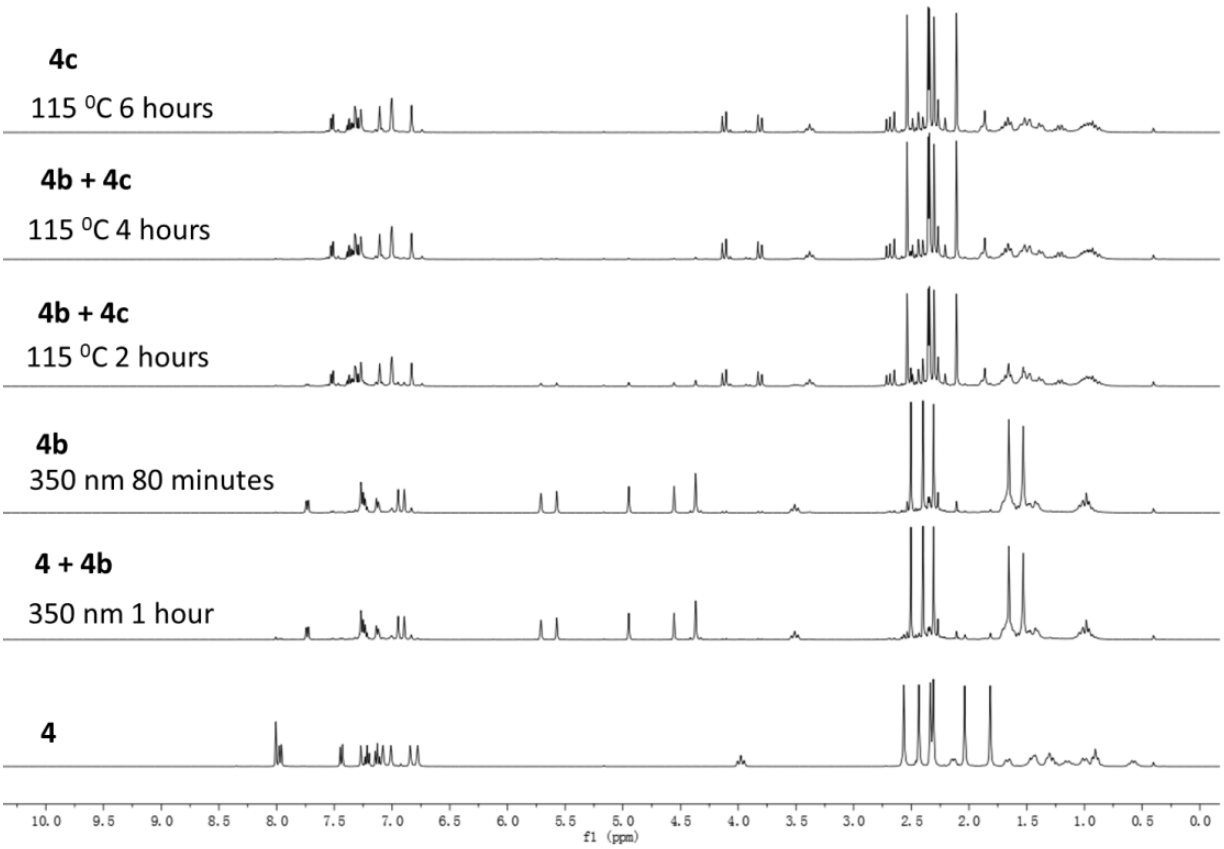


Figure S53. ^{1}H NMR spectra showing the photo conversion of **4** → **4b** and thermos conversion of **4b** → **4c** (0.08M in C_6D_6).

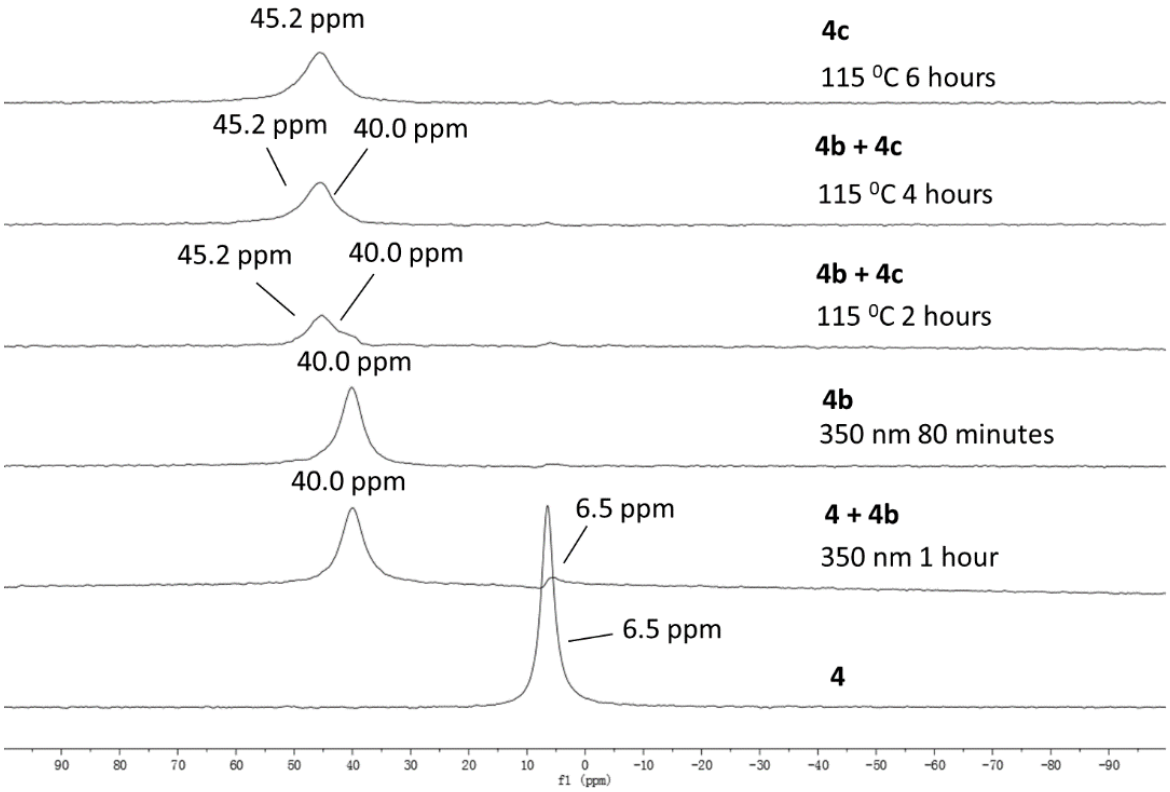


Figure S54. ^{11}B NMR spectra showing the photo conversion of **4** → **4b** and thermos conversion of **4b** → **4c** (0.08M in C_6D_6).

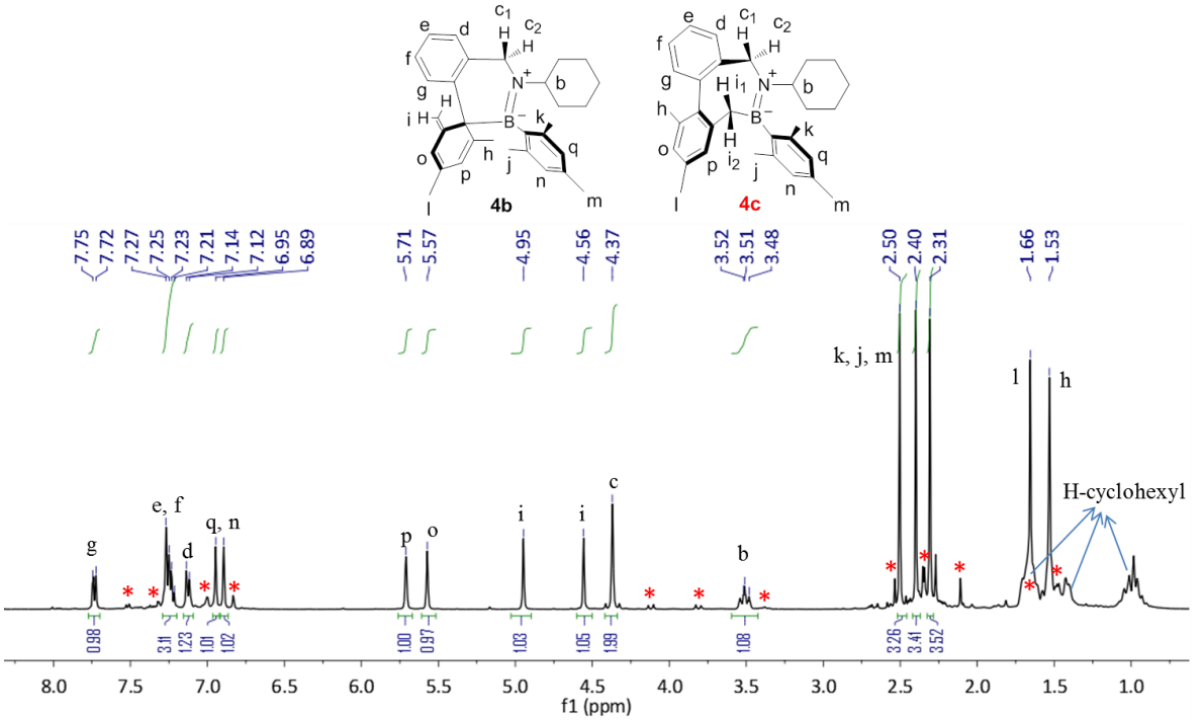


Figure S55. ^{1}H NMR spectra of **4b** (mixed with some **4c** and labeled with *) in C_6D_6 with the assignment of all

peaks.

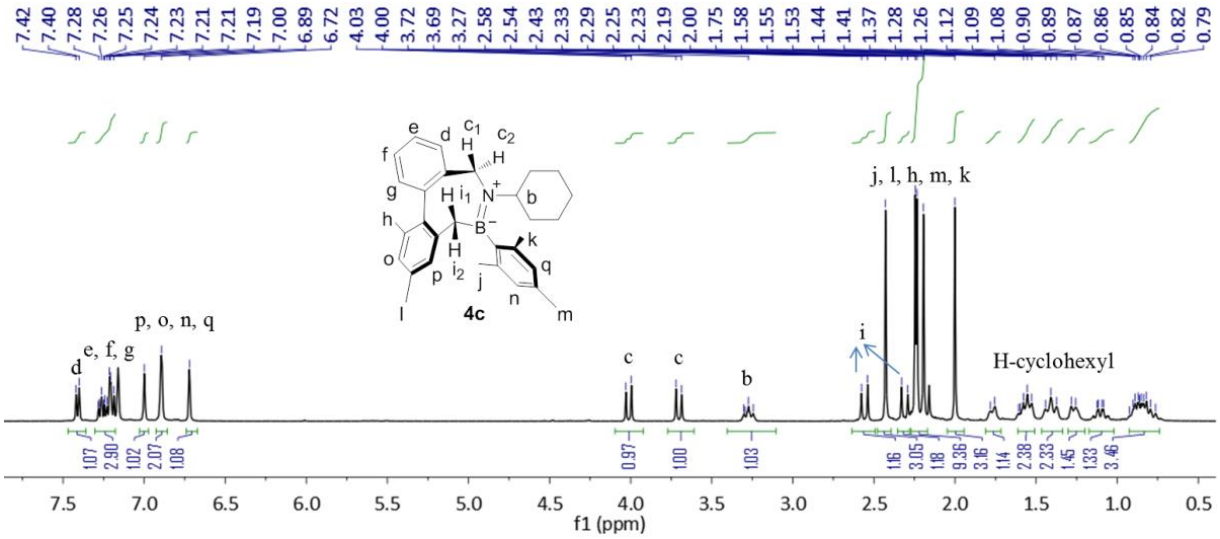


Figure S56. ^{1}H NMR spectra of **4c** in C_6D_6 with the assignment of all peaks.

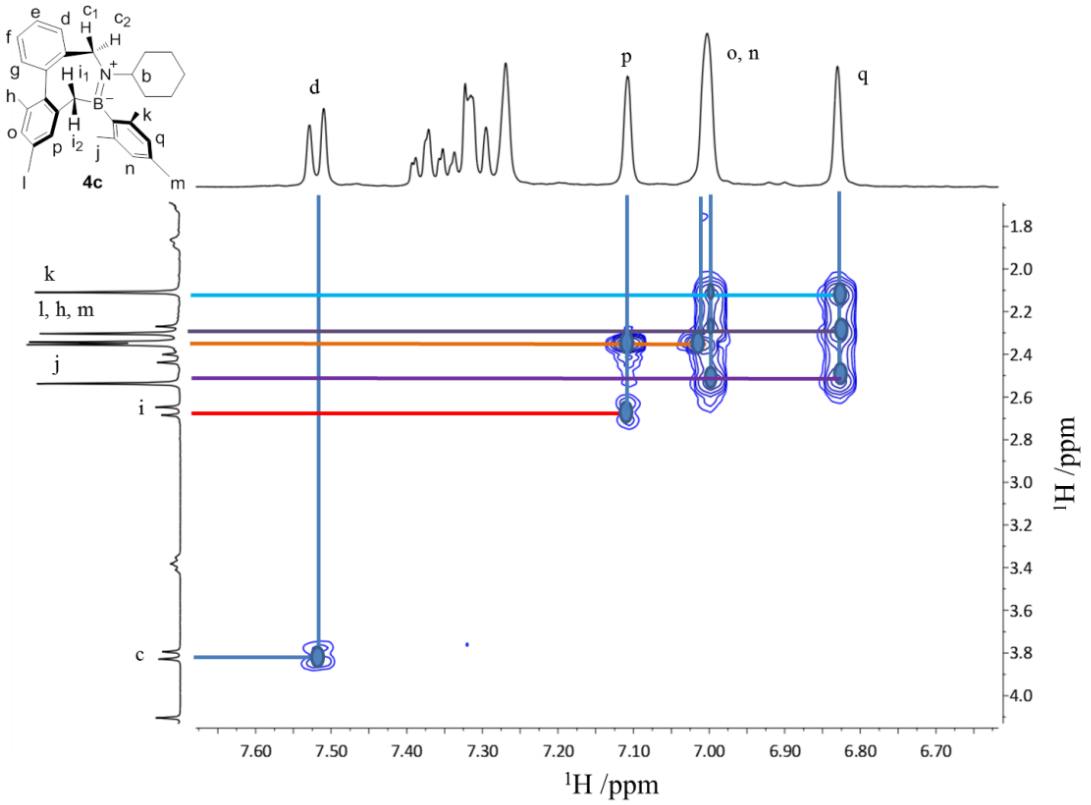


Figure S57. ^{1}H-^{1}H COSY NMR spectra of **4c** in C_6D_6 with the assignment of part of the peaks.

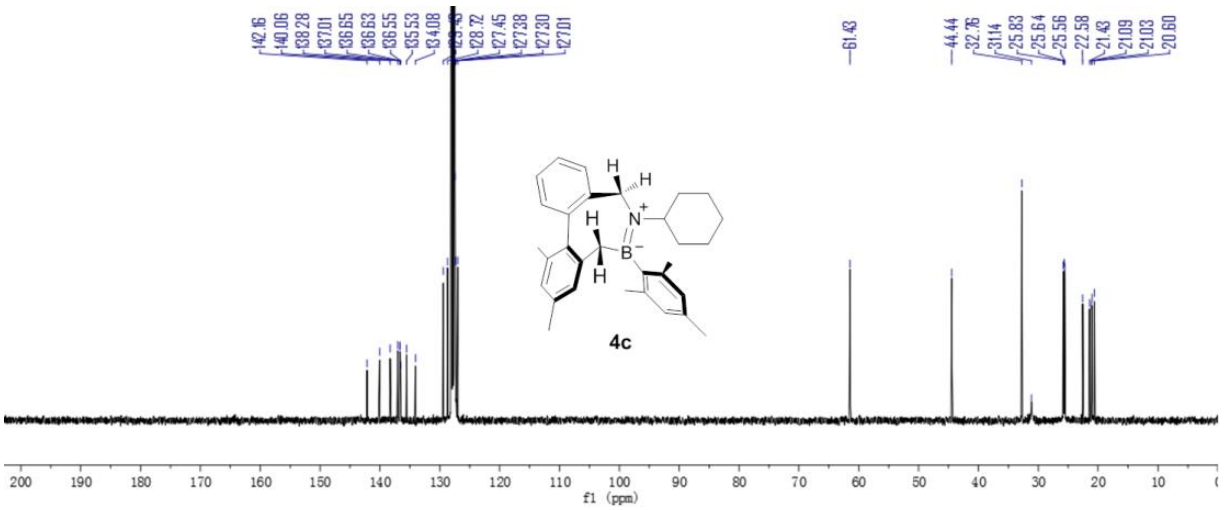


Figure S58. ^{13}C NMR spectra of **4c** in C_6D_6.

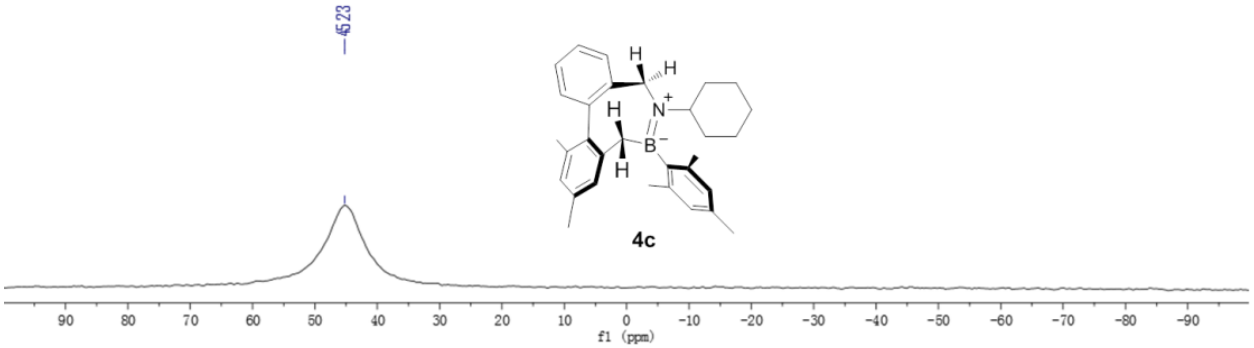
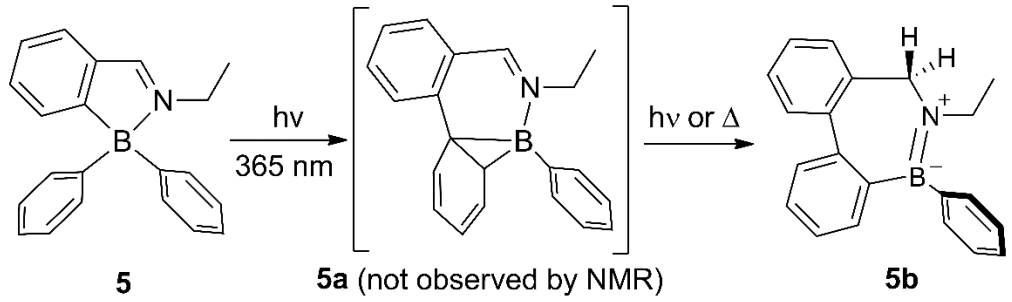


Figure S59. ^{11}B NMR spectra of **4c** in C_6D_6.

3.1.5. **5 → 5b**



Scheme S6. The structures of **5** - **5b**

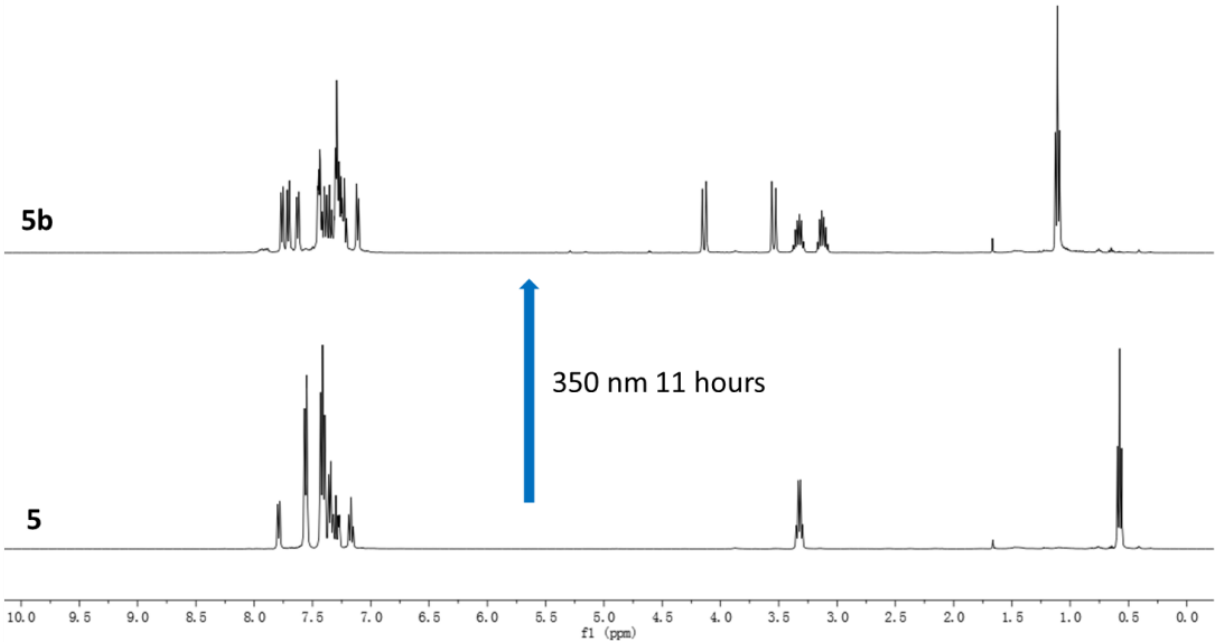


Figure S60. ^{1}H NMR spectra showing the conversion of **5** → **5b** (0.1M in C_6D_6).

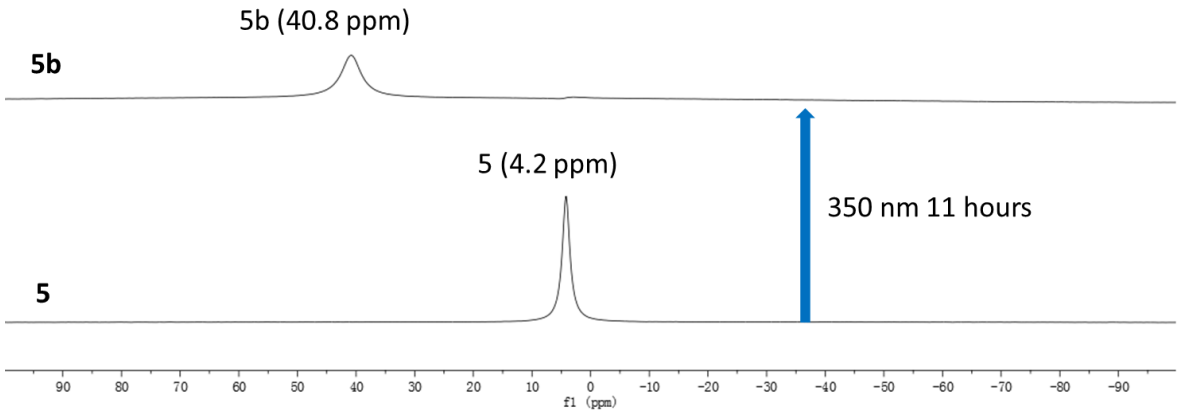


Figure S61. ^{11}B NMR spectra showing the conversion of **5** → **5b** (0.1M in C_6D_6).

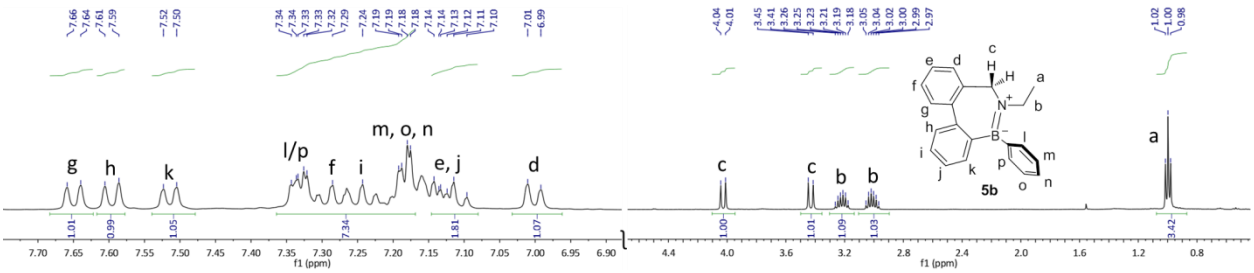


Figure S62. ^{1}H NMR spectra of **5b** in C_6D_6 with the assignment of all peaks.

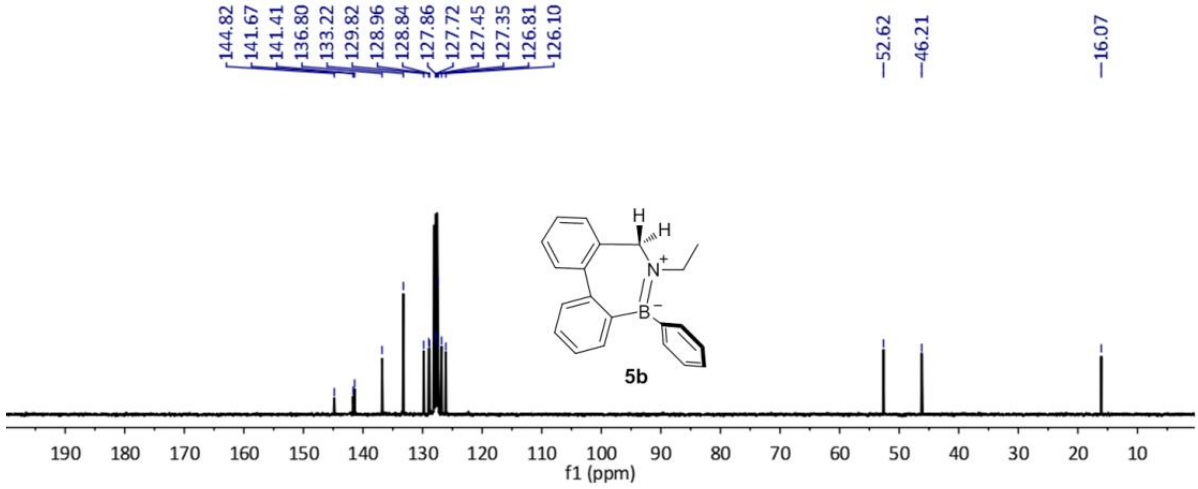


Figure S63. ^{13}C NMR spectra of **5b** in C_6D_6.

