Supplementary Information

BNN-1,3-Dipoles: Isolation and Intramolecular Cycloaddition with Unactivated Arenes

Contents

Method

General. All reactions were performed under an atmosphere of nitrogen by using standard Schlenk or dry box techniques; solvents were dried over Na metal, K metal or CaH_2. ^1H, ^{11}B, ^{13}C and ^{19}F spectra were obtained with BRUKER AVANCE III HD 500MHz spectrometer at 298 K. NMR multiplicities are abbreviated as follows: s = singlet, d = doublet, t = triplet, m = multiplet, br = broad signal. Coupling constants *J* are given in Hz. UV-vis spectra were measured on a SHIMADZU UV-1900 spectrometer. Electrospray ionization (ESI) mass spectra were obtained at the Agilent Q-TOF6510 Mass Spectrometer. Melting points were measured on a X4 Melting Point apparatus (Beijing Tech, CN) in sealed capillaries and are uncorrected. DppI,[S1] Mes*BBr_2,[S2] DmpBBr_2,[S3] 1,2-bis(trimethylsilyl)-hydrazine,[S4] 1,3-diisopropyl-4,5-dimethylimidazol-2-ylidene (IPr_2Me_2),[S5] and 1,3-di-tert-butylimidazol-2-ylidene (I^tBu)[S6] were synthesized according to literature procedures.

DppBBr_2: 5.981 g (16.8 mmol) DppI were dissolved in toluene (60 mL) and 7.40 mL of a 2.5 M solution (18.5 mmol) of n-butyllithium were added. The mixture turned to yellow and was stirred overnight at room temperature. 2.23 mL (23.6 mmol) of BBr_3 was injected and the mixture was stirred for another 12 h. After filtration at 50 °C, the filtrate was concentrated under reduced pressure until incipient crystallization was observed and then stored at –20 °C overnight. The mother liquor was removed and **DppBBr_2** was obtained in form of yellow crystals (2.434 g, 36 % yield).

Mp: 126.2 °C (dec); ^1H NMR (500 MHz, $CDCl_3$): δ = 7.54 (t, J = 7.6 Hz, 1H, Ar-*H*), 7.44 (m, 12H, Ar-*H*); ^{13}C NMR (126 MHz, C_6D_6): δ = 144.2 (C^q), 142.6 (C^q), 130.2 (*C*H), 129.4 (*C*H), 128.6 (*C*H), 128.5 (*C*H), 128.1 (*C*H), B-*C* was not observed; ^{11}B NMR (160 MHz, C_6D_6): δ =

60.0 (br); HRMS (ESI): m/z calcd for $C_{18}H_{14}BBr_2$: 398.9571 $[(M + H)]^+$; found: 398.9563.

Compound 1: 2.308 g (5.8 mmol) **DppBBr₂** was dissolved in 20 mL of toluene and 0.511 g (2.9 mmol) 1,2-bis(trimethylsilyl)-hydrazine was added at room temperature. The mixture was stirred for 12 h and concentrated under reduced pressure until precipitate was observed and then stored at –20 ºC overnight. The mother liquor was removed and colorless crystals of **1** were obtained in 52 % yield (1.002 g).

Mp: 134.5 ºC (dec); ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.51 (m, 3H, Ar-*H*), 7.37 (m, 23H, Ar-*H*), 6.22 (s, 2H, N-*H*); ^{13}C NMR (126 MHz, C_6D_6): δ = 146.6 (C^q), 143.5 (C^q), 129.6 (*C*H), 129.4 (*C*H), 128.6 (*C*H), 128.4 (*C*H), 127.4 (*C*H), B-*C* was not observed; ^{11}B NMR (160 MHz, C_6D_6): δ = 36.3 (br); HRMS (ESI): m/z calcd for $C_{36}H_{29}B_2Br_2N_2$: 670.0903 $[(M + H)]^+$; found: 670.0918.

Compound 2: 10.122 g (21.0 mmol) **DmpBBr₂** was dissolved in 50 mL of DCM and 1.849 g (10.5 mmol) 1,2-bis(trimethylsilyl)-hydrazine was added at room temperature. The mixture was stirred for 12 h and the resulted precipitate was collected by filtration and dried under vacuum to afford a white powder of **2** in 59 % yield (5.154 g).

Mp: 273.9 ºC; ^{1}H NMR (500 MHz, C_6D_6): δ = 7.03 (m, 2H, Ar-*H*), 6.99 (m, 4H, Ar-*H*), 6.85 (s, 8H, Ar-*H*), 6.85 (s, 8H, Ar-*H*), 6.76 (s, 2H, N-*H*), 2.26 (s, 12H, CH_3), 2.05 (s, 24H, CH_3); ^{13}C NMR (126 MHz, C_6D_6): δ = 138.3 (C^q), 138.1 (C^q), 136.5 (C^q), 136.0 (C^q), 135.9 (C^q), 130.0 (*C*H), 128.9 (*C*H), 126.5 (*C*H), 21.3 (CH_3), 20.8 (CH_3); ^{11}B NMR (160 MHz, C_6D_6): δ = 32.4 (br); HRMS (ESI): m/z calcd for $C_{48}H_{53}B_2Br_2N_2$: 839.2756 $[(M + H)]^+$; found: 839.2744.

Compound 3: A benzene solution (10 mL) of **I^{t}Bu** (0.270 g, 1.5 mmol) was added into **1** (0.334 g, 0.5 mmol) at room temperature. The resulting suspension was stirred 2 min at room temperature. After filtration, filtrate was vacuumed and the residue was washed with cold n-hexane to afford a yellow powder, which was recrystallized from benzene at 10 ºC to give product **3** in 50 % yield (0.172 g).

Mp: 212.8 ºC; ^{1}H NMR (500 MHz, C_6D_6): δ = 7.90 (d, *J* = 6.9 Hz, 2H, Ar-*H*), 7.78 (d, *J* = 7.1 Hz, 2H, Ar-*H*), 7.49 (dd, J = 7.6, 1.2 Hz, 2H, Ar-*H*), 7.44 (m, 1H, Ar-*H*), 7.33 (m, 2H, Ar-*H*), 7.16 (m, 6H, Ar-*H*), 7.12 (m, 3H, Ar-*H*), 6.96 (dd, *J* = 7.6, 1.2 Hz, 2H, Ar-*H*), 6.82 (m, 1H, Ar-*H*), 6.22 (d, *J* = 2.2 Hz, 1H, C_2H_2), 6.16 (d, *J* = 5.8 Hz, 1H, C-*H*), 6.01 (d, *J* = 2.2 Hz, 1H, C_2H_2), 5.93 (dd, *J* = 9.4, 4.1 Hz, 1H, C-*H*), 5.80–5.76 (m, 1H, C-*H*), 4.42 (d, *J* = 16.5 Hz, 1H, N-C*H*), 2.70–2.65 (m, 1H, B-C*H*), 1.06 (s, 9H, CH_3), 1.03 (s, 9H, CH_3); ^{11}B NMR (160 MHz, C_6D_6): δ = 43.0 (br), 23.0 (br); satisfactory ^{13}C NMR data was not obtained because of its limited solubility in C_6D_6, $C_6D_5CD_3$ and THF-D_8 and instability in CD_3CN, CD_2Cl_2, and $CDCl_3$. HRMS (ESI): m/z calcd for $C_{47}H_{47}B_2N_4$: 689.3996 $[(M + H)]^+$; found: 689.3997.

Compound 4: A toluene solution (10 mL) of **2** (3.178 g, 3.8 mmol) was added into **IPr$_2$Me$_2$** (2.126 g, 11.8 mmol) at room temperature. The resulting suspension was stirred overnight at room temperature. After filtration, filtrate was vacuumed and the residue was washed with cold n-hexane to afford a yellow powder of **4** in 89 % yield (2.903 g).

Mp: 122.0 ºC (dec); ^{1}H NMR (500 MHz, C_6D_6): δ = 7.34 (dd, *J* = 7.5, 1.1 Hz, 1H, Ar-*H*), 7.27 (t, *J* = 7.5 Hz, 1H, Ar-*H*), 7.17 (dd, *J* = 7.5, 1.3 Hz, 1H, Ar-*H*), 7.14 (t, *J* = 7.5 Hz, 1H, Ar-*H*), 6.96 (m, 2H, Ar-*H*), 6.88 (s, 1H, Ar-*H*), 6.78 (s, 1H, Ar-*H*), 6.67 (s, 1H, Ar-*H*), 6.61 (dd, *J* = 7.6, 1.1 Hz, 1H, Ar-*H*), 6.55 (s, 1H, Ar-*H*), 6.38 (s, 1H, Ar-*H*), 5.47 (s, 1H, C-*H*), 3.97 (sept, 1H, C*H*(CH_3)$_2$), 3.89 (sept, 1H, C*H*(CH_3)$_2$), 2.50 (d, *J* = 3.1 Hz, 6H, CH_3), 2.28 (s, 3H, CH_3), 2.23 (s, 3H, CH_3), 2.19 (s, 6H, CH_3), 2.11 (s, 3H, CH_3), 2.02 (s, 1H, C-*H*), 1.98 (s, 3H, CH_3), 1.94 (s, 3H, CH_3), 1.90 (s, 3H, CH_3), 1.74 (s, 3H, CH_3), 1.70 (s, 3H, CH_3), 1.59 (s, 3H, CH_3), 1.55 (d, *J* = 6.9 Hz, 3H, , CH(CH_3)$_2$), 0.94 (s, 3H, CH_3), 0.82 (d, *J* = 6.9 Hz, 3H, CH(CH_3)$_2$), 0.69 (d, J = 6.9 Hz, 3H, CH(CH_3)$_2$), 0.30 (d, J = 6.9 Hz, 3H, CH(CH_3)$_2$); ^{13}C NMR (126 MHz, C_6D_6): δ = 145.9 (C^q), 145.7 (C^q), 144.4 (C^q), 143.9 (C^q), 143.4 (C^q), 142.6 (C^q), 142.3 (C^q), 142.0 (C^q), 139.6 (C^q), 138.1 (C^q), 137.6 (C^q), 136.0 (C^q), 135.8 (C^q), 135.4 (C^q), 135.3 (C^q), 134.8 (C^q), 133.1 (C^q), 131.2 (C^q), 129.0 (*C*H), 128.7 (*C*H), 128.6 (*C*H), 128.5 (*C*H), 128.5 (*C*H), 128.1 (*C*H), 127.7 (*C*H), 127.6 (*C*H), 127.5 (*C*H), 127.4 (*C*H), 127.0 (*C*H), 126.0 (*C*H), 125.0 (C^q), 124.4 (C^q), 123.9 (C^q), 117.2 (*C*H), 66.7 (N-C^q), 54.3 (*C*H(CH$_3$)$_2$), 53.0 (*C*H(CH$_3$)$_2$), 30.2 (*C*H$_3$), 30.2 (*C*H$_3$), 26.2 (*C*H$_3$), 23.1 (*C*H$_3$), 22.7 (*C*H$_3$), 22.4 (*C*H$_3$), 22.4 (*C*H$_3$), 22.1 (*C*H$_3$), 21.5 (*C*H$_3$), 21.5 (*C*H$_3$), 21.1 (*C*H$_3$), 21.1 (*C*H$_3$), 21.0 (*C*H$_3$), 20.9 (*C*H$_3$), 20.9 (*C*H$_3$),19.8 (*C*H$_3$), 10.6 (*C*H$_3$), 10.0 (*C*H$_3$), B-*C* was not observed; ^{11}B NMR (160 MHz, C_6D_6): δ = 41.3 (br), 22.3 (br); HRMS (ESI): m/z calcd for $C_{59}H_{71}B_2N_4$: 857.5878 [(M + H)]$^+$; found: 857.5837.

Compound 5: 2.081 g (5.0 mmol) **Mes*BBr$_2$** was dissolved in 20 mL of hexane and 0.440 g (2.5 mmol) 1,2-bis(trimethylsilyl)-hydrazine was added at room temperature. The mixture was stirred for 12 h and the resulted precipitate was collected by filtration and dried under vacuum to afford a white powder of **5** in 30 % yield (1.058 g).

Mp: 171.4 ºC (dec); ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.49 (s, 4H, Ar-*H*), 7.39 (s, 2H, N-*H*), 1.51 (s, 36H, CH_3), 1.35 (s, 18H, CH_3); ^{13}C NMR (126 MHz, $CDCl_3$): δ = 153.7 (C^q), 150.8 (C^q), 122.3 (*C*H), 38.5 (C^q), 35.0 (C^q), 34.1 (*C*H$_3$), 31.3 (*C*H$_3$), B-*C* was not observed; ^{11}B NMR (160 MHz, $CDCl_3$): δ = 36.4 (br); HRMS (ESI): m/z calcd for $C_{36}H_{61}B_2Br_2N_2$: 702.3407 [(M + H)]$^+$; found: 702.3439.

Compound 6: A toluene solution (10 mL) of **IPr$_2$Me$_2$** (0.540 g, 3 mmol) was added into **5** (0.700 g, 1 mmol) at room temperature. The resulting suspension was stirred 30 min at room temperature. After filtration, filtrate was vacuumed and the residue was was recrystallized from n-hexane to give product **6** in 31 % yield (0.236 g).

Mp: 155.4 ºC; ^{1}H NMR (500 MHz, C_6D_6): δ = 8.38 (sept, 1H, C*H*(CH_3)$_2$), 7.61 (s, 2H, Ar-*H*), 7.56 (s, 2H, Ar-*H*), 5.22 (sept, 1H, C*H*(CH_3)$_2$), 1.80 (s, 18H, C(C*H*$_3$)$_3$), 1.70 (s, 18H, C(C*H*$_3$)$_3$), 1.64 (s, 3H, CH_3), 1.46 (s, 9H, C(C*H*$_3$)$_3$), 1.45 (s, 3H, CH_3), 1.32 (s, 9H, C(C*H*$_3$)$_3$), 1.33 (d, *J* = 7.1 Hz, 6H, CH(C*H*$_3$)$_2$), 0.80 (d, *J* = 7.1 Hz, 6H, CH(C*H*$_3$)$_2$); ^{13}C NMR (126 MHz, C_6D_6): δ = 158.0 (C^q), 152.0 (C^q), 149.6 (C^q), 146.8 (C^q), 128.4 (*C*H), 127.3 (C^q), 124.3 (C^q), 123.0 (*C*H), 119.5 (*C*H), 49.7 (*C*H(CH_3)$_2$), 49.1 (*C*H(CH_3)$_2$), 39.1 (*C*H$_3$), 37.6 (*C*H$_3$), 34.7 (*C*H$_3$), 32.3 (*C*(CH_3)$_3$), 31.8 (*C*H$_3$), 31.6 (*C*H$_3$), 21.6 (*C*H$_3$), 21.2 (*C*H$_3$), 10.5 (*C*H$_3$), 10.5 (*C*H$_3$), B-*C* was not observed; ^{11}B NMR (160 MHz, C_6D_6): δ = 33.7 (br), 2.8 (br); HRMS (ESI): m/z calcd for $C_{47}H_{79}B_2N_4$: 721.6500 [(M + H)]$^+$; found: 721.6496.

Compound 7: 0.503 g (0.7 mmol) **6** were dissolved in toluene (10 mL) and CO_2 was passed for 5 min at room temperature. After filtration, the filtrate was removed under vacuum and the residue was washed by CH_3CN to afford a white solid of **7** in 32 % yield (0.141 g).

Mp: 185.6 ºC ; ^{1}H NMR(500 MHz, $CDCl_3$): δ = 7.47 (s, 4H, Ar-*H*), 1.40 (s, 36H, C(C*H*$_3$)$_3$), 1.35 (s, 18H, C(C*H*$_3$)$_3$); ^{13}C NMR (126 MHz, $CDCl_3$): δ = 155.5 (*C*=O), 152.7 (C^q), 146.1 (C^q), 121.9 (*C*H), 37.7 (*C*(*C*H$_3$)$_3$), 35.3 (*C*(*C*H$_3$)$_3$), 33.0 (C(*C*H$_3$)$_3$), 31.3 (C(*C*H$_3$)$_3$), B-C was not observed; ^{11}B NMR (160 MHz, $CDCl_3$): δ = 36.0 (br); HRMS (ESI): m/z calcd for $C_{38}H_{59}B_2N_2O_4$: 628.4695 [(M + H)]$^+$; found: 628.4719.

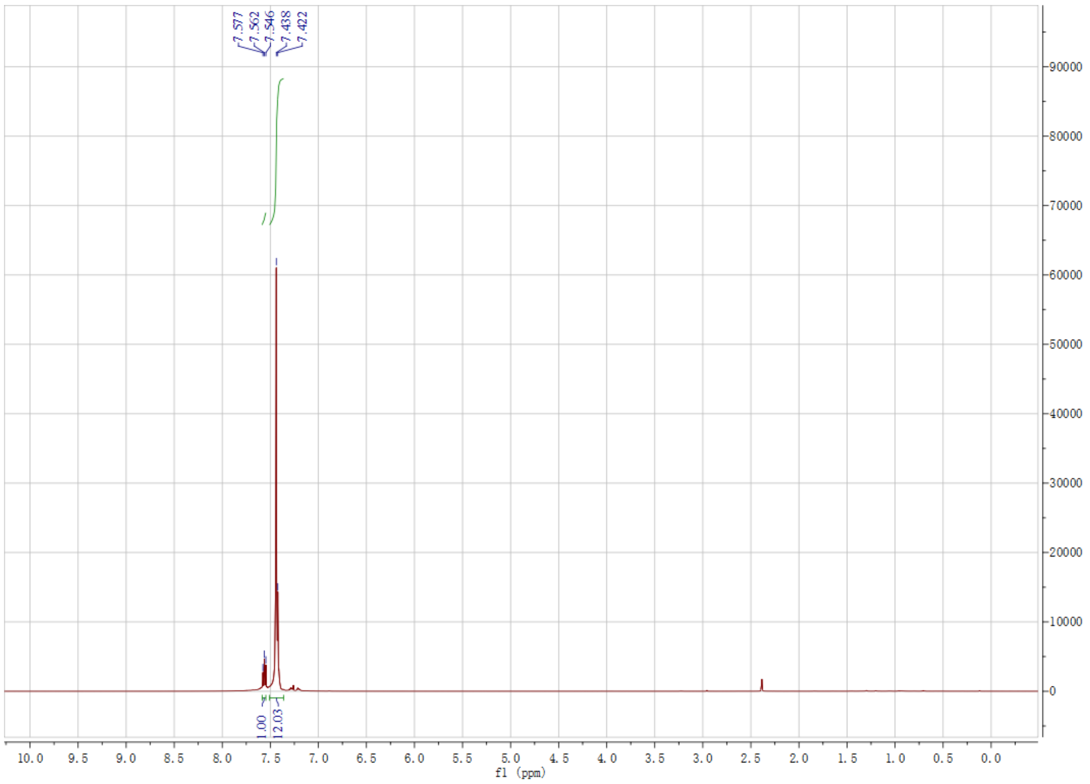


Fig. S1 ^{1}H NMR spectrum of **DppBBr$_2$** in $CDCl_3$ (500 MHz).