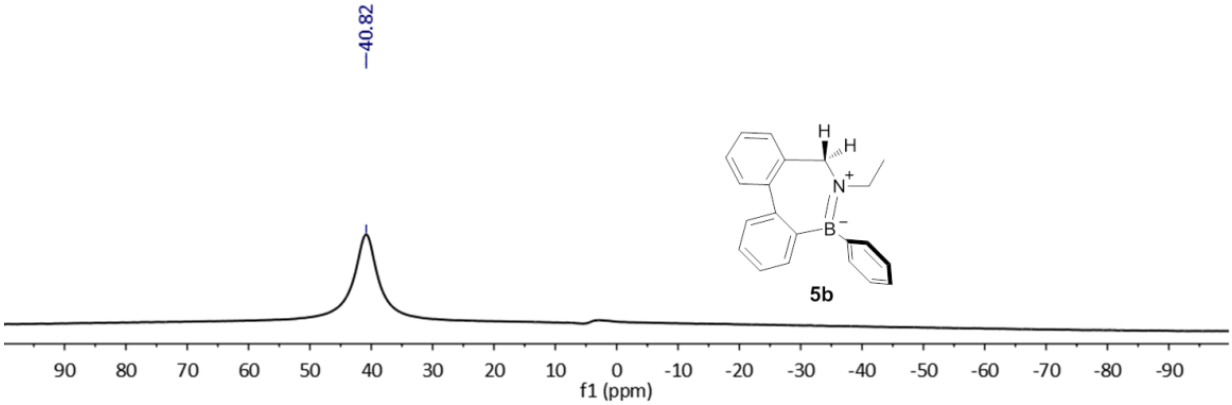
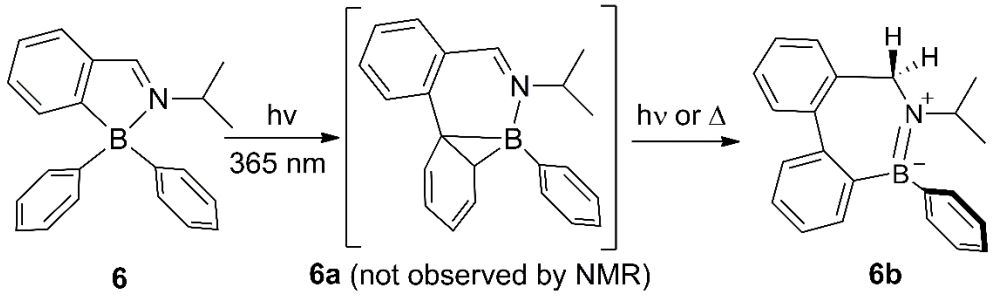


Figure S64. ^{11}B NMR spectra of **5b** in C_6D_6.

3.1.6. **6 → 6b**



Scheme S7. The structures of **6** - **6b**

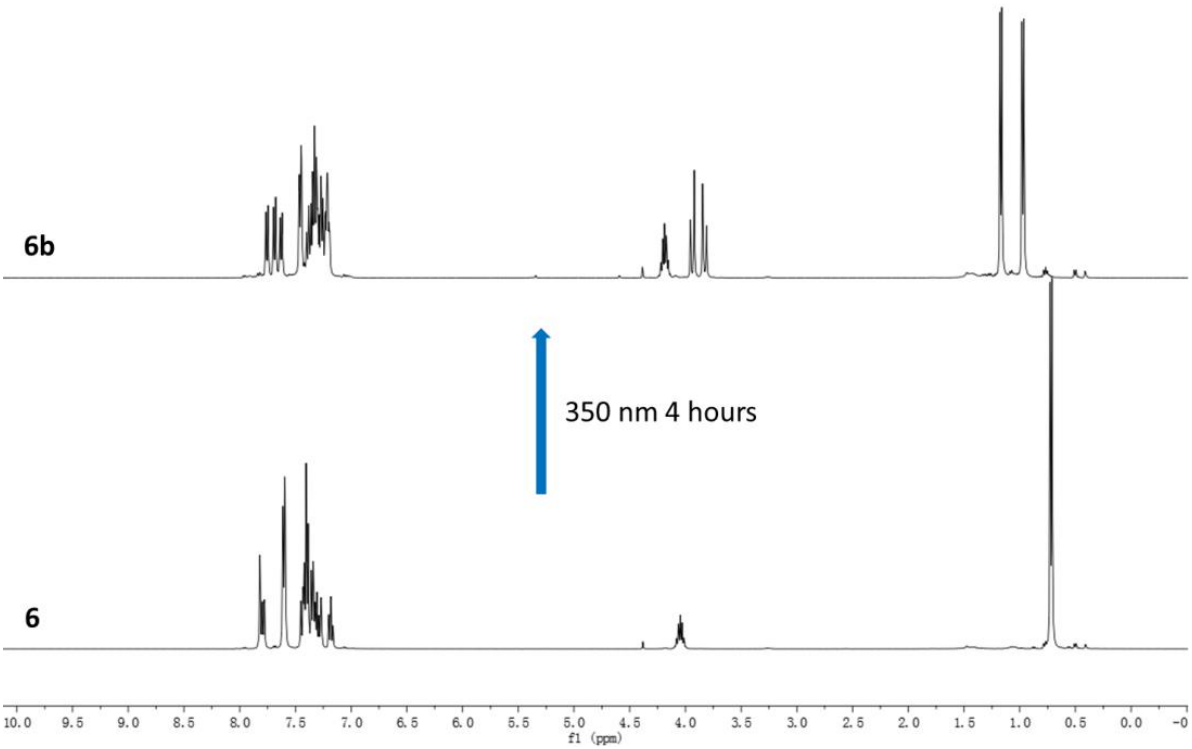


Figure S65. ^{1}H NMR spectra showing the conversion of **6** → **6b** (0.2M in C_6D_6).

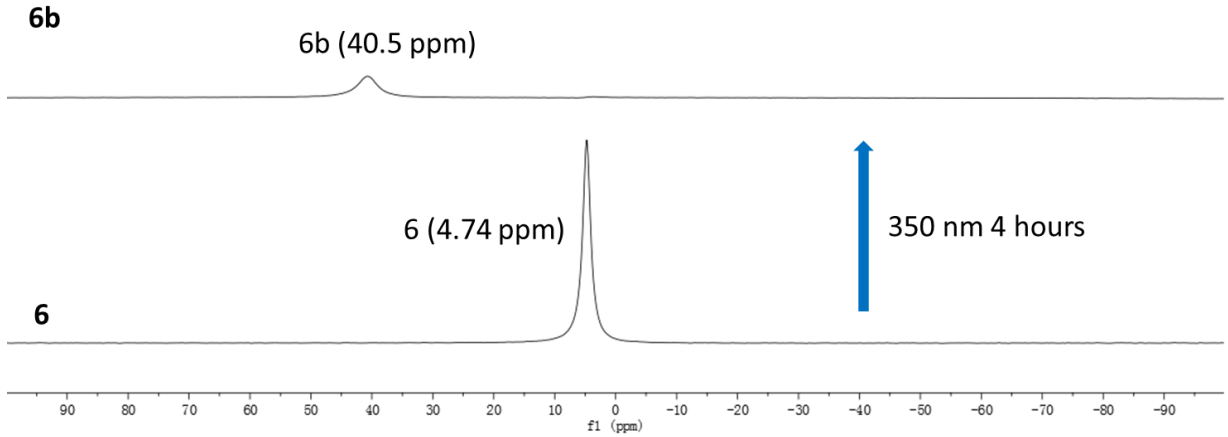


Figure S66. ^{11}B NMR spectra showing the conversion of **6** → **6b** (0.2M in C_6D_6).

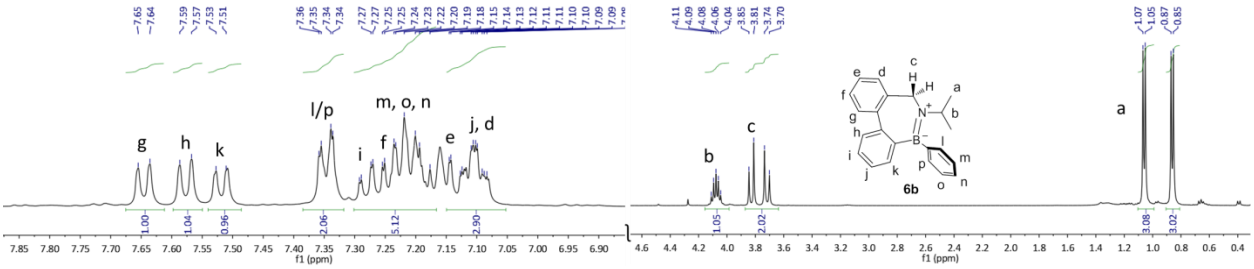


Figure S67. ^{1}H NMR spectra of **6b** in C_6D_6 with the assignment of all peaks.

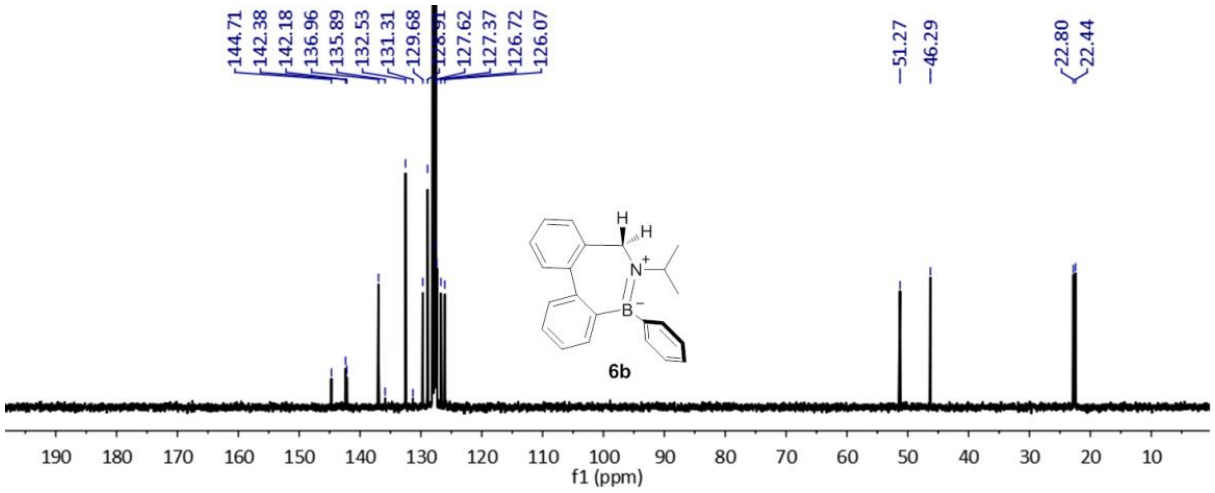


Figure S68. ^{13}C NMR spectra of **6b** in C_6D_6.

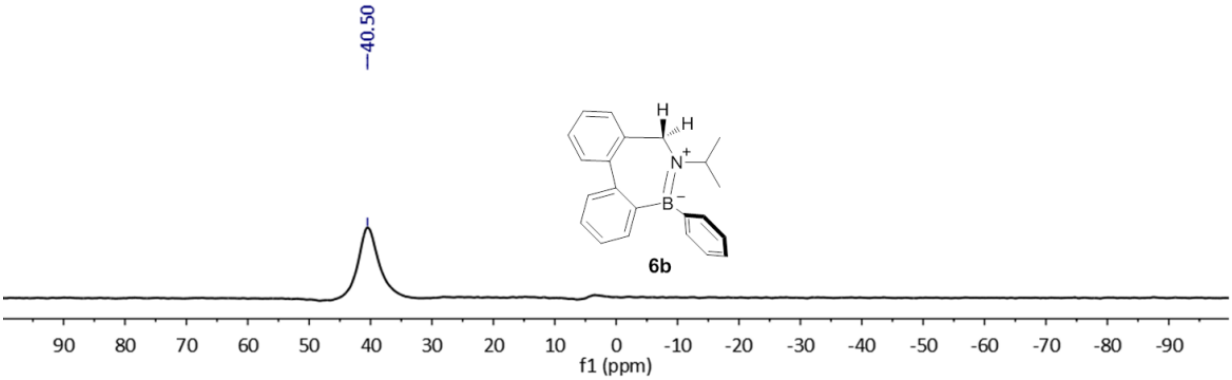
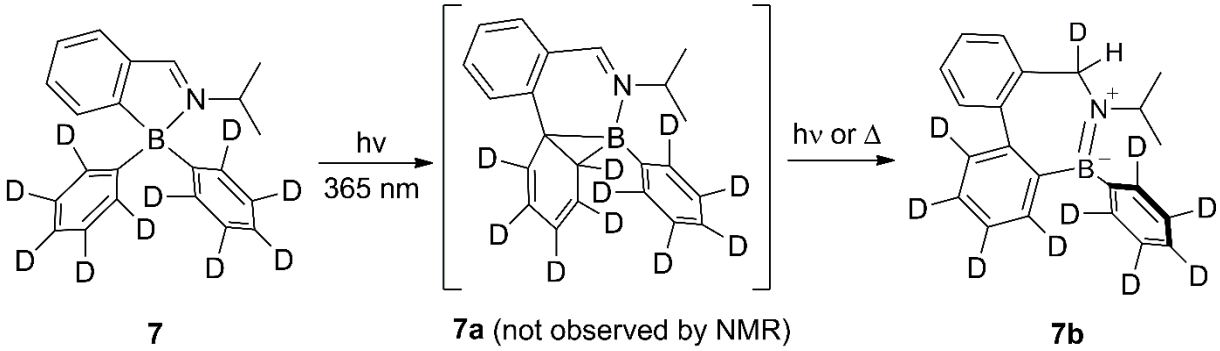


Figure S69. ^{11}B NMR spectra of **6b** in C_6D_6.

3.1.7. **7 → 7b**



Scheme S8. The structures of different isomers of **7** - **7b**

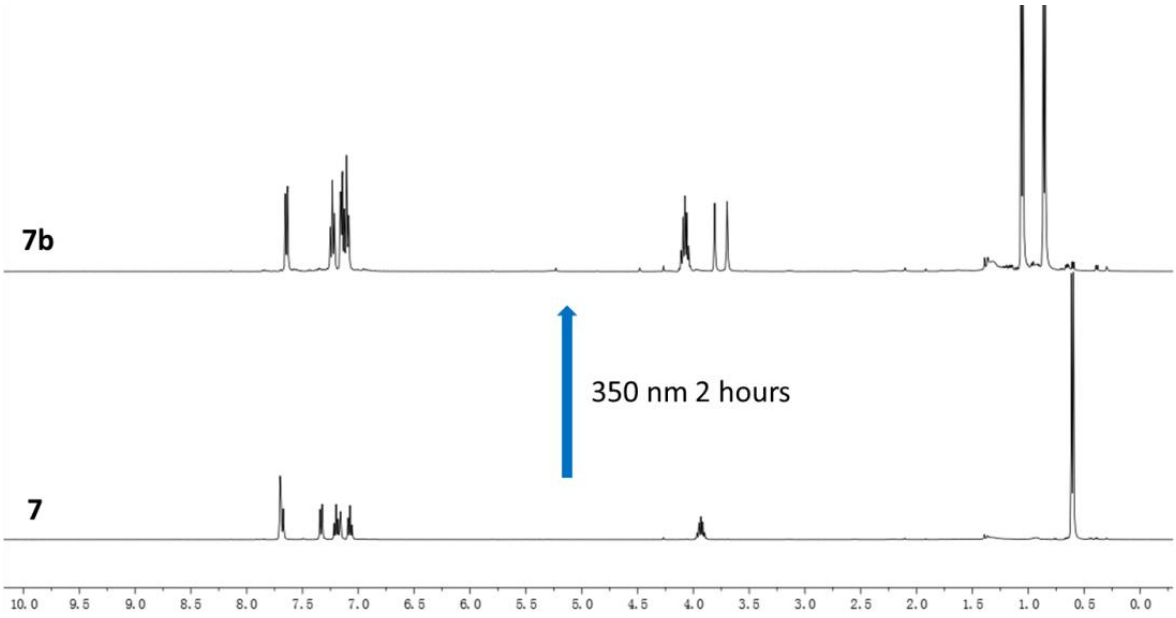


Figure S70. ^{1}H NMR spectra showing the conversion of **7** → **7b** (0.1M in C_6D_6).

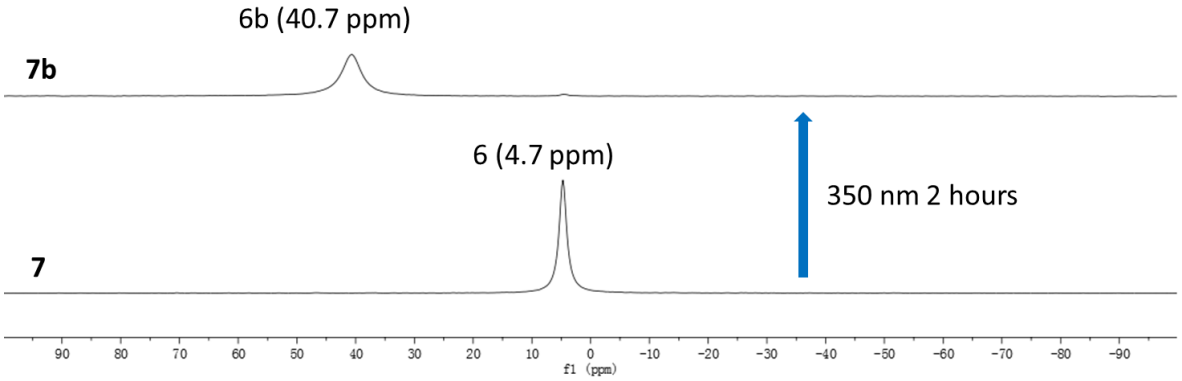


Figure S71. ^{11}B NMR spectra showing the conversion of **7** → **7b** (0.1M in C_6D_6).

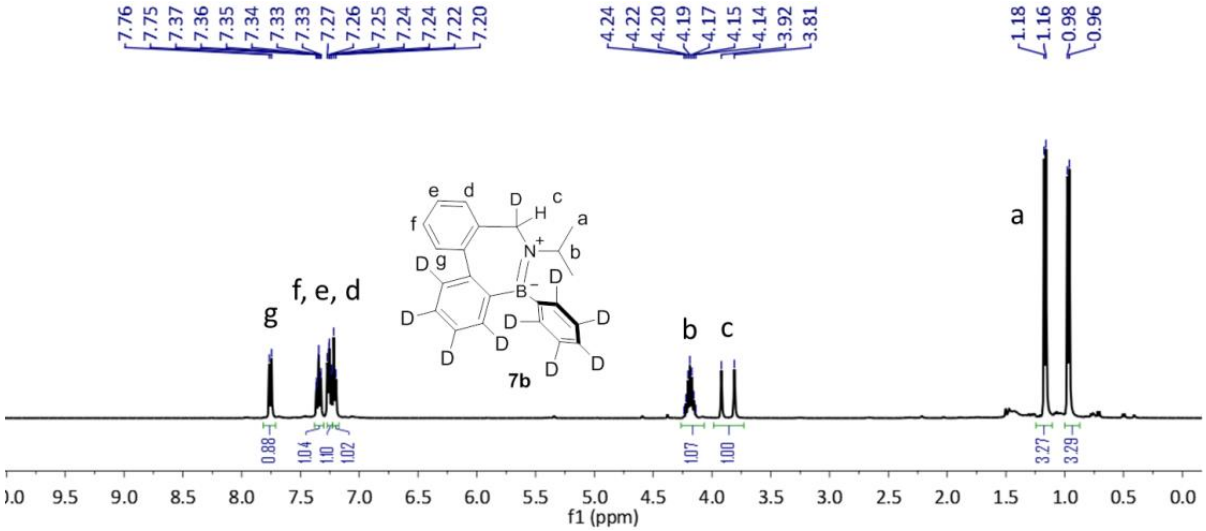


Figure S72. ^{1}H NMR spectra of **7b** in C_6D_6 with the assignment of all peaks.

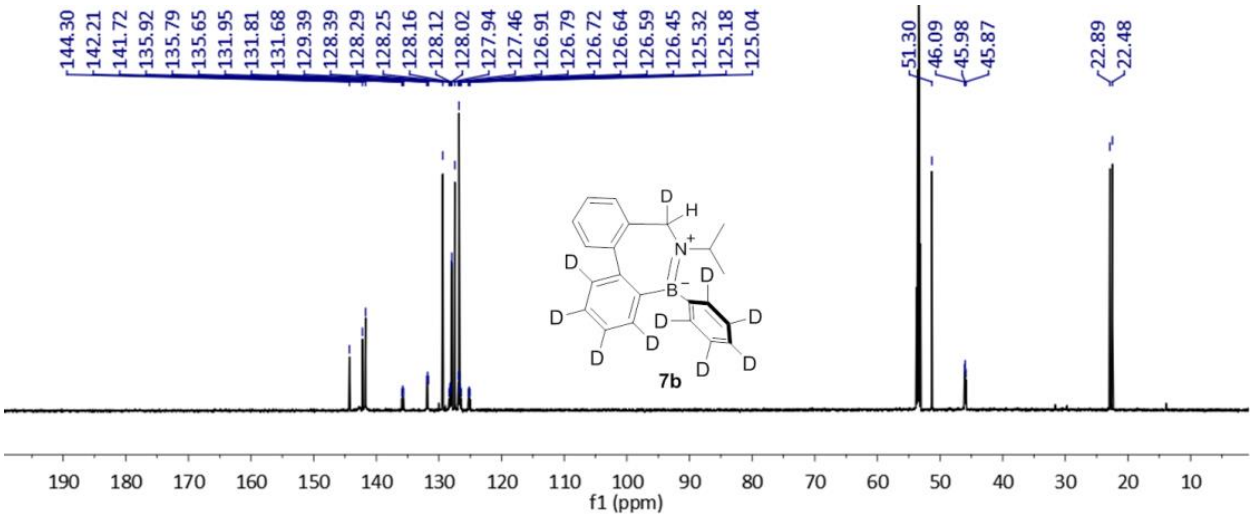


Figure S73. ^{13}C NMR spectra of **7b** in CD_2Cl_2.

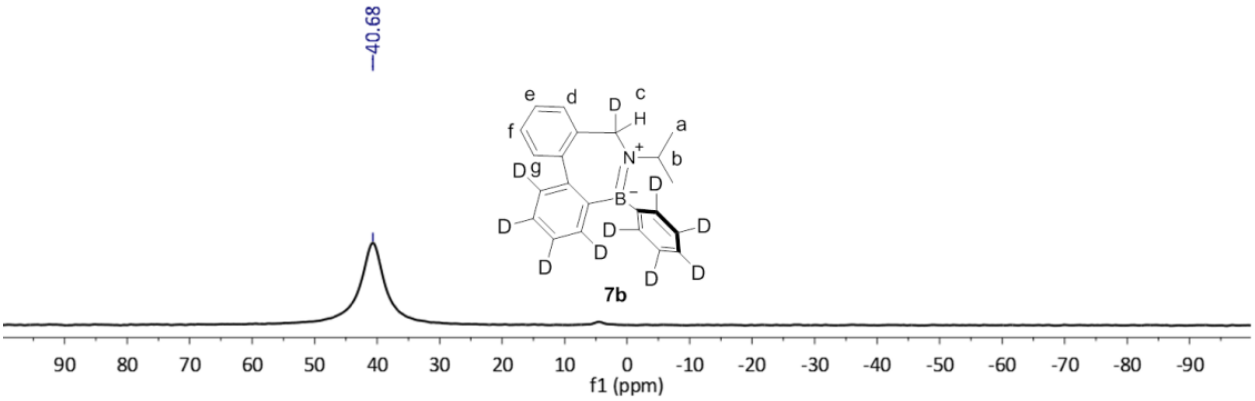


Figure 74. ^{11}B NMR spectra of **7b** in C_6D_6.

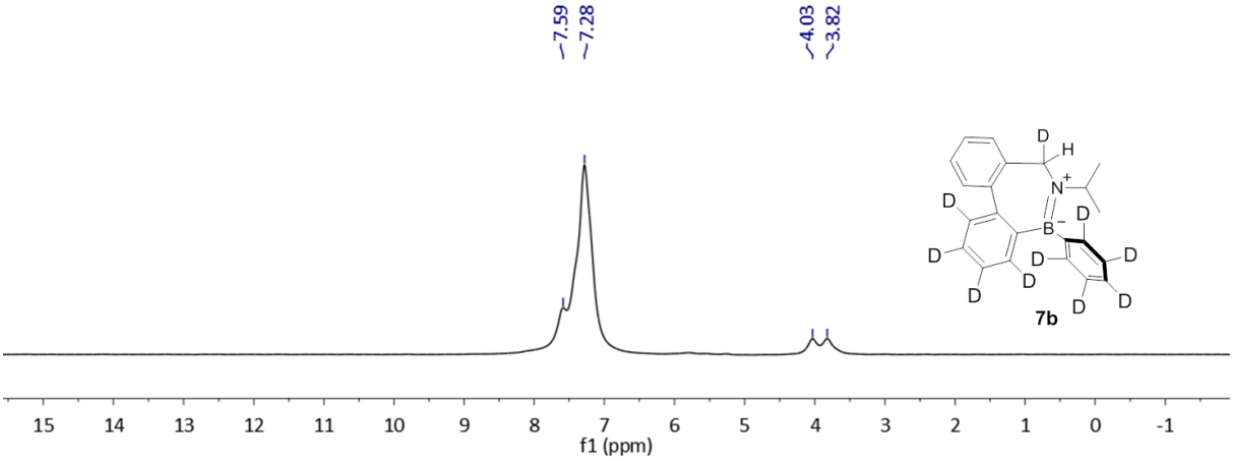


Figure S75. ^{2}H NMR spectra of **7b** in CH_2Cl_2.

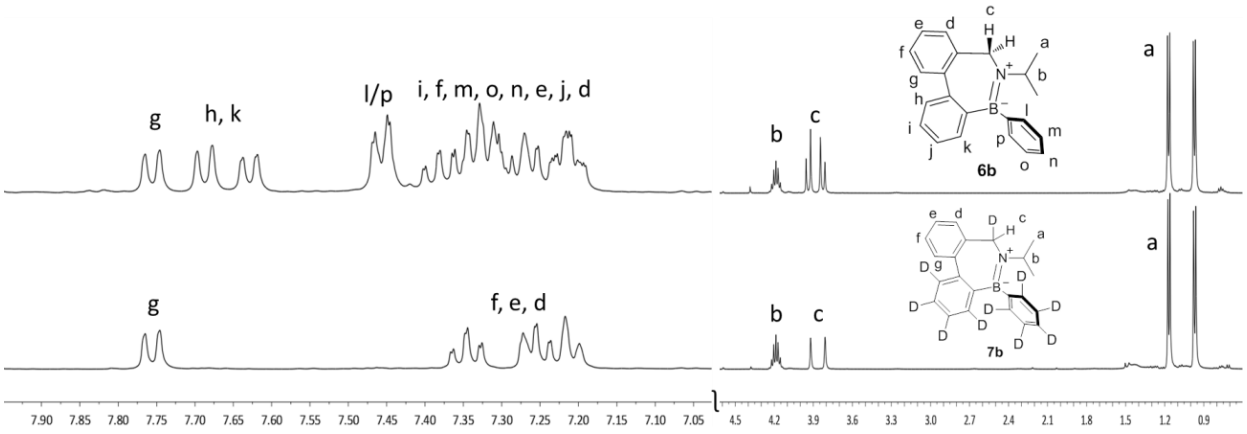


Figure S76. Comparison of the ^{1}H NMR spectrum of **6b** and **7b** in C_6D_6.

S4. Photophysical Properties

UV-Visible spectra were recorded on a Varian Cary 50 spectrometer. Excitation and emission spectra were recorded using a Photon Technologies International QuantaMaster Model 2 spectrometer.

Table S1. Photophysical properties of **1**-**7**

Compound	λ_{abs}(nm), $\varepsilon(10^4\ M^{-1}\ cm^{-1})$[a]	λ_{em} (nm)
1	281, 0.893; 332, 0.229	497
2	282, 1.065; 332, 0.304	504
3	281, 0.872; 332, 0.236	507
4	282, 1.011; 332, 0.290	502
5	277, 1.144 318, 0.288	462
6	278, 1.178 318, 0.332	464
7	278, 1.094 318, 0.293	464

[a] 10^{-5} M in CH_2Cl_2 at 298 K

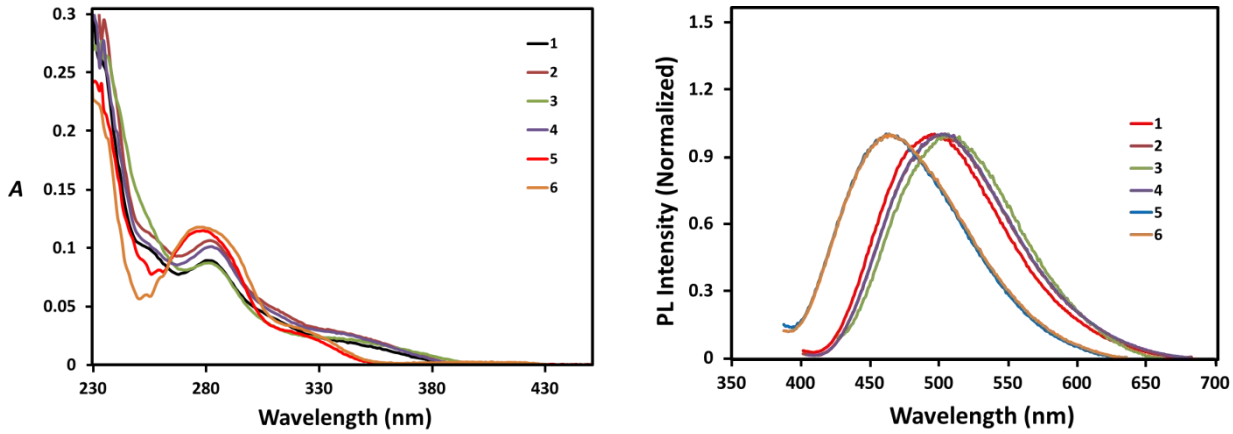


Figure S77. Absorption (10^{-5} M, left) and emission spectra (5×10^{-5}, right) of **1-6** in dichloromethane.

Table S2. Absorption spectral data summary **1c**, **2a**, **2c**, **3c**, **4c 5b** and **6b**

Compound	λ_{abs}(nm), $\varepsilon(10^4\ M^{-1}\ cm^{-1})$
1c[a]	250, 1.035 280, 0.221
2a[b]	355, 0.150 536, 0.350
2c[a]	250, 0.875 280, 0.122
3c[a]	250, 1.273 280, 0.172
4c[a]	250, 1.123 280, 0.202
5b[a]	262, 1.225 293, 0.246
6b[a]	262, 1.447 293, 0.206

[a] 10^{-5} M in CH_2Cl_2 at 298 K; [b] 5 x 10^{-5}M in toluene

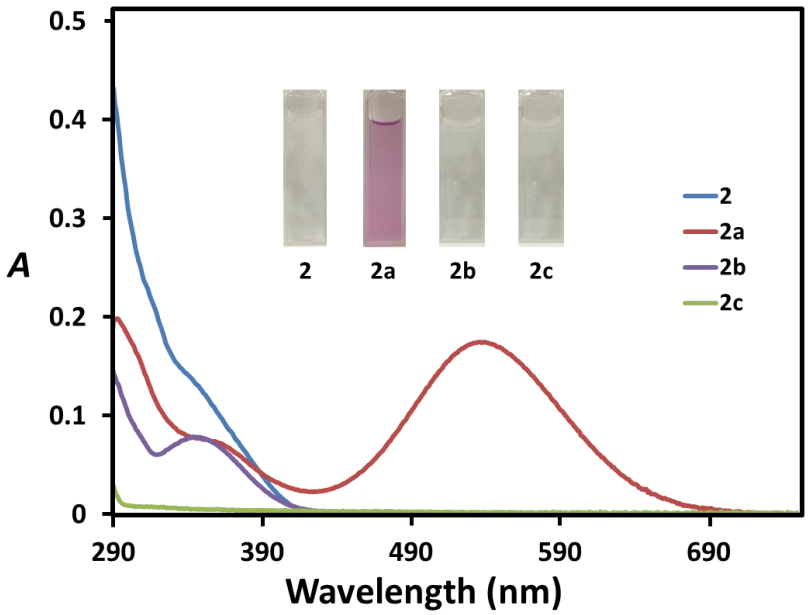


Figure S78. Absorption spectra of **2**, **2a**, **2b**, **2c** in toluene (5×10^{-5} M). Inset: Photographs showing the color of the solution.

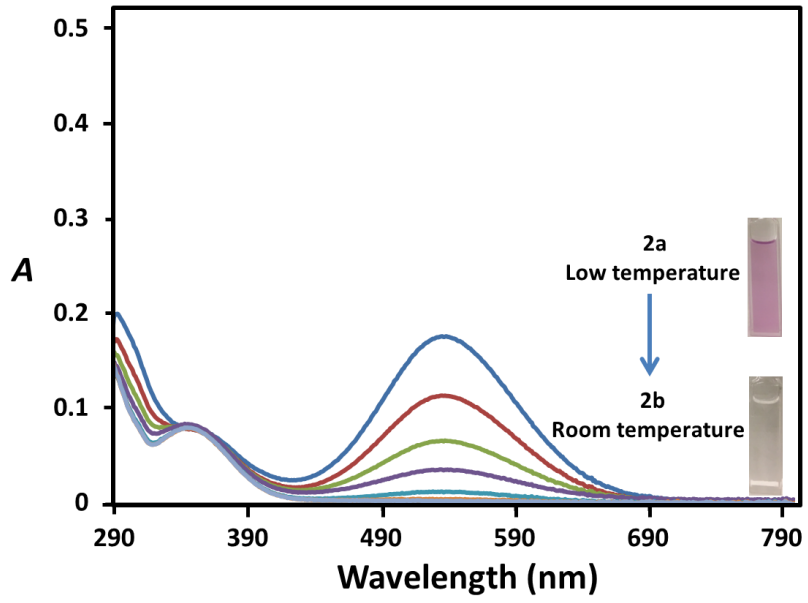


Figure S79. Absorption spectra showing the conversion of **2a**-**2b** in toluene (5×10^{-5} M) during the sample reach room temperature. Inset: Photographs showing the solution color change of **2a**-**2b**.

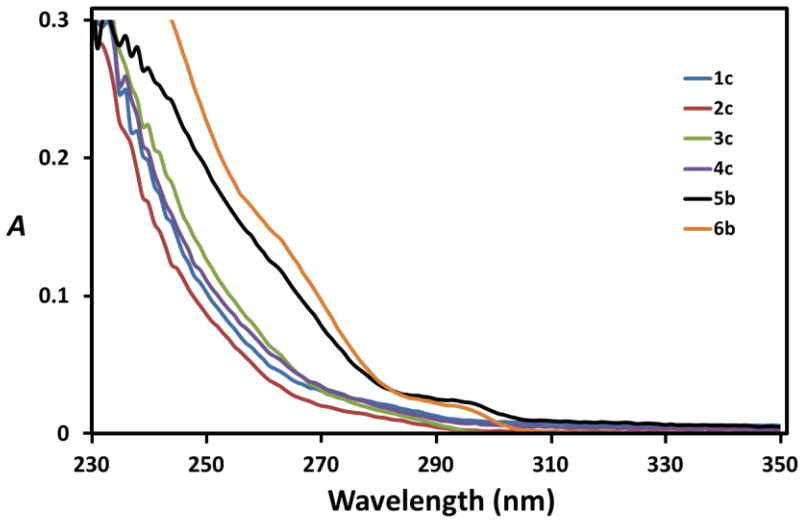


Figure S80. Absorption spectra of **1c**, **2c**, **3c**, **4c, 5b** and **6b** in dichloromethane (10^{-5} M).

S5. TD-DFT Calculation Data of 1-7

DFT and TD-DFT calculations were performed using the Gaussian 09 suite of programs[3S] on the High Performance Computing Virtual Laboratory (HPCVL) at Queen's University. Geometry optimizations and vertical excitations of all compounds were obtained at the B3LYP[4S]/6-31g(d)[5S] level of theory, with the resulting structures confirmed to be stationary points through vibrational frequency analysis.

Table S3. TD-DFT calculated electronic transitions for **1** along with their corresponding excitation energies and oscillator strengths.

Compound	Spin State	Transition Configuration	Excitation Energy (nm, eV)	Oscillator Strength
1	S_1	HOMO → LUMO (99%)	418.61 (2.96)	0.0194
	S_2	HOMO-2 → LUMO (12%)	385.99 (3.21)	0.0086
		HOMO-1 → LUMO (87%)		
	S_3	HOMO-2 → LUMO (87%)	374.06 (3.31)	0.0132
		HOMO-1 → LUMO (12%)		
	S_4	HOMO-3 → LUMO (99%)	355.21 (3.49)	0.0044
	S_5	HOMO-4 → LUMO (95%)	307.52 (4.03)	0.0567
		HOMO-5 → LUMO+1 (3%)		

Table S4. TD-DFT calculated electronic transitions for **2** along with their corresponding excitation energies and oscillator strengths.

Compound	Spin State	Transition Configuration	Excitation Energy (nm, eV)	Oscillator Strength
2	S_1	HOMO → LUMO (99%)	422.23 (2.94)	0.0205
	S_2	HOMO-2 → LUMO (10%)	386.80 (3.21)	0.0175
		HOMO-1 → LUMO (89%)		
	S_3	HOMO-2 → LUMO (89%)	376.15 (3.30)	0.0092
		HOMO-1 → LUMO (12%)		
	S_4	HOMO-3 → LUMO (100%)	355.01 (3.49)	0.0018
	S_5	HOMO-4 → LUMO (95%)	309.30 (4.01)	0.0617
		HOMO-5 → LUMO+1 (2%)		

Table S5. TD-DFT calculated electronic transitions for **3** along with their corresponding excitation energies and oscillator strengths.

Compound	Spin State	Transition Configuration	Excitation Energy (nm, eV)	Oscillator Strength
3	S_1	HOMO → LUMO (99%)	418.37 (2.96)	0.0295
	S_2	HOMO-2 → LUMO (29%)	378.82 (3.27)	0.0122
		HOMO-1 → LUMO (70%)		
	S_3	HOMO-2 → LUMO (70%)	372.39 (3.33)	0.0083
		HOMO-1 → LUMO (29%)		
	S_4	HOMO-3 → LUMO (9%)	353.47 (3.51)	0.0125
	S_5	HOMO-4 → LUMO (94%)	306.56 (4.04)	0.0470
		HOMO-5 → LUMO+1 (2%)		

Table S6. TD-DFT calculated electronic transitions for **4** along with their corresponding excitation energies and oscillator strengths.

Compound	Spin State	Transition Configuration	Excitation Energy (nm, eV)	Oscillator Strength
4	S_1	HOMO → LUMO (99%)	420.04 (2.95)	0.0223
	S_2	HOMO-1 → LUMO (90%)	384.30 (3.23)	0.0182
		HOMO-2 → LUMO (9%)		
	S_3	HOMO-2 → LUMO (90%)	373.74 (3.32)	0.0093
		HOMO-1 → LUMO (9%)		
	S_4	HOMO-3 → LUMO (100%)	351.96 (3.52)	0.0019

	S_5	HOMO-4 → LUMO (95%) HOMO-5 → LUMO+1 (2%)	308.61 (4.02)	0.0590

Table S7. TD-DFT calculated electronic transitions for **4c** along with their corresponding excitation energies and oscillator strengths.

Compound	Spin State	Transition Configuration	Excitation Energy (nm, eV)	Oscillator Strength
4c	S_1	HOMO → LUMO (75%) HOMO-3 → LUMO (9%) HOMO-1 → LUMO+1 (5%) HOMO → LUMO+1 (2%)	262.39 (4.73)	0.0314
	S_2	HOMO-1 → LUMO+1 (15%) HOMO → LUMO+1 (59%) HOMO-4 → LUMO (4%) HOMO-3 → LUMO (5%) HOMO-1 → LUMO (5%) HOMO → LUMO (8%)	251.86 (4.92)	0.0333
	S_3	HOMO-3 → LUMO (16%) HOMO-1 → LUMO (48%) HOMO-5 → LUMO (2%) HOMO-1 → LUMO+2 (4%) HOMO-1 → LUMO+4 (3%) HOMO → LUMO+1 (7%) HOMO → LUMO+2 (6%) HOMO → LUMO+4 (4%)	246.71 (5.03)	0.0789
	S_4	HOMO-3 → LUMO (17%) HOMO-1 → LUMO (21%) HOMO-1 → LUMO+1 (14%) HOMO → LUMO (10%) HOMO → LUMO+1 (13%) HOMO-3 → LUMO+1 (5%) HOMO-2 → LUMO+2 (3%) HOMO → LUMO+3 (6%)	242.88 (5.10)	0.0050

	S_5	HOMO-2 → LUMO+2 (22%)	242.59 (5.11)	0.0025
		HOMO → LUMO+3 (21%)		
		HOMO → LUMO+4 (10%)		
		HOMO-3 → LUMO+3 (4%)		
		HOMO-2 → LUMO (4%)		
		HOMO-2 → LUMO+1 (7%)		
		HOMO-2 → LUMO+3 (2%)		
		HOMO-2 → LUMO+4 (5%)		
		HOMO-2 → LUMO+5 (2%)		
		HOMO-1 → LUMO+1 (4%)		
		HOMO-1 → LUMO+3 (7%)		
		HOMO → LUMO+1 (3%)		

Table S8. TD-DFT calculated electronic transitions for **5** along with their corresponding excitation energies and oscillator strengths.

Compound	Spin State	Transition Configuration	Excitation Energy (nm, eV)	Oscillator Strength
5	S_1	HOMO → LUMO (98%)	366.58 (3.38)	0.0062
	S_2	HOMO-1 → LUMO (97%)	343.62 (3.61)	0.01
	S_3	HOMO-2 → LUMO (97%)	330.59 (3.75)	0.0004
	S_4	HOMO-3 → LUMO (100%)	321.48 (3.86)	0.0001
	S_5	HOMO-4 → LUMO (89%)	298.97 (4.15)	0.0514
		HOMO-5 → LUMO (7%)		
		HOMO-5 → LUMO+1 (3%)		

Table S9. TD-DFT calculated electronic transitions for **6** along with their corresponding excitation energies and oscillator strengths.

Compound	Spin State	Transition Configuration	Excitation Energy (nm, eV)	Oscillator Strength
6	S_1	HOMO → LUMO (98%)	373.32 (3.32)	0.0048
	S_2	HOMO-2 → LUMO (3%)	348.47 (3.56)	0.0130
		HOMO-1 → LUMO (95%)		
	S_3	HOMO-2 → LUMO (96%)	334.61 (3.71)	0.0021
		HOMO-1 → LUMO (3%)		
	S_4	HOMO-3 → LUMO (100%)	324.06 (3.83)	0.0012

	S_5	HOMO-4 → LUMO (95%) HOMO-5 → LUMO+1 (3%)	300.41 (4.13)	0.0593

Table S10. TD-DFT calculated electronic transitions for **6c** along with their corresponding excitation energies and oscillator strengths.

Compound	Spin State	Transition Configuration	Excitation Energy (nm, eV)	Oscillator Strength
6c	S_1	HOMO-1 → LUMO (24%) HOMO → LUMO (42%) HOMO → LUMO+1 (20%) HOMO-1 → LUMO+1 (6%)	269.52 (4.60)	0.0504
	S_2	HOMO-1 → LUMO (53%) HOMO → LUMO (38%) HOMO → LUMO+2 (2%)	261.50 (4.74)	0.0790
	S_3	HOMO-4 → LUMO (25%) HOMO-3 → LUMO (14%) HOMO → LUMO+1 (11%) HOMO → LUMO+2 (26%) HOMO-4 → LUMO+1 (2%) HOMO-2 → LUMO (3%) HOMO-1 → LUMO+1 (3%) HOMO → LUMO+3 (9%)	249.23 (4.97)	0.0064
	S_4	HOMO-3 → LUMO (26%) HOMO-2 → LUMO (19%) HOMO-1 → LUMO (12%) HOMO → LUMO+1 (25%) HOMO → LUMO (5%) HOMO → LUMO+2 (5%)	246.72 (5.03)	0.0662
	S_5	HOMO-4 → LUMO (12%) HOMO-1 → LUMO+1 (43%) HOMO-3 → LUMO (8%) HOMO-3 → LUMO+1 (3%) HOMO-2 → LUMO (7%)	242.15 (5.12)	0.1258

		HOMO-2 → LUMO+3 (3%)		
		HOMO-1 → LUMO+4 (5%)		
		HOMO → LUMO (5%)		

Table S11. Primary orbitals which contribute to the calculated transitions of **1** (iso = 0.03). Most H atoms have been omitted for clarity.

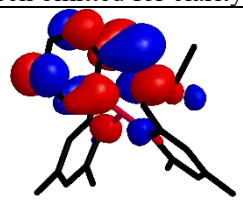
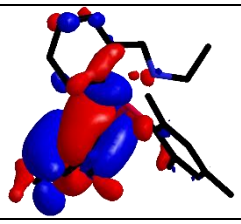
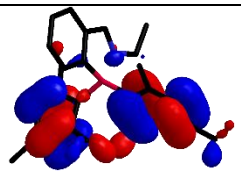
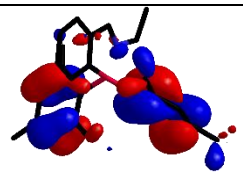
			
LUMO	HOMO	HOMO-1	HOMO-2

Table S12. Primary orbitals which contribute to the calculated transitions of **2** (iso = 0.03). Most H atoms have been omitted for clarity.

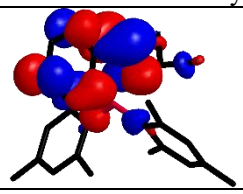
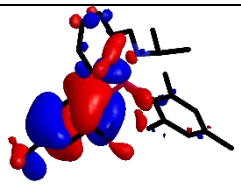
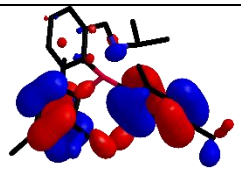
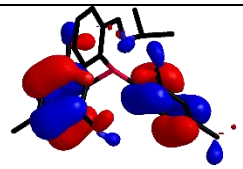
			
LUMO	HOMO	HOMO-1	HOMO-2

Table S13. Primary orbitals which contribute to the calculated transitions of **3** (iso = 0.03). Most H atoms have been omitted for clarity.

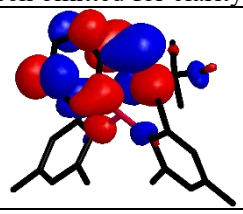
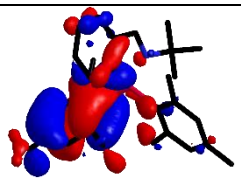
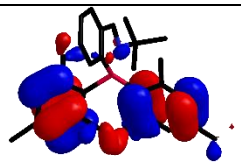
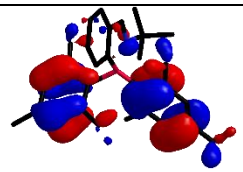
			
LUMO	HOMO	HOMO-1	HOMO-2

Table S14. Primary orbitals which contribute to the calculated transitions of **4** (iso = 0.03). Most H atoms have been omitted for clarity.

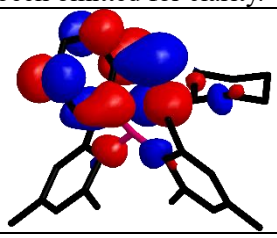
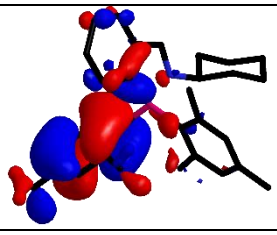
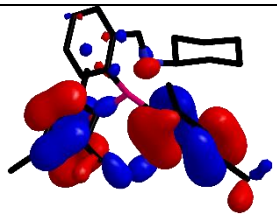
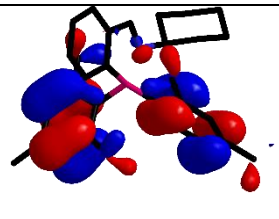
			
LUMO	HOMO	HOMO-1	HOMO-2

Table S15. Primary orbitals which contribute to the calculated transitions of **4c** (iso = 0.03). Most H atoms have been omitted for clarity.

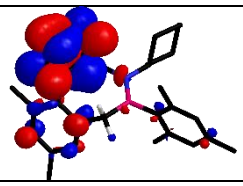
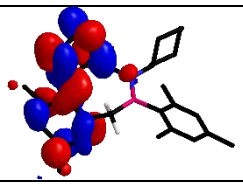
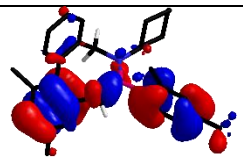
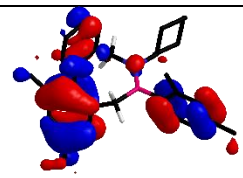
			
LUMO+1	LUMO	HOMO	HOMO-1

Table S16. Primary orbitals which contribute to the calculated transitions of **5** (iso = 0.03). Most H atoms have been omitted for clarity.

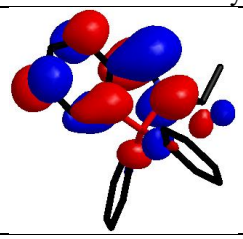
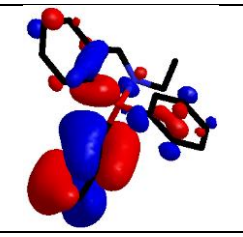
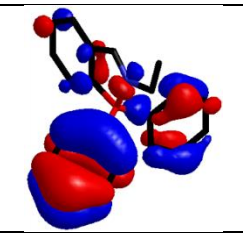
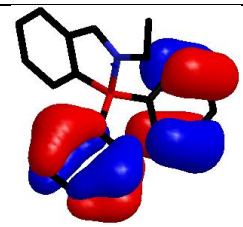
			
LUMO	HOMO	HOMO-1	HOMO-2

Table S17. Primary orbitals which contribute to the calculated transitions of **6** (iso = 0.03). Most H atoms have been omitted for clarity.

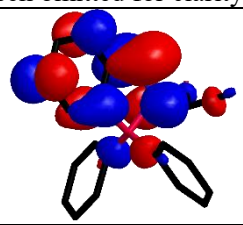
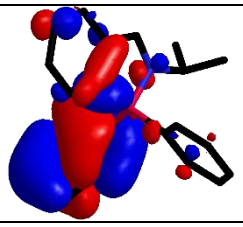
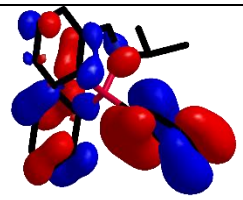
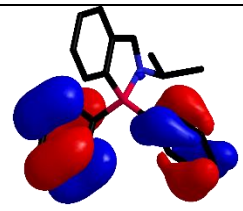
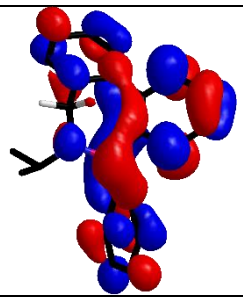
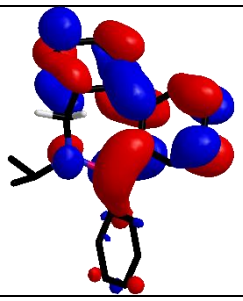
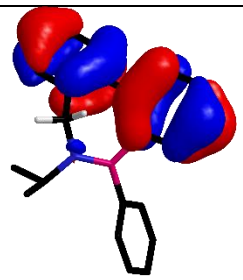
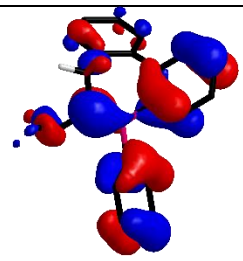
			
LUMO	HOMO	HOMO-1	HOMO-2

Table S18. Primary orbitals which contribute to the calculated transitions of **6b** (iso = 0.03). Most H atoms have been omitted for clarity.

			
LUMO+1	LUMO	HOMO	HOMO-1

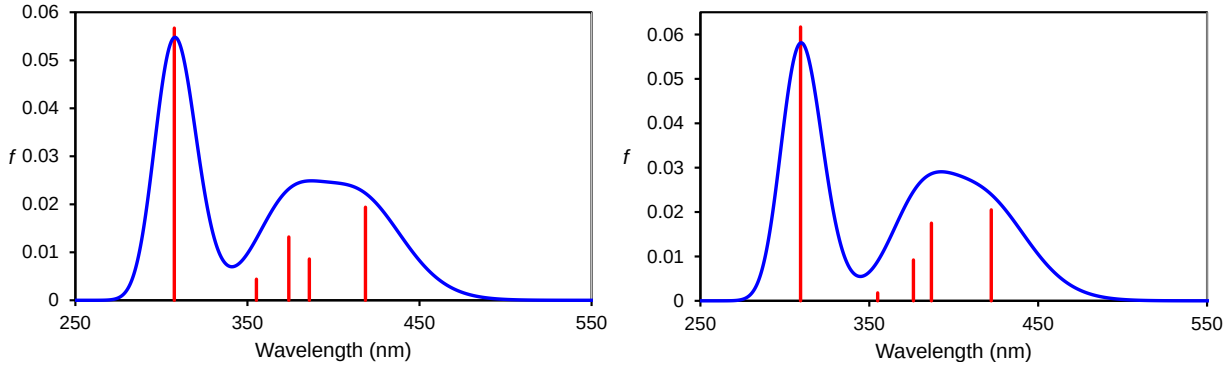


Figure S81. Predicted UV/Vis spectra of **1** (left) and **2** (right) for their first five excited states.[6S]

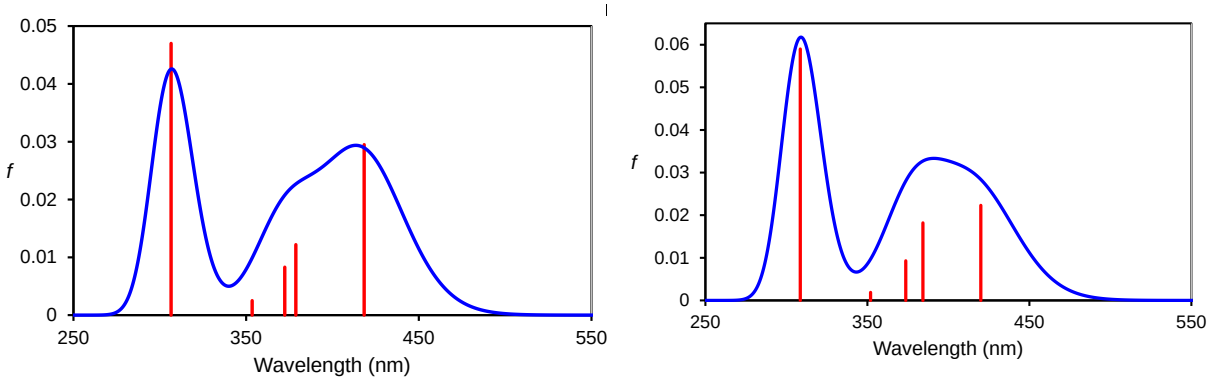


Figure S82. Predicted UV/Vis spectra of **3** (left) and **4** (right) for their first five excited states.[6S]

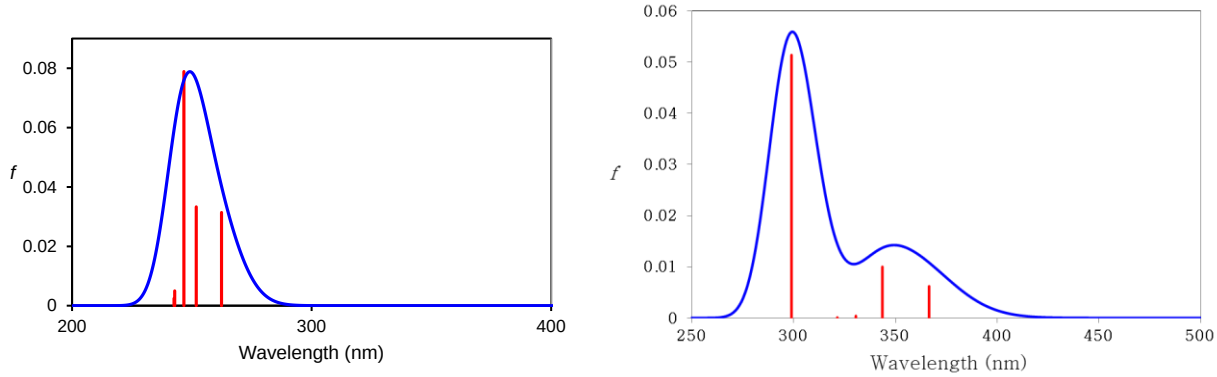


Figure S83. Predicted UV/Vis spectra of **4c** (left) and **5** (right) for their first five excited states.[6S]