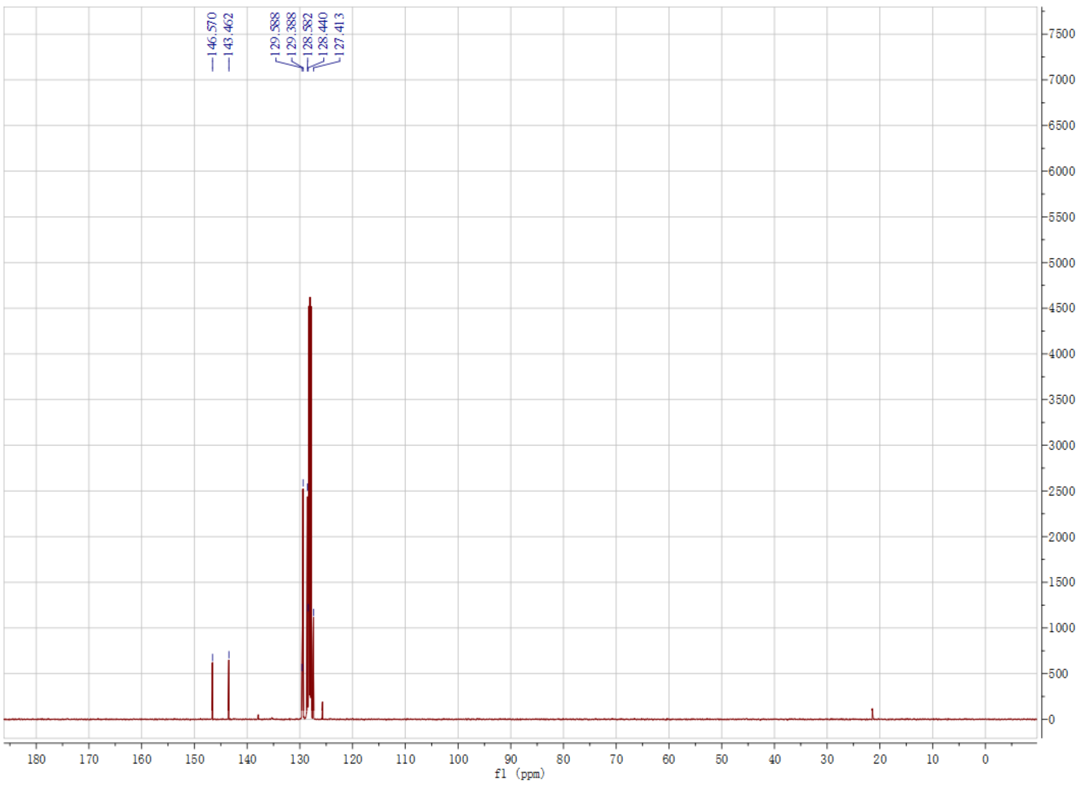


Fig. S2 ^{13}C NMR spectrum of **DppBBr$_2$** in C_6D_6 (126 MHz).

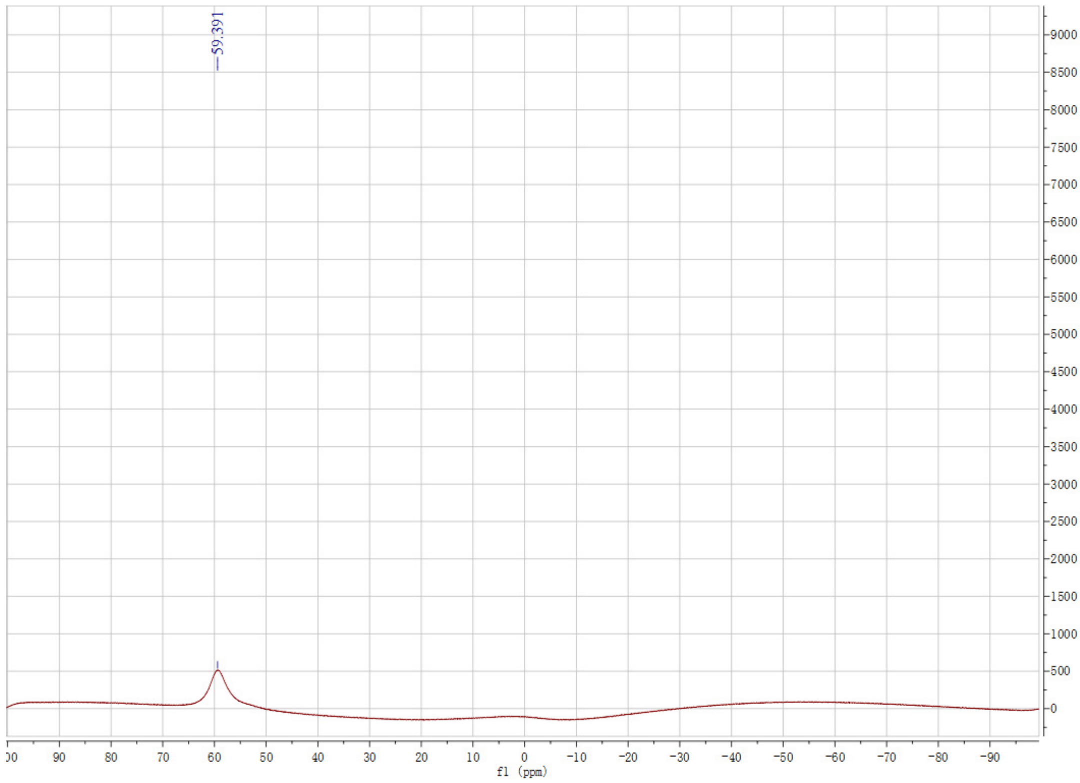


Fig. S3 ^{11}B NMR spectrum of **DppBBr₂** in C_6D_6 (160 MHz).

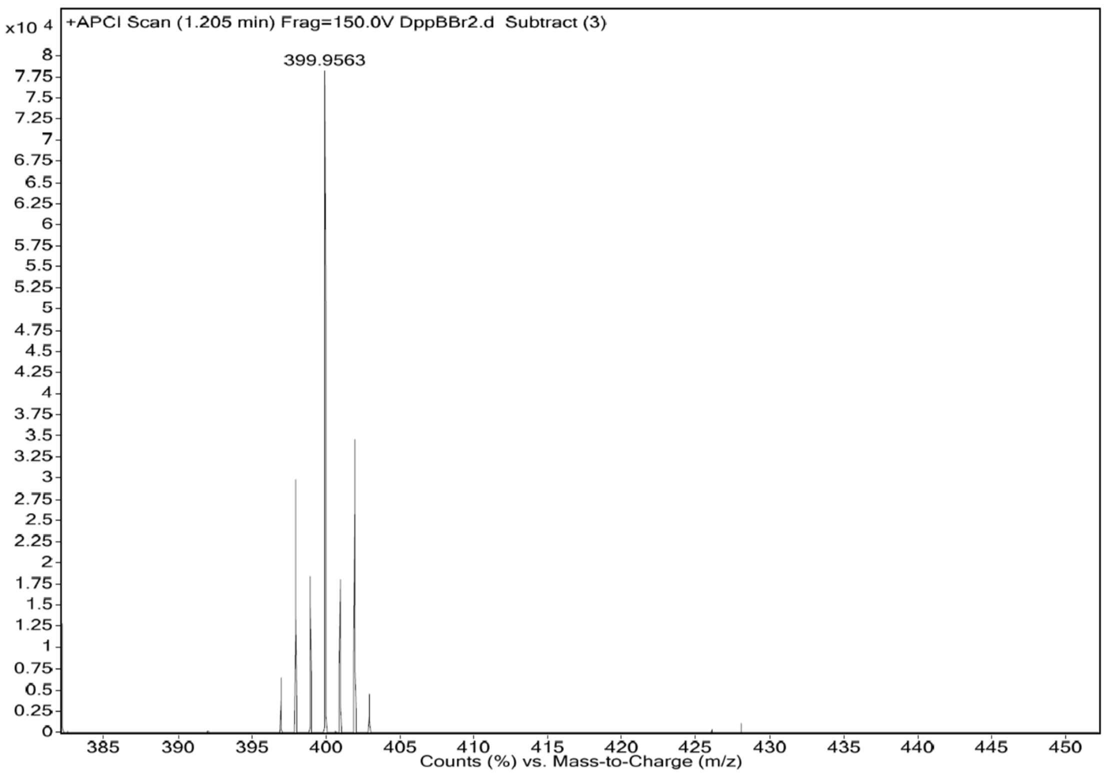


Fig. S4 HRMS spectrum of **DppBBr$_2$**.

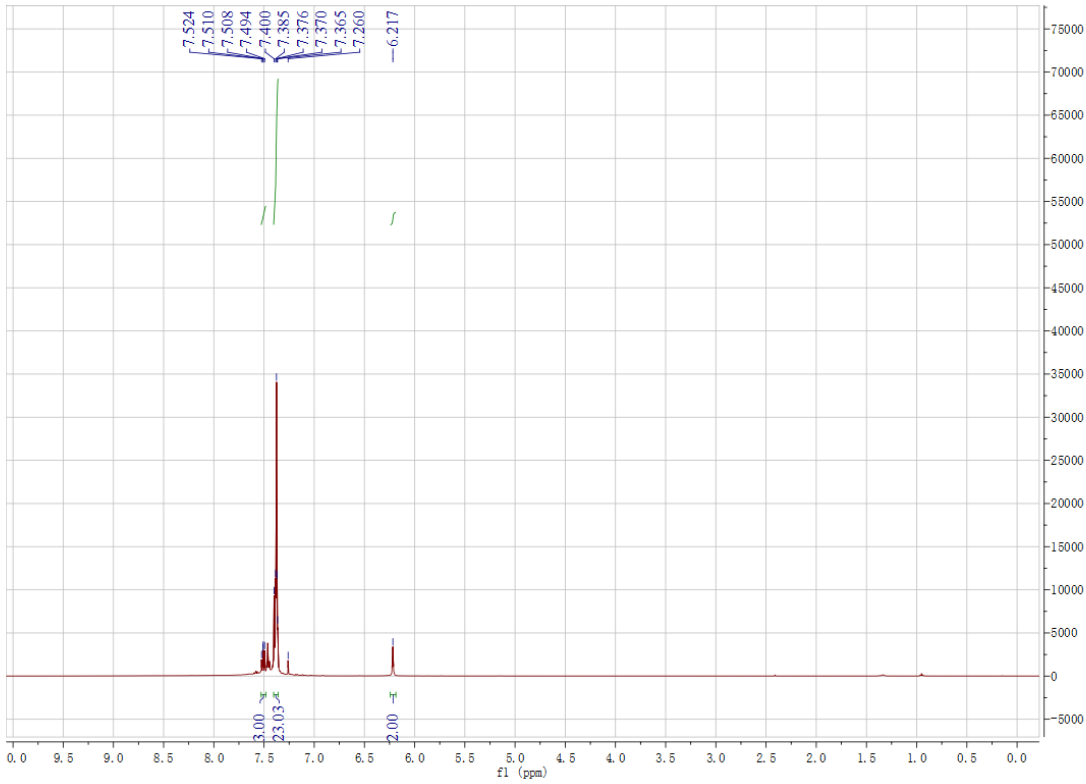


Fig. S5 ^{1}H NMR spectrum of **1** in $CDCl_3$ (500 MHz).

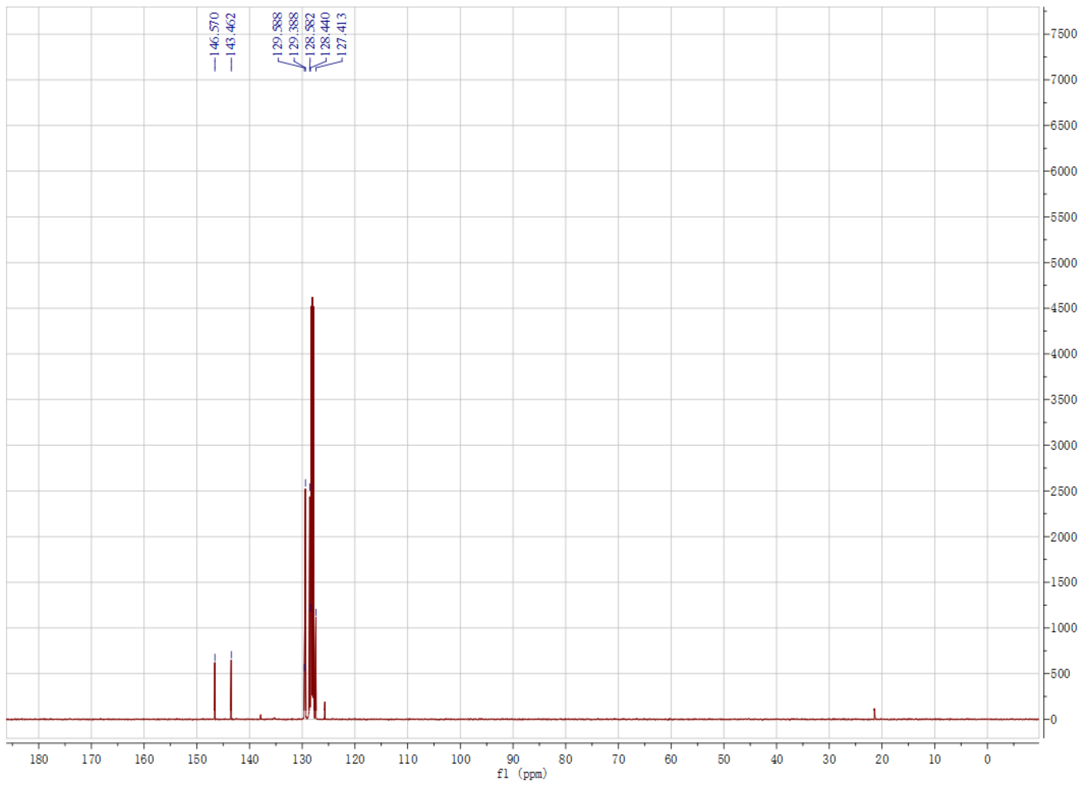


Fig. S6 ^{13}C NMR spectrum of **1** in C_6D_6 (126 MHz).

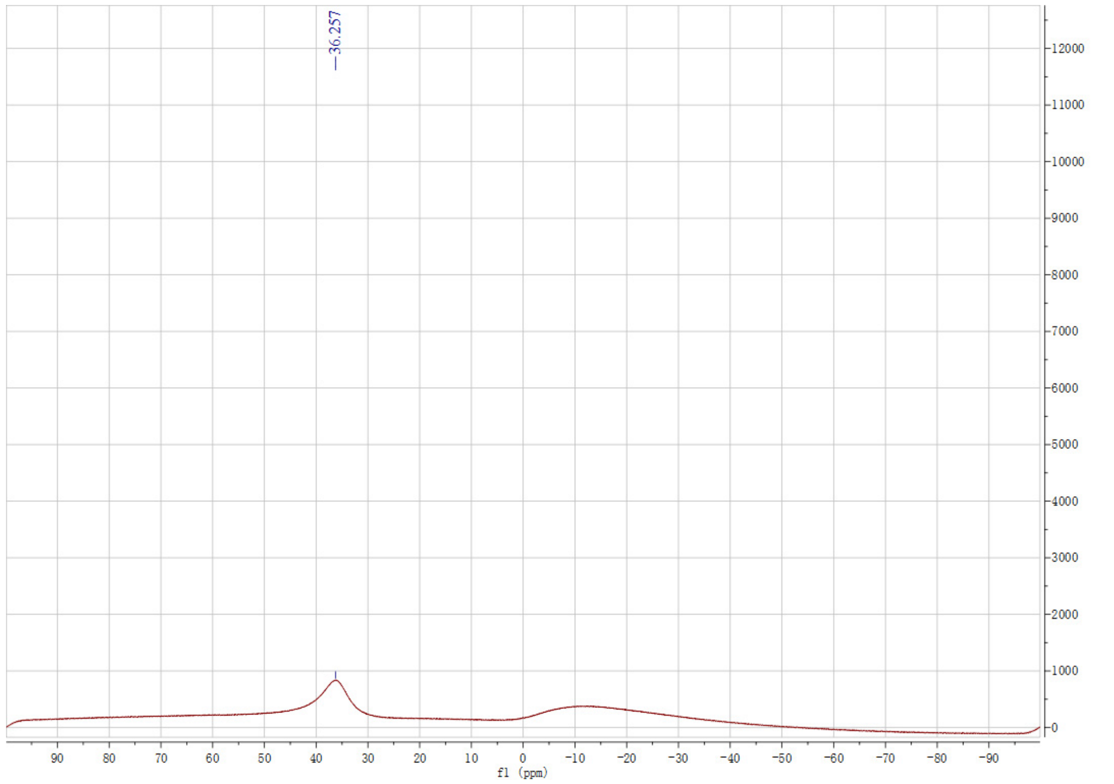


Fig. S7 [11]B NMR spectrum of **1** in C_6D_6 (160 MHz).

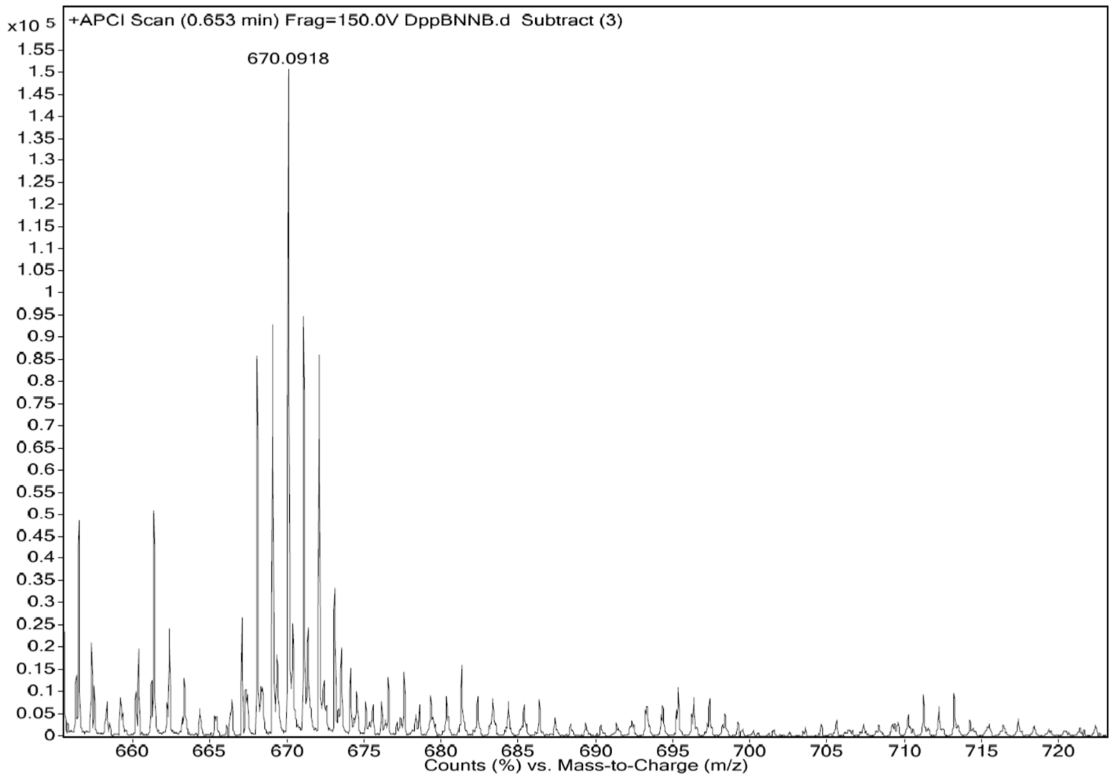


Fig. S8 HRMS spectrum of **1**.