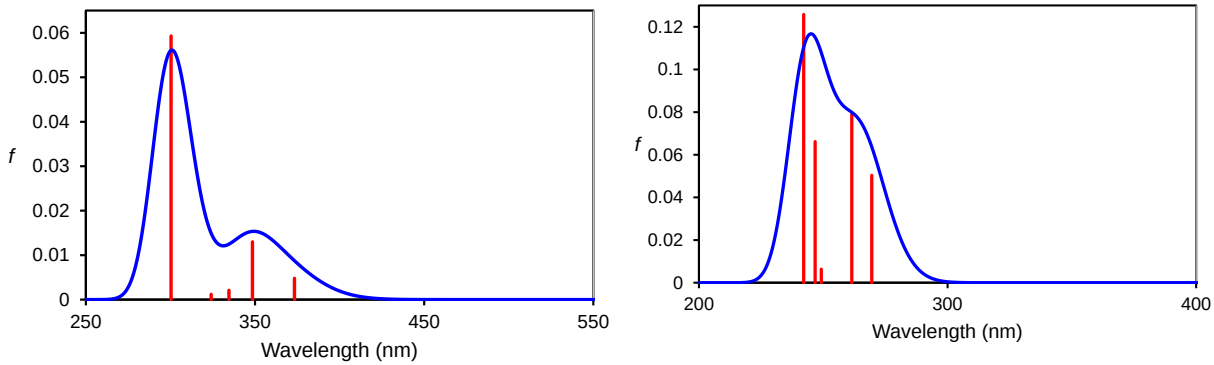


Figure S84. Predicted UV/Vis spectra of **6** (left) and **6c** (right) for their first five excited states.[6S]

Calculated Energy of **4c** relative to **4** = -124.72 kJ/mol
Calculated Energy of **6c** relative to **6** = -69.45 kJ/mol

1; E = -1127.79318187:

N	-0.21778900	1.19540200	1.52479300
C	1.54022200	4.15411600	-1.64454800
C	1.05601900	4.03824700	-0.34829900
H	1.06322400	4.88911100	0.32964400
C	0.56949100	2.78948300	0.06792300
C	0.53187800	1.64321200	-0.76316400
C	1.29899900	-0.68661100	0.05335900
C	2.41904300	-0.65291800	0.92951300
C	3.47633200	-1.56127600	0.78112500
H	4.30898400	-1.51083900	1.48130400
C	3.51295700	-2.50755100	-0.24043400
C	4.64557500	-3.49975800	-0.36015100
H	4.42925600	-4.42545100	0.19103000
H	5.57965500	-3.09440000	0.04493400
H	4.82403900	-3.78113500	-1.40409700
C	-5.46007600	-2.12273000	-0.66789900
H	-5.51319200	-2.65459500	-1.62774500
H	-6.25728800	-1.37056300	-0.67361600
H	-5.68697900	-2.85090500	0.11852800
C	-4.10317400	-1.49153500	-0.46265600
C	-3.79524900	-0.23886500	-0.99017100
H	-4.56507600	0.30664600	-1.53401000
C	-2.53483600	0.35343000	-0.83664900
C	-1.48689100	-0.31807000	-0.14226500
C	-1.81984400	-1.58275800	0.42555700
C	-0.85975200	-2.45227200	1.22436900
H	-1.42256200	-3.09988200	1.90649600
H	-0.13822500	-1.88732700	1.81340300
H	-0.26763200	-3.10369600	0.57116400
C	-3.09968900	-2.13383400	0.25647000
H	-3.31167100	-3.10362400	0.70506300
C	0.05440200	2.45471800	1.36848200
H	-0.10346200	3.18158300	2.16192500
C	-0.84526000	0.66481800	2.74210400
H	-0.19785600	-0.13252400	3.12056200
H	-1.77421300	0.18073100	2.42709400
C	-1.12430800	1.67241100	3.85330300
H	-0.20913300	2.14720700	4.22525900
H	-1.58652000	1.14475100	4.69365800
H	-1.82003900	2.45645400	3.53426300
C	1.54661900	3.02812200	-2.48412600
H	1.93920500	3.12299600	-3.49390100
C	1.06590900	1.79090500	-2.05031100
H	1.11251300	0.94436100	-2.72885300
C	2.45736700	-2.49005800	-1.14909700
H	2.47283500	-3.18480300	-1.98817000
C	1.37356400	-1.60969600	-1.02947700
C	0.31762500	-1.73607700	-2.11780400
H	0.77164200	-2.14012900	-3.02985400
H	-0.16087300	-0.78969100	-2.37285600
H	-0.49132200	-2.41677700	-1.82745700
C	2.59471200	0.37207800	2.03586900
H	2.57241800	1.39633400	1.64795800
H	3.56429000	0.23384000	2.52516800
H	1.83313700	0.30153900	2.81924300
C	-2.38898200	1.73549300	-1.44615300
H	-3.34477500	2.06484800	-1.86711200
H	-1.64751000	1.76254600	-2.25021700
H	-2.07936900	2.48701400	-0.71293100
B	0.01007500	0.35527700	0.09923300
H	1.92472300	5.10403400	-2.00482500

2; E = -167.10472212:

N	-0.30363500	1.33077300	1.32171000
C	1.68684900	3.96827800	-2.00080700
C	1.10335400	3.97709800	-0.74153300
H	1.05114900	4.89174200	-0.15475300
C	0.59363100	2.76998800	-0.23818800
C	0.62871600	1.54300200	-0.94464900
C	1.36418300	-0.68740800	0.10339400
C	2.42325500	-0.59925100	1.04483900
C	3.52253800	-1.46700300	0.98530900
H	4.30686600	-1.36744700	1.73432100
C	3.65458600	-2.43786800	-0.00347300
C	4.83116500	-3.38455000	-0.03607700
H	4.59200200	-4.34082800	0.44943800
H	5.69832100	-2.96460200	0.48543700
H	5.13408000	-3.61412600	-1.06416400
C	-5.23826400	-2.43363800	-0.92007200
H	-5.20394800	-3.03770900	-1.83702300
H	-6.06271600	-1.72079300	-1.03655200
H	-5.48903300	-3.10991000	-0.09560400
C	-3.92473700	-1.72841800	-0.67743300
C	-3.62093100	-0.52059000	-1.30543400
H	-4.36329100	-0.06536100	-1.95940000
C	-2.39904000	0.13705500	-1.11612600
C	-1.38885500	-0.41709500	-0.27670200
C	-1.71567100	-1.63625700	0.38308100
C	-0.78731100	-2.38760000	1.32685100
H	-1.37670900	-2.97803200	2.03796300
H	-0.11694800	-1.74310100	1.89552400
H	-0.13938800	-3.08523200	0.78269800
C	-2.95833300	-2.25518800	0.17431800
H	-3.17070700	-3.18550600	0.69978600
C	-0.02834600	2.56861000	1.04025600
H	-0.27362900	3.37982900	1.72418500
C	-1.09660600	1.00848200	2.54107200
H	-0.98933500	-0.06741800	2.68019900
C	-0.57851400	1.71905400	3.80203800
H	0.49468300	1.57758800	3.94995700
H	-1.09884000	1.31155300	4.67516400
H	-0.78524300	2.79525800	3.78106600
C	1.76692300	2.76180100	-2.71578400
H	2.23645000	2.75795500	-3.69675000
C	1.26396400	1.56824400	-2.19449200
H	1.37398100	0.65826400	-2.77578900
C	2.64492500	-2.49603800	-0.96177600
H	2.72648300	-3.22310700	-1.76906900
C	1.52503100	-1.65419900	-0.93361100
C	0.52766200	-1.88403700	-2.06045900
H	1.03889500	-2.32591900	-2.92346100

H	0.02677000	-0.97615100	-2.39751900
H	-0.26814400	-2.57746100	-1.76390500
C	2.45332400	0.41811700	2.16575500
H	2.37458200	1.44646100	1.79837800
H	3.39153300	0.34199700	2.72510700
H	1.64017300	0.26013500	2.88174700
C	-2.24723800	1.45883500	-1.84525800
H	-3.17745600	1.71308700	-2.36423900
H	-1.44803900	1.43569800	-2.59272300
H	-2.01439800	2.28667700	-1.16788300
B	0.05777800	0.33416100	0.00311400
C	-2.58703200	1.32778400	2.33359800
H	-2.73371300	2.40646100	2.19710300
H	-2.99266400	0.80598900	1.46643200
H	-3.15239600	1.02259400	3.22135700
H	2.09181500	4.88196700	-2.42640500

3; E = -1206.40487381:

N	-0.28116700	1.48230900	1.12599600
C	1.66040600	3.60329600	-2.60186200
C	1.16238200	3.77581600	-1.31872400
H	1.17725200	4.75163400	-0.83775100
C	0.64128500	2.65542300	-0.65143100
C	0.58971100	1.35687900	-1.20640700
C	1.41406200	-0.65029300	0.11183100
C	2.47712400	-0.40449400	1.02673400
C	3.59950700	-1.24323500	1.07418700
H	4.38020300	-1.02557900	1.80161200
C	3.76654600	-2.32298200	0.21080600
C	4.96772700	-3.23377400	0.30251300
H	4.78029300	-4.07994200	0.97804500
H	5.84610300	-2.70318800	0.68697300
H	5.22825300	-3.65405200	-0.67536900
C	-5.17820800	-2.64368200	-0.98106700
H	-5.14134400	-3.20334000	-1.92572100
H	-6.02759900	-1.95439200	-1.04919700
H	-5.39048300	-3.36580900	-0.18509900
C	-3.88447100	-1.90648000	-0.72856500
C	-3.64465400	-0.64617200	-1.27438900
H	-4.42328600	-0.17369300	-1.87131300
C	-2.44023400	0.04064900	-1.07735200
C	-1.37931200	-0.52596000	-0.30420300
C	-1.64401800	-1.80536700	0.26952300
C	-0.68396800	-2.60701700	1.14109900
H	-1.24539800	-3.12624800	1.92744400
H	0.09166000	-2.01188200	1.61380600
H	-0.17070800	-3.37996300	0.55662500
C	-2.87084500	-2.45299500	0.05048800
H	-3.03014300	-3.42666000	0.51276500
C	0.06079800	2.64651600	0.65771400
H	-0.10879900	3.56176200	1.21935300
C	-1.07542900	1.45833600	2.41861800
C	-0.53136900	2.49675000	3.42720200
H	0.54160700	2.37185400	3.60110300
H	-1.04629400	2.35605600	4.38246500
H	-0.71588000	3.53176100	3.12267900
C	1.63931500	2.32308600	-3.17931100
H	2.03111900	2.18914000	-4.18499900
C	1.13126500	1.21816800	-2.49416400
H	1.15762800	0.25164100	-2.98430900
C	2.77364200	-2.51386800	-0.74587700
H	2.88828500	-3.31824400	-1.47227200
C	1.62843600	-1.71044900	-0.81990900
C	0.68040200	-2.08901400	-1.95197300
H	1.26063400	-2.34407100	-2.84725700
H	-0.03046400	-1.31084700	-2.21890800
H	0.08386000	-2.97429000	-1.69904700
C	2.52323900	0.78329400	1.96671900
H	2.50374900	1.73416100	1.42218600
H	3.44777900	0.76518000	2.55290700
H	1.69217500	0.80001400	2.67482500
C	-2.36470800	1.40798600	-1.73193000
H	-3.33558800	1.67261800	-2.16388000
H	-1.62503100	1.44448700	-2.53737900
H	-2.09739400	2.19942100	-1.02545900
B	0.04866600	0.28471100	-0.08910500
C	-2.54398900	1.80103000	2.08925600
H	-2.62596700	2.80233800	1.65094400
H	-2.96817600	1.07883000	1.38846500
H	-3.13970100	1.78549700	3.00908000
C	-1.02050300	0.07428400	3.07540800
H	-1.53490600	-0.66722000	2.46868100
H	0.00477800	-0.26109200	3.25043500
H	-1.52707500	0.12498400	4.04518300
H	2.06885100	4.44503700	-3.15367400

4; E = -1283.84175491:

C	-0.43595300	-2.33777800	0.87931700
C	0.60291000	-2.10257700	1.84243800
C	1.10901900	-0.78997200	1.68072000
C	2.17147500	-0.42929200	2.52187500
C	2.63937000	-1.31000400	3.49877700
C	2.09293300	-2.59481700	3.65276400
C	1.06918400	-3.00597200	2.81052800
H	2.64554600	0.54221600	2.42537500
H	3.44938600	-0.99711300	4.15358500
H	2.47973200	-3.26356400	4.41642100
H	0.64483700	-4.00449100	2.89095100
B	0.41500800	-0.07710500	0.37963500
N	-0.59986100	-1.38494200	0.01105500
C	-0.66193900	1.17196300	0.50155200
C	-1.33528200	1.49808000	1.71474500
C	-1.02438000	1.93419600	-0.64614400
C	-2.26934200	2.54086800	1.76401400
C	-1.97777400	2.96044500	-0.55481600
C	-2.60579200	3.29645900	0.64109600
H	-2.75717700	2.76120900	2.71244400
H	-2.22996300	3.51795500	-1.45606000
C	1.72806500	0.22425800	-0.59306700
C	2.30496000	-0.68397000	-1.51988100
C	2.44262500	1.43959400	-0.37665800
C	3.47252000	-0.36021000	-2.22351100
C	3.61347800	1.72039600	-1.09449600
C	4.14526500	0.84509400	-2.03862900
H	3.87357300	-1.08595100	-2.92973300
H	4.12658800	2.66189600	-0.90153700
C	-0.42010200	1.75401900	-2.03176100
H	0.50679800	2.32904600	-2.14227200
H	-0.15996700	0.72282900	-2.27308800
H	-1.12046400	2.11419400	-2.79417200
C	-1.11527500	0.75206400	3.01708200
H	-1.29733600	-0.32289100	2.91847000
H	-0.09345500	0.86026200	3.39408800
H	-1.79405300	1.13005100	3.78890000

C	-3.59580000	4.43440200	0.72304200
H	-4.39675800	4.22139200	1.44028000
H	-3.11038000	5.36408500	1.05017900
H	-4.05723200	4.63553100	-0.24998600
C	1.71893600	-2.04850900	-1.81137600
H	1.64346800	-2.67076500	-0.91326800
H	0.71640400	-1.97631600	-2.24371200
H	2.34325100	-2.58792400	-2.53125300
C	2.01466600	2.52651300	0.59891200
H	2.88590500	3.11909600	0.90081800
H	1.29243300	3.21682800	0.14724600
H	1.54128900	2.14351600	1.50336600
C	5.38749400	1.18759400	-2.82691500
H	5.95884400	0.28907000	-3.08614800
H	5.13942600	1.69527200	-3.76938600
H	6.04786800	1.85706300	-2.26446000
H	-1.06287900	-3.22799500	0.87757700
C	-1.76532400	-1.41903600	-0.91101800
C	-1.92611600	-2.75544500	-1.66557300
C	-3.07874300	-1.08657500	-0.16725900
H	-1.58229000	-0.63260000	-1.64562200
C	-3.09857900	-2.67652700	-2.65839700
H	-2.12801200	-3.56696000	-0.95233000
H	-1.00213800	-3.01718700	-2.18998000
C	-4.26442900	-1.01774100	-1.14160000
H	-3.26236600	-1.87063400	0.58319700
H	-2.97069800	-0.14204100	0.36971500
C	-4.41337900	-2.31081900	-1.95503200
H	-3.19769000	-3.63439200	-3.18378400
H	-2.87187000	-1.92252900	-3.42599500
H	-5.18485100	-0.80743000	-0.58314700
H	-4.11587100	-0.16873300	-1.82407400
H	-5.22150500	-2.21017600	-2.69024800
H	-4.70254800	-3.13192000	-1.28230500

5; E = -891.92614308:

C	-3.86323300	-1.79339600	-1.07748000
C	-3.40642800	-1.67532700	0.23133100
C	-2.14636700	-1.09818700	0.43862600
C	-1.32344500	-0.63153300	-0.61334800
C	-1.81355900	-0.76036500	-1.91477400
C	-3.06745900	-1.33738700	-2.14028100
H	-4.83489600	-2.23550300	-1.27901200
H	-4.01168200	-2.02060100	1.06677500
H	-1.22411500	-0.41105500	-2.75926800
H	-3.43794200	-1.43472500	-3.15813900
C	-1.47812800	-0.87069300	1.69995800
H	-1.88552100	-1.15283900	2.66885300
C	0.10973200	1.60364800	-0.24553900
C	0.84876000	2.13169200	-1.32068000
C	-0.62491400	2.52572200	0.52285800
C	0.86121200	3.49827300	-1.60856800
C	-0.61404200	3.89544600	0.25099000
C	0.13242400	4.38946200	-0.81960500
H	1.44578300	3.86744700	-2.44848900
H	-1.19200800	4.57591700	0.87273800
C	1.40475200	-0.82553600	-0.33447600
C	1.38603000	-2.12497700	-0.87437000
C	2.67340100	-0.28608500	-0.04185400
C	2.55891600	-2.84634100	-1.10975300
C	3.85324900	-0.99850600	-0.26849100
C	3.80009500	-2.28574600	-0.80560700
H	2.50274500	-3.84686300	-1.53325900
H	4.81368400	-0.54513700	-0.03286300
C	0.56387300	0.04992000	2.69104400
H	1.52390600	-0.43469000	2.48183300
H	0.74331900	1.12953300	2.62185900
C	0.06755800	-0.32094700	4.08438200
H	-0.07988600	-1.40129500	4.19345000
H	0.81694800	-0.01372700	4.82055500
H	-0.87071800	0.18626000	4.33644600
N	-0.32364900	-0.29283800	1.57940700
B	0.03771200	-0.00531200	0.00197900
H	0.14449800	5.45468500	-1.03716400
H	1.43425500	1.45880600	-1.94236800
H	-1.23488200	2.16887300	1.35171300
H	4.71547100	-2.84324800	-0.98928300
H	0.43234700	-2.58451600	-1.12229900
H	2.74110600	0.72428500	0.35598700

6; E = -931.24053890:

N	-0.08578200	-0.37462500	1.45603300
C	-3.05407500	-3.13725000	-0.87000000
C	-2.54542400	-2.83633100	0.38930200
H	-2.88763900	-3.37244300	1.27189900
C	-1.58076600	-1.82392700	0.48456500
C	-1.10543500	-1.09625200	-0.63254700
C	-0.60617200	1.52012600	-0.35772900
C	-1.59553200	2.08010600	0.47201000
C	-2.14510300	3.34018700	0.22871000
H	-2.90429500	3.73882300	0.89836100
C	-1.72586400	4.08443800	-0.87512500
C	4.21727200	-0.69799200	-1.36259100
C	3.26280500	-1.70613600	-1.50690700
H	3.55191400	-2.67673700	-1.90422900
C	1.93393900	-1.47107800	-1.14627300
C	1.50627900	-0.23144900	-0.63345900
C	2.49272300	0.76655700	-0.50491100
C	3.82547800	0.54342300	-0.85927000
H	4.55612000	1.34166200	-0.74766100
C	-0.91518100	-1.34770800	1.67520200
H	-1.07177700	-1.76011600	2.67167600
C	0.75839700	0.22766700	2.51027000
H	1.20226800	1.10855700	2.03955100
C	-0.06200700	0.68974000	3.72092100
H	-0.85453500	1.38084100	3.41985300
H	0.59346900	1.20950600	4.42770900
H	-0.51582200	-0.15336600	4.25512900
C	-2.60083600	-2.43023300	-1.99509600
H	-3.00803100	-2.67554500	-2.97326200
C	-1.64114400	-1.41927600	-1.88130000
H	-1.31621200	-0.88568900	-2.77146100
C	-0.75956400	3.54900900	-1.72733800
H	-0.42703300	4.11285800	-2.59623500
C	-0.21232400	2.28999000	-1.46799800
B	-0.02925000	0.01040800	-0.13972800
C	1.88798500	-0.73463700	2.90688300
H	1.48738800	-1.62943600	3.39887600
H	2.45971500	-1.04514900	2.02884100
H	2.56825400	-0.23986100	3.60867500
H	-2.14980900	5.06645700	-1.07033000
H	0.54361000	1.89830100	-2.14385500
H	-1.96298700	1.51274400	1.32509200
H	2.20956800	1.74957900	-0.13518200

H	5.25235800	-0.87558900	-1.64440400	H	-3.80233200	-3.91641100	-0.98499800
H	1.20984100	-2.27249600	-1.27154700				

S6. DFT Mechanistic Calculation Data of 2 and 3

DFT calculations were performed using the Gaussian 09 suite of programs[3S] on the High Performance Computing Virtual Laboratory (HPCVL) at Queen's University. Geometry optimizations of all initial, transition state, intermediate, and final structures were obtained at the cam-B3LYP[4S] level of theory employing the SVP[7S] basis set, with the resulting structures confirmed to be stationary points through vibrational frequency analysis (the transition state contained one true imaginary frequency).

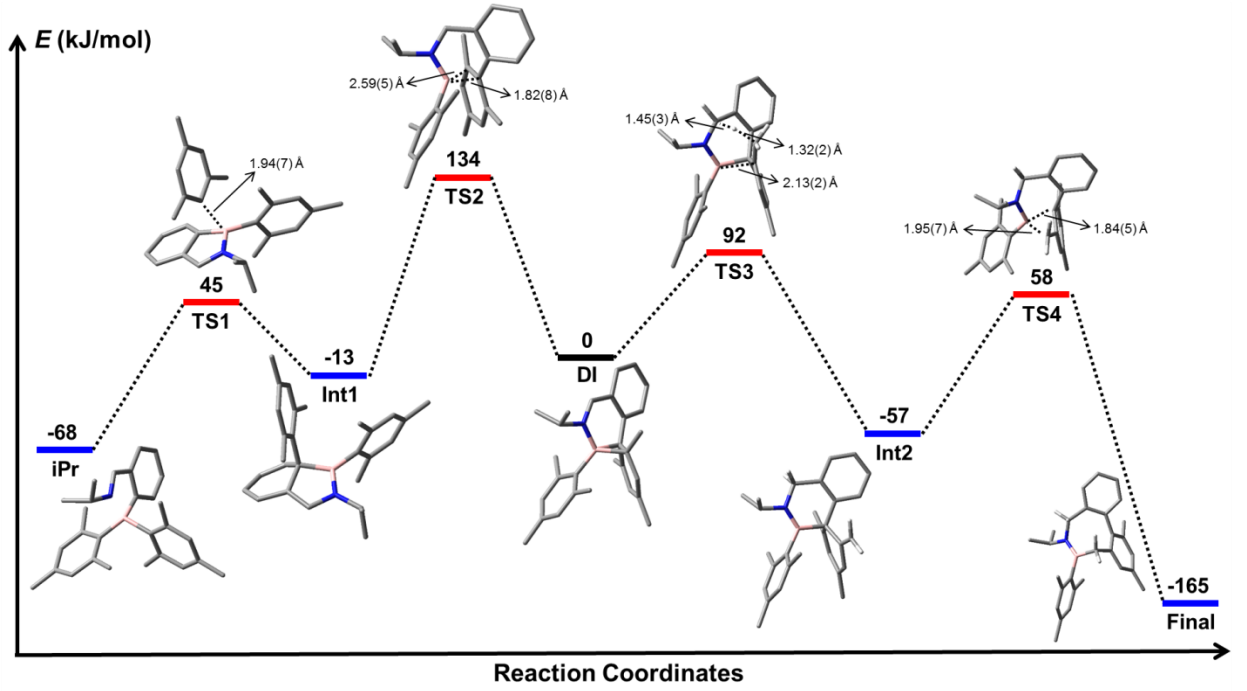


Figure S85. Calculated ground-state reaction profile showing the various starting, transition state, intermediate, and final structures of the conversion from **iPr** to **Final**.

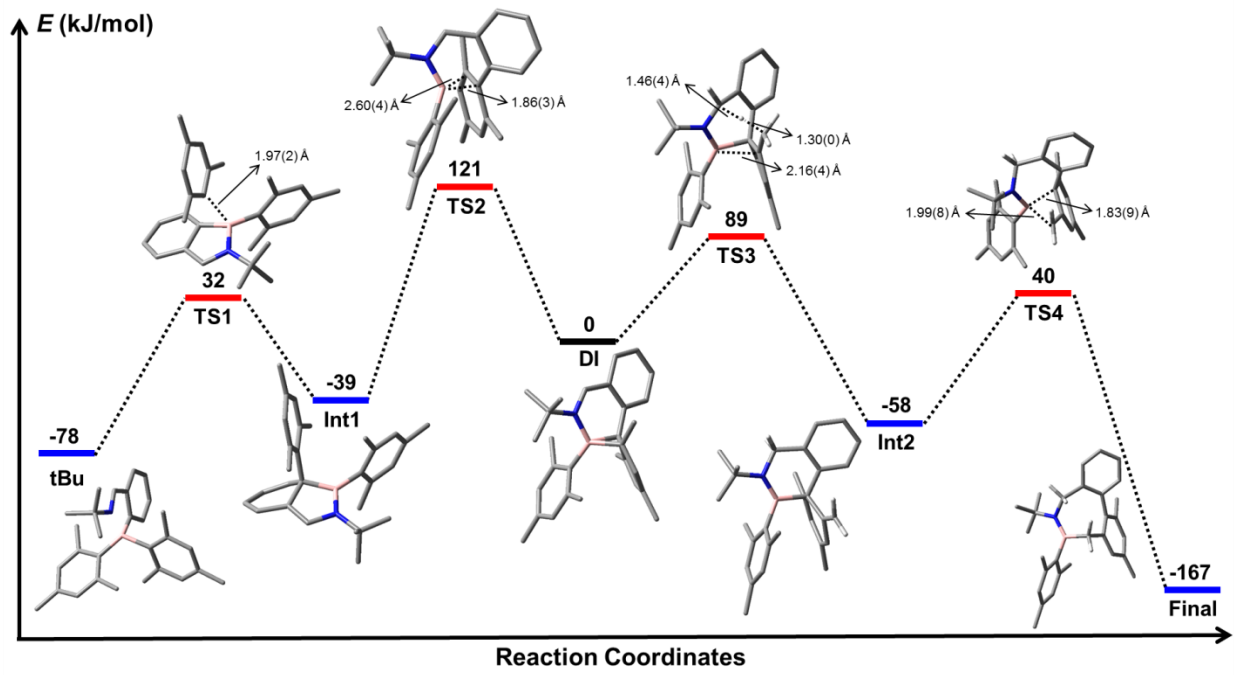


Figure S86. Calculated ground-state reaction profile showing the various starting, transition state, intermediate, and final structures of the conversion from **tBu** to **Final**.

iPr; E = -1165.56528236:

C	-0.01625200	2.53283600	1.07636100
C	0.61055600	2.75627800	-0.19954600
C	0.63687200	1.55003300	-0.92424800
C	1.27005700	1.59046000	-2.17250900
C	1.78184600	2.78490600	-2.66945600
C	1.71007500	3.97686500	-1.93500800
C	1.12669800	3.96630100	-0.67956600
H	1.37094400	0.68553000	-2.77330300
H	2.25602900	2.79454300	-3.65405700
H	2.12363500	4.89959300	-2.34645100
H	1.07772600	4.87518800	-0.07424200
B	0.05736800	0.33342600	0.00534400
N	-0.30517500	1.30231200	1.32550300
C	-1.38281400	-0.41049900	-0.29457100
C	-2.38678600	0.16500300	-1.11676300
C	-1.71196500	-1.63305300	0.34424500
C	-3.61453800	-0.47362000	-1.30648900
C	-2.95996300	-2.23489800	0.13665300
C	-3.92682500	-1.68431800	-0.69436500
H	-4.35983500	0.00241800	-1.95046500
H	-3.17900100	-3.17544000	0.65106100
C	1.35696100	-0.68604600	0.09961400
C	2.39624500	-0.62582000	1.05639600
C	1.52572300	-1.62321400	-0.95531700
C	3.49400500	-1.49036000	0.98843500
C	2.64179800	-2.46388500	-0.99229300
C	3.63857000	-2.43128400	-0.02308800
H	4.27082700	-1.41214800	1.75472600
H	2.73280200	-3.17299600	-1.82094100
C	-0.78226400	-2.39950000	1.26338300
H	-0.11722400	-3.06684100	0.69448000
H	-0.11963000	-1.76353500	1.85813700
H	-1.36597800	-3.02669300	1.95287700
C	-2.21822100	1.49240900	-1.81792400
H	-1.97195400	2.30540300	-1.12126700
H	-1.41235300	1.47081200	-2.56380600
H	-3.14563400	1.77187400	-2.33676600
C	-5.24665700	-2.36625500	-0.93569000
H	-6.07181800	-1.64063700	-0.99100600
H	-5.23825200	-2.91929200	-1.88940300
H	-5.47921900	-3.08852700	-0.14014900
C	2.40151900	0.35811800	2.19962800
H	2.36169300	1.40037200	1.85200200
H	1.55035400	0.19967900	2.87517700
H	3.31518700	0.24711600	2.79948800
C	0.53686100	-1.81761900	-2.08711200
H	1.04796100	-2.23984700	-2.96455800
H	-0.26492400	-2.51722800	-1.80592600
H	0.03464500	-0.89667400	-2.39845300
C	4.81056700	-3.37471700	-0.06836100
H	5.66236000	-2.98758300	0.50918000
H	4.54765700	-4.35864900	0.35435700
H	5.14938500	-3.54723000	-1.10077700
H	-0.24974400	3.33546700	1.78389700
C	-1.08498800	0.94956900	2.53253000
H	-0.94054400	-0.12801800	2.66976300
C	-0.59724900	1.67076000	3.78918200
H	-0.85784800	2.73989300	3.77657800
H	-1.09297400	1.23386300	4.66751500
H	0.48709900	1.58009400	3.93109900
C	-2.57738300	1.21433900	2.32525900

H	-2.76002700	2.29097500	2.17879300
H	-2.97283400	0.66979300	1.46093800
H	-3.13382900	0.89869000	3.22000200

TS1; E = -1165.522158:

C	-0.91532300	-2.52213300	0.74669000
C	-1.60741500	-2.17977300	-0.38765200
C	-0.99633700	-0.98428100	-0.99564200
C	-1.40531200	-0.78268200	-2.38740900
C	-2.41597600	-1.49916900	-2.94067900
C	-3.13325900	-2.51717200	-2.21969200
C	-2.72087500	-2.86111900	-0.97322600
H	-0.90784900	-0.04145300	-3.00665000
H	-2.68692400	-1.30778500	-3.98214000
H	-3.97116900	-3.02856600	-2.69700700
H	-3.20650700	-3.66999500	-0.42004200
B	0.18523100	-0.61668400	-0.03601100
N	0.08685700	-1.65855200	1.02598400
C	1.60614100	0.08760200	-0.18582900
C	2.51321800	-0.43231800	-1.13987700
C	2.05152500	1.12871200	0.65258400
C	3.79135200	0.10928400	-1.26467700
C	3.34267400	1.64866300	0.49937100
C	4.22623900	1.16283800	-0.45850600
H	4.47407300	-0.30918800	-2.01047400
H	3.66800100	2.45674400	1.16132100
C	-1.33584000	0.59711800	-0.07998900
C	-2.32202800	0.69026000	0.94415600
C	-1.03445400	1.77572700	-0.81445900
C	-2.93883000	1.91776900	1.19441800
C	-1.68600100	2.97386900	-0.51305200
C	-2.64842900	3.07585000	0.48079800
H	-3.68506700	1.96387400	1.99193600
H	-1.41936900	3.86445700	-1.08975000
C	-0.02556800	1.90890200	-1.93530600
H	-0.53623800	2.23220600	-2.85585700
H	0.70615800	2.68848500	-1.67725400
H	0.54303000	1.00729700	-2.15253800
C	-2.77151400	-0.43335900	1.84112100
H	-3.51339800	-0.05712800	2.55748600
H	-3.23106300	-1.25320200	1.27651600
H	-1.94120500	-0.86078300	2.41469500
C	-3.36506900	4.36721800	0.76159800
H	-4.35294600	4.38159700	0.27268700
H	-3.53510600	4.50673400	1.83921700
H	-2.79975600	5.23228000	0.38745400
C	1.17766400	1.72425900	1.73098100
H	0.51583500	2.50618100	1.32841000
H	0.52172300	0.97695100	2.19616800
H	1.79003900	2.18279100	2.52069700
C	2.11844400	-1.57496300	-2.04423400
H	1.70037100	-2.42102400	-1.47903500
H	1.34032400	-1.27704900	-2.76360600
H	2.98074900	-1.94198600	-2.61789900
C	5.60754600	1.73882300	-0.62267700
H	6.37681400	0.95188100	-0.58988300
H	5.71272000	2.25036200	-1.59291900
H	5.83652500	2.46935200	0.16578700
C	1.05516900	-1.92843500	2.09467200
H	1.75751700	-1.08623800	2.07473100
C	0.40432400	-1.96769500	3.47598300
H	-0.33133000	-2.78289000	3.55917600
H	1.16886600	-2.13441400	4.24885500
H	-0.10543800	-1.02129800	3.70555700
C	1.85395000	-3.19926800	1.80878500
H	2.34679400	-3.13652100	0.82857200
H	2.63095700	-3.34526400	2.57373900
H	1.20781700	-4.09102700	1.81166800
H	-1.14519500	-3.35926900	1.40904000

Int1; E = -1165.544384:

C	-0.58600700	2.78928100	-0.47066600
C	-1.45044200	2.18130500	0.35517300
C	-0.98339200	0.85433600	2.31222400
C	-1.95374500	1.52601300	2.95516100
C	-2.90805800	2.37768600	2.25040400
C	-2.63634800	2.74338800	0.98295900
H	-0.25982300	0.29518900	2.90021800
H	-2.00828500	1.47880100	4.04621900
H	-3.77151300	2.77919700	2.78499500
H	-3.24723000	3.48184200	0.45579900
B	0.52258600	0.82287700	0.03454000
N	0.55971700	2.01384500	-0.73433600
C	1.70612800	-0.21660300	0.06821200
C	1.83005300	-1.26430600	-0.86939500
C	2.69440900	-0.08245000	1.06387100
C	2.90024700	-2.15447100	-0.77423300
C	3.74732700	-0.99764000	1.13482000
C	3.86515200	-2.04815000	0.22805900
H	2.98392600	-2.95973500	-1.51027600
H	4.50188500	-0.87993100	1.91831800
C	2.66988300	1.07350000	2.03568500
H	1.65152000	1.43236300	2.24049300
H	3.13040100	0.80095100	2.99626300
H	3.23735000	1.93104200	1.63811500
C	0.81962800	-1.45977400	-1.97284600
H	0.44300600	-0.50205100	-2.35913500
H	1.25621300	-2.01701200	-2.81387100
H	-0.05627900	-2.02306700	-1.61647500
C	4.98620800	-3.04786900	0.32960400
H	5.82414800	-2.65631300	0.92347000
H	4.64440300	-3.97715500	0.81418100
H	5.37029300	-3.32395200	-0.66355200
C	1.61955900	2.49560000	-1.61838000
H	2.38657500	1.70797100	-1.60721500
C	2.25521700	3.78232300	-1.09378600
H	1.54020500	4.61961400	-1.09851700
H	2.61645100	3.65119000	-0.06399200
H	3.10895900	4.07263000	-1.72373700
C	1.12461900	2.65555900	-3.05520100
H	0.70206800	1.71402400	-3.43430600
H	0.34753400	3.43247100	-3.12987400
H	1.95223800	2.94982500	-3.71734300
H	-0.69616700	3.77874100	-0.91705700
C	-0.91695000	0.81873200	0.78994000
C	-1.67962400	-0.43809600	0.23091600
C	-1.49230200	-1.70578800	0.84569200
C	-2.51836300	-0.39319300	-0.91402000
C	-2.18417200	-2.82541100	0.37677100
C	-3.18781900	-1.54859800	-1.33444200
C	-3.05932300	-2.77559900	-0.69992300
H	-2.01725900	-3.78159500	0.88025800
H	-3.83334700	-1.47571600	-2.21358900
C	-0.55730300	-1.98831400	2.00164600

H	0.39437500	-1.45265500	1.92236400
H	-1.01529600	-1.73378800	2.96834300
H	-0.32212300	-3.06094400	2.02507100
C	-2.74893100	0.81303700	-1.79805000
H	-3.29339000	1.61574000	-1.28659400
H	-1.81175900	1.24228000	-2.17299200
H	-3.34635700	0.51256400	-2.66927000
C	-3.82761600	-3.98737700	-1.15168500
H	-3.25182100	-4.91127800	-0.99543500
H	-4.76886100	-4.09118900	-0.58707700
H	-4.09119500	-3.92406700	-2.21722100

TS2; E = -1165.488468:

C	2.06670900	-1.35535900	1.19063400
C	2.65749800	-1.01171700	0.00564900
C	1.91949300	-0.14650200	-0.91847600
C	2.34585700	-0.21921000	-2.29607500
C	3.46836600	-0.89142700	-2.67933200
C	4.29758800	-1.54852900	-1.71356000
C	3.91237400	-1.58295200	-0.41297100
H	1.82744000	0.36234700	-3.05350000
H	3.77535200	-0.86814500	-3.72722200
H	5.22805100	-2.02467900	-2.03050100
H	4.50971400	-2.11356700	0.33363100
B	0.10641300	-0.28468100	0.30119300
N	0.72579500	-1.02644100	1.33542400
C	1.12666700	1.03227600	-0.45079100
C	0.12994100	1.66471000	-1.31939800
C	1.54803200	1.83908800	0.68546400
C	-0.40632200	2.89479900	-1.00167200
C	0.91445900	3.05338800	0.97051400
C	-0.04398200	3.61486100	0.14492500
H	-1.16105800	3.31525200	-1.67165300
H	1.24776000	3.60925900	1.85032500
C	-1.42201600	-0.48369400	-0.05872500
C	-1.76269800	-1.58418300	-0.88708100
C	-2.46955900	0.29460000	0.47028700
C	-3.09728500	-1.82859500	-1.20764700
C	-3.79635800	0.02181700	0.12235600
C	-4.13330700	-1.02591300	-0.72785400
H	-3.33814500	-2.68009600	-1.85125100
H	-4.59205900	0.64236600	0.54589300
C	2.73809900	1.50656300	1.52085800
H	3.00071400	2.35926400	2.16050700
H	2.56963900	0.62161700	2.15592400
H	3.60051600	1.24608900	0.88943500
C	-0.39922800	1.01976400	-2.57142600
H	0.11802400	1.41831100	-3.45893000
H	-0.26964000	-0.06456700	-2.57755000
H	-1.46855600	1.24168700	-2.68471400
C	-0.68997000	4.93145000	0.46103000
H	-1.72416600	4.78471200	0.81484000
H	-0.14412400	5.47285000	1.24585000
H	-0.74451400	5.57402200	-0.43058800
C	-2.22454700	1.39519600	1.47106100
H	-2.73244900	1.16744800	2.42212000
H	-1.15840200	1.53323700	1.68452100
H	-2.62584600	2.35658700	1.11671000
C	-0.71588800	-2.51218000	-1.45826000
H	0.16173300	-2.61104900	-0.80703900
H	-1.13765500	-3.51271000	-1.63161000
H	-0.33812500	-2.15026400	-2.42802700
C	-5.56195700	-1.29707000	-1.11661300
H	-5.80782200	-2.36548300	-1.02123600
H	-6.26559400	-0.72822800	-0.49284600
H	-5.74642200	-1.01684800	-2.16638300
C	-0.04230500	-1.68203000	2.40953500
H	-1.08390800	-1.37125800	2.25987000
C	0.40227500	-1.17660600	3.78098100
H	1.43838100	-1.47284100	4.00613600
H	0.34175100	-0.07969100	3.83178000
H	-0.24111600	-1.59381600	4.56999300
C	0.00083300	-3.20588300	2.32225700
H	-0.34599100	-3.55442100	1.33987100
H	1.01507000	-3.59877700	2.48493200
H	-0.65439500	-3.64329400	3.09024900
H	2.55659400	-1.94680900	1.96252000

DI; E = -1165.539447:

C	2.04722400	1.80401900	0.16875500
C	2.94834400	0.74501200	-0.15573100
C	2.48712800	-0.58468800	-0.31331900
C	3.43188300	-1.53768600	-0.74838000
C	4.75371500	-1.20604700	-0.97891100
C	5.20135600	0.11298200	-0.80492400
C	4.30283100	1.07158300	-0.39563100
H	3.12367700	-2.57792400	-0.84140200
H	5.46065900	-1.98570500	-1.27168300
H	6.24656600	0.37149500	-0.98383700
H	4.62710300	2.10632600	-0.25733300
B	0.03569300	0.33570900	0.37156600
N	0.75867400	1.66727400	0.32889300
C	-1.48989700	0.36862800	-0.12654900
C	-1.80220800	0.40273400	-1.50570500
C	-2.57890500	0.39846700	0.77743900
C	-3.12946300	0.36736400	-1.94068200
C	-3.89488000	0.36680800	0.31013400
C	-4.19668300	0.32567600	-1.04864900
H	-3.33398900	0.38388100	-3.01612400
H	-4.71361000	0.38903400	1.03661500
C	1.09857100	-0.96420000	0.00972700
C	0.61534700	-0.72544300	1.44734000
C	0.50242300	-2.10709400	-0.73692500
C	-0.31831300	-1.75530300	1.95505900
C	-0.44286200	-2.88348000	-0.16787600
C	-0.84960800	-2.74760200	1.22053700
H	-0.57500200	-1.68502900	3.01594200
H	-0.91371200	-3.67038900	-0.76495600
C	1.61247300	-0.30299600	2.51168800
H	2.39413800	-1.06681000	2.65916600
H	2.12606900	0.64413000	2.30375400
H	1.08655800	-0.17658100	3.47086200
C	0.89726700	-2.37623500	-2.17264800
H	1.62060000	-3.20168000	-2.26076500
H	0.01219000	-2.66561100	-2.75708500
H	1.35118000	-1.50160200	-2.65466900
C	-1.83637900	-3.73456700	1.77526800
H	-2.80624600	-3.65282000	1.25663700
H	-1.48833700	-4.77160500	1.63819100
H	-2.01237300	-3.57281600	2.84819500
C	-2.40003000	0.53224500	2.27248700
H	-2.72497500	-0.37798800	2.79787200
H	-1.35812800	0.72333000	2.55214400
H	-3.01539500	1.36152900	2.65619700

C	-0.74533200	0.53139800	-2.57832000
H	-0.82315700	-0.28035700	-3.31643800
H	-0.87826000	1.47416400	-3.13391000
H	0.27153900	0.52183300	-2.17290400
C	-5.61986900	0.24106900	-1.53194000
H	-5.73866900	0.70321000	-2.52277600
H	-5.94539900	-0.80871600	-1.62086200
H	-6.31287500	0.73762200	-0.83708500
C	-0.03064900	2.91558700	0.52467900
H	-1.07008800	2.58138400	0.59509300
C	0.34143500	3.59365700	1.83978100
H	1.36485500	3.99897500	1.82228500
H	-0.34368800	4.43226500	2.03103700
H	0.26392800	2.89044000	2.68106800
C	0.07463000	3.85131200	-0.67386700
H	1.08850300	4.26296700	-0.79330600
H	-0.19986500	3.33184500	-1.60195300
H	-0.61320800	4.69890500	-0.54122300
H	2.46292500	2.81360800	0.22614300

TS3; E = -1165.50429:

C	2.19621600	1.53282700	0.63752400
C	2.99065400	0.53899600	-0.07507600
C	2.42594400	-0.72485200	-0.35108400
C	3.24190100	-1.69324300	-0.95501200
C	4.56300800	-1.42739300	-1.28654300
C	5.11281400	-0.17258000	-1.01420500
C	4.33254900	0.79299500	-0.40230200
H	2.85192700	-2.69506000	-1.12608300
H	5.17653500	-2.21056600	-1.73696800
H	6.15211800	0.04279800	-1.27150000
H	4.75489000	1.77471400	-0.17304800
B	0.10518900	0.39791700	0.12935800
N	0.83341800	1.58715700	0.36053800
C	-1.43552700	0.44022500	-0.26268700
C	-1.77859300	0.39307200	-1.63398300
C	-2.49039800	0.55774800	0.66865600
C	-3.11511700	0.34476100	-2.03071800
C	-3.81914800	0.50342700	0.23692100
C	-4.15753700	0.36921000	-1.10651200
H	-3.34894200	0.30205100	-3.09917500
H	-4.61763600	0.58736700	0.98086000
C	1.01519900	-1.01449100	0.11247900
C	0.84171000	-0.95273700	1.60603200
C	0.24907600	-2.12531600	-0.55151900
C	-0.31146000	-1.58979200	2.18846400
C	-0.74556400	-2.74799600	0.11787200
C	-1.08168800	-2.46481100	1.49581100
H	-0.49104100	-1.42811700	3.25439300
H	-1.34470500	-3.49824800	-0.40647000
C	1.84680800	-0.37571000	2.42410300
H	2.87327500	-0.71394100	2.22637000
H	2.11209500	0.80541800	1.89251100
H	1.60821200	-0.31499600	3.49222400
C	0.49370100	-2.49688700	-1.99396000
H	1.08662700	-3.42124700	-2.07982200
H	-0.46256000	-2.68113800	-2.50339700
H	1.03343100	-1.71999300	-2.54613200
C	-2.25547900	-3.16677600	2.11123500
H	-3.19347500	-2.85030100	1.62467800
H	-2.18210200	-4.25886200	1.98355600
H	-2.34081200	-2.95219400	3.18565000
C	-2.26587800	0.82204400	2.13868500
H	-2.69804200	0.02575900	2.76228800
H	-1.20386200	0.90719200	2.39095000
H	-2.75985600	1.76305700	2.43020500
C	-0.73561400	0.48984400	-2.72283200
H	-0.88939400	-0.26779600	-3.50477500
H	-0.79925800	1.47415200	-3.21489400
H	0.28799300	0.38952800	-2.34322400
C	-5.59298700	0.26392100	-1.54697900
H	-6.27400800	0.72832000	-0.81940600
H	-5.75265500	0.74664400	-2.52226800
H	-5.89703500	-0.79058400	-1.65324000
C	0.19374600	2.91803200	0.40835000
H	-0.87826900	2.73127200	0.27587800
C	0.38349800	3.60121900	1.76113700
H	1.42911100	3.89393900	1.93777300
H	-0.22478100	4.51674400	1.80246600
H	0.06822500	2.94505800	2.58453000
C	0.65891600	3.79826300	-0.74877200
H	1.73231100	4.03075800	-0.67827000
H	0.48098600	3.30228800	-1.71339100
H	0.10878700	4.75105200	-0.74543800
H	2.67755200	2.50124400	0.79209500

Int2; E = -1165.561203:

C	-2.21496200	1.88478600	0.39471600
C	-3.02694400	0.69476700	-0.03796300
C	-2.46880200	-0.56943700	-0.21861800
C	-3.32433600	-1.63902500	-0.52599300
C	-4.69152200	-1.46034800	-0.66531000
C	-5.24128600	-0.18733200	-0.50564700
C	-4.40911900	0.87524400	-0.19420100
H	-2.89384900	-2.63261500	-0.66163500
H	-5.33260000	-2.31217000	-0.90266700
H	-6.31536800	-0.02840100	-0.62309800
H	-4.83211800	1.87505300	-0.06119400
B	-0.10766900	0.55211100	0.03729100
N	-0.77584700	1.77074200	0.22161500
C	1.48256700	0.52318400	-0.08553200
C	2.30217400	0.36905700	1.05359700
C	2.11637900	0.66585400	-1.33840400
C	3.68857200	0.27698000	0.91598600
C	3.50574600	0.56786200	-1.43932700
C	4.31387700	0.35045000	-0.32653000
H	4.30129500	0.15833500	1.81525700
H	3.97183600	0.67901800	-2.42351700
C	-0.97438800	-0.83329100	-0.03671700
C	-0.42055400	-1.64846600	-1.21459000
C	-0.75695700	-1.53785200	1.30494300
C	0.62429600	-2.63311300	-0.93750000
C	0.13270200	-2.53536300	1.42910600
C	0.90455000	-3.06456700	0.30471000
H	1.15206600	-3.05484900	-1.79704500
H	0.29244000	-2.98801000	2.41259900
C	-0.83946700	-1.46220500	-2.47678600
H	-1.63769600	-0.76313800	-2.73069200
H	-2.57990500	2.76751100	-0.15322900
H	-0.38309000	-2.01864500	-3.29890400
C	-1.55348000	-1.05999400	2.48617600
H	-2.61624700	-1.32827200	2.38393900
H	-1.17666200	-1.50132400	3.41895700
H	-1.51958300	0.03630500	2.58790000

C	1.95901600	-4.08973800	0.59604900
H	2.74051000	-3.66911800	1.25036300
H	1.53291500	-4.95715000	1.12674100
H	2.44150700	-4.44983200	-0.32275100
C	1.35324400	0.97986600	-2.60404400
H	1.47430800	0.18411500	-3.35346900
H	0.27791900	1.10008200	-2.43031600
H	1.72999500	1.91226400	-3.05441900
C	1.74330700	0.34375200	2.45740300
H	1.80617800	-0.66105100	2.90007300
H	2.31118200	1.02595600	3.10877200
H	0.69100700	0.64962700	2.49468200
C	5.80599000	0.20279400	-0.46017600
H	6.32938200	0.55898500	0.43902200
H	6.08683300	-0.85374100	-0.60368000
H	6.19150200	0.76206500	-1.32491200
C	-0.06076400	3.05849700	0.32275000
H	1.00469500	2.80296200	0.29612500
C	-0.33642900	3.97596900	-0.86941100
H	-1.37699000	4.33420600	-0.89421500
H	0.30983500	4.86448600	-0.81310600
H	-0.12624900	3.46309300	-1.81786700
C	-0.32723400	3.77084800	1.64880200
H	-1.35775300	4.15049000	1.72120300
H	-0.14458400	3.10253600	2.50316900
H	0.34525700	4.63553100	1.74743600
H	-2.44576000	2.08487700	1.45778000

TS4; E = -1165.517423:

C	1.96153900	1.58370300	-0.93691900
C	2.97375200	0.54860400	-0.51867300
C	2.51373000	-0.67958000	-0.04116200
C	3.44342200	-1.64207500	0.36905700
C	4.81025800	-1.39943800	0.29308200
C	5.26557700	-0.17756400	-0.19706300
C	4.34782000	0.78798700	-0.59531300
H	3.08102700	-2.59906700	0.75382300
H	5.52015900	-2.16245000	0.61962400
H	6.33673400	0.02713000	-0.25818700
H	4.70108700	1.75387200	-0.96628000
B	0.04491300	0.48122900	0.38156700
N	0.82319300	1.64844900	-0.05469700
C	-1.54708200	0.48125800	0.09065700
C	-1.96182600	0.46392200	-1.26688800
C	-2.57643100	0.58456900	1.05965700
C	-3.31494300	0.42583100	-1.60968900
C	-3.92233500	0.55900700	0.67630400
C	-4.32182400	0.45075200	-0.65053300
H	-3.58805400	0.39399900	-2.66874000
H	-4.68821100	0.64028800	1.45311300
C	1.04128900	-1.03190200	0.03239600
C	0.46363300	-1.10608000	1.37231000
C	0.60002500	-2.03241100	-0.94381200
C	-0.56128700	-2.07627300	1.63372200
C	-0.42781900	-2.87220000	-0.64789200
C	-1.01370200	-2.91658700	0.66138700
H	-0.97684100	-2.12681900	2.64145300
H	-0.77484600	-3.58727100	-1.39797000
C	0.66967400	0.01717400	2.17733200
H	1.62675900	0.53251000	2.14210000
H	2.45922800	2.56231700	-0.98089400
H	0.12024200	0.09333600	3.11263300
C	1.34233000	-2.16931600	-2.24437900
H	0.73990700	-2.71147800	-2.98580800
H	1.63101900	-1.19668300	-2.66598300
H	2.27947700	-2.72680800	-2.09208200
C	-2.10879500	-3.90716700	0.92321900
H	-3.00058900	-3.64622700	0.33141800
H	-1.80509900	-4.92075300	0.61858200
H	-2.39627800	-3.93050600	1.98266900
C	-2.32789200	0.77508000	2.53802900
H	-3.24963200	1.10779700	3.03473000
H	-2.01486400	-0.15480800	3.03442100
H	-1.55311700	1.52686200	2.73561300
C	-0.98467700	0.57009700	-2.41027200
H	-1.45906400	0.29108600	-3.36126700
H	-0.62101000	1.60410100	-2.50790200
H	-0.10228700	-0.05903000	-2.27696200
C	-5.77485700	0.37408900	-1.03512900
H	-5.97230200	0.91073200	-1.97491200
H	-6.09101800	-0.67136400	-1.18707200
H	-6.42189900	0.80118800	-0.25552400
C	0.45848800	2.95551500	0.49030500
H	-0.43071900	2.77884100	1.11364000
C	1.53765500	3.54936300	1.40222400
H	2.46198200	3.77329600	0.84682000
H	1.19248900	4.49260400	1.85280600
H	1.79361600	2.85701000	2.21663100
C	0.04104700	3.95102900	-0.59484000
H	0.87112300	4.17177100	-1.28463500
H	-0.79822100	3.55406700	-1.18334500
H	-0.27577800	4.90604900	-0.14826500
H	1.65744800	1.36480800	-1.98190900

Final; E = -1165.602212:

C	1.46359600	-2.19197300	-0.26574900
C	2.73299800	-1.34750000	-0.31985300
C	2.86425800	0.05333900	-0.41876200
C	4.14764900	0.56600700	-0.69884000
C	5.27435000	-0.22865400	-0.82385300
C	5.14886800	-1.60479100	-0.66281300
C	3.89301500	-2.13546200	-0.42300200
H	4.24617800	1.64409000	-0.83198900
H	6.24307200	0.22440500	-1.04446200
H	6.01856300	-2.26095800	-0.73785200
H	3.78986800	-3.21994300	-0.32615200
B	-0.57237700	-0.80947600	-0.59741000
N	0.19483000	-1.66513000	0.21214700
C	-2.09953300	-0.49217900	-0.30447900
C	-2.55722700	0.35493500	0.71947200
C	-3.05789700	-1.09147400	-1.15743700
C	-3.92932700	0.60295200	0.86014800
C	-4.41378400	-0.83301600	-0.98194500
C	-4.87407400	0.02323900	0.02266500
H	-4.26469500	1.27042000	1.65996600
H	-5.13746800	-1.31309800	-1.64778600
C	1.80777800	1.11460300	-0.26876700
C	0.65749200	1.16113900	-1.08935100
C	2.03874000	2.17842100	0.62895900
C	-0.14105500	2.30436400	-1.09306000
C	1.19387300	3.29374000	0.61135500
C	0.12274900	3.39739800	-0.26852100
H	-1.01969400	2.32312000	-1.74316600
H	1.38727000	4.10784900	1.31555000