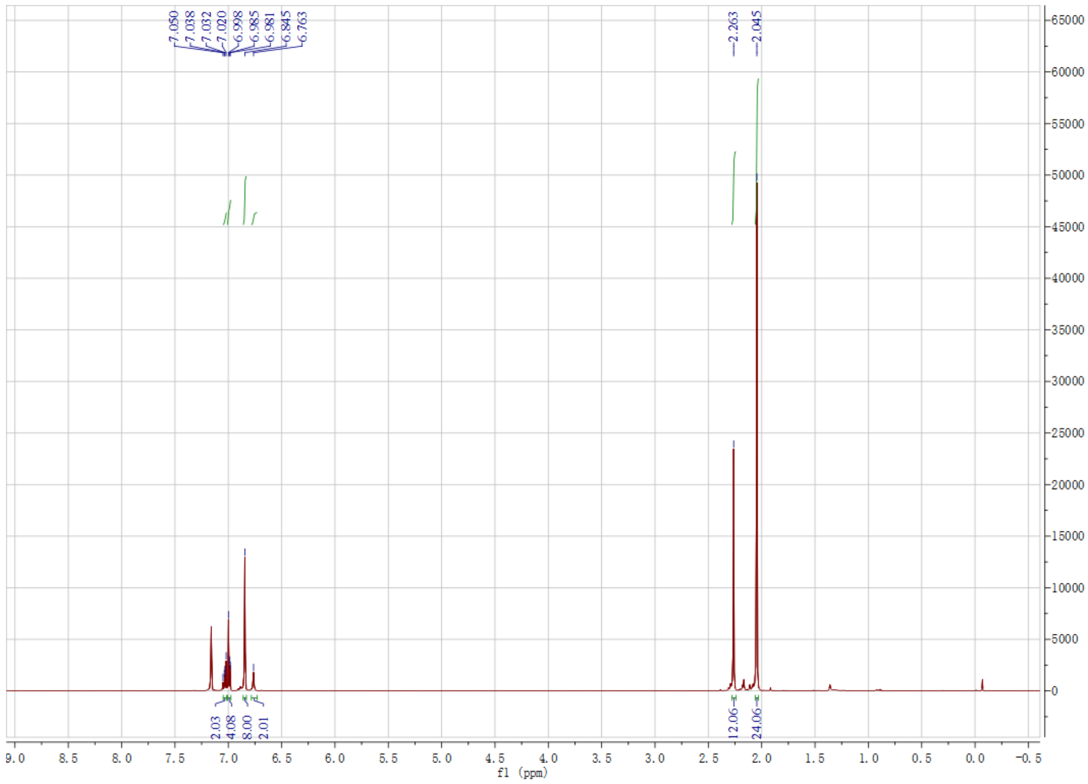


Fig. S9 [1]H NMR spectrum of **2** in C_6D_6 (500 MHz).

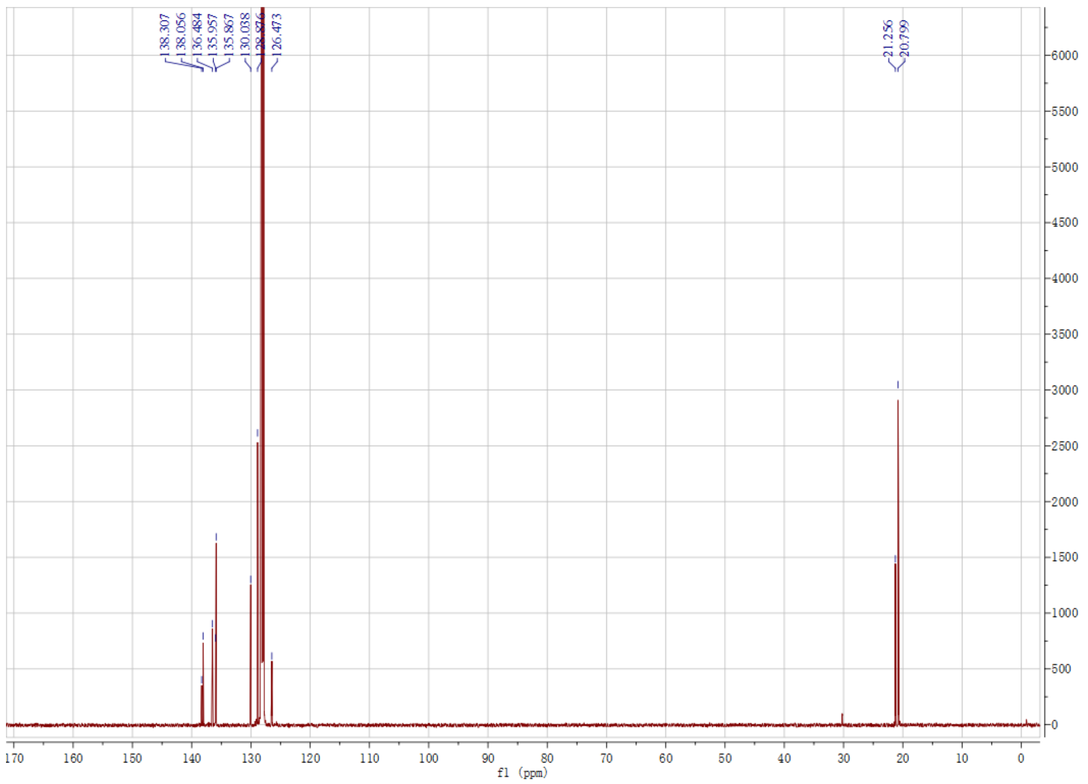


Fig. S10 [13]C NMR spectrum of **2** in C_6D_6 (126 MHz).

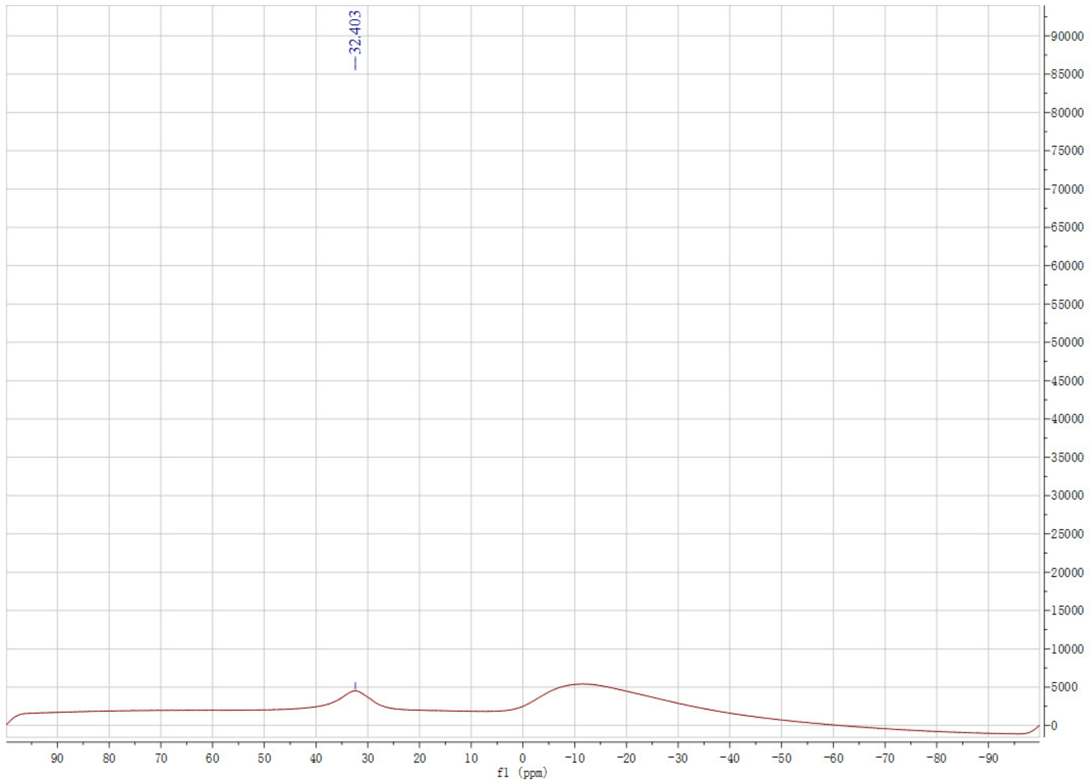


Fig. S11 ^{11}B NMR spectrum of **2** in C_6D_6 (160 MHz).

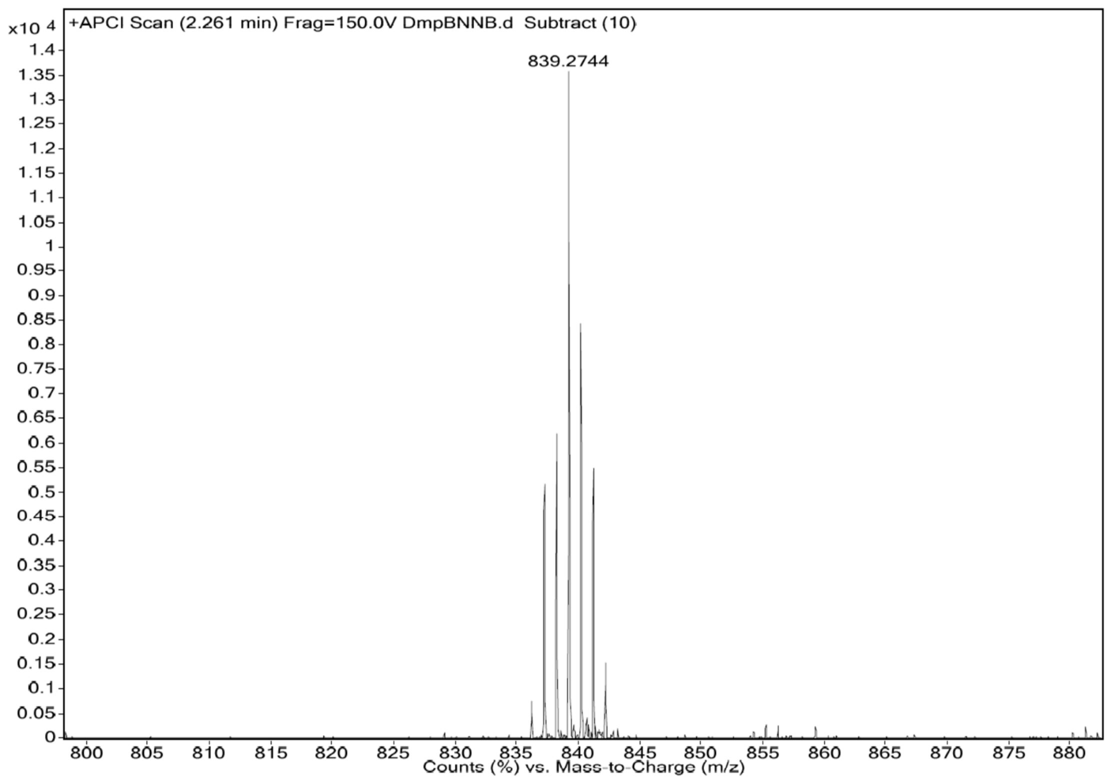


Fig. S12 HRMS spectrum of **2**.

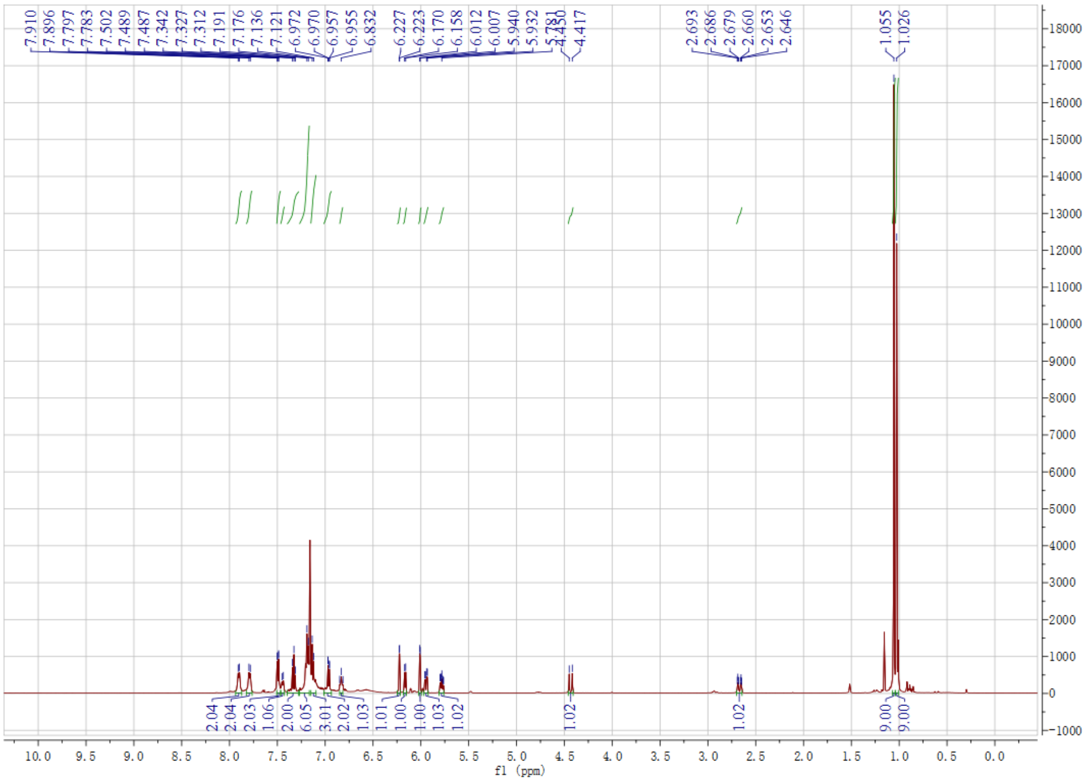


Fig. S13 ^{1}H NMR spectrum of **3** in C_6D_6 (500 MHz).

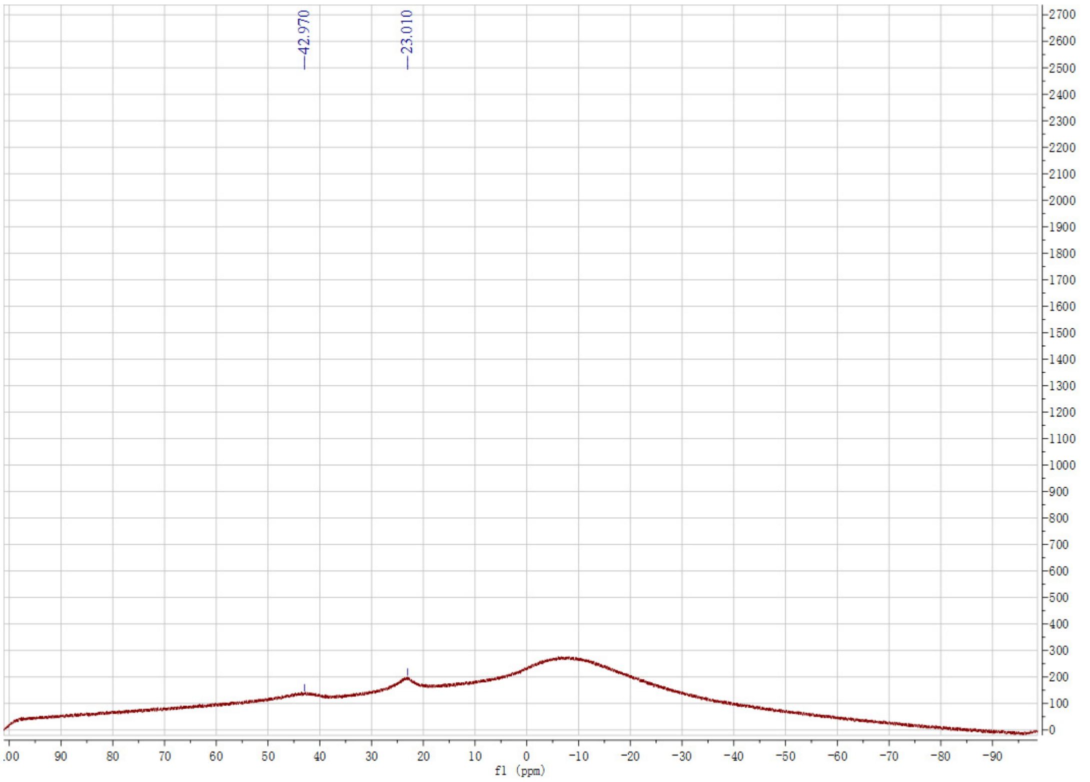


Fig. S14 ^{11}B NMR spectrum of **3** in C_6D_6 (160 MHz).