C	0.16267700	-0.06664400	-1.81326700
H	0.98768300	-0.63325200	-2.26463800
H	1.32049900	-2.57207800	-1.29102100
H	-0.53617600	0.22326600	-2.60822400
C	3.15084600	2.16298000	1.65301800
H	4.06625100	2.65068000	1.28396900
H	2.83679700	2.70979400	2.55380200
H	3.42788100	1.14349500	1.94946200
C	-0.75371300	4.61986300	-0.30858700
H	-1.81526300	4.35348000	-0.18874200
H	-0.48942500	5.33275600	0.48483000
H	-0.66054600	5.14269900	-1.27374700
C	-2.62342000	-2.02213700	-2.26501600
H	-2.10129700	-1.48035000	-3.06951200
H	-1.92930900	-2.79531500	-1.89998700
H	-3.48405300	-2.53387400	-2.71722800
C	-1.62291100	0.99580300	1.71770300
H	-1.84272000	2.06721500	1.83378800
H	-1.74224700	0.53578800	2.71292700
H	-0.56857500	0.90706800	1.43032000
C	-6.34580600	0.29838600	0.18133400
H	-6.54470400	0.93972200	1.05126500
H	-6.75563700	0.80276500	-0.70821700
H	-6.91547600	-0.63487800	0.31222000
C	-0.28758400	-2.22043900	1.48632200
H	-1.21472000	-1.68077100	1.71059000
C	-0.65506900	-3.70106900	1.38186200
H	0.22023200	-4.33729600	1.17794000
H	-1.09797200	-4.05050600	2.32658200
H	-1.39177300	-3.86286000	0.58152700
C	0.69174900	-1.95232200	2.62787000
H	1.64151300	-2.49314100	2.49469500
H	0.92118300	-0.87969300	2.70233900
H	0.25972300	-2.27962200	3.58536500
H	1.70768400	-3.08473700	0.32317000

tBu; E = -1204.81323673:

C	0.10539900	2.61275100	0.71941900
C	0.66023000	2.65376100	-0.60340500
C	0.57687800	1.37905700	-1.18810200
C	1.08411800	1.26214300	-2.48942300
C	1.59395300	2.37246400	-3.15422600
C	1.64662700	3.63491800	-2.54674100
C	1.18041800	3.78112500	-1.25212500
H	1.08186900	0.30233900	-3.00503800
H	1.96535700	2.25774200	-4.17568100
H	2.05707700	4.48849100	-3.08947100
H	1.21856700	4.74918200	-0.74574300
B	0.04520300	0.29610700	-0.07982300
N	-0.24947100	1.44825900	1.14653000
C	-1.38572700	-0.50263400	-0.29944000
C	-2.44964500	0.10200100	-1.02996800
C	-1.65008700	-1.79404500	0.22815100
C	-3.66029400	-0.56239800	-1.23294000
C	-2.88431200	-2.42169900	0.00498600
C	-3.90375000	-1.83808000	-0.73111700
H	-4.44726400	-0.05698700	-1.80043600
H	-3.04575100	-3.41562400	0.43351900
C	1.40407800	-0.64424000	0.08590900
C	2.47495500	-0.42055800	0.98849200
C	1.59490300	-1.69033300	-0.85858900
C	3.58172000	-1.27683200	1.02023800
C	2.72240900	-2.51307100	-0.80053600
C	3.72251700	-2.35060600	0.15041700
H	4.37578700	-1.07600000	1.74531300
H	2.82000300	-3.31393000	-1.54066900
C	-0.68650200	-2.63249300	1.04829200
H	-0.21753100	-3.40926400	0.42553700
H	0.12722200	-2.06764500	1.50319000
H	-1.23483900	-3.15543600	1.84668900
C	-2.36666700	1.49113200	-1.61971300
H	-2.06836800	2.24479300	-0.87953200
H	-1.63903100	1.55359600	-2.43963300
H	-3.34426500	1.79386800	-2.01957700
C	-5.20897000	-2.54288200	-0.98452100
H	-6.06685800	-1.87244400	-0.82369700
H	-5.27115500	-2.90122200	-2.02506000
H	-5.33027300	-3.41523300	-0.32686200
C	2.55282600	0.76435600	1.92187700
H	2.55830700	1.71494400	1.36781800
H	1.72068800	0.80755300	2.63210600
H	3.48098700	0.72578900	2.50813200
C	0.63935100	-2.02528100	-1.98905400
H	1.21162900	-2.24993700	-2.90205600
H	0.04415500	-2.92211100	-1.75788600
H	-0.07754100	-1.23558400	-2.22071600
C	4.90144200	-3.28295900	0.22457200
H	5.76765400	-2.80105800	0.70067600
H	4.66164000	-4.18254300	0.81557000
H	5.20826200	-3.62516300	-0.77491600
H	-0.03229200	3.51457800	1.32139700
C	-1.00775500	1.36923300	2.44400800
C	-0.48118600	2.39877100	3.45741500
H	-0.70776100	3.43633700	3.17610700
H	-0.97378300	2.22260000	4.42303300
H	0.60308600	2.30646500	3.61026200
C	-2.48604600	1.66911800	2.15793300
H	-2.61010700	2.67866300	1.73760800
H	-2.90927200	0.94301600	1.45303800
H	-3.05923100	1.61978500	3.09549900
C	-0.89145600	-0.02098500	3.06264100
H	-1.39753600	-0.76682300	2.44753400
H	0.15214200	-0.32927600	3.20260900
H	-1.37783700	-0.01220100	4.04804100

TS1Bu; E = -1204.77164225:

C	-0.83424100	-2.61196200	0.25309300
C	-1.47923300	-2.10401700	-0.84270100
C	-0.90267700	-0.79898100	-1.18273100
C	-1.20186500	-0.39714900	-2.56034300
C	-2.14169300	-1.04268100	-3.29608800
C	-2.87348400	-2.17868600	-2.80098400
C	-2.52502700	-2.71504900	-1.60376200
H	-0.67012600	0.42775300	-3.02398900
H	-2.33373300	-0.70361100	-4.31745200
H	-3.65809100	-2.62622500	-3.41372300
H	-3.00720900	-3.62169500	-1.22721200
B	0.19634200	-0.54766500	-0.09764900
N	0.10676000	-1.78297100	0.76800700
C	1.56247800	0.27900300	-0.18063400
C	2.49895100	-0.17221100	-1.14916900
C	1.92735000	1.38326600	0.61444400
C	3.73037700	0.46205000	-1.29406100
C	3.17568000	1.99619200	0.43831300

C	4.09293600	1.55728300	-0.50694000
H	4.43282500	0.08920700	-2.04562900
H	3.43391600	2.85028400	1.07199700
C	-1.43164700	0.56465600	-0.04266500
C	-2.43532000	0.39881600	0.95642400
C	-1.25349200	1.87061700	-0.58118700
C	-3.19900700	1.49875300	1.35814600
C	-2.04861200	2.92645200	-0.13440300
C	-3.03920100	2.77156900	0.82546800
H	-3.95538000	1.34251600	2.13160700
H	-1.87550100	3.91790300	-0.56344400
C	-0.24854100	2.29143800	-1.63371700
H	-0.77480500	2.57470400	-2.55849900
H	0.28950300	3.18429700	-1.28384500
H	0.50536100	1.54459700	-1.87602100
C	-2.75242500	-0.87690600	1.69110900
H	-3.52841700	-0.68515300	2.44312500
H	-3.11734600	-1.66402200	1.02068000
H	-1.87207500	-1.27543500	2.20935600
C	-3.91047400	3.91952300	1.25283600
H	-4.80067900	3.99686300	0.60705900
H	-4.26616200	3.79367900	2.28540200
H	-3.37573400	4.87791400	1.18649300
C	1.03046800	1.99265300	1.66821600
H	0.15546900	1.37784400	1.89623600
H	1.58950700	2.16024100	2.60181100
H	0.65637200	2.97444300	1.33930600
C	2.18604400	-1.33709400	-2.05809400
H	1.79107900	-2.20105100	-1.50611100
H	1.42011800	-1.07352000	-2.80241300
H	3.08320900	-1.66340200	-2.60222600
C	5.43190400	2.22254800	-0.68146700
H	5.56617100	2.58519700	-1.71262300
H	5.54745100	3.08068500	-0.00474500
H	6.25599500	1.52037700	-0.47850100
C	0.98526000	-2.25102900	1.88257000
C	0.33292200	-3.40678000	2.65559800
H	0.24806700	-4.32477000	2.05799300
H	0.96263800	-3.64770500	3.52274600
H	-0.66530500	-3.13869300	3.03210400
C	2.32165800	-2.74845100	1.31574800
H	2.86522400	-1.94205200	0.80805700
H	2.95757400	-3.13090500	2.12843100
H	2.15878800	-3.56688000	0.59863300
H	-1.08197500	-3.55861300	0.72777400
C	1.23671500	-1.11731000	2.87747900
H	1.81698700	-0.30885900	2.42520700
H	0.29200200	-0.70393900	3.25868000
H	1.81043500	-1.50194100	3.73296300

Int1Bu; E = -1204.79862872:

C	0.09838500	-2.85578000	-0.09487500
C	1.06990500	-2.29611800	0.63535400
C	0.80264100	-0.67724700	2.38325800
C	1.63462800	-1.41123200	3.14166200
C	2.45524400	-2.48201400	2.57975400
C	2.14828900	-2.95704300	1.35773700
H	0.16447400	0.05867000	2.86656900
H	1.67094800	-1.24156600	4.22129600
H	3.23811700	-2.93966400	3.18832600
H	2.64484600	-3.83815800	0.94137600
B	-0.64566400	-0.68012700	0.09333400
N	-0.91372000	-1.95013900	-0.49642300
C	-1.53758300	0.61884000	0.06993600
C	-1.39233500	1.63131500	-0.89946700
C	-2.48229200	0.80175800	1.10078000
C	-2.15858700	2.79453200	-0.80589000
C	-3.22518100	1.98174100	1.16846000
C	-3.07198600	2.99858100	0.22751500
H	-2.03843800	3.56842300	-1.57015500
H	-3.95159400	2.10615200	1.97707900
C	-2.75946900	-0.29099400	2.10613200
H	-1.86297400	-0.87514400	2.35731200
H	-3.16744200	0.11799300	3.04143700
H	-3.50366600	-1.00414200	1.71355100
C	-0.42493400	1.49722100	-2.05021400
H	-0.23604800	0.44639900	-2.31094400
H	-0.80882700	2.00508700	-2.94722400
H	0.55096100	1.94408900	-1.80672400
C	-3.85337800	4.28138200	0.32993900
H	-4.78415600	4.14326800	0.89836600
H	-3.26743200	5.06098300	0.84412800
H	-4.11406300	4.67455100	-0.66356300
C	-2.01816400	-2.47977800	-1.33343200
C	-2.74565800	-3.59689800	-0.57048800
H	-2.08530600	-4.44456600	-0.34013000
H	-3.14959400	-3.21466000	0.37816900
H	-3.58273000	-3.98224900	-1.17061500
C	-1.43539300	-3.02989400	-2.64398800
H	-0.93404700	-2.22996800	-3.20854800
H	-0.70548900	-3.83317900	-2.47061400
H	-2.23794100	-3.44095500	-3.27356400
H	0.03650900	-3.90535200	-0.38038100
C	0.78215800	-0.82092200	0.86456200
C	1.78554800	0.18491700	0.19471100
C	1.91351900	1.51158600	0.68724000
C	2.55858200	-0.15622000	-0.94699700
C	2.83753800	2.38898200	0.11209000
C	3.46938900	0.76416500	-1.47700000
C	3.65008000	2.03797800	-0.95718700
H	2.91177400	3.39926400	0.52353300
H	4.05441300	0.46292800	-2.35004000
C	1.09627700	2.11686700	1.80863800
H	0.03726700	1.84215500	1.75954800
H	1.48013700	1.82959900	2.79777500
H	1.14855400	3.21206900	1.74396500
C	2.46748400	-1.45485900	-1.71815200
H	2.86850400	-2.30920000	-1.15908000
H	1.43714500	-1.70388700	-1.99900000
H	3.04974600	-1.36548900	-2.64518000
C	4.67136400	2.98729600	-1.52158500
H	4.36004400	4.03472600	-1.39824100
H	5.64144800	2.87314500	-1.01019900
H	4.84421100	2.80483400	-2.59211500
C	-3.03307600	-1.39313100	-1.68241100
H	-3.52081300	-0.98086400	-0.79113600
H	-2.57108600	-0.56213000	-2.22930800
H	-3.81106800	-1.83173000	-2.32387000

TS2Bu; E = -1204.73751441:

C	2.14873400	-1.42168600	0.80212400
C	2.62065800	-0.92579400	-0.37870700
C	1.81622600	0.05317200	-1.10366300
C	2.11907500	0.16873000	-2.51134100

C	3.19658800	-0.44331700	-3.07994600
C	4.10169100	-1.22317600	-2.28916500
C	3.83114700	-1.43223100	-0.97682800
H	1.54518000	0.84688900	-3.13584900
H	3.41132500	-0.27544400	-4.13755600
H	4.99706200	-1.64843300	-2.74784100
H	4.48689800	-2.05451000	-0.36154500
B	0.11267000	-0.28195100	0.27698300
N	0.82657400	-1.14656800	1.15400900
C	1.08344600	1.15262700	-0.41002500
C	0.04579700	1.91192100	-1.11646600
C	1.60109200	1.79262900	0.78805200
C	-0.41548100	3.10960800	-0.61649100
C	1.02005700	2.97211700	1.27379000
C	0.03998400	3.66519800	0.58865000
H	-1.19285500	3.63588000	-1.17736200
H	1.42420900	3.39774600	2.19558400
C	-1.40802100	-0.42695900	-0.12822600
C	-1.71485600	-1.46882800	-1.04339400
C	-2.47212200	0.34831700	0.37055100
C	-3.03410400	-1.68437600	-1.43912000
C	-3.78107800	0.10855000	-0.05908200
C	-4.08687500	-0.89871100	-0.96772000
H	-3.24763500	-2.49259200	-2.14489000
H	-4.59041900	0.72226700	0.34825500
C	2.84906300	1.35088100	1.47657300
H	3.16372000	2.10694500	2.20764400
H	2.72939700	0.38438500	1.99068200
H	3.65955600	1.19117700	0.74961500
C	-0.59758600	1.44828000	-2.39772900
H	-0.14765300	1.95932600	-3.26408600
H	-0.50167800	0.37294100	-2.56284700
H	-1.66698500	1.69761600	-2.38801900
C	-0.53785000	4.94876000	1.10786600
H	-1.56858600	4.79661400	1.46931900
H	0.05224300	5.35041600	1.94295300
H	-0.58508500	5.71333100	0.31761200
C	-2.28254800	1.40751100	1.42604600
H	-2.85436900	1.14872700	2.33164800
H	-1.23230900	1.53057700	1.71296600
H	-2.65489200	2.38326400	1.08079000
C	-0.64300400	-2.34199000	-1.65120100
H	-1.07278700	-3.27952000	-2.03157800
H	-0.15036200	-1.83747400	-2.49743600
H	0.15852600	-2.58705900	-0.94374100
C	-5.49739900	-1.13898500	-1.43454700
H	-6.22441200	-0.58008300	-0.82893400
H	-5.62632200	-0.82575200	-2.48323100
H	-5.75975900	-2.20655600	-1.38369000
C	0.28930000	-1.98666600	2.27852000
C	1.14776800	-1.72344000	3.52766100
H	2.19652700	-2.01911500	3.39604300
H	1.12309400	-0.65513400	3.78909600
H	0.75015600	-2.29333900	4.37970900
C	0.34219400	-3.47360300	1.90354100
H	-0.31177000	-3.68040400	1.04490900
H	1.35767400	-3.80088500	1.64428600
H	-0.00505400	-4.08524500	2.74929800
H	2.73766200	-2.08209700	1.43264400
C	-1.15006700	-1.63650400	2.65076200
H	-1.25686500	-0.56931300	2.88134000
H	-1.86475200	-1.89914800	1.86435400
H	-1.41901600	-2.20247400	3.55397800

DIBu; E = -1204.78368516:

C	2.22111300	1.50688700	0.00608300
C	2.93653500	0.33096500	-0.37987900
C	2.30106600	-0.92786500	-0.42367200
C	3.05857300	-2.01494300	-0.90613800
C	4.37998700	-1.86589900	-1.28433400
C	5.00870800	-0.61204200	-1.21819800
C	4.28863700	0.47118000	-0.76629800
H	2.60073700	-3.00471200	-0.92662600
H	4.94738100	-2.73968900	-1.61325800
H	6.05332200	-0.50057500	-1.51392000
H	4.75613700	1.45783300	-0.70994000
B	0.05501400	0.34472600	0.41823300
N	0.95200200	1.60248400	0.29637800
C	-1.44149200	0.41368500	-0.16112200
C	-1.61573100	0.55715100	-1.56245100
C	-2.61235200	0.28373900	0.61661300
C	-2.88409600	0.48391600	-2.13891400
C	-3.86926000	0.20881700	0.00587800
C	-4.03171900	0.28535800	-1.37217800
H	-2.98022700	0.58878600	-3.22406200
H	-4.75556100	0.10178600	0.63966100
C	0.91554200	-1.08357000	0.04120400
C	0.59233500	-0.73192000	1.50442600
C	0.13253900	-2.19225500	-0.58616100
C	-0.32637300	-1.69410200	2.16519600
C	-0.73561600	-2.92429600	0.13667100
C	-0.95196400	-2.71561600	1.56055500
H	-0.45962200	-1.55831400	3.24308000
H	-1.32092000	-3.70306100	-0.36228000
C	1.73162600	-0.38845500	2.45286600
H	2.41273700	-1.24551700	2.58471800
H	2.34843000	0.46445700	2.14690900
H	1.31649500	-0.14115500	3.44241700
C	0.21040300	-2.42940700	-2.07875700
H	0.18054000	-3.50391200	-2.31295800
H	-0.65849300	-1.96524600	-2.57062100
H	1.10856000	-2.00880600	-2.54529000
C	-1.87614100	-3.65060800	2.28628600
H	-2.89867100	-3.59051800	1.87642700
H	-1.55301800	-4.69898900	2.17662100
H	-1.92707800	-3.42000500	3.35991600
C	-2.61566400	0.30878600	2.12758300
H	-2.98546000	-0.63794900	2.54658100
H	-1.61997200	0.48944800	2.54455300
H	-3.28756800	1.10567100	2.48634900
C	-0.45672000	0.86132300	-2.48340900
H	-0.70514200	0.62061900	-3.52668500
H	-0.20593200	1.93394700	-2.45383100
H	0.45525600	0.31727400	-2.21427700
C	-5.38684800	0.15527700	-2.01461400
H	-5.47322800	0.79064500	-2.90849300
H	-5.57516300	-0.88279800	-2.33545500
H	-6.19196800	0.43255700	-1.31890200
C	0.51444200	3.01673200	0.66372300
C	1.18808500	3.37129800	1.99760000
H	2.28496000	3.36990100	1.92621600
H	0.87501600	4.37564400	2.31678900
H	0.89518900	2.65617100	2.77933800
C	0.92906300	4.00829700	-0.43254100

H	2.01623600	4.11374100	-0.54440300
H	0.50943600	3.71333200	-1.40408100
H	0.53491800	5.00303500	-0.18273700
H	2.81435700	2.42215400	0.03223900
C	-0.99344200	3.14873500	0.85428800
H	-1.55204400	2.96167200	-0.06854800
H	-1.36895500	2.47495600	1.62945600
H	-1.19718500	4.17960600	1.17745200

TS3Bu; E = -1204.749673:

C	2.36537700	1.25180600	0.57970700
C	3.02175200	0.16000500	-0.12042700
C	2.30772300	-1.03045300	-0.35585200
C	2.98326100	-2.10321600	-0.95684400
C	4.31968200	-2.00603300	-1.31702200
C	5.02355700	-0.82232700	-1.07843600
C	4.37962600	0.24288000	-0.47407200
H	2.46886100	-3.05230900	-1.10003900
H	4.82527000	-2.86589800	-1.76161400
H	6.07627100	-0.74067100	-1.35758400
H	4.92338400	1.16981700	-0.27389300
B	0.14300400	0.40531500	0.14673000
N	1.01607900	1.51591200	0.31751500
C	-1.39292900	0.46165000	-0.26256000
C	-1.69612000	0.39191500	-1.64296500
C	-2.47417700	0.52588300	0.63960800
C	-3.01650400	0.27678800	-2.07564300
C	-3.78684200	0.40281900	0.17234700
C	-4.08346300	0.24920500	-1.17836200
H	-3.21959700	0.22027500	-3.14958800
H	-4.60795700	0.44962700	0.89474600
C	0.89006600	-1.12780400	0.15267300
C	0.76014600	-1.02969800	1.64496000
C	-0.00440500	-2.16262600	-0.47465200
C	-0.41423100	-1.56996000	2.27531700
C	-1.01113900	-2.71106900	0.23879400
C	-1.26949900	-2.39796000	1.62560300
H	-0.54178200	-1.38216300	3.34458600
H	-1.68766500	-3.41261400	-0.25831600
C	1.83841300	-0.54117400	2.43093800
H	2.81678700	-0.99857300	2.22503800
H	2.20686900	0.57030900	1.86598000
H	1.62947500	-0.43809600	3.50212300
C	0.13407400	-2.54212500	-1.93037700
H	0.54911700	-3.55600800	-2.04527700
H	-0.85267400	-2.54060100	-2.41495400
H	0.78832700	-1.86384700	-2.48728500
C	-2.46392900	-3.00971200	2.29449500
H	-3.39590000	-2.63201400	1.84054700
H	-2.47306600	-4.10521400	2.17582200
H	-2.49141000	-2.78120300	3.36911700
C	-2.30688000	0.82991800	2.11007600
H	-2.74796800	0.04465100	2.74033100
H	-1.25589400	0.94463000	2.39747900
H	-2.82902200	1.76891200	2.35803600
C	-0.62467300	0.55588800	-2.69530000
H	-0.83408100	-0.04948200	-3.58861200
H	-0.57918900	1.60833600	-3.02362000
H	0.37754500	0.29963800	-2.33181100
C	-5.49941100	0.06920900	-1.65617400
H	-6.22324900	0.48253300	-0.93920800
H	-5.66306100	0.55798400	-2.62788300
H	-5.74034200	-0.99890500	-1.78607800
C	0.69158400	2.98999100	0.33139200
C	1.01413900	3.55825400	1.72237800
H	2.07548100	3.46852900	1.98748200
H	0.75417300	4.62614500	1.75707700
H	0.42541900	3.03878200	2.49268600
C	1.52750800	3.69154800	-0.75157800
H	2.60832200	3.60729800	-0.58348800
H	1.30499700	3.26439400	-1.74023500
H	1.27821400	4.76206000	-0.77684500
H	2.98944400	2.12952300	0.73837000
C	-0.77245100	3.31273500	0.03689100
H	-1.09268500	2.95543000	-0.94753400
H	-1.45251500	2.90580100	0.78981800
H	-0.87901100	4.40693400	0.04886700

Int2Bu; E = -1204.80594809:

C	-2.44709800	1.50746300	0.44049100
C	-3.07747100	0.25366900	-0.09219000
C	-2.35451600	-0.92195500	-0.25937200
C	-3.04414300	-2.08731300	-0.62653300
C	-4.41349300	-2.07898300	-0.84351000
C	-5.12912600	-0.88869500	-0.70510700
C	-4.45938300	0.26494200	-0.33017600
H	-2.48447100	-3.01584100	-0.74823000
H	-4.92665800	-3.00055200	-1.12692500
H	-6.20565800	-0.86481200	-0.88739400
H	-5.01387400	1.19988900	-0.20953300
B	-0.17365000	0.54548400	0.06697000
N	-1.00133900	1.67088000	0.25876200
C	1.41276500	0.57603200	-0.10279100
C	2.27470000	0.37790300	0.99474500
C	1.99390000	0.71263100	-1.38117200
C	3.64984100	0.24255900	0.79376300
C	3.37242100	0.57115300	-1.54714300
C	4.22201400	0.31234300	-0.47382700
H	4.29740500	0.09093400	1.66331900
H	3.79709000	0.67825000	-2.55030500
C	-0.85175500	-0.96273200	0.00158900
C	-0.14938700	-1.73805200	-1.12744400
C	-0.61736700	-1.60877700	1.37106800
C	0.95308000	-2.63287200	-0.78089000
C	0.34362900	-2.52734200	1.55579400
C	1.20497500	-3.01970700	0.48108900
H	1.55404600	-3.02406300	-1.60600000
H	0.49771200	-2.93991100	2.55766100
C	-0.51068900	-1.60899400	-2.41421500
H	-1.35049400	-0.98692200	-2.72705900
H	-2.96869000	2.35576200	-0.02077700
H	0.03676800	-2.13728800	-3.19842400
C	-1.48839200	-1.17063100	2.51504400
H	-2.53497300	-1.47585400	2.36219700
H	-1.13977000	-1.60625900	3.46125100
H	-1.49524700	-0.07483900	2.62915500
C	2.31816500	-3.95582800	0.84427300
H	3.03423000	-3.46511600	1.52428100
H	1.93368600	-4.84314100	1.37392100
H	2.86966000	-4.29540900	-0.04299500
C	1.18486100	1.09784000	-2.59695900
H	1.37547800	0.41840800	-3.43984100
H	0.10582400	1.09219100	-2.40623400
H	1.45900000	2.11336400	-2.92957500

C	1.78706800	0.38999400	2.42498100
H	2.03778600	-0.54373600	2.94854700
H	2.26589900	1.21251600	2.98139000
H	0.70304300	0.53042600	2.50219300
C	5.70049100	0.11431100	-0.67653500
H	6.27554600	0.43595500	0.20395800
H	5.93685700	-0.94867400	-0.84972600
H	6.06752100	0.67513300	-1.54834000
C	-0.62173700	3.12784400	0.32645700
C	-1.06988200	3.82722100	-0.96733500
H	-2.15092000	3.74351200	-1.14589600
H	-0.82976500	4.89954100	-0.91763700
H	-0.54707600	3.40116900	-1.83436500
C	-1.30027400	3.79068400	1.54103900
H	-2.39278000	3.84498300	1.45834600
H	-1.04882100	3.25375600	2.46822800
H	-0.93392500	4.82157100	1.64129800
H	-2.68880200	1.56789300	1.51658200
C	0.87846900	3.37875700	0.49056400
H	1.27902900	2.89586100	1.38934700
H	1.46542800	3.04403000	-0.36874500
H	1.02755300	4.46291500	0.59595500

TS4Bu; E = -1204.768338:

C	-2.00258500	1.26153400	1.08974400
C	-2.97094200	0.21685900	0.60855500
C	-2.42676900	-0.93812600	0.05181600
C	-3.28053500	-1.93605900	-0.42732300
C	-4.66181400	-1.79203800	-0.34192100
C	-5.20245800	-0.64045100	0.22605000
C	-4.35637100	0.35951500	0.69566200
H	-2.85154200	-2.83792300	-0.87202600
H	-5.31756700	-2.57877900	-0.72127700
H	-6.28564500	-0.51757900	0.29452400
H	-4.77663800	1.26987600	1.13169300
B	-0.05332600	0.44236700	-0.32021100
N	-0.93820300	1.53670700	0.13927900
C	1.54831000	0.47699300	-0.03471000
C	1.95844500	0.52164600	1.32606900
C	2.59318400	0.51181800	-0.99748000
C	3.30844800	0.51069600	1.68296000
C	3.93517300	0.50912100	-0.59638500
C	4.32524000	0.48678200	0.73618800
H	3.56983500	0.53402300	2.74500500
H	4.70809900	0.53684600	-1.36960600
C	-0.92829200	-1.14717100	-0.01921300
C	-0.36970000	-1.18081200	-1.37328600
C	-0.41144000	-2.12909800	0.94256900
C	0.67746400	-2.11569100	-1.66851000
C	0.65290700	-2.90991500	0.62017900
C	1.19630500	-2.93225500	-0.70908400
H	1.04949900	-2.16888600	-2.69239000
H	1.05486500	-3.60935500	1.35751800
C	-0.65311800	-0.06408000	-2.15761800
H	-1.63094200	0.40675400	-2.09013000
H	-2.55513300	2.17845600	1.32116800
H	-0.12477000	0.06277200	-3.10037000
C	-1.12610700	-2.32471000	2.25089800
H	-0.48241900	-2.83802600	2.97812400
H	-1.47030000	-1.37812400	2.68911200
H	-2.02845500	-2.93806700	2.10181100
C	2.31693800	-3.88288700	-1.00759500
H	3.22100800	-3.58183600	-0.45452100
H	2.06589900	-4.90453400	-0.68269500
H	2.56249800	-3.90477700	-2.07762300
C	2.38863300	0.59555100	-2.49320800
H	3.33945100	0.83852500	-2.98651100
H	2.04060500	-0.35222800	-2.92290500
H	1.66585500	1.36806400	-2.77443800
C	0.97950000	0.63639200	2.46644500
H	1.49321500	0.53502100	3.43192400
H	0.47479400	1.61236400	2.45260800
H	0.19776600	-0.12735900	2.42704300
C	5.77455500	0.44284900	1.13881600
H	5.96908400	1.08072300	2.01389800
H	6.08089700	-0.58078700	1.41108600
H	6.43062500	0.77525700	0.32167900
C	-0.90951800	2.93359700	-0.36356800
C	-2.24961600	3.30733200	-1.02643900
H	-3.09680700	3.25860200	-0.32829800
H	-2.20996600	4.33479900	-1.41874300
H	-2.46843600	2.63188800	-1.86639500
C	-0.61697900	3.90440200	0.79508900
H	-1.35894600	3.82851100	1.60275500
H	0.37505200	3.69695300	1.22203100
H	-0.62552100	4.94640900	0.44048400
H	-1.58928500	0.92511700	2.05779900
C	0.18424300	3.13747200	-1.41069900
H	1.17679300	2.89386700	-1.01369500
H	0.00105900	2.52759000	-2.30350400
H	0.19091900	4.19146900	-1.72304100

FinalBu; E = -1204.84738287:

C	1.44561700	-2.07441500	-0.56426600
C	2.72481700	-1.24701900	-0.52139100
C	2.87279200	0.15654700	-0.47408800
C	4.16173100	0.67665600	-0.71363300
C	5.27865200	-0.11401200	-0.92519500
C	5.13833200	-1.49685500	-0.90074800
C	3.87595500	-2.03268000	-0.70840100
H	4.27449000	1.76054600	-0.74580800
H	6.25065600	0.34898300	-1.10747600
H	5.99910600	-2.15309300	-1.04523000
H	3.76114200	-3.12002800	-0.71961800
B	-0.58607000	-0.71100900	-0.54199400
N	0.21811300	-1.66699400	0.11966100
C	-2.12162400	-0.38068700	-0.28957700
C	-2.63579400	0.57986500	0.59704700
C	-3.03044800	-1.05883000	-1.13991500
C	-4.01274400	0.84010300	0.62249000
C	-4.39253300	-0.78054300	-1.08227100
C	-4.90962700	0.17567100	-0.20382900
H	-4.39172700	1.59071800	1.32311700
H	-5.07407700	-1.32219300	-1.74530100
C	1.83592800	1.21974800	-0.22501800
C	0.65666600	1.32910500	-0.99886700
C	2.12179900	2.24241000	0.70540000
C	-0.08389000	2.50947000	-0.96429000
C	1.32742600	3.39415800	0.73391700
C	0.25349600	3.57420400	-0.12956100
H	-0.97646000	2.58143800	-1.59123200
H	1.56860300	4.17730200	1.45834600
C	0.09467100	0.14063600	-1.73498500
H	0.87815100	-0.38265000	-2.29717700

H	1.21849000	-2.22501300	-1.63007500
H	-0.66530300	0.47848800	-2.45183600
C	3.23972700	2.14909100	1.72000400
H	4.15169600	2.66973100	1.38935800
H	2.92492700	2.62259800	2.66138300
H	3.52073100	1.11106600	1.93650200
C	-0.54812100	4.84739600	-0.14029100
H	-1.62934500	4.64198800	-0.11697000
H	-0.30292200	5.48708600	0.71910600
H	-0.35200600	5.42937200	-1.05528000
C	-2.53486200	-2.09699900	-2.11870500
H	-1.80401300	-1.67374400	-2.82605000
H	-2.03198800	-2.93213200	-1.60736900
H	-3.36115800	-2.51629600	-2.70883100
C	-1.77713800	1.33941500	1.57972700
H	-1.91482100	2.42436700	1.46690800
H	-2.06277900	1.08876900	2.61422200
H	-0.70661200	1.13298500	1.46288200
C	-6.38567600	0.47040500	-0.17051300
H	-6.63555800	1.18881000	0.62264800
H	-6.72931900	0.89475000	-1.12744900
H	-6.97325400	-0.44426800	0.00449200
C	-0.06290900	-2.48511800	1.34101700
C	-0.34390800	-3.94758600	0.95363100
H	0.49480800	-4.42711900	0.43039200
H	-0.54425500	-4.54294500	1.85642600
H	-1.23081100	-4.00913200	0.30628300
C	1.15021000	-2.40823200	2.28345300
H	2.06653100	-2.82229300	1.84222900
H	1.35237400	-1.36269600	2.55888100
H	0.94447700	-2.97286300	3.20435800
H	1.72047800	-3.07221600	-0.21252400
C	-1.27358100	-1.98878400	2.12889800
H	-1.14954900	-0.94747900	2.44359500
H	-2.20747700	-2.07475100	1.56332000
H	-1.36944900	-2.60279700	3.03587900

S7. X-Ray Crystal Structure Data of 2, 6, 4c and 6b

The crystal data of **2**, **6**, **4c**, and **6b** were collected on a Bruker D8-Venture diffractometer with Mo-target (λ = 0.71073 Å) at 180 K. Data were processed on a PC with the aid of the Bruker SHELXTL software package22 and corrected for absorption effects. The crystals of **2**, **6**, and **4c** belong to the monoclinic space group P21/c while that of **6b** belongs to the orthorhombic space group Pbca. ll non-hydrogen atoms were refined anisotropically. The positions of hydrogen atoms were calculated and their contributions in structural factors were included. The details of crystal data, collection parameters and results of analyses are provided in the supporting materials. The crystal data of **2**, **6**, **4c**, and **6b** were deposited to the Cambridge Crystallographic Data Center with deposition numbers of CCDC 1847798-1847801 for **2**, **6**, **4c**, and **6b**, respectively. This data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Crystal data of compound 2

Table S19. Crystal data and structure refinement for **2**.

Identification code	**2**	
Empirical formula	C28 H34 B N	
Formula weight	395.37	
Temperature	180(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 8.4716(3) Å	α= 90°.
	b = 27.7566(10) Å	β= 100.2570(10)°.
	c = 11.7695(4) Å	γ = 90°.
Volume	2723.29(17) $Å^3$	
Z	4	
Density (calculated)	0.964 Mg/m^3	
Absorption coefficient	0.054 mm^{-1}	
F(000)	856	
Crystal size	0.120 x 0.100 x 0.050 mm^3	
Theta range for data collection	2.443 to 27.359°.	
Index ranges	-10<=h<=10, -35<=k<=35, -15<=l<=15	
Reflections collected	40531	
Independent reflections	6147 [R(int) = 0.0765]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.745 and 0.685	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6147 / 0 / 279	
Goodness-of-fit on F^2	1.066	
Final R indices [I>2sigma(I)]	R1 = 0.0693, wR2 = 0.1702	
R indices (all data)	R1 = 0.1100, wR2 = 0.1921	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.230 and -0.227 $e.Å^{-3}$	

Table S20. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **2**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
B(1)	3657(3)	6587(1)	5777(2)	34(1)
N(1)	4396(2)	6807(1)	7066(1)	36(1)
C(1)	2510(2)	7048(1)	5362(2)	37(1)
C(2)	1555(2)	7179(1)	4319(2)	44(1)
C(3)	850(3)	7631(1)	4178(2)	52(1)
C(4)	1083(3)	7969(1)	5054(3)	60(1)
C(5)	2061(3)	7864(1)	6080(2)	54(1)
C(6)	2759(3)	7406(1)	6226(2)	42(1)
C(7)	3811(3)	7226(1)	7220(2)	42(1)
C(8)	5328(3)	6538(1)	8058(2)	44(1)
C(9)	6652(4)	6834(1)	8754(2)	85(1)
C(10)	4229(3)	6343(1)	8829(2)	74(1)
C(11)	3016(2)	6053(1)	6066(2)	34(1)
C(12)	1445(2)	5972(1)	6271(2)	39(1)
C(13)	910(3)	5514(1)	6465(2)	48(1)
C(14)	1892(3)	5111(1)	6499(2)	49(1)
C(15)	3458(3)	5190(1)	6370(2)	45(1)
C(16)	4035(2)	5645(1)	6149(2)	39(1)
C(17)	269(3)	6381(1)	6312(2)	56(1)
C(18)	1277(4)	4613(1)	6677(3)	73(1)
C(19)	5777(3)	5659(1)	6003(2)	48(1)
C(20)	4819(2)	6586(1)	4782(2)	33(1)
C(21)	4271(2)	6331(1)	3741(2)	39(1)
C(22)	5165(3)	6332(1)	2853(2)	45(1)
C(23)	6598(3)	6577(1)	2923(2)	42(1)
C(24)	7095(2)	6841(1)	3910(2)	40(1)
C(25)	6247(2)	6854(1)	4822(2)	35(1)
C(26)	2740(3)	6037(1)	3519(2)	51(1)
C(27)	7581(3)	6557(1)	1975(2)	60(1)
C(28)	6954(3)	7163(1)	5838(2)	45(1)

Table S21. Bond lengths [Å] and angles [°] for **2**.

B(1)-C(1)	1.629(3)	C(6)-C(7)	1.427(3)
B(1)-C(11)	1.636(3)	C(8)-C(9)	1.510(3)
B(1)-N(1)	1.651(3)	C(8)-C(10)	1.511(3)
B(1)-C(20)	1.658(3)	C(11)-C(12)	1.412(3)
N(1)-C(7)	1.291(2)	C(11)-C(16)	1.416(3)
N(1)-C(8)	1.488(3)	C(12)-C(13)	1.382(3)
C(1)-C(2)	1.393(3)	C(12)-C(17)	1.517(3)
C(1)-C(6)	1.409(3)	C(13)-C(14)	1.390(3)
C(2)-C(3)	1.386(3)	C(14)-C(15)	1.379(3)
C(3)-C(4)	1.382(4)	C(14)-C(18)	1.507(3)
C(4)-C(5)	1.369(4)	C(15)-C(16)	1.395(3)
C(5)-C(6)	1.401(3)	C(16)-C(19)	1.516(3)

C(20)-C(25)	1.414(3)	N(1)-C(8)-C(10)	110.64(19)
C(20)-C(21)	1.419(3)	C(9)-C(8)-C(10)	110.3(2)
C(21)-C(22)	1.396(3)	C(12)-C(11)-C(16)	116.30(17)
C(21)-C(26)	1.514(3)	C(12)-C(11)-B(1)	122.48(17)
C(22)-C(23)	1.381(3)	C(16)-C(11)-B(1)	121.21(17)
C(23)-C(24)	1.376(3)	C(13)-C(12)-C(11)	121.40(19)
C(23)-C(27)	1.507(3)	C(13)-C(12)-C(17)	116.47(19)
C(24)-C(25)	1.394(3)	C(11)-C(12)-C(17)	122.12(17)
C(25)-C(28)	1.506(3)	C(12)-C(13)-C(14)	122.1(2)
		C(15)-C(14)-C(13)	116.87(19)
C(1)-B(1)-C(11)	124.92(17)	C(15)-C(14)-C(18)	121.6(2)
C(1)-B(1)-N(1)	95.37(14)	C(13)-C(14)-C(18)	121.5(2)
C(11)-B(1)-N(1)	103.25(15)	C(14)-C(15)-C(16)	122.7(2)
C(1)-B(1)-C(20)	100.84(15)	C(15)-C(16)-C(11)	120.44(19)
C(11)-B(1)-C(20)	113.88(15)	C(15)-C(16)-C(19)	115.08(18)
N(1)-B(1)-C(20)	118.33(16)	C(11)-C(16)-C(19)	124.48(18)
C(7)-N(1)-C(8)	120.45(17)	C(25)-C(20)-C(21)	115.95(17)
C(7)-N(1)-B(1)	111.66(17)	C(25)-C(20)-B(1)	125.92(17)
C(8)-N(1)-B(1)	126.61(15)	C(21)-C(20)-B(1)	117.84(16)
C(2)-C(1)-C(6)	116.25(19)	C(22)-C(21)-C(20)	120.50(19)
C(2)-C(1)-B(1)	133.68(19)	C(22)-C(21)-C(26)	115.72(19)
C(6)-C(1)-B(1)	109.39(18)	C(20)-C(21)-C(26)	123.76(18)
C(3)-C(2)-C(1)	120.8(2)	C(23)-C(22)-C(21)	123.0(2)
C(4)-C(3)-C(2)	121.6(2)	C(24)-C(23)-C(22)	116.50(18)
C(5)-C(4)-C(3)	119.8(2)	C(24)-C(23)-C(27)	121.2(2)
C(4)-C(5)-C(6)	118.5(2)	C(22)-C(23)-C(27)	122.3(2)
C(5)-C(6)-C(1)	123.0(2)	C(23)-C(24)-C(25)	122.77(19)
C(5)-C(6)-C(7)	127.3(2)	C(24)-C(25)-C(20)	121.10(19)
C(1)-C(6)-C(7)	109.73(17)	C(24)-C(25)-C(28)	116.00(18)
N(1)-C(7)-C(6)	113.53(18)	C(20)-C(25)-C(28)	122.90(17)
N(1)-C(8)-C(9)	113.00(19)		

Table S22. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
B(1)	32(1)	34(1)	36(1)	-4(1)	7(1)	-2(1)
N(1)	39(1)	36(1)	36(1)	-3(1)	12(1)	-3(1)
C(1)	31(1)	38(1)	44(1)	4(1)	13(1)	-2(1)
C(2)	36(1)	47(1)	51(1)	7(1)	11(1)	-3(1)
C(3)	39(1)	54(1)	65(2)	24(1)	11(1)	2(1)
C(4)	53(2)	40(1)	90(2)	14(1)	22(1)	5(1)
C(5)	60(2)	38(1)	69(2)	-3(1)	23(1)	2(1)
C(6)	45(1)	34(1)	50(1)	1(1)	18(1)	1(1)
C(7)	50(1)	37(1)	44(1)	-9(1)	18(1)	-3(1)
C(8)	47(1)	48(1)	35(1)	-4(1)	5(1)	1(1)
C(9)	87(2)	113(2)	45(2)	16(2)	-15(1)	-45(2)
C(10)	67(2)	99(2)	58(2)	30(2)	11(1)	-10(2)
C(11)	34(1)	34(1)	35(1)	-4(1)	7(1)	-3(1)
C(12)	35(1)	38(1)	44(1)	4(1)	7(1)	-2(1)

C(13)	41(1)	48(1)	54(1)	7(1)	8(1)	-9(1)
C(14)	59(2)	37(1)	49(1)	4(1)	5(1)	-8(1)
C(15)	56(1)	34(1)	44(1)	-2(1)	7(1)	4(1)
C(16)	40(1)	39(1)	38(1)	-5(1)	7(1)	1(1)
C(17)	38(1)	52(1)	82(2)	15(1)	23(1)	3(1)
C(18)	84(2)	42(1)	93(2)	10(1)	18(2)	-16(1)
C(19)	44(1)	45(1)	56(1)	-4(1)	14(1)	10(1)
C(20)	32(1)	32(1)	34(1)	1(1)	4(1)	1(1)
C(21)	41(1)	40(1)	37(1)	-1(1)	6(1)	-3(1)
C(22)	57(1)	46(1)	33(1)	0(1)	8(1)	6(1)
C(23)	50(1)	42(1)	39(1)	10(1)	15(1)	9(1)
C(24)	37(1)	40(1)	45(1)	10(1)	12(1)	2(1)
C(25)	33(1)	33(1)	38(1)	5(1)	7(1)	3(1)
C(26)	54(1)	55(1)	41(1)	-9(1)	1(1)	-14(1)
C(27)	78(2)	61(2)	49(1)	12(1)	32(1)	11(1)
C(28)	38(1)	48(1)	48(1)	-7(1)	10(1)	-10(1)

Table S23. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **2**.

	x	y	z	U(eq)
H(2)	1384	6956	3697	53
H(3)	191	7710	3462	63
H(4)	565	8273	4944	72
H(5)	2263	8097	6679	65
H(7)	4056	7399	7926	51
H(8)	5839	6256	7737	52
H(9A)	7234	7006	8230	128
H(9B)	7393	6621	9256	128
H(9C)	6187	7067	9227	128
H(10A)	3379	6151	8368	112
H(10B)	3749	6612	9187	112
H(10C)	4846	6141	9432	112
H(13)	-164	5473	6579	57
H(15)	4173	4924	6434	54
H(17A)	-51	6517	5537	84
H(17B)	779	6632	6840	84
H(17C)	-681	6258	6587	84
H(18A)	103	4611	6483	109
H(18B)	1614	4518	7487	109
H(18C)	1715	4384	6179	109
H(19A)	5842	5612	5187	71
H(19B)	6372	5402	6464	71
H(19C)	6244	5972	6261	71
H(22)	4769	6156	2169	54
H(24)	8055	7024	3973	48
H(26A)	2327	6026	2687	76
H(26B)	1940	6187	3913	76
H(26C)	2963	5709	3812	76
H(27A)	7066	6340	1363	90
H(27B)	8659	6438	2290	90

H(27C)	7659	6881	1657	90
H(28A)	7934	7317	5684	67
H(28B)	7211	6962	6531	67
H(28C)	6176	7410	5960	67

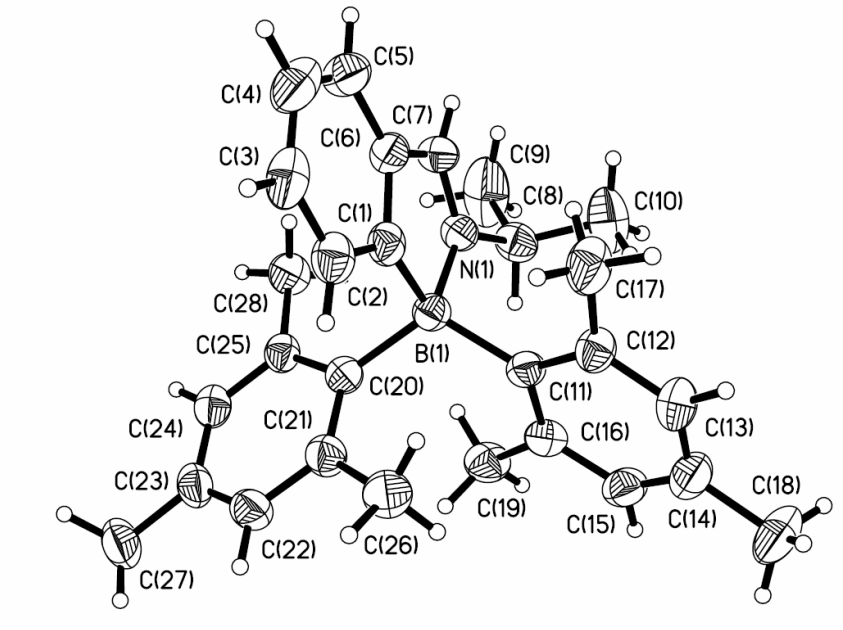


Figure S87. The crystal structure of **2** with labeling schemes.

Crystal data of compound 6

Table S24. Crystal data and structure refinement for **6**.

Identification code	**6**	
Empirical formula	C22 H22 B N	
Formula weight	311.21	
Temperature	180(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 14.0764(16) Å	α= 90°.
	b = 13.7022(14) Å	β= 110.47°.
	c = 9.8458(11) Å	γ = 90°.
Volume	1779.1(3) $Å^3$	
Z	4	
Density (calculated)	1.162 Mg/m^3	
Absorption coefficient	0.066 mm^{-1}	
F(000)	664	
Crystal size	0.100 x 0.100 x 0.100 mm^3	
Theta range for data collection	2.973 to 27.200°.	
Index ranges	-15<=h<=18, -17<=k<=17, -12<=l<=12	
Reflections collected	16761	
Independent reflections	3451 [R(int) = 0.1723]	
Completeness to theta = 25.242°	84.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.780 and 0.670	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3451 / 0 / 219	
Goodness-of-fit on F^2	1.004	
Final R indices [I>2sigma(I)]	R1 = 0.0984, wR2 = 0.1815	
R indices (all data)	R1 = 0.2138, wR2 = 0.2329	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.171 and -0.184 $e.Å^{-3}$	

Table S25. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **6**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
B(1)	2614(3)	4233(3)	6404(4)	38(1)
N(1)	1909(2)	3433(2)	6825(3)	37(1)
C(1)	3543(2)	3504(3)	6551(4)	40(1)
C(2)	4444(3)	3597(3)	6291(4)	48(1)
C(3)	5094(3)	2813(3)	6459(5)	59(1)
C(4)	4866(3)	1914(3)	6902(5)	63(1)
C(5)	3969(3)	1774(3)	7143(4)	54(1)
C(6)	3325(2)	2573(3)	6957(4)	42(1)
C(7)	2357(2)	2598(3)	7143(4)	41(1)
C(8)	962(2)	3660(3)	7100(4)	42(1)
C(9)	91(3)	2990(3)	6279(4)	51(1)
C(10)	1181(3)	3627(3)	8728(4)	52(1)
C(11)	2815(2)	5088(2)	7592(4)	38(1)
C(12)	3516(3)	4988(3)	8988(4)	43(1)
C(13)	3652(3)	5695(3)	10055(4)	52(1)
C(14)	3077(3)	6527(3)	9730(4)	53(1)
C(16)	2248(3)	5943(3)	7307(4)	46(1)
C(15)	2376(3)	6656(3)	8371(4)	54(1)
C(17)	2101(3)	4617(2)	4751(4)	40(1)
C(18)	2675(3)	5259(3)	4240(4)	52(1)
C(19)	2346(3)	5588(3)	2815(4)	56(1)
C(20)	1426(4)	5294(3)	1863(4)	55(1)
C(21)	832(3)	4681(3)	2325(4)	52(1)
C(22)	1169(3)	4351(2)	3752(4)	42(1)

Table S26. Bond lengths [Å] and angles [°] for **6**.

B(1)-C(11)	1.609(5)	C(13)-C(14)	1.370(5)
B(1)-C(1)	1.612(5)	C(14)-C(15)	1.368(5)
B(1)-C(17)	1.620(5)	C(16)-C(15)	1.398(5)
B(1)-N(1)	1.626(5)	C(17)-C(22)	1.385(5)
N(1)-C(7)	1.291(4)	C(17)-C(18)	1.401(5)
N(1)-C(8)	1.484(4)	C(18)-C(19)	1.390(5)
C(1)-C(2)	1.385(5)	C(19)-C(20)	1.368(6)
C(1)-C(6)	1.403(5)	C(20)-C(21)	1.370(6)
C(2)-C(3)	1.383(5)	C(21)-C(22)	1.392(5)
C(3)-C(4)	1.382(6)		
C(4)-C(5)	1.377(6)	C(11)-B(1)-C(1)	117.1(3)
C(5)-C(6)	1.392(5)	C(11)-B(1)-C(17)	113.4(3)
C(6)-C(7)	1.437(5)	C(1)-B(1)-C(17)	110.7(3)
C(8)-C(9)	1.518(5)	C(11)-B(1)-N(1)	105.9(3)
C(8)-C(10)	1.524(5)	C(1)-B(1)-N(1)	96.1(3)
C(11)-C(16)	1.388(5)	C(17)-B(1)-N(1)	112.2(3)
C(11)-C(12)	1.391(5)	C(7)-N(1)-C(8)	122.3(3)
C(12)-C(13)	1.392(5)	C(7)-N(1)-B(1)	111.7(3)

C(8)-N(1)-B(1)	124.9(3)	C(16)-C(11)-B(1)	121.6(3)
C(2)-C(1)-C(6)	116.2(3)	C(12)-C(11)-B(1)	122.0(3)
C(2)-C(1)-B(1)	133.9(3)	C(11)-C(12)-C(13)	122.7(4)
C(6)-C(1)-B(1)	109.8(3)	C(14)-C(13)-C(12)	119.3(4)
C(3)-C(2)-C(1)	121.1(4)	C(15)-C(14)-C(13)	120.1(4)
C(4)-C(3)-C(2)	120.9(4)	C(11)-C(16)-C(15)	121.6(3)
C(5)-C(4)-C(3)	120.4(4)	C(14)-C(15)-C(16)	120.2(4)
C(4)-C(5)-C(6)	117.5(4)	C(22)-C(17)-C(18)	115.6(3)
C(5)-C(6)-C(1)	123.8(3)	C(22)-C(17)-B(1)	127.4(3)
C(5)-C(6)-C(7)	127.2(4)	C(18)-C(17)-B(1)	117.0(3)
C(1)-C(6)-C(7)	109.0(3)	C(19)-C(18)-C(17)	122.4(4)
N(1)-C(7)-C(6)	113.2(3)	C(20)-C(19)-C(18)	119.8(4)
N(1)-C(8)-C(9)	112.7(3)	C(19)-C(20)-C(21)	119.7(4)
N(1)-C(8)-C(10)	108.7(3)	C(20)-C(21)-C(22)	120.1(4)
C(9)-C(8)-C(10)	111.8(3)	C(17)-C(22)-C(21)	122.4(4)
C(16)-C(11)-C(12)	116.2(3)		

Table S27. Anisotropic displacement parameters ($Å^2$x 10^3) for **6**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
B(1)	40(2)	38(2)	40(2)	-2(2)	19(2)	-6(2)
N(1)	38(2)	37(2)	38(2)	0(1)	17(1)	-1(1)
C(1)	38(2)	48(2)	35(2)	-8(2)	15(2)	1(2)
C(2)	44(2)	53(2)	54(2)	-9(2)	23(2)	-3(2)
C(3)	42(2)	74(3)	64(3)	-19(2)	21(2)	3(2)
C(4)	52(2)	67(3)	65(3)	-19(2)	14(2)	20(2)
C(5)	51(2)	48(2)	60(3)	-5(2)	17(2)	11(2)
C(6)	43(2)	41(2)	40(2)	-4(2)	12(2)	2(2)
C(7)	44(2)	37(2)	43(2)	1(2)	16(2)	5(2)
C(8)	36(2)	44(2)	51(2)	1(2)	21(2)	4(2)
C(9)	42(2)	53(2)	62(3)	5(2)	24(2)	-3(2)
C(10)	54(2)	59(3)	51(2)	5(2)	29(2)	5(2)
C(11)	42(2)	35(2)	40(2)	-1(2)	19(2)	-3(2)
C(12)	46(2)	42(2)	44(2)	1(2)	20(2)	-5(2)
C(13)	56(2)	61(3)	40(2)	-10(2)	19(2)	-14(2)
C(14)	68(3)	47(2)	56(3)	-15(2)	36(2)	-15(2)
C(16)	49(2)	45(2)	45(2)	2(2)	18(2)	0(2)
C(15)	66(3)	40(2)	67(3)	-5(2)	36(2)	1(2)
C(17)	46(2)	39(2)	38(2)	-3(2)	20(2)	4(2)
C(18)	57(2)	56(3)	47(2)	3(2)	25(2)	-3(2)
C(19)	67(3)	58(3)	54(3)	7(2)	35(2)	5(2)
C(20)	86(3)	42(2)	41(2)	6(2)	29(2)	14(2)
C(21)	62(2)	41(2)	44(2)	-3(2)	5(2)	11(2)
C(22)	46(2)	36(2)	40(2)	-3(2)	12(2)	6(2)

Table S28. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **6**.

	x	y	z	U(eq)

H(2)	4619	4210	5994	58
H(3)	5706	2893	6267	71
H(4)	5332	1389	7042	75
H(5)	3797	1155	7425	64
H(7)	2075	2055	7468	50
H(8)	759	4342	6763	50
H(9A)	-10	3010	5243	77
H(9B)	-529	3206	6426	77
H(9C)	251	2320	6638	77
H(10A)	566	3796	8925	78
H(10B)	1719	4095	9215	78
H(10C)	1401	2968	9091	78
H(12)	3920	4414	9222	52
H(13)	4137	5601	10998	62
H(14)	3165	7015	10449	63
H(16)	1762	6045	6366	55
H(15)	1975	7232	8151	65
H(18)	3312	5477	4891	62
H(19)	2760	6016	2502	67
H(20)	1199	5514	887	66
H(21)	188	4481	1670	63
H(22)	746	3927	4051	50

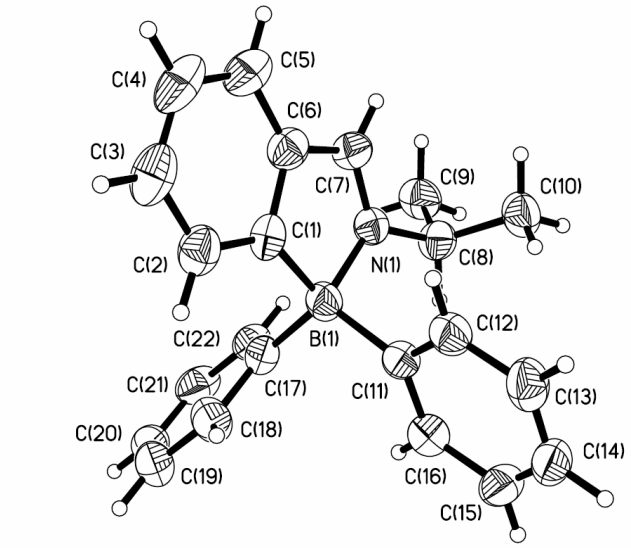


Figure S88. The crystal structure of **6** with labeling schemes.