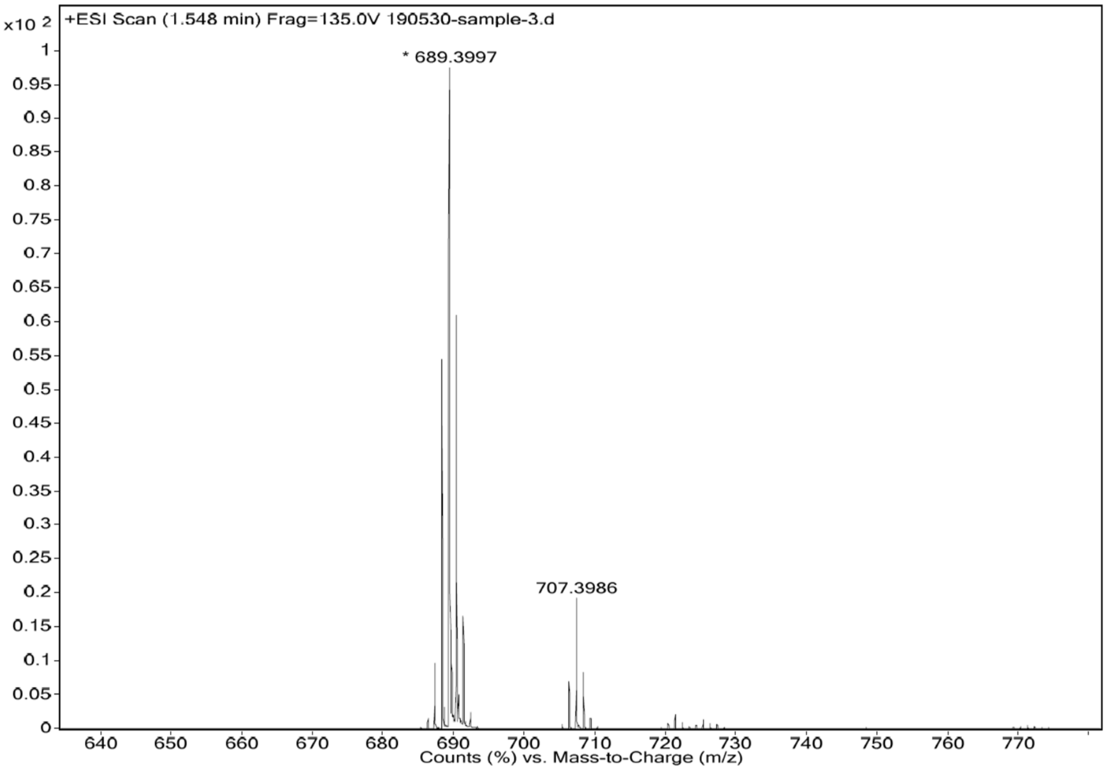


Fig. S15 HRMS spectrum of **3**.

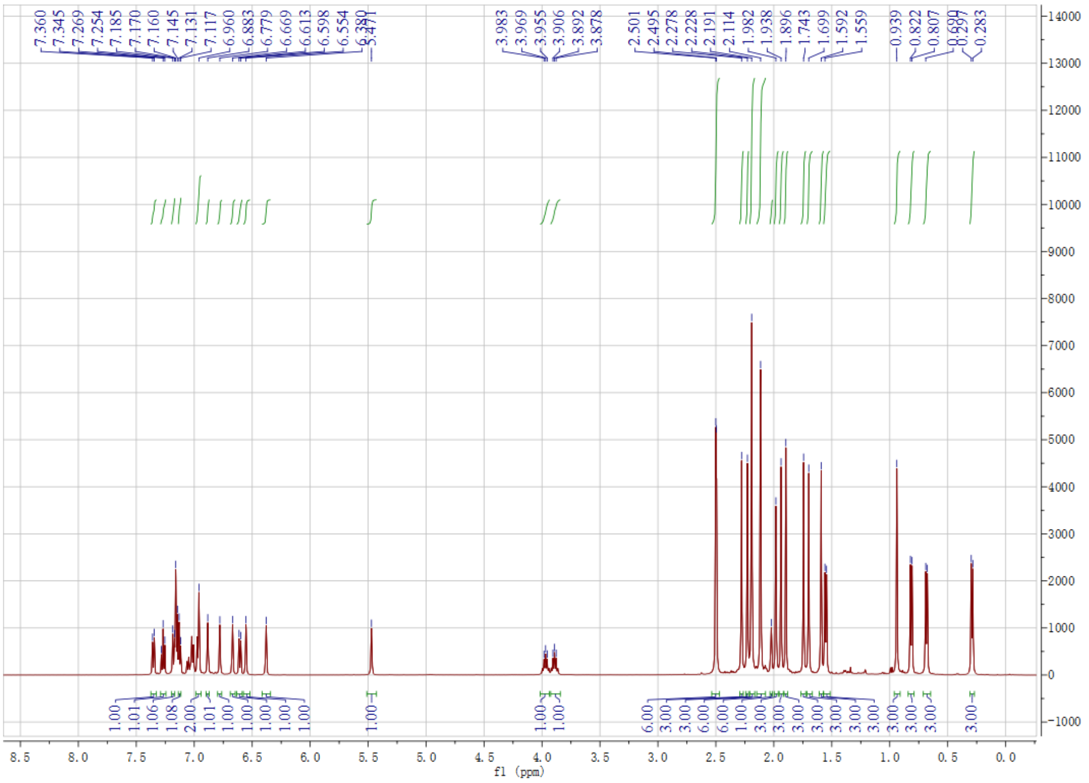


Fig. S16 ^{1}H NMR spectrum of **4** in C_6D_6 (500 MHz).

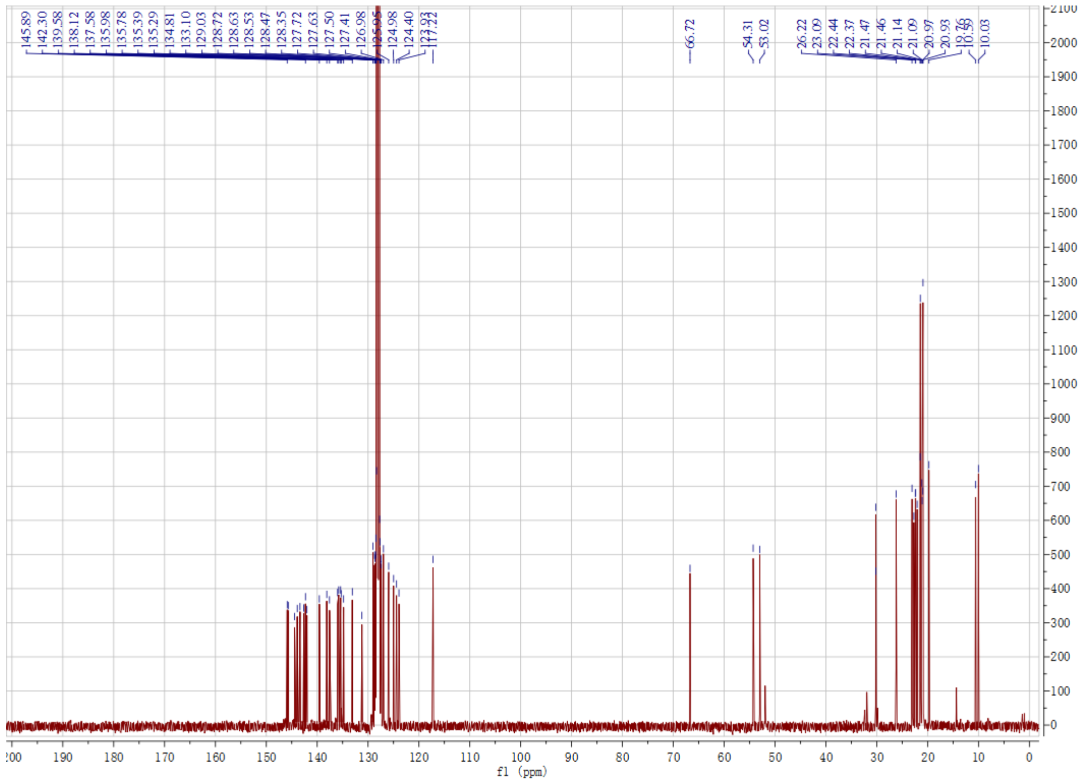


Fig S17 ^{13}C NMR spectrum of **4** in C_6D_6 (126 MHz).

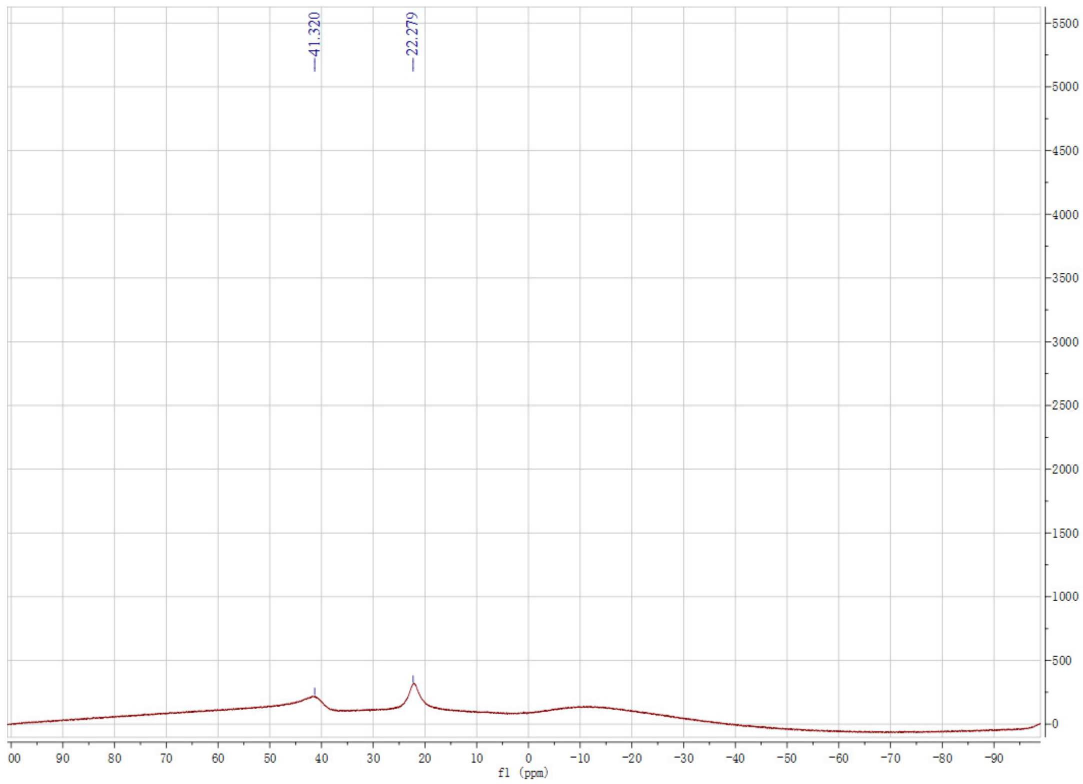


Fig. S18 ^{11}B NMR spectrum of **4** in C_6D_6 (160 MHz).

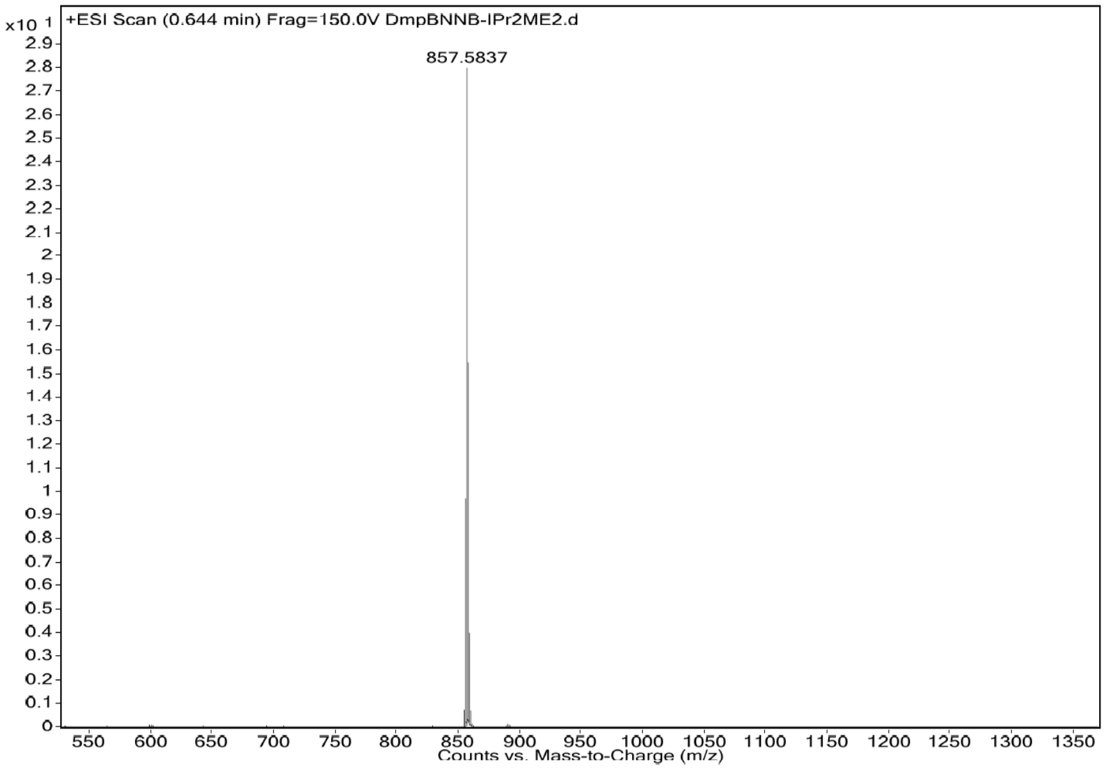


Fig. S19 HRMS spectrum of **4**.

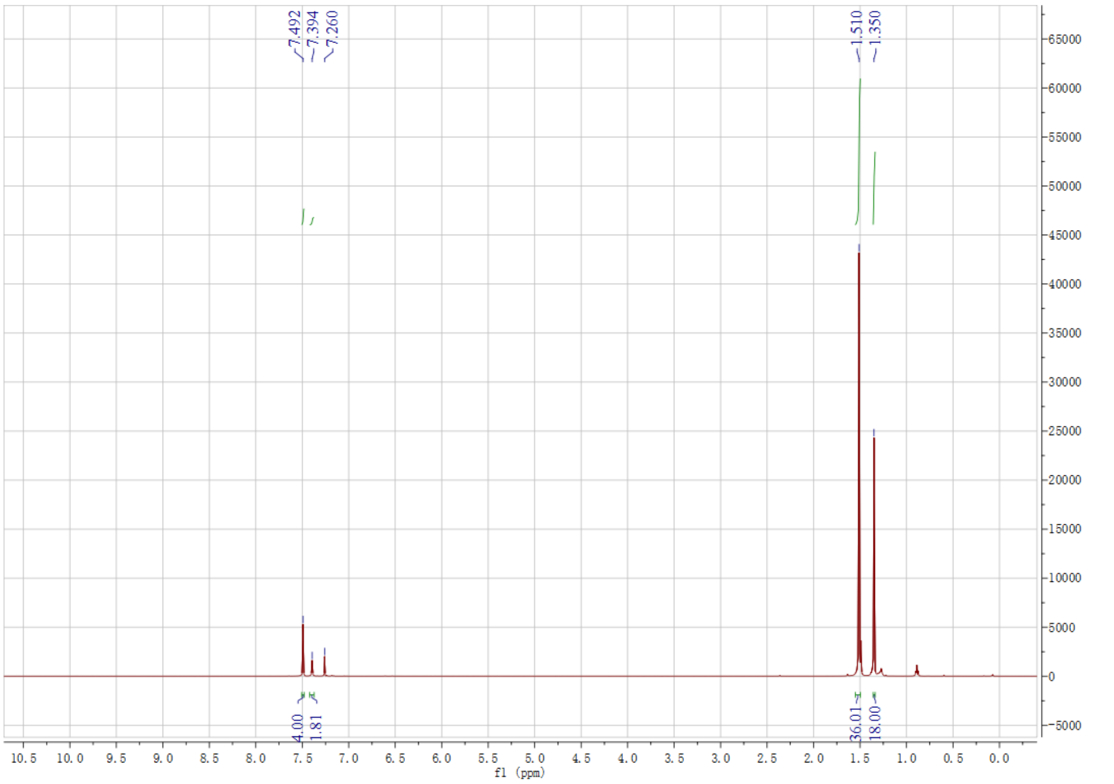


Fig. S20 ^{1}H NMR spectrum of **5** in $CDCl_3$ (500 MHz).

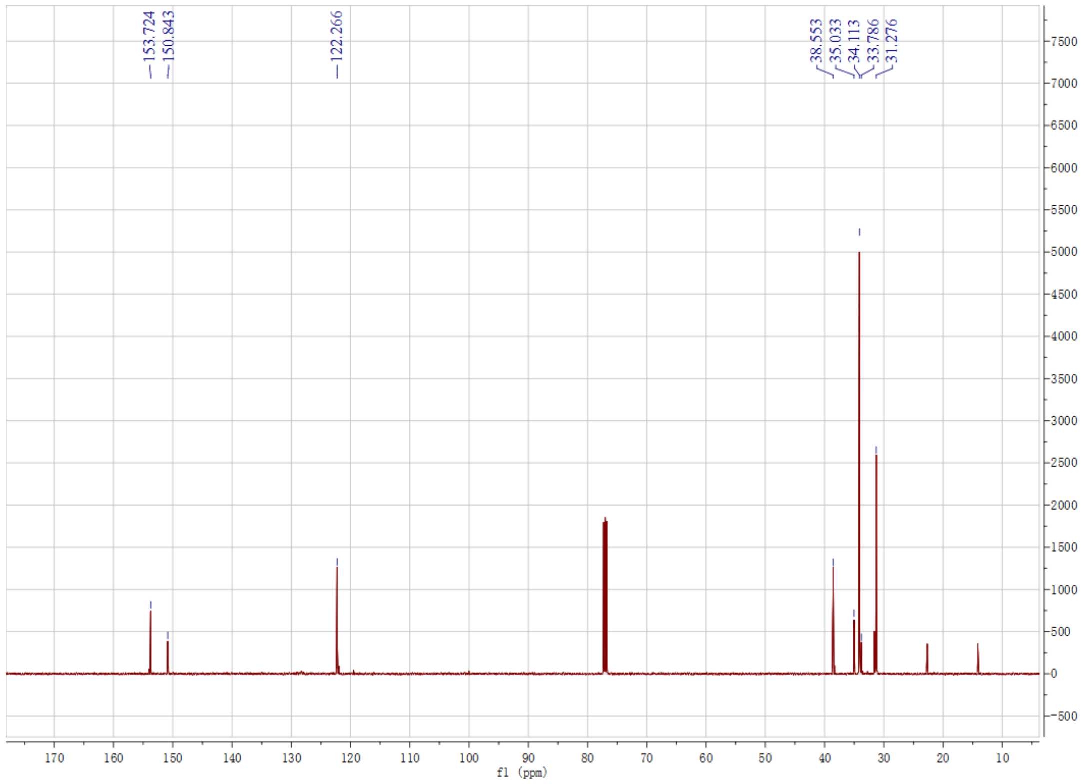


Fig. S21 ^{13}C NMR spectrum of **5** in $CDCl_3$ (126 MHz).