Crystal data of compound 4c

Table S29. Crystal data and structure refinement for **4c**.

Identification code	**4c**	
Empirical formula	C34 H41 B N	
Formula weight	474.49	
Temperature	180(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 7.9902(4) Å	α= 90°.
	b = 21.3281(10) Å	β= 102.778(2)°.
	c = 17.0355(7) Å	γ = 90°.
Volume	2831.2(2) $Å^3$	
Z	4	
Density (calculated)	1.113 Mg/m^3	
Absorption coefficient	0.063 mm^{-1}	
F(000)	1028	
Crystal size	0.180 x 0.150 x 0.120 mm^3	
Theta range for data collection	2.269 to 27.136°.	
Index ranges	-10<=h<=10, -27<=k<=27, -21<=l<=21	
Reflections collected	96859	
Independent reflections	6245 [R(int) = 0.1388]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.766 and 0.658	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6245 / 0 / 331	
Goodness-of-fit on F^2	1.169	
Final R indices [I>2sigma(I)]	R1 = 0.0576, wR2 = 0.1392	
R indices (all data)	R1 = 0.1423, wR2 = 0.2048	
Extinction coefficient	0.0058(13)	
Largest diff. peak and hole	0.218 and -0.213 e.$Å^{-3}$	

Table S30. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **4c**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
B(1)	4444(4)	6199(1)	7074(2)	37(1)
C(1)	4755(3)	6939(1)	7125(2)	42(1)
N(1)	5313(3)	5766(1)	7631(1)	37(1)
C(2)	6549(3)	7204(1)	7401(2)	42(1)
C(3)	7458(3)	7395(1)	6838(2)	47(1)
C(4)	9090(4)	7648(1)	7066(2)	54(1)
C(5)	9814(4)	7704(1)	7877(2)	53(1)
C(6)	8956(4)	7519(1)	8461(2)	48(1)
C(7)	7305(3)	7271(1)	8218(2)	42(1)
C(8)	9836(4)	7567(1)	9341(2)	59(1)
C(9)	10043(5)	7847(2)	6437(2)	80(1)
C(10)	6316(3)	7059(1)	8812(2)	44(1)
C(11)	5957(3)	6421(1)	8876(2)	43(1)
C(12)	4978(4)	6234(2)	9415(2)	54(1)
C(13)	4325(4)	6672(2)	9867(2)	64(1)
C(14)	4636(4)	7302(2)	9788(2)	63(1)
C(15)	5633(4)	7492(1)	9272(2)	54(1)
C(16)	6619(3)	5943(1)	8363(1)	41(1)
C(17)	2973(3)	5996(1)	6329(1)	34(1)
C(18)	3340(3)	5908(1)	5566(1)	37(1)
C(19)	2004(3)	5816(1)	4892(2)	42(1)
C(20)	305(3)	5810(1)	4948(2)	45(1)
C(21)	-44(3)	5885(1)	5700(2)	44(1)
C(22)	1244(3)	5973(1)	6388(2)	39(1)
C(23)	765(4)	6034(1)	7193(2)	54(1)
C(24)	5165(3)	5908(1)	5471(2)	49(1)
C(25)	-1118(4)	5734(1)	4206(2)	59(1)
C(26)	5067(3)	5081(1)	7513(2)	39(1)
C(27)	6685(3)	4758(1)	7385(2)	45(1)
C(28)	6355(4)	4064(1)	7198(2)	56(1)
C(29)	5661(4)	3746(1)	7856(2)	58(1)
C(30)	4057(4)	4064(1)	7988(2)	52(1)
C(31)	4376(3)	4760(1)	8172(2)	45(1)
C(32)	136(5)	5637(2)	67(2)	72(1)
C(33)	-717(4)	5310(2)	546(2)	72(1)
C(34)	846(4)	5330(2)	-479(2)	70(1)

Table S31. Bond lengths [Å] and angles [°] for **4c**.

B(1)-N(1)	1.394(3)	C(2)-C(3)	1.386(4)
B(1)-C(17)	1.588(4)	C(2)-C(7)	1.398(3)
B(1)-C(1)	1.598(4)	C(3)-C(4)	1.385(4)
C(1)-C(2)	1.515(3)	C(4)-C(5)	1.380(4)
N(1)-C(26)	1.481(3)	C(4)-C(9)	1.506(4)
N(1)-C(16)	1.487(3)	C(5)-C(6)	1.384(4)

C(6)-C(7)	1.396(4)
C(6)-C(8)	1.512(4)
C(7)-C(10)	1.485(4)
C(10)-C(11)	1.399(4)
C(10)-C(15)	1.399(4)
C(11)-C(12)	1.391(4)
C(11)-C(16)	1.513(4)
C(12)-C(13)	1.384(4)
C(13)-C(14)	1.380(5)
C(14)-C(15)	1.371(4)
C(17)-C(18)	1.407(3)
C(17)-C(22)	1.408(3)
C(18)-C(19)	1.398(3)
C(18)-C(24)	1.503(4)
C(19)-C(20)	1.382(4)
C(20)-C(21)	1.379(4)
C(20)-C(25)	1.510(3)
C(21)-C(22)	1.392(3)
C(22)-C(23)	1.508(4)
C(26)-C(31)	1.520(3)
C(26)-C(27)	1.523(4)
C(27)-C(28)	1.526(4)
C(28)-C(29)	1.514(4)
C(29)-C(30)	1.511(4)
C(30)-C(31)	1.526(4)
C(32)-C(34)	1.360(5)
C(32)-C(33)	1.364(5)
C(33)-C(34)#1	1.372(5)
C(34)-C(33)#1	1.372(5)

N(1)-B(1)-C(17)	122.1(2)
N(1)-B(1)-C(1)	124.7(2)
C(17)-B(1)-C(1)	113.1(2)
C(2)-C(1)-B(1)	120.6(2)
B(1)-N(1)-C(26)	122.0(2)
B(1)-N(1)-C(16)	123.6(2)
C(26)-N(1)-C(16)	114.28(18)
C(3)-C(2)-C(7)	118.8(2)
C(3)-C(2)-C(1)	120.0(2)
C(7)-C(2)-C(1)	121.2(2)
C(4)-C(3)-C(2)	121.7(3)
C(5)-C(4)-C(3)	118.3(3)
C(5)-C(4)-C(9)	121.5(3)
C(3)-C(4)-C(9)	120.2(3)
C(4)-C(5)-C(6)	122.0(3)
C(5)-C(6)-C(7)	118.7(2)
C(5)-C(6)-C(8)	119.8(2)
C(7)-C(6)-C(8)	121.4(3)
C(6)-C(7)-C(2)	120.4(3)
C(6)-C(7)-C(10)	121.6(2)
C(2)-C(7)-C(10)	118.0(2)
C(11)-C(10)-C(15)	119.2(3)
C(11)-C(10)-C(7)	119.9(2)
C(15)-C(10)-C(7)	120.8(3)
C(12)-C(11)-C(10)	119.0(3)
C(12)-C(11)-C(16)	120.5(2)
C(10)-C(11)-C(16)	120.5(2)
C(13)-C(12)-C(11)	120.6(3)
C(14)-C(13)-C(12)	120.4(3)
C(15)-C(14)-C(13)	119.6(3)
C(14)-C(15)-C(10)	121.2(3)
N(1)-C(16)-C(11)	112.7(2)
C(18)-C(17)-C(22)	118.1(2)
C(18)-C(17)-B(1)	120.4(2)
C(22)-C(17)-B(1)	121.1(2)
C(19)-C(18)-C(17)	120.0(2)
C(19)-C(18)-C(24)	119.7(2)
C(17)-C(18)-C(24)	120.3(2)
C(20)-C(19)-C(18)	121.9(2)
C(21)-C(20)-C(19)	117.8(2)
C(21)-C(20)-C(25)	121.3(3)
C(19)-C(20)-C(25)	120.9(3)
C(20)-C(21)-C(22)	122.3(2)
C(21)-C(22)-C(17)	119.9(2)
C(21)-C(22)-C(23)	119.3(2)
C(17)-C(22)-C(23)	120.9(2)
N(1)-C(26)-C(31)	113.8(2)
N(1)-C(26)-C(27)	112.0(2)
C(31)-C(26)-C(27)	111.1(2)
C(26)-C(27)-C(28)	110.9(2)
C(29)-C(28)-C(27)	110.8(2)
C(30)-C(29)-C(28)	111.8(2)
C(29)-C(30)-C(31)	111.0(2)
C(26)-C(31)-C(30)	111.1(2)
C(34)-C(32)-C(33)	120.2(3)
C(32)-C(33)-C(34)#1	119.7(3)
C(32)-C(34)-C(33)#1	120.1(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z

Table S32. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **4c**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
B(1)	37(2)	36(2)	39(2)	1(1)	10(1)	1(1)
C(1)	43(1)	35(1)	46(1)	1(1)	3(1)	-1(1)
N(1)	40(1)	30(1)	38(1)	0(1)	4(1)	-1(1)
C(2)	44(1)	28(1)	50(2)	-2(1)	4(1)	0(1)
C(3)	52(2)	40(2)	47(2)	3(1)	4(1)	-5(1)
C(4)	57(2)	44(2)	60(2)	3(1)	12(1)	-10(1)
C(5)	47(2)	45(2)	64(2)	-1(1)	4(1)	-10(1)
C(6)	52(2)	33(1)	55(2)	-2(1)	3(1)	-6(1)
C(7)	45(1)	32(1)	48(2)	-2(1)	4(1)	-2(1)
C(8)	56(2)	52(2)	60(2)	-5(1)	-5(1)	-11(1)
C(9)	76(2)	90(3)	75(2)	8(2)	21(2)	-28(2)
C(10)	43(2)	46(2)	41(1)	-6(1)	2(1)	-4(1)
C(11)	43(1)	46(2)	37(1)	-2(1)	1(1)	-3(1)
C(12)	55(2)	63(2)	43(2)	0(1)	7(1)	-11(1)
C(13)	56(2)	91(3)	44(2)	-12(2)	12(1)	-11(2)
C(14)	56(2)	78(2)	55(2)	-25(2)	10(2)	-2(2)
C(15)	54(2)	53(2)	53(2)	-14(1)	5(1)	-1(1)
C(16)	41(1)	39(1)	40(1)	1(1)	-1(1)	-3(1)
C(17)	35(1)	28(1)	38(1)	2(1)	5(1)	2(1)
C(18)	38(1)	32(1)	42(1)	4(1)	7(1)	1(1)
C(19)	50(2)	39(1)	36(1)	2(1)	6(1)	-1(1)
C(20)	41(2)	38(1)	49(2)	3(1)	-2(1)	-2(1)
C(21)	31(1)	42(2)	57(2)	3(1)	5(1)	-1(1)
C(22)	35(1)	35(1)	46(1)	0(1)	9(1)	1(1)
C(23)	47(2)	57(2)	60(2)	-2(1)	19(1)	1(1)
C(24)	41(2)	56(2)	49(2)	4(1)	12(1)	-1(1)
C(25)	53(2)	54(2)	58(2)	2(1)	-13(1)	-1(1)
C(26)	41(1)	31(1)	43(1)	1(1)	2(1)	-2(1)
C(27)	52(2)	36(1)	46(2)	3(1)	13(1)	2(1)
C(28)	75(2)	38(2)	56(2)	1(1)	17(2)	10(1)
C(29)	73(2)	34(2)	64(2)	7(1)	12(2)	3(1)
C(30)	55(2)	39(2)	60(2)	8(1)	7(1)	-7(1)
C(31)	46(2)	35(1)	55(2)	4(1)	12(1)	-1(1)

C(32)	76(2)	59(2)	81(2)	-4(2)	16(2)	-2(2)
C(33)	68(2)	80(3)	73(2)	-14(2)	25(2)	5(2)
C(34)	66(2)	83(3)	65(2)	6(2)	20(2)	-12(2)

Table S33. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **4c**.

	x	y	z	U(eq)
H(1A)	4273	7113	6584	50
H(1B)	4057	7110	7489	50
H(3)	6949	7351	6281	57
H(5)	10935	7875	8040	64
H(8A)	10886	7816	9397	88
H(8B)	10129	7145	9558	88
H(8C)	9065	7769	9638	88
H(9A)	10870	8176	6658	120
H(9B)	9225	8009	5965	120
H(9C)	10652	7486	6279	120
H(12)	4754	5801	9474	65
H(13)	3658	6538	10233	76
H(14)	4163	7603	10089	76
H(15)	5865	7926	9227	65
H(16A)	7639	6116	8198	50
H(16B)	6983	5562	8688	50
H(19)	2272	5757	4381	51
H(21)	-1205	5877	5749	53
H(23A)	-390	6212	7117	80
H(23B)	1588	6310	7543	80
H(23C)	786	5619	7443	80
H(24A)	5705	5507	5658	73
H(24B)	5797	6250	5791	73
H(24C)	5184	5968	4903	73
H(25A)	-1903	5402	4299	89
H(25B)	-627	5619	3747	89
H(25C)	-1749	6129	4091	89
H(26)	4179	5025	7003	47
H(27A)	7609	4803	7876	53
H(27B)	7072	4962	6934	53
H(28A)	5519	4018	6678	67

H(28B)	7438	3858	7150	67
H(29A)	5401	3302	7708	69
H(29B)	6549	3754	8363	69
H(30A)	3682	3860	8442	63
H(30B)	3127	4016	7501	63
H(31A)	3290	4963	8220	54
H(31B)	5211	4807	8692	54
H(32A)	234	6080	115	87
H(33A)	-1220	5525	925	108
H(34A)	1433	5559	-814	105

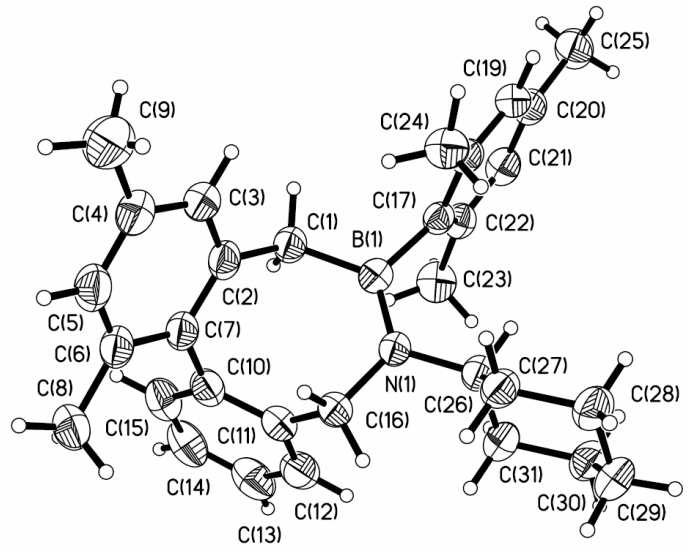


Figure S89. The crystal structure of **4c** with labeling schemes.

Crystal data of compound 6b

Table S34. Crystal data and structure refinement for **6b**.

Identification code	**6b**	
Empirical formula	C22 H22 B N	
Formula weight	311.21	
Temperature	180(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 19.0048(7) Å	α= 90°.
	b = 7.9860(3) Å	β= 90°.
	c = 23.0446(10) Å	γ = 90°.
Volume	3497.5(2) $Å^3$	
Z	8	
Density (calculated)	1.182 Mg/m^3	
Absorption coefficient	0.067 mm^{-1}	
F(000)	1328	
Crystal size	0.294 x 0.141 x 0.130 mm^3	
Theta range for data collection	2.904 to 27.138°.	
Index ranges	-24<=h<=22, -10<=k<=8, -29<=l<=29	
Reflections collected	27021	
Independent reflections	3865 [R(int) = 0.0999]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.780 and 0.658	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3865 / 0 / 219	
Goodness-of-fit on F^2	1.060	
Final R indices [I>2sigma(I)]	R1 = 0.0571, wR2 = 0.1110	
R indices (all data)	R1 = 0.1105, wR2 = 0.1348	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.181 and -0.205 $e.Å^{-3}$	

Table S35. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **6b**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	4500(1)	4889(2)	3558(1)	30(1)
C(1)	4222(1)	7693(2)	4068(1)	32(1)
C(2)	4341(1)	8452(3)	4608(1)	37(1)
C(3)	3902(1)	9650(3)	4837(1)	46(1)
C(4)	3325(1)	10172(3)	4526(1)	53(1)
C(5)	3199(1)	9517(3)	3982(1)	48(1)
C(6)	3634(1)	8275(3)	3746(1)	35(1)
C(7)	3489(1)	7704(3)	3143(1)	35(1)
C(8)	3324(1)	8884(3)	2715(1)	43(1)
C(9)	3201(1)	8413(3)	2147(1)	49(1)
C(10)	3223(1)	6734(3)	1997(1)	47(1)
C(11)	3376(1)	5553(3)	2416(1)	41(1)
C(12)	3521(1)	6011(3)	2987(1)	33(1)
C(13)	3743(1)	4731(3)	3431(1)	37(1)
C(14)	4958(1)	3525(2)	3342(1)	34(1)
C(15)	4861(1)	1922(3)	3690(1)	52(1)
C(16)	4867(1)	3195(3)	2697(1)	40(1)
C(17)	5548(1)	6384(2)	4050(1)	29(1)
C(18)	6010(1)	7543(2)	3806(1)	32(1)
C(19)	6715(1)	7603(3)	3964(1)	37(1)
C(20)	6975(1)	6518(3)	4375(1)	39(1)
C(21)	6533(1)	5376(3)	4629(1)	47(1)
C(22)	5833(1)	5313(3)	4466(1)	44(1)
B(1)	4745(1)	6275(3)	3867(1)	29(1)

Table S36. Bond lengths [Å] and angles [°] for **6b**.

N(1)-B(1)	1.396(3)	C(3)-C(4)	1.375(3)
N(1)-C(13)	1.474(2)	C(4)-C(5)	1.380(3)
N(1)-C(14)	1.481(2)	C(5)-C(6)	1.401(3)
C(1)-C(2)	1.402(3)	C(6)-C(7)	1.490(3)
C(1)-C(6)	1.418(3)	C(7)-C(8)	1.399(3)
C(1)-B(1)	1.577(3)	C(7)-C(12)	1.400(3)
C(2)-C(3)	1.375(3)	C(8)-C(9)	1.381(3)

C(9)-C(10)	1.385(3)	C(1)-C(6)-C(7)	122.26(17)
C(10)-C(11)	1.381(3)	C(8)-C(7)-C(12)	118.6(2)
C(11)-C(12)	1.391(3)	C(8)-C(7)-C(6)	119.55(19)
C(12)-C(13)	1.507(3)	C(12)-C(7)-C(6)	121.8(2)
C(14)-C(16)	1.519(3)	C(9)-C(8)-C(7)	121.5(2)
C(14)-C(15)	1.523(3)	C(8)-C(9)-C(10)	119.6(2)
C(17)-C(18)	1.393(3)	C(11)-C(10)-C(9)	119.6(2)
C(17)-C(22)	1.394(3)	C(10)-C(11)-C(12)	121.5(2)
C(17)-B(1)	1.585(3)	C(11)-C(12)-C(7)	119.2(2)
C(18)-C(19)	1.387(3)	C(11)-C(12)-C(13)	121.26(19)
C(19)-C(20)	1.376(3)	C(7)-C(12)-C(13)	119.51(19)
C(20)-C(21)	1.372(3)	N(1)-C(13)-C(12)	110.52(16)
C(21)-C(22)	1.384(3)	N(1)-C(14)-C(16)	112.92(16)
		N(1)-C(14)-C(15)	111.70(17)
B(1)-N(1)-C(13)	119.65(16)	C(16)-C(14)-C(15)	110.90(18)
B(1)-N(1)-C(14)	124.02(16)	C(18)-C(17)-C(22)	116.07(18)
C(13)-N(1)-C(14)	116.33(16)	C(18)-C(17)-B(1)	122.43(18)
C(2)-C(1)-C(6)	116.69(18)	C(22)-C(17)-B(1)	121.50(18)
C(2)-C(1)-B(1)	117.96(18)	C(19)-C(18)-C(17)	121.75(19)
C(6)-C(1)-B(1)	125.34(18)	C(20)-C(19)-C(18)	120.34(19)
C(3)-C(2)-C(1)	123.0(2)	C(21)-C(20)-C(19)	119.47(19)
C(4)-C(3)-C(2)	119.6(2)	C(20)-C(21)-C(22)	119.8(2)
C(3)-C(4)-C(5)	119.9(2)	C(21)-C(22)-C(17)	122.5(2)
C(4)-C(5)-C(6)	121.2(2)	N(1)-B(1)-C(1)	120.59(17)
C(5)-C(6)-C(1)	119.6(2)	N(1)-B(1)-C(17)	119.97(18)
C(5)-C(6)-C(7)	117.95(19)	C(1)-B(1)-C(17)	119.34(17)

Table S37. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **6b**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	25(1)	29(1)	34(1)	0(1)	1(1)	-2(1)
C(1)	28(1)	33(1)	34(1)	-2(1)	4(1)	-7(1)
C(2)	39(1)	39(1)	33(1)	-2(1)	5(1)	-8(1)
C(3)	46(1)	53(2)	41(1)	-16(1)	12(1)	-9(1)
C(4)	42(1)	54(2)	62(2)	-26(1)	18(1)	-2(1)
C(5)	30(1)	51(2)	62(2)	-18(1)	1(1)	1(1)
C(6)	25(1)	36(1)	44(1)	-9(1)	4(1)	-4(1)

C(7)	19(1)	41(1)	45(1)	-8(1)	-4(1)	2(1)
C(8)	33(1)	41(1)	56(2)	-7(1)	-12(1)	9(1)
C(9)	38(1)	53(2)	55(2)	0(1)	-17(1)	11(1)
C(10)	38(1)	58(2)	46(2)	-11(1)	-14(1)	7(1)
C(11)	29(1)	44(1)	51(2)	-13(1)	-9(1)	2(1)
C(12)	22(1)	37(1)	40(1)	-6(1)	-2(1)	-2(1)
C(13)	28(1)	35(1)	48(1)	-5(1)	2(1)	-9(1)
C(14)	34(1)	28(1)	39(1)	2(1)	0(1)	2(1)
C(15)	68(2)	32(1)	55(2)	9(1)	-3(1)	3(1)
C(16)	42(1)	35(1)	43(1)	-3(1)	3(1)	4(1)
C(17)	31(1)	31(1)	27(1)	-1(1)	-1(1)	0(1)
C(18)	32(1)	31(1)	31(1)	1(1)	2(1)	1(1)
C(19)	31(1)	35(1)	45(1)	-2(1)	7(1)	-5(1)
C(20)	28(1)	46(1)	44(1)	-7(1)	-5(1)	4(1)
C(21)	43(1)	53(2)	45(2)	12(1)	-11(1)	2(1)
C(22)	40(1)	48(1)	43(1)	18(1)	-4(1)	-8(1)
B(1)	31(1)	31(1)	27(1)	5(1)	2(1)	-5(1)

Table S38. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **6b**.

	x	y	z	U(eq)
H(2)	4743	8125	4824	44
H(3)	3997	10113	5209	56
H(4)	3015	10983	4686	63
H(5)	2809	9915	3763	57
H(8)	3297	10034	2817	52
H(9)	3102	9236	1861	58
H(10)	3134	6398	1609	57
H(11)	3382	4402	2313	50
H(13A)	3469	4894	3792	44
H(13B)	3643	3592	3283	44
H(14)	5456	3895	3401	41
H(15A)	4383	1494	3632	78
H(15B)	4935	2157	4103	78
H(15C)	5202	1082	3560	78
H(16A)	4898	4255	2484	60
H(16B)	4406	2683	2628	60
H(16C)	5238	2436	2563	60

H(18)	5839	8311	3526	38
H(19)	7018	8398	3786	44
H(20)	7458	6561	4482	47
H(21)	6707	4630	4916	56
H(22)	5535	4509	4644	52

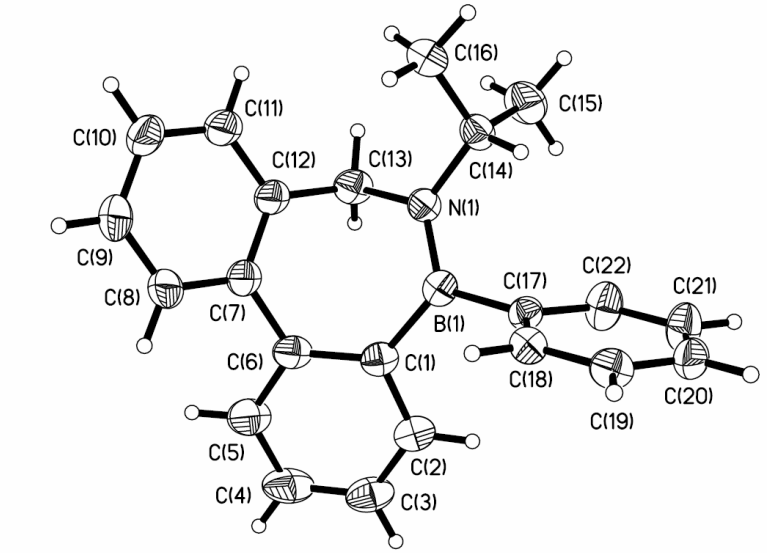


Figure S90. The crystal structure of **6b** with labeling schemes.

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