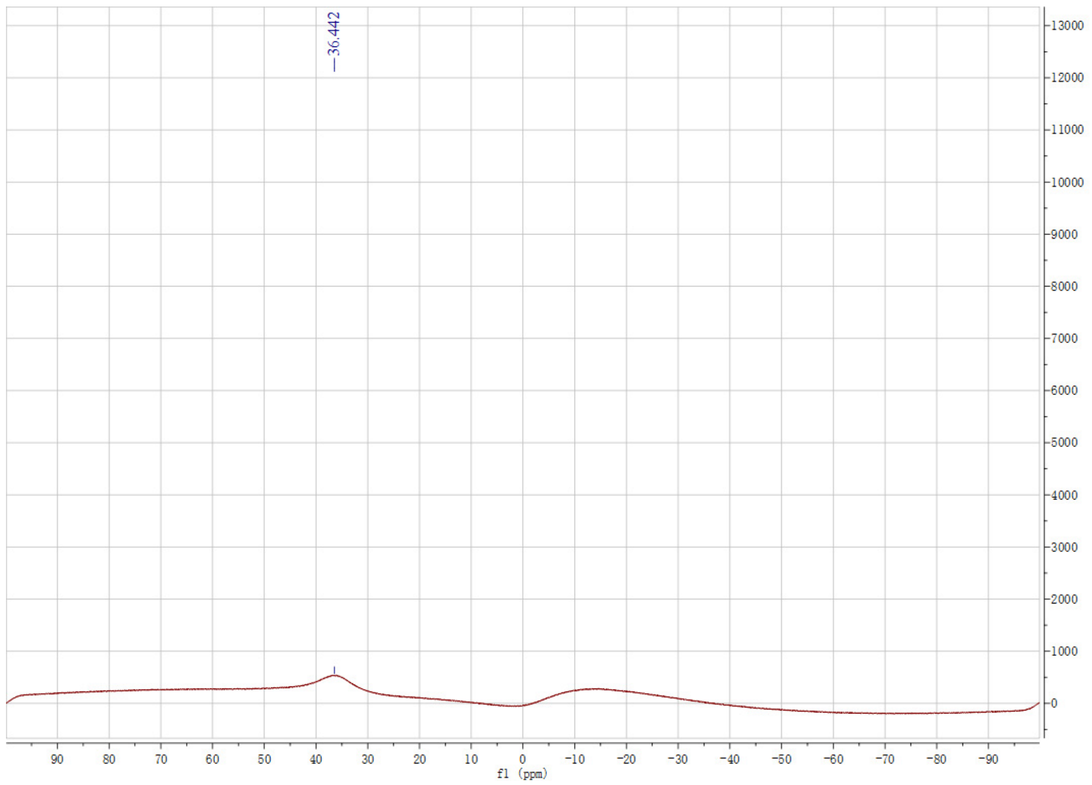


Fig. S22 ^{11}B NMR spectrum of **5** in $CDCl_3$ (160 MHz).

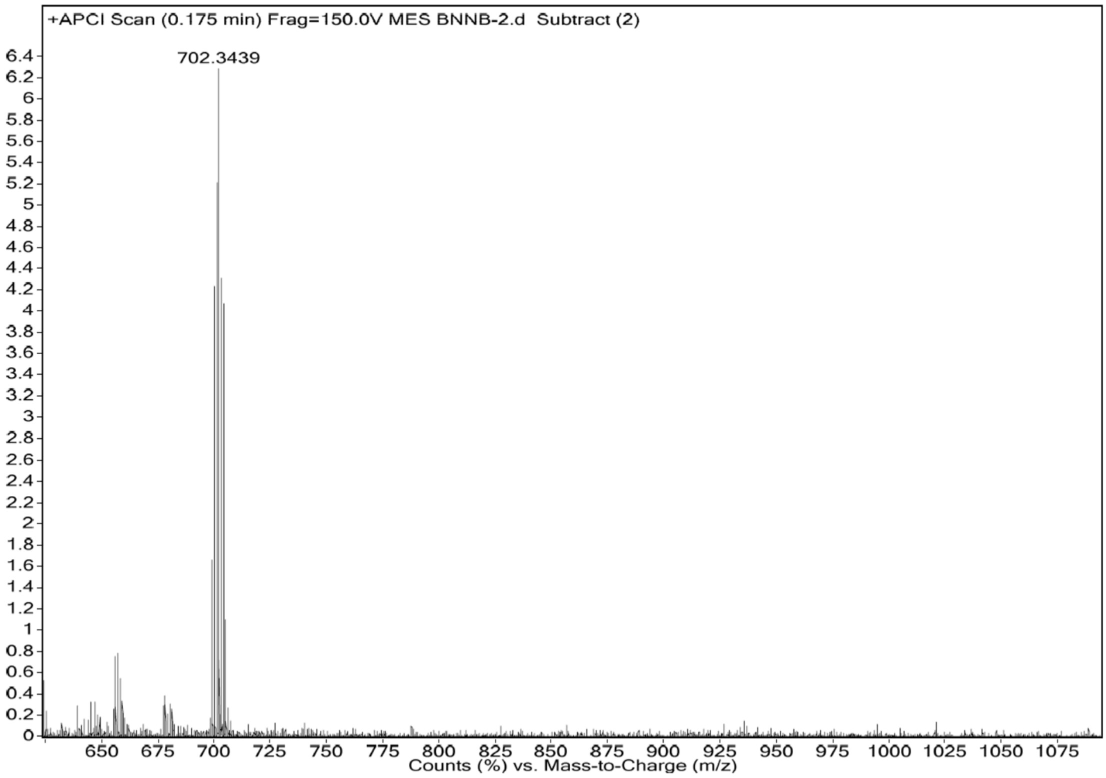


Fig. S23 HRMS spectrum of **5**.

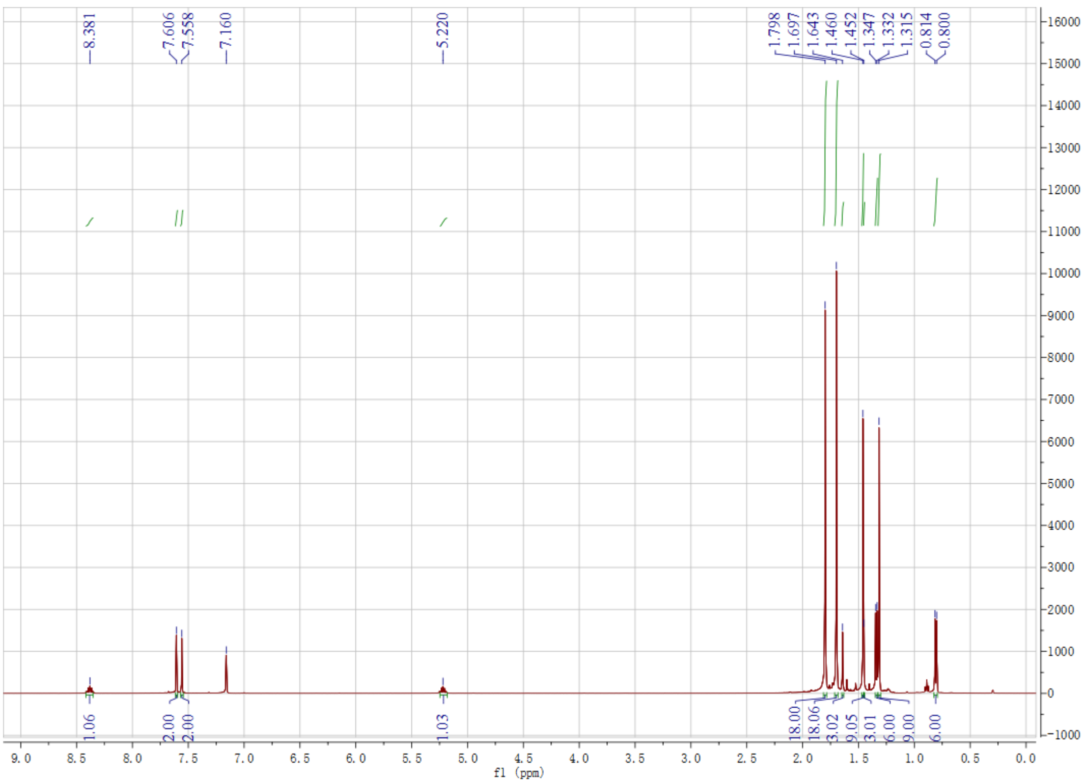


Fig. S24 ^{1}H NMR spectrum of **6** in C_6D_6 (500 MHz).

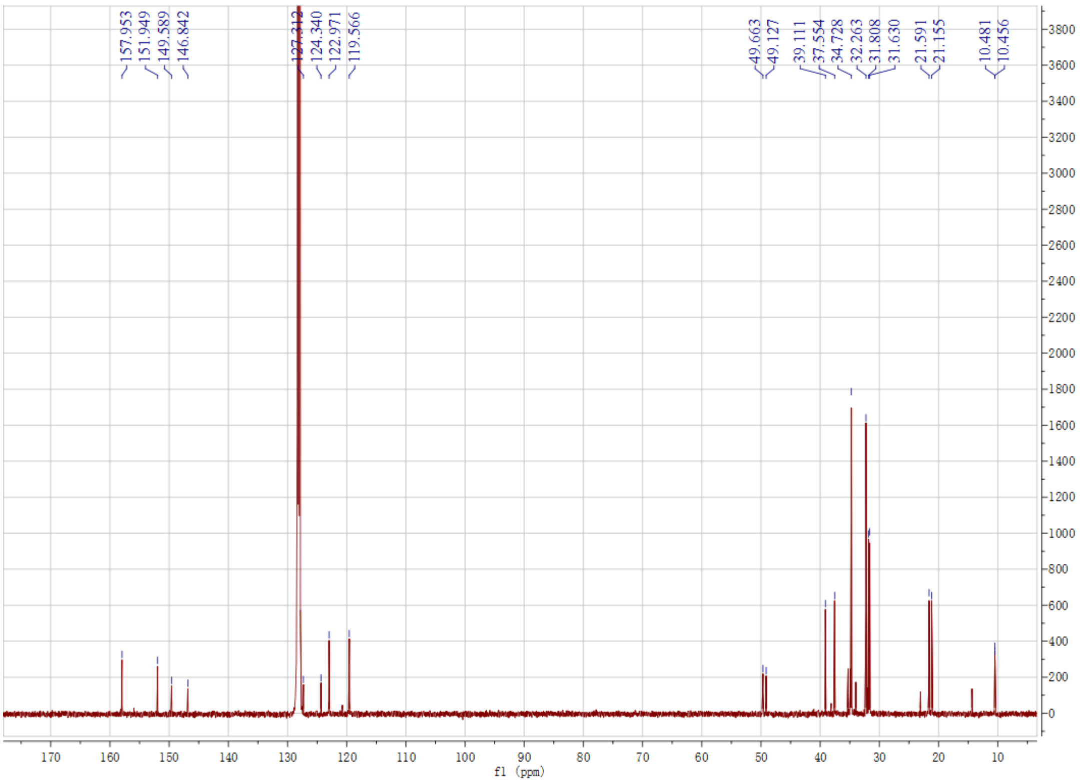


Fig. S25 ^{13}C NMR spectrum of **6** in C_6D_6 (126MHz).

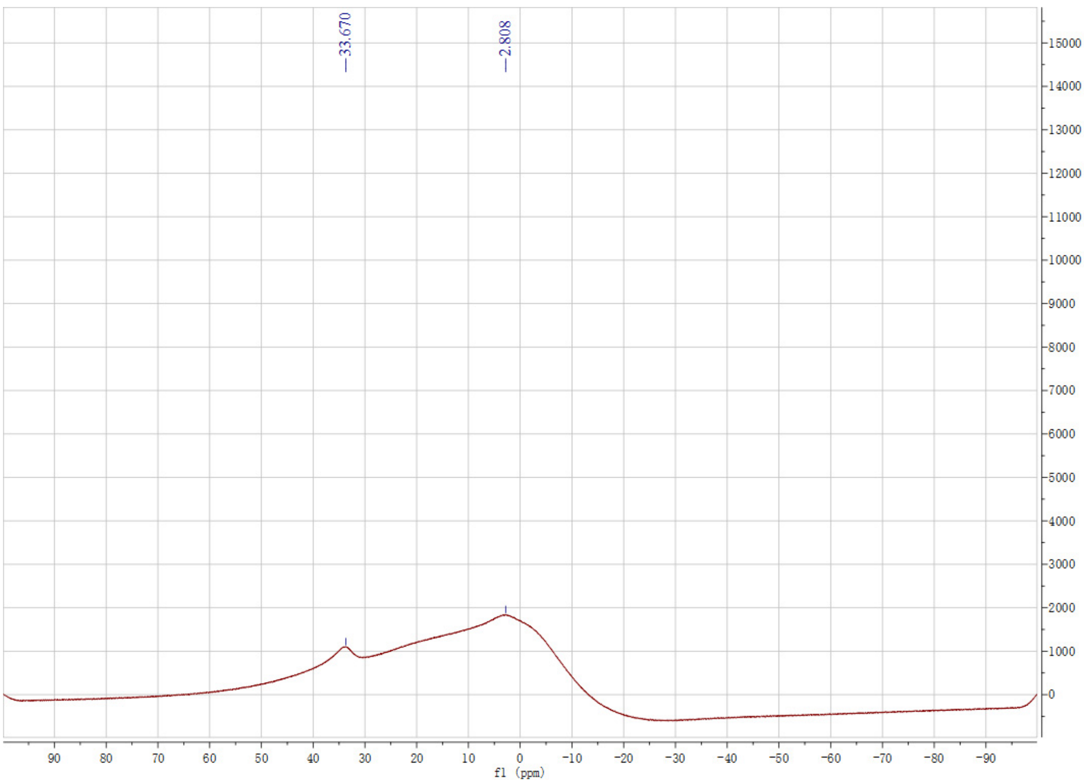


Fig. S26 ^{11}B NMR spectrum of **6** in C_6D_6 (160 MHz).

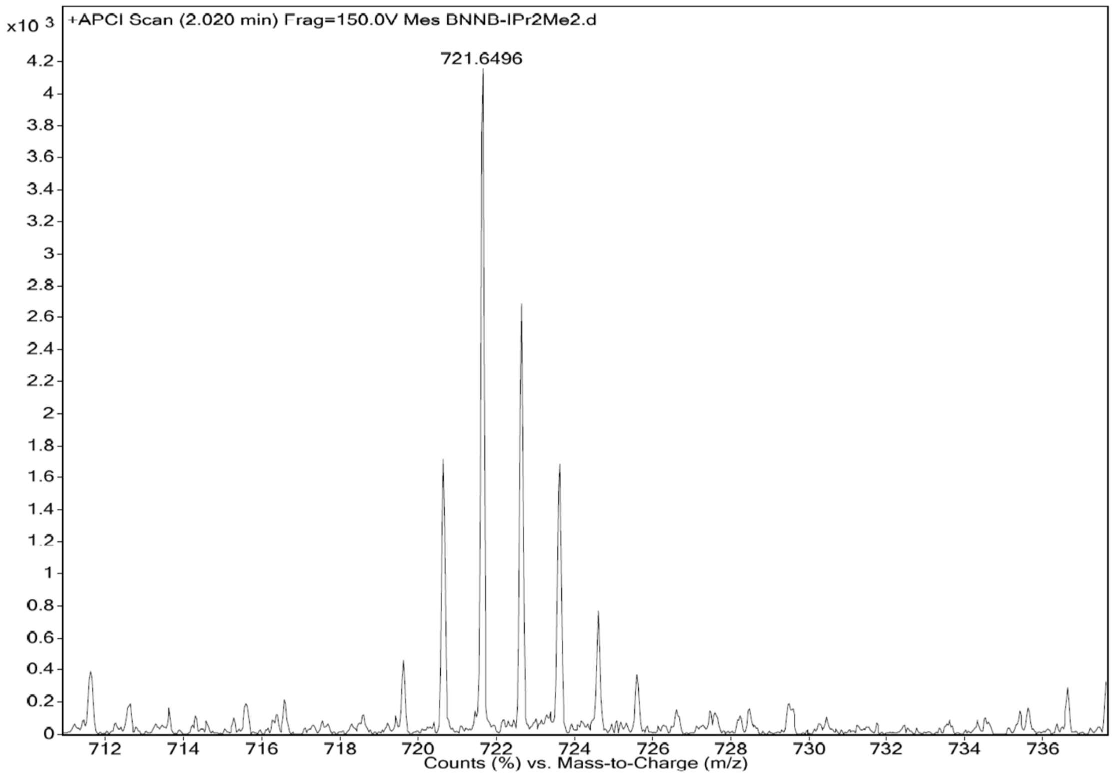


Fig. S27 HRMS spectrum of **6**.

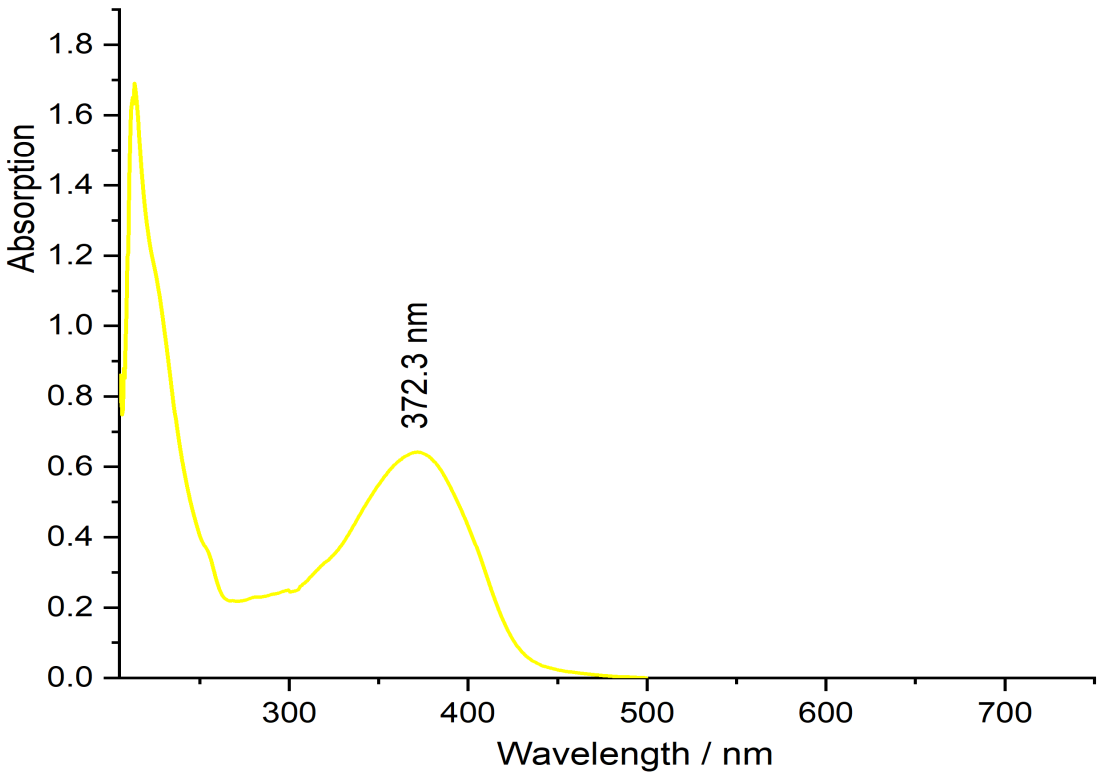


Fig. S28 UV-vis spectrum of **6** in n-hexane at room temperature.

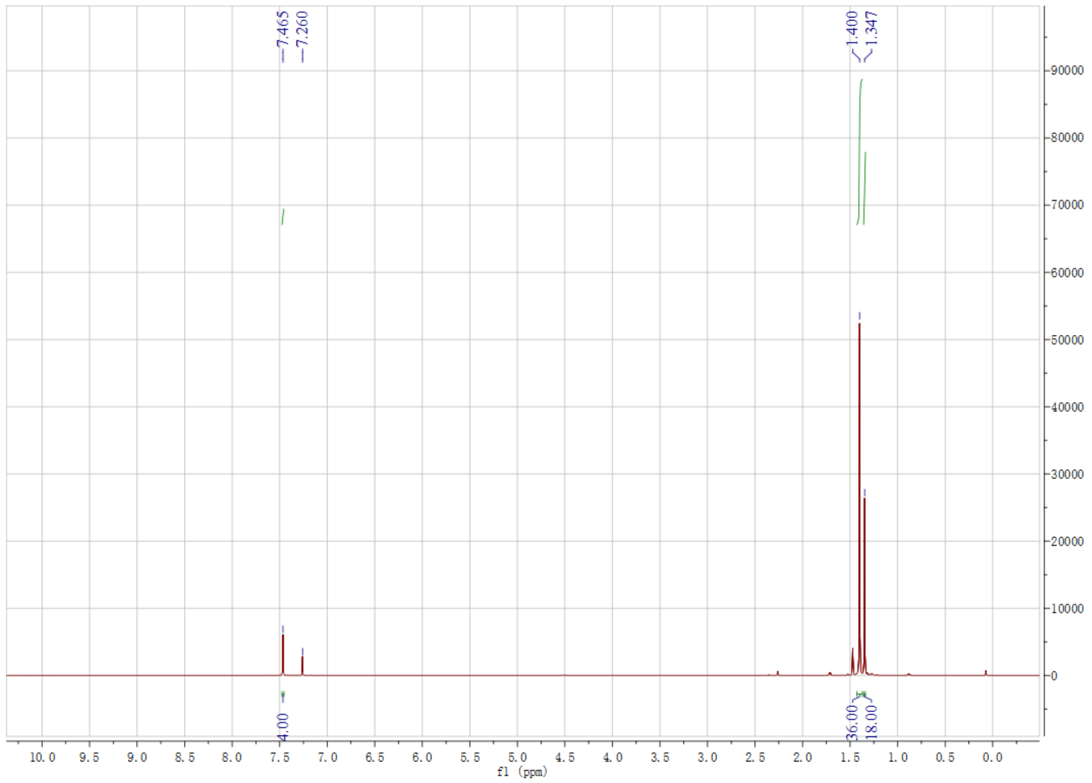


Fig. S29 [1]H NMR spectrum of **7** in $CDCl_3$ (500 MHz).

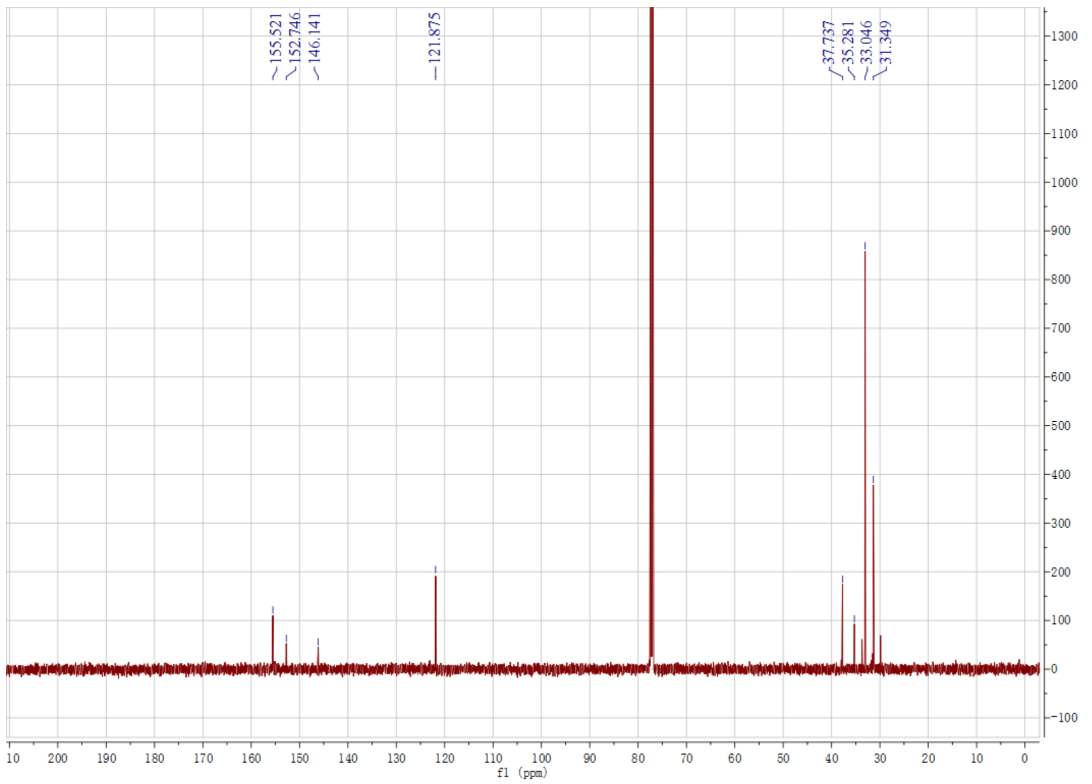


Fig. S30 [13]C NMR spectrum of **7** in $CDCl_3$ (126 MHz).

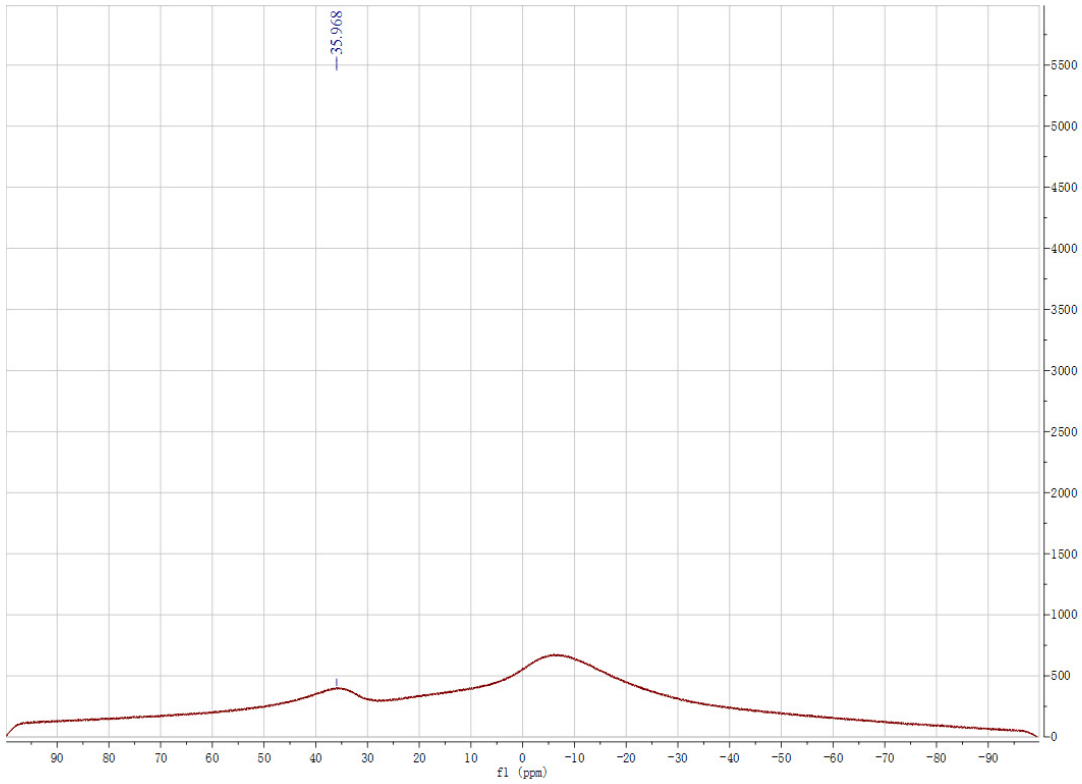


Fig. S31 [11]B NMR spectrum of **7** in $CDCl_3$ (160 MHz).

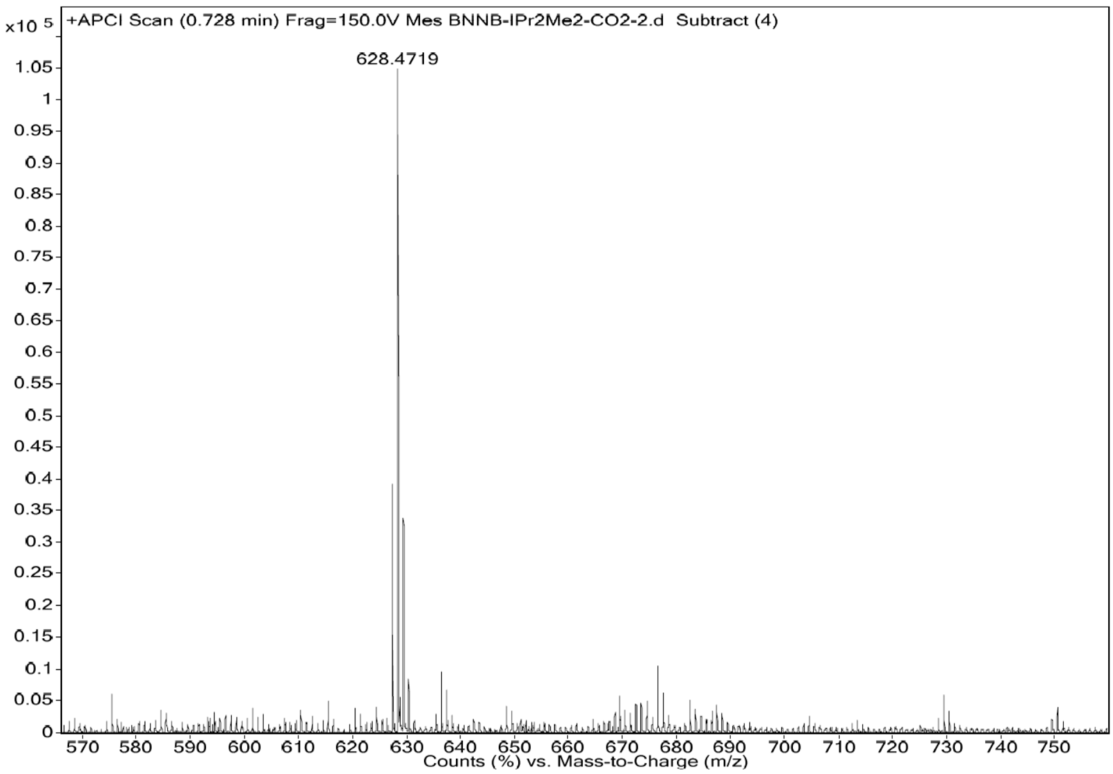


Fig. S32 HRMS spectrum of **7**.

Crystallographic details

All crystallographic intensity data was collected using a Rigaku Oxford Diffraction XtaLAB Synergy-S diffractometer equipped with a HyPix-6000HE Hybrid Photon Counting (HPC) detector, and PhotonJet-S microfocus sealed tube X-ray sources for generating Mo Ka radiation (λ = 0.71 Å, for **3**) and Cu Kα radiation (λ = 1.54184 Å, for the others). A suitable single crystal identified by microscopy was mounted on a Nylon loop with paratone oil, and then quickly placed onto the instrument. The crystal temperature was held at 173 K using an Oxford Cryosystems CryostreamPlus 800 open-flow N_2 cryostat. Reflections were recorded, indexed and corrected for absorption with the *CrysAlis*^{pro} software suit. [S7] All structures were solved by intrinsic phasing (ShelXT-2015) [S8, S9], and refined to convergence by full-matrix least squares methods based on F^2 (SHELX-2014/2018)[S10] embedded in the Olex2[S11]. All non-hydrogen atoms were refined with anisotropic displacement parameters (ADPs). Hydrogen atoms attached to carbon (CH) were placed in calculated positions and included using riding model with isotropic thermal parameters, U_{iso} = 1.2 U_{eq} (C) for aromatic hydrogen and U_{iso} = 1.5 U_{eq} (C) for methyl hydrogen. Hydrogen atoms bonded to nitrogen (NH) were located in geometrically idealized positions and then fixed with d(N-H) = 0.90 Å and U_{iso}(H) = 1.2 Ueq (N). Due to non-ideal solvent masking, beam stop clipping and the minor presence of diffuse scattering, OMIT instruction was applied during structure refinement. In the crystal structure of **3,** one phenyl ring was found to be disordered. Based on the residual electron density located in this region, the disorder was successfully divided into two components (C31A-C36A, and C31B-C36B) using PART command, and a free variable was introduced for the occupancy refinements.

The occupancies of both components were constrained to sum to 1.0. In order to get reasonable geometry and ADPs for the disorder atoms, some structural and thermal parameter restraints (SADI, SIMU and ISOR) were adopted in the refinements. In the unit cell of compound **5**, there exists a large region of disordered solvent molecules, which could not be modeled as discrete atomic sites. PLATON/SQUEEZE[S12] was used to calculate the diffraction contribution of the solvent molecules to produce a set of solvent-free diffraction intensities. The SQUEEZE calculations showed a total solvent accessible area volume of 1013 $Å^3$ and the residual electron density amounted to 258 electron per unit cell, corresponding to nearly 5 molecules of n-hexane (about 0.55 n-hexane molecules per asymmetric unit). For comparison, the residual factors (R_1/wR_2) were 0.0677/0.2147 for the best disorder model, and 0.0559/0.1691 for the model squeezed, respectively. Details of the SQUEEZE calculations are included in its CIF file. Additionally, two tertiary butyl groups and one bromine atom were disordered, which were resolved with PART command and some restraints in geometry (DFIX and SADI) and thermal parameters (SIMU and ISOR) in the refinement. In cases of **6** and **7**, tertiary butyl groups were also disordered over two positions similar to the disorder model for **5.** These groups was treated analogously to that of **5**. In **6,** toluene is disordered and PART instruction was applied for solving this problem. Furthermore, the molecule, **7**, is fully disordered over two conformations across an inversion center, which give rise to the heavy disorder of the bicyclic moiety. PART -1 instruction was used to solve this problem. Restraints including ISOR and SIMU on displacement parameters were applied. The refinement results are summarized in **Table S1**.

Table S1. X-ray data for compounds **1-7**.

Compounds	**1**	**2**	**3**	**4•toluene**	**5**	**5-sq**	**6•(toluene)$_{1.5}$**	**7**
Formula	$C_{36}H_{28}B_2Br_2N_2$	$C_{24}H_{26}BBrN$	$C_{47}H_{46}B_2N_4$	$C_{66}H_{78}B_2N_4$	$C_{36}H_{60}B_2Br_2N_2$	$C_{36}H_{60}B_2Br_2N_2$	$C_{57.5}H_{90}B_2N_4$	$C_{38}H_{58}B_2N_2O_4$
Formula weight	670.04	419.18	688.50	949.94	702.30	702.30	858.95	628.48
Temperature (K)	173.00(10)	173.00(10)	172.98(10)	173.00(10)	173.00(10)	173.00(10)	172.99(10)	172.99(10)
Wavelength (Å)	1.54184	1.54184	0.71	1.54184	1.54184	1.54184	1.54184	1.54184
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic	trigonal	trigonal	triclinic	triclinic
Space group	I2/a	P21/n	P21/n	P21/n	R-3	R-3	P-1	P-1
a (Å)	18.5040(3)	13.4204(6)	11.2493(3)	11.75034(11)	32.9585(3)	32.9585(3)	11.7577(4)	9.0716(10)
b (Å)	17.9348(3)	13.4075(4)	26.0979(7)	23.8044(3)	32.9585(3)	32.9585(3)	13.9324(4)	9.8412(13)
c (Å)	19.6933(7)	13.5682(5)	13.6593(4)	19.95734(18)	9.9663(2)	9.9663(2)	18.6526(5)	11.5149(12)
α (°)	90	90	90	90	90	90	102.637(2)	76.803(10)
β (°)	108.694(2)	118.076(5)	109.818(3)	98.1553(9)	90	90	99.834(2)	82.173(9)
γ (°)	90	90	90	90	120	120	105.896(3)	68.411(11)
V (°)	6190.7(3)	2154.09(17)	3772.6(2)	5525.81(9)	9375.6(3)	9375.6(3)	2779.50(15)	929.1(2)
Z	8	4	4	4	9	9	2	1
Density (calcd. g/cm^{-3})	1.438	1.293	1.212	1.141	1.119	1.119	1.026	1.123
Absorption coeff. (mm^{-1})	3.526	2.635	0.069	0.489	2.621	2.621	0.432	0.549
Reflections collected	14639	11490	21327	31156	20723	20723	26499	8347
Independent reflections	5361	3751	6608	9650	3651	3651	9752	3616
	[R_{int} = 0.0876]	[R_{int} = 0.0480]	[R_{int} = 0.0449]	[R_{int} = 0.0359]	[R_{int} = 0.0194]	[R_{int} = 0.0194]	[R_{int} = 0.0545]	[R_{int} = 0.0532]
Data/restraints/parameters	5361/14/385	3751/1/253	6608/204/527	9650/0/668	3651/139/271	3651/139/271	9752/272/641	3616/1042/434
R_1 [I>2sigma(I)]	0.0730	0.0403	0.0451	0.0440	0.0677	0.0559	0.0752	0.0803
wR_2 [all data]	0.2527	0.1161	0.1224	0.1211	0.2147	0.1691	0.1965	0.2121
GOF	1.208	1.044	1.026	1.109	1.049	1.051	1.031	1.079
CCDC No	1977878	1977879	1977880	1977881		1977882	1977883	1977884

Computational details

Geometry optimizations were carried out with the Gaussian 09 package[S13] with the M06-2X functional.[S14] The Def2-SVP basis set was used for all the atoms. Frequency calculations at the same level of theory were performed to identify the number of imaginary frequencies (zero for local minimum and one for transition states) and provide the thermal corrections of Gibbs free energy. Transition states were submitted to intrinsic reaction coordinate (IRC) calculations to determine two corresponding minima.

The single-point energy calculations were performed at the M06-2X/Def2-TZVP level of theory for solution-phase (benzene). The gas-phase geometry was used for all the solution phase calculations. The SMD method was used with the corresponding solvent, while Bondi radii[S15] were chosen as the atomic radii to define the molecular cavity. The correction of Gibbs free energy from frequency calculations was added to the single-point energy to obtain the Gibbs free energy in solution. All the energies reported in the paper correspond to the reference state of 1 mol/L, 298K. Natural bond orbital (NBO) calculations were carried out using NBO 6.0 program[S16] at the M06-2X/TZVP level of theory. Intrinsic bond orbitals (IBOs) were carried out using ORCA program[S17] at the PBE/Def2-TZVP//M06-2X/Def2-SVP level of theory. The IEFPCM solvation model with n-hexane was used for these TD-DFT calculations.

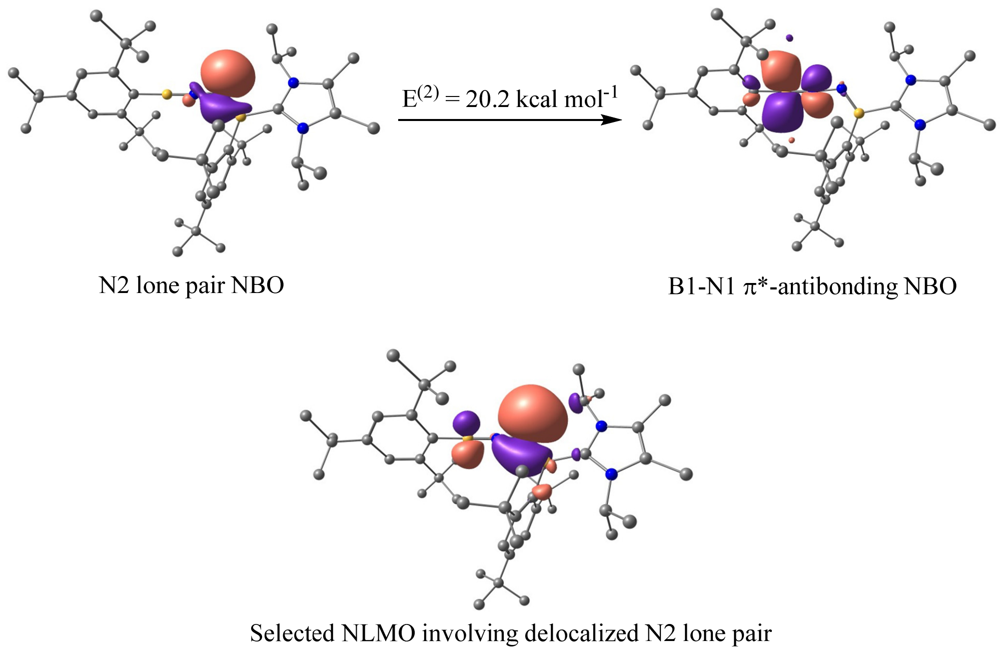


Fig. S33 Hyperconjugative delocalization and NLMO analysis of **6**.

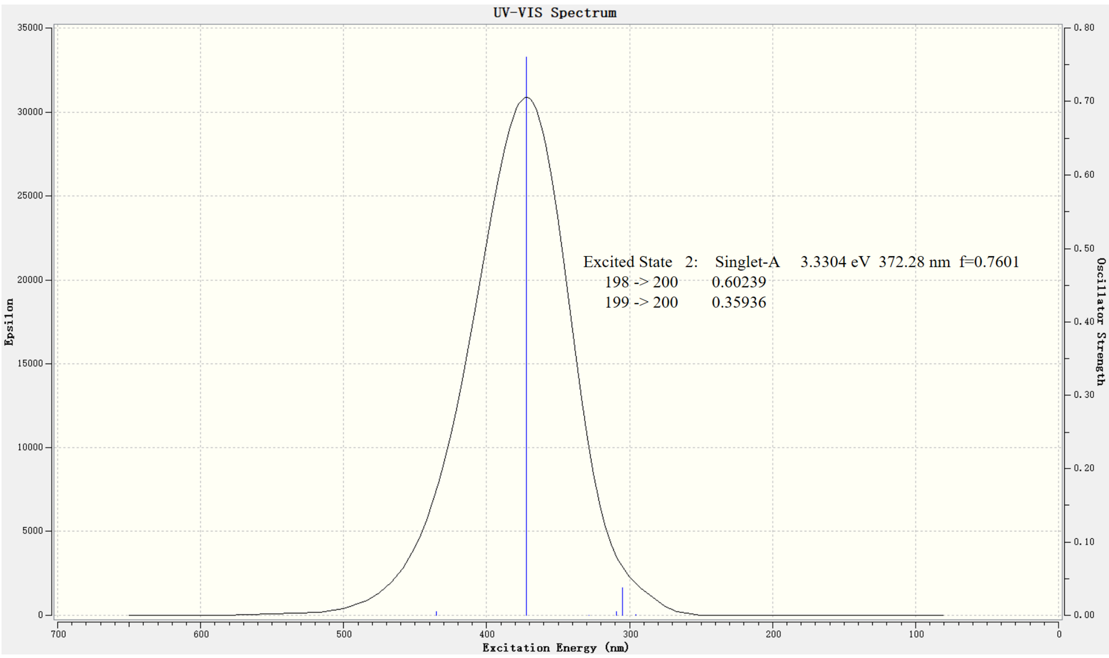


Fig. S34 Calculated UV-vis spectrum of **6** at TD-PBE1PBE/6-311G (d) and the IEFPCM solvation model with n-hexane was used for calculation.

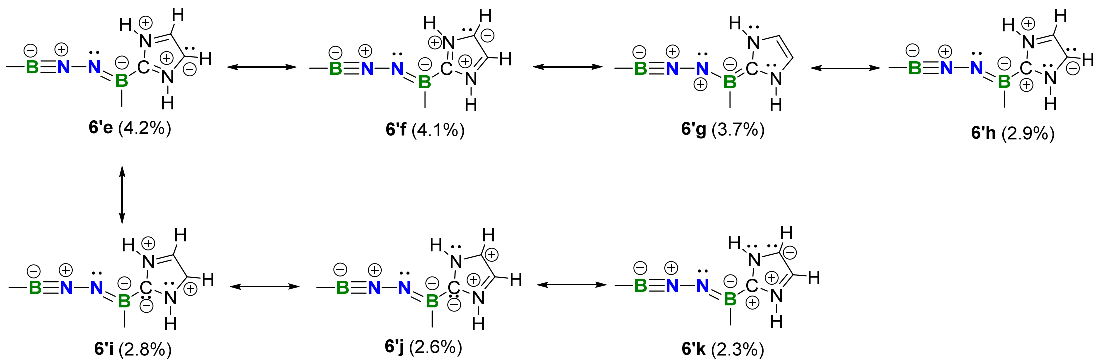


Fig. S35 Selected resonance structures and their weights for **6'** (continued).

Table S2. Selected Wiberg bond index of **6**.

Atom		1	2	3	4	5	6	7	8	9
1.	N	0.0000	0.0552	0.0023	0.0187	0.0002	0.0000	0.0050	0.0000	1.2809
2.	N	0.0552	0.0000	0.0025	0.0213	0.0002	0.0000	0.0012	0.0000	1.2718
3.	N	0.0023	0.0025	0.0000	1.1349	0.0278	0.0080	0.0030	0.0012	0.0176
4.	N	0.0187	0.0213	**1.1349**	0.0000	0.0052	0.0075	0.0200	0.0002	0.0365

Atom		37	38	39	40	41	42	43	44	45
1.	N	0.0080	0.0063	0.0000	0.0013	0.0039	0.0098	0.0000	0.0083	0.0018
2.	N	0.0011	0.0063	0.0000	0.0084	0.0039	0.0020	0.0000	0.0090	0.0107
3.	N	0.0001	0.0342	0.0066	0.0001	**1.8649**	0.0004	0.0000	0.0000	0.0001
4.	N	0.0018	**1.3535**	0.0014	0.0005	0.1440	0.0030	0.0001	0.0001	0.0007

Table S3. Selected NPA charges of **6**.

Atom No		Natural Charge	Natural Population Core	Valence	Rydberg	Total
N	3	**-0.65025**	1.99892	5.63360	0.01773	7.65025
N	4	**-0.72354**	1.99925	5.69619	0.02810	7.72354
B	38	**0.72712**	1.99859	2.24788	0.02641	4.27288
B	41	**0.81539**	1.99781	2.17036	0.01644	4.18461

Table S4. Energies of Intermediates and Transition States

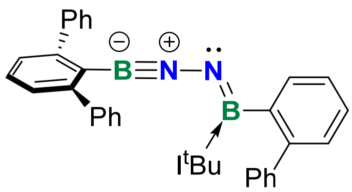
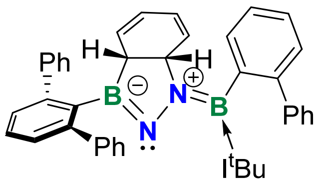
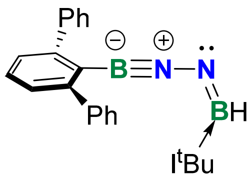
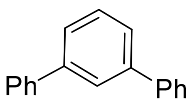
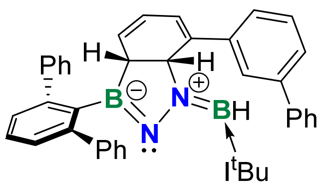
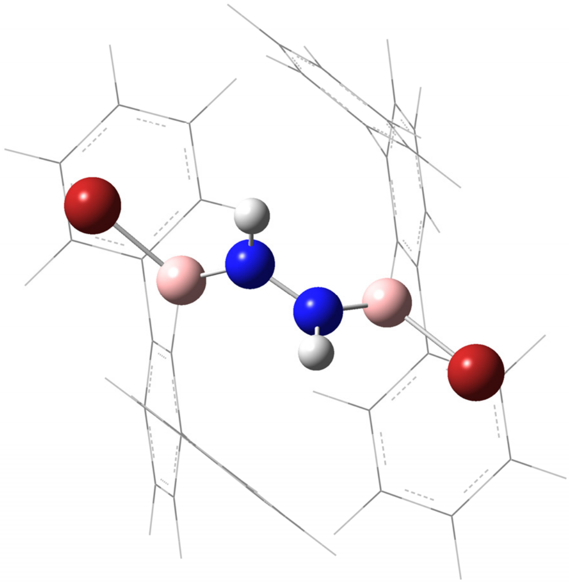
Species	Thermal Corrections of Gibbs Free Energies (Hartree)	Solvation Energies (Hartree)
1	0.485711	-6696.43869
I^{t}Bu	0.254943	-540.6494961
[I^{t}BuH][Br]	0.264865	-3115.517504
IN-3	0.750797	-2087.363379
TS	0.748181	-2087.335464
3	0.754881	-2087.390953
	0.673734	-1856.329993
benzene	0.074005	-232.2317873
TSa	0.769966	-2088.521796
	0.776209	-2088.56767
	0.518615	-1394.225975
	0.222868	-694.3287952
TSb	0.766153	-2088.524264
	0.771496	-2088.571862

Table S5. Calculated geometries (atom, x-, y-, z-positions in Å).

1.

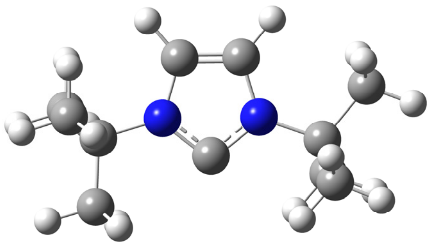


Br	3.38457900	0.80446500	1.12618200
N	0.69194900	0.02967200	1.47354100
C	0.94981300	1.86166300	-0.41549700
C	1.45483200	1.79049900	-1.73384300
C	0.99522500	2.67625900	-2.71484600
C	0.03003700	3.63087900	-2.41123700
C	-0.48084900	3.70764500	-1.11984000
C	-0.03003700	2.83781500	-0.11931800
C	-0.62656500	2.95545500	1.23872500
C	-2.02096800	2.94585600	1.38678800
C	-2.60095800	2.97722300	2.65343700
C	-1.79355800	3.02820200	3.79051300
C	-0.40502000	3.05835200	3.65259000
C	0.17523800	3.02601700	2.38527400
C	2.45954200	0.76151000	-2.12352200
C	3.69411000	1.15054000	-2.65665400
C	4.65295900	0.19701000	-2.98981200
C	4.38408400	-1.15939100	-2.80702400
C	3.14780100	-1.55605400	-2.29937400
C	2.19001700	-0.60239800	-1.95843200
B	1.48033200	0.87353700	0.69113700
N	-0.69194900	-0.02967200	1.47354100

Br	-3.38457900	-0.80446500	1.12618200
B	-1.48033200	-0.87353700	0.69113700
C	-0.94981300	-1.86166300	-0.41549700
C	-1.45483200	-1.79049900	-1.73384300
C	0.03003700	-2.83781500	-0.11931800
C	-0.99522500	-2.67625900	-2.71484600
C	-2.45954200	-0.76151000	-2.12352200
C	0.48084900	-3.70764500	-1.11984000
C	0.62656500	-2.95545500	1.23872500
C	-0.03003700	-3.63087900	-2.41123700
C	-3.69411000	-1.15054000	-2.65665400
C	-2.19001700	0.60239800	-1.95843200
C	2.02096800	-2.94585600	1.38678800
C	-0.17523800	-3.02601700	2.38527400
C	-4.65295900	-0.19701000	-2.98981200
C	-3.14780100	1.55605400	-2.29937400
C	2.60095800	-2.97722300	2.65343700
C	0.40502000	-3.05835200	3.65259000
C	-4.38408400	1.15939100	-2.80702400
C	1.79355800	-3.02820200	3.79051300
H	1.12341700	-0.57654200	2.17020700
H	-1.12341700	0.57654200	2.17020700
H	1.38864000	2.59105500	-3.72949600
H	-0.32742200	4.31416000	-3.18328800
H	-1.22871700	4.46248400	-0.86770600
H	-2.65269300	2.85758200	0.49962700
H	-3.68670800	2.93970200	2.75189800
H	-2.24534100	3.04602400	4.78336600
H	0.23155500	3.10908600	4.53734100
H	1.26279300	3.05395900	2.28128500
H	3.91009600	2.21391800	-2.77960000
H	5.61844400	0.51541900	-3.38638000
H	5.13587700	-1.90651100	-3.06612000
H	2.91756900	-2.61584100	-2.17322600
H	1.21796700	-0.91937200	-1.57231100
H	-1.38864000	-2.59105500	-3.72949600
H	1.22871700	-4.46248400	-0.86770600
H	0.32742200	-4.31416000	-3.18328800
H	-3.91009600	-2.21391800	-2.77960000
H	-1.21796700	0.91937200	-1.57231100
H	2.65269300	-2.85758200	0.49962700
H	-1.26279300	-3.05395900	2.28128500
H	-5.61844400	-0.51541900	-3.38638000

H	-2.91756900	2.61584100	-2.17322600
H	3.68670800	-2.93970200	2.75189800
H	-0.23155500	-3.10908600	4.53734100
H	-5.13587700	1.90651100	-3.06612000
H	2.24534100	-3.04602400	4.78336600

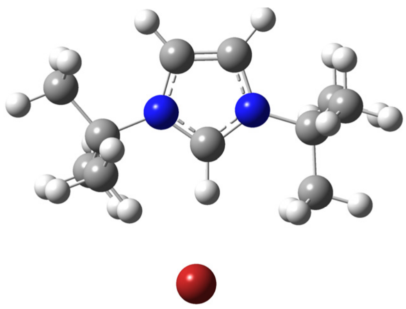
I^tBu



C	-2.17828200	0.80930700	5.47251500
C	-2.11239800	-0.54415700	5.52573300
H	-2.24476800	1.53109400	6.27872000
H	-2.11114100	-1.20870200	6.38437900
N	-2.14703700	1.14284100	4.12831100
N	-2.04259600	-0.97945800	4.21114900
C	-2.06355800	0.04778900	3.32431300
C	-1.97560400	-2.40936100	3.84266200
C	-1.86344100	-2.54036600	2.32696900
C	-0.74288300	-3.03057500	4.50680400
C	-3.25408100	-3.09898900	4.32832900
H	-2.72417800	-2.07799000	1.82887100
H	-0.96177900	-2.03738200	1.95597600
H	-1.81905100	-3.60839000	2.06801500
H	-0.80348900	-2.98005200	5.60371300
H	-0.65476100	-4.08873400	4.22214600
H	0.16630000	-2.50280100	4.18533500
H	-3.23679700	-4.16387500	4.05501200
H	-3.35963100	-3.02997200	5.42093700
H	-4.13403100	-2.63059500	3.86482400
C	-2.19705500	2.51169200	3.56286400
C	-0.91169000	2.75112600	2.76826800
C	-3.41612800	2.60689700	2.64352400
C	-2.31168100	3.53689900	4.68829600
H	-0.03469800	2.68372100	3.42906100
H	-0.81579500	1.98900200	1.98416300
H	-0.92979600	3.74962800	2.30730600

H	-4.33978600	2.42489600	3.21261200
H	-3.47247500	3.60680700	2.18892100
H	-3.34013100	1.84910900	1.85331800
H	-2.35061600	4.54367700	4.25039800
H	-3.22933700	3.38921100	5.27639800
H	-1.44390100	3.49613100	5.36288600

[I^{t}BuH][Br]



C	-0.27947600	-2.62934900	-0.00173700
C	-1.56575000	-2.18116100	-0.00191400
H	0.10394700	-3.64251600	-0.00258800
H	-2.49911900	-2.73403700	-0.00291300
N	0.53409200	-1.51865900	-0.00004800
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C	-2.70471200	0.09492300	0.00042700
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C	-3.51546400	-0.20650600	1.26194700
H	-1.61950000	1.78529500	0.88090300
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H	-3.11780600	2.19592800	0.00255600
H	-3.87122400	-1.24407800	-1.28537200
H	-4.39315900	0.45525400	-1.29220900
H	-2.90993700	-0.01565400	-2.15997500
H	-4.39378700	0.45243200	1.29303000
H	-3.87174700	-1.24686700	1.28284900
H	-2.91095100	-0.02026800	2.16051400
C	2.03456800	-1.47810200	0.00044500
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C	2.48433400	-0.73715200	1.26032900
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H	2.10904800	-1.24233000	-2.16174400
H	2.14408500	0.31045400	-1.23869100
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H	2.10758600	-1.24157000	2.16261600
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H	2.14352400	0.31091000	1.23907200
H	3.65227500	-2.87562700	0.00162600
H	2.23877500	-3.46280800	0.89874800
H	2.24003300	-3.46300200	-0.89726900
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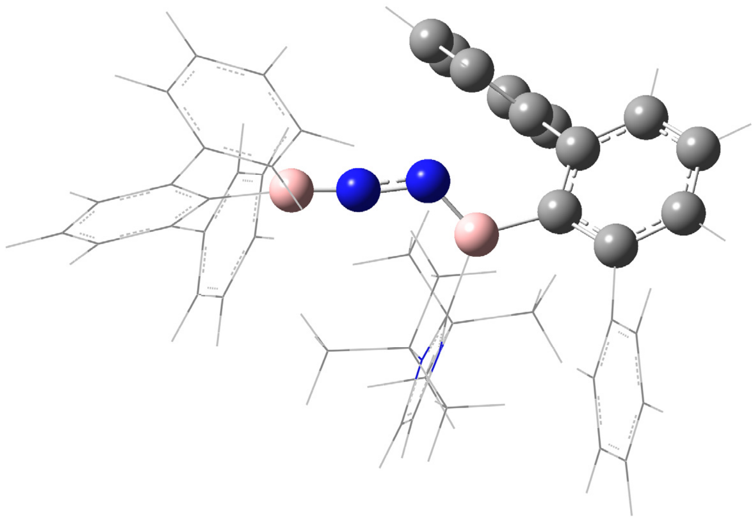

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C	-0.37585300	4.16381000	-3.24704500
C	0.92725400	3.75020300	-3.51181200
H	-2.40716800	3.53479600	-2.87117700
H	-0.61347100	5.22717200	-3.17860800
H	1.72046700	4.48775800	-3.64984800
N	1.04320400	-0.42897400	-0.56484800
N	-0.06525600	-0.28335600	-1.24570500
C	-2.26208200	0.90049300	-2.93985900
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C	-2.50799200	0.20251500	-1.72150100

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C	-4.69637000	-0.41712000	-2.65014600
H	-5.10853900	0.16486200	-4.68537000
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C	-1.49478900	1.08403600	2.95115100
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H	-1.53763400	1.86131800	3.70180000
H	-1.49655800	-0.85394300	4.01105000
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C	-4.33864000	-0.93839400	-0.29689600
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H	-4.94541000	-2.82406900	-1.14966600
C	-5.09060600	-0.56000900	1.99027000
H	-3.94447000	0.85025300	0.83041400
C	-5.74377700	-1.79186100	1.99811100
H	-6.18185800	-3.57596400	0.86306000
H	-5.13538100	0.09163400	2.86488500
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B	2.16989900	-0.58819100	-0.04725300
C	3.48301300	-0.83047500	0.72772900
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C	4.12391900	-2.09495000	0.75872100
C	5.11582000	-0.00959200	2.34844300
C	5.21259300	-2.29701600	1.61843200
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C	-2.53487700	3.06995300	0.21800200
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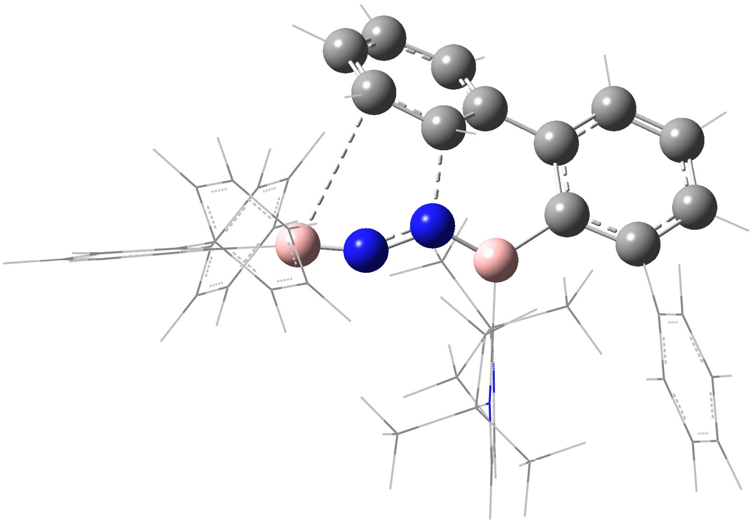
TS



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C	-1.98162600	1.27260200	-2.62525900
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H	-2.54574400	2.73144700	-4.11194900
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B	-1.34266400	-0.02896800	-0.51910900
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C	-2.22641900	0.74027600	3.08391600
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H	-4.47342500	-2.27343600	-1.79041100
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C	-5.97142900	-2.34726600	1.27217200
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C	3.01303800	4.16268000	2.16531100
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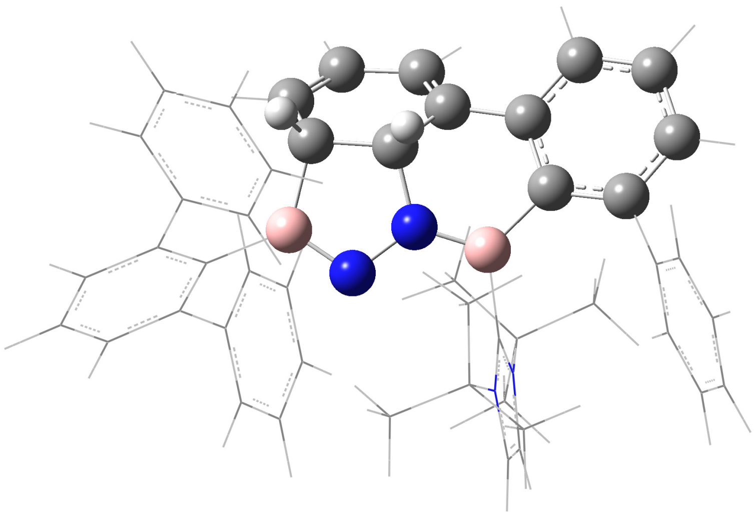
3



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H	-0.39489600	2.72564000	-3.90764000
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C	-1.87762600	0.71602500	-2.78512100
C	-2.71103100	1.03249300	-3.86226900
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C	-2.06848600	1.12506200	3.14794600
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H	-2.10891900	-0.80243800	4.22963400
N	-1.83705500	1.37207300	1.81228300
N	-1.75239700	-0.78147500	2.09504700
C	-1.66255200	0.19311500	1.16928500
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B	2.19051700	-0.14143700	-0.51672900
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H	4.81498600	-4.25894800	-3.79588300
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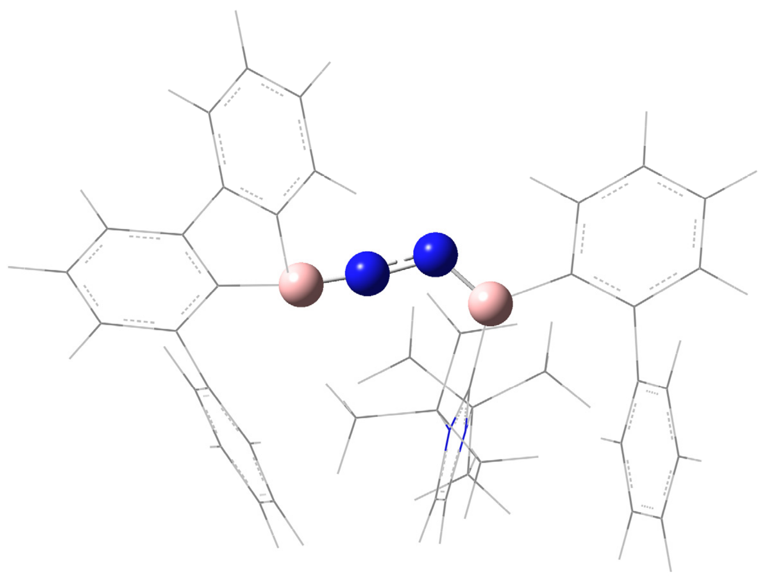

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C	-4.96938700	-0.30534700	0.74806600
C	-6.03100500	-0.43090600	-0.16867400
H	-6.68439900	-0.36741100	-2.22038900
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H	-1.93724200	-0.02769100	5.86249400
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C	-6.05407400	-1.67628800	2.54013900
C	-5.17387200	0.46994600	3.16412500
C	-6.55834800	-1.84905800	3.82816700
H	-6.20709700	-2.45145800	1.78602800
C	-5.66661100	0.29628800	4.45775500
H	-4.66929900	1.39757200	2.89812900
C	-6.36765900	-0.86120400	4.79436300
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B	1.20736500	-0.24730600	1.47136300
C	2.69792100	-0.43586700	1.82392700
C	3.40715700	0.53602400	2.56310300
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C	4.79600500	0.43880200	2.70573900
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H	5.33564000	-2.46512600	1.02700100
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C	1.56379200	-3.21255300	1.02583700
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C	1.42402300	-4.65643200	-0.90441200
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H	0.19206400	-1.66481500	3.62076000
H	-2.93609500	-3.44477500	4.81933400
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C	-2.00584300	3.02232600	2.33002900
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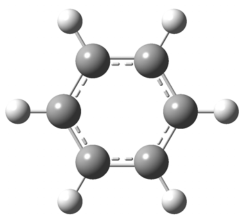

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C	0.16345400	5.01756800	-0.09962700
C	-1.23115600	5.01759900	-0.10002100
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H	0.70952000	5.96186600	-0.10008900
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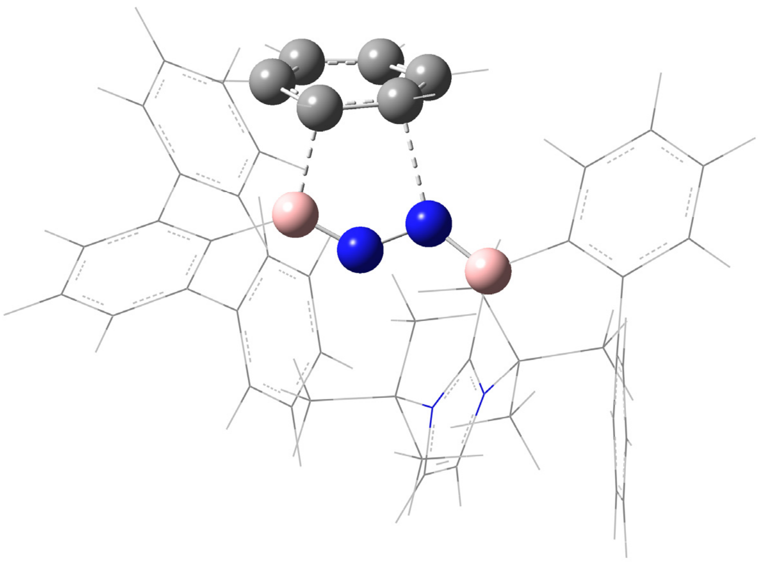
TSa



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H	1.70989900	3.91769800	-3.44679000
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C	-4.04685100	-0.57562200	-1.52514700
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H	-5.96936600	-1.05726900	-2.36750800
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H	0.18458100	-0.08667100	-3.59068500
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C	-1.48557400	-0.55612300	2.98660300
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H	5.72804400	-2.15640100	-2.34161800
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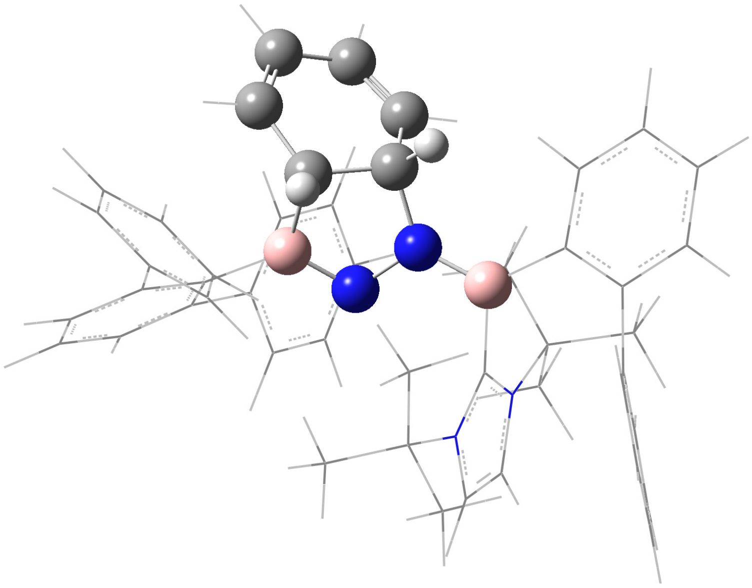

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C	2.62154100	-0.19458700	-3.10048000
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C	-3.83627800	1.49379500	-3.31691800
C	-2.84657700	0.66882200	-1.21278900
C	-5.06757400	0.94073300	-2.98129400
H	-3.70592000	2.03434200	-4.25565300

C	-4.12036000	0.13875800	-0.87367700
C	-5.19542700	0.27333700	-1.76867700
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H	-6.16263100	-0.14608600	-1.48430700
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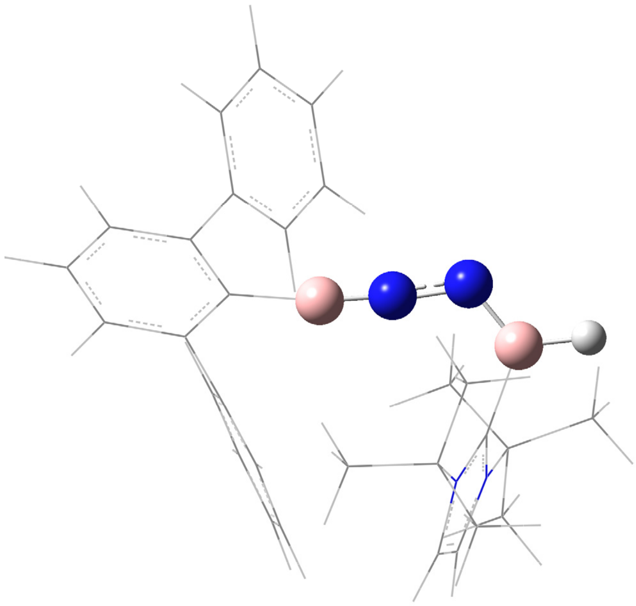

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H	0.04597900	1.69618100	8.53960000
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C	4.82312000	-0.72463700	5.07354400
C	4.44738800	-2.62890500	3.60651300
C	6.19466200	-1.00360800	5.06771700
C	5.82154400	-2.89549800	3.63138900
C	6.69475300	-2.08353300	4.34753600
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C	1.56673200	-4.87542600	2.56388400

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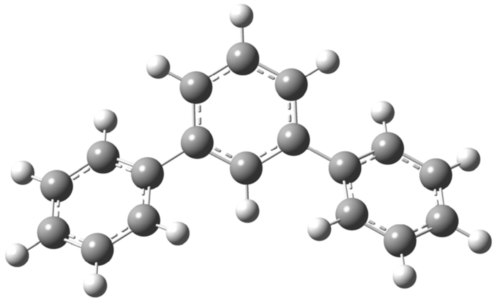

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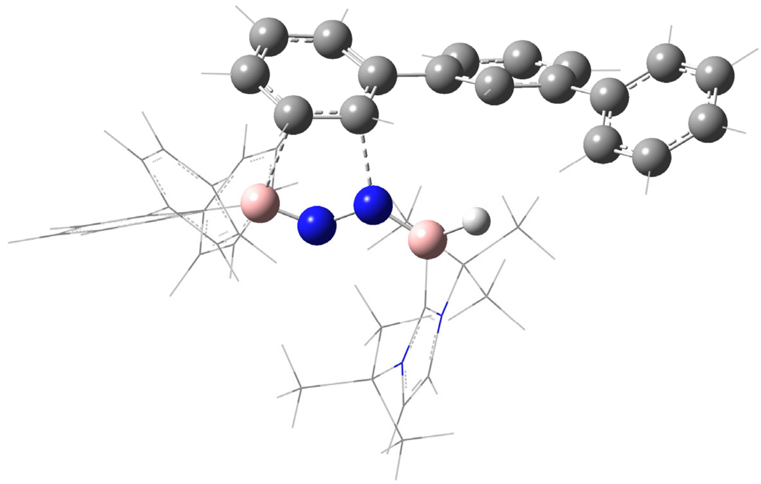
TSb



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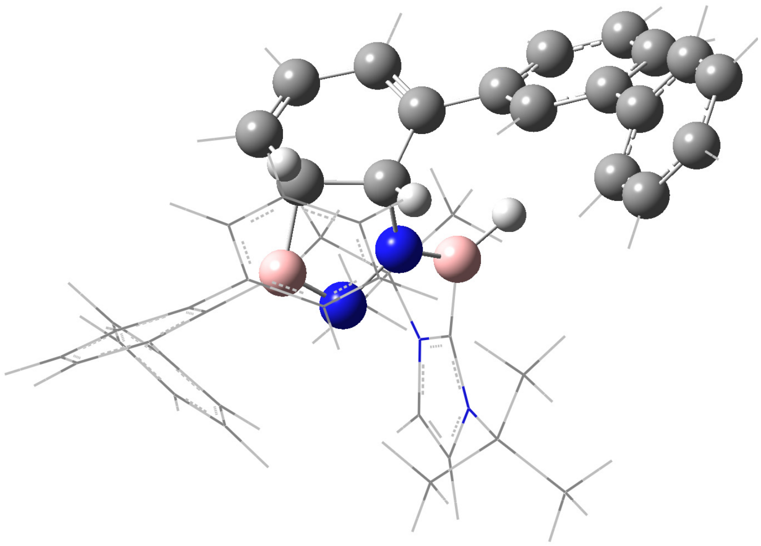

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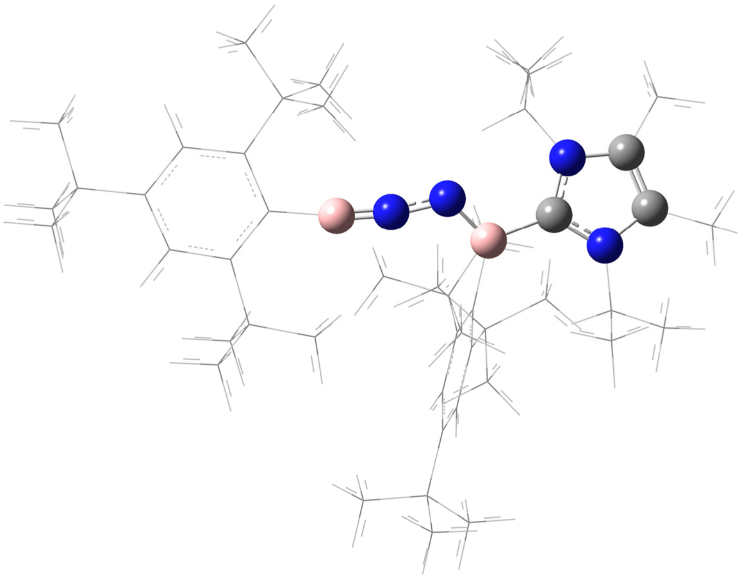
6



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H	9.07435025	-1.31520699	1.26431673
H	7.94955427	-2.48638295	0.54008931

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