Electronic Supplementary Material (ESI) for ChemComm.

Consecutive reduction, radical-cyclization, and oxidative-dehydrogenation reaction of ortho-substituted diboryl compound

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Contents

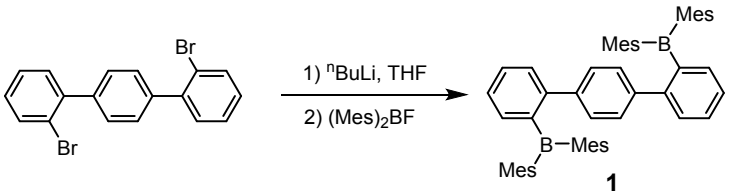
Experimental Section

All reactions and manipulations were carried out under an argon atmosphere by using standard Schlenk techniques and a glovebox. CD_3CN was dried by 4Å molecular sieve (2-3 days). Prior to use, the THF were dried by refluxing with sodium and benzophenone and degassed by applying four freeze-pump-thaw cycles. The 2,2"-dibromo-1,1':4',1"-terphenyl was synthesized according to literature methods.[S1] The ^{1}H and ^{13}C NMR spectra were performed using a JEOL JNM-ECS-400 or INOVA 600NB (Bruker) at room temperature in ppm downfield from Me_4Si. The ^{11}B NMR spectra were also recorded using a JEOL JNM-ECS-400 at room temperature in ppm downfield from external aqueous BF_3•Et_2O. The cyclic voltammetry experiment was conducted in an argon-filled atmosphere using a CHI 760e Electrochemical Workstation. Freshly distilled THF was used as solvent and $^{n}Bu_4NPF_6$ (10^{-1} M) was used as electrolyte. A standard three-electrode cell configuration was employed using a platinum-disk working electrode, a platinum-wire counter electrode, and a silver wire serving as the reference electrode. Formal redox potentials were referenced to the ferrocene/ferrocenium redox couple [$E(Fc/Fc^{+}) = 0$ V]. EPR spectra were obtained using Bruker ER200DSRC10/12 apparatus. The ESI mass spectra were recorded on a Thermo Scientific Orbitrap Elite mass spectrometer (LTQ Orbittrap Elite). UV-vis-NIR spectra were recorded on Agilent Carry 5000 UV-Vis-NIR spectrometer. The IR spectra were performed with a Nicolet 360 FTIR spectrometer in the region 4000–400 cm^{-1} using KBr pellets. Elemental analyses for C and H were carried out with a German Elementary Vario EL cube instrument.

X-ray Crystallography

The data were collected with a SuperNova (Dual) X-ray diffractometer that equipped with Cu/Mo Kα radiation (λ = 1.54184/0.71073 Å) at low temperature (173 K). Data reduction was performed using CrysAlis^{Pro} (Version 1. 171. 37. 35). The data sets were corrected by empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.[S2] Crystals structures were solved by direct methods using Olex 2-1.2. Subsequent difference Fourier analyses and least squares refinement with SHELXL-2014/7 program package[S3] allowed for the location of the atom positions. Non-hydrogen atoms were refined with anisotropic displacement parameters during the final cycles. All hydrogen atoms were found in difference maps and refined using a riding model. More details on the crystallographic studies as well as atomic displacement parameters are given in CIF files. The crystallographic details for compounds **1**, **1a**, **1b** and **2a** are

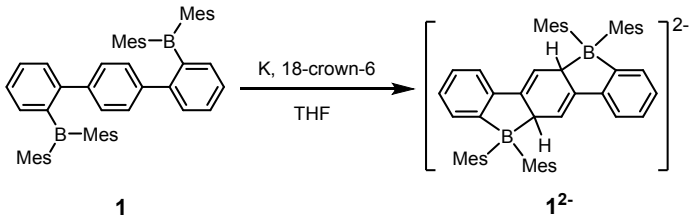
summarized in Table S1. The data have been deposited in the Cambridge Crystallographic Data Centre (CCDC), deposition numbers CCDC 1544754–1544757 for compounds **1**, **1a**, **1b** and **2a**.



Scheme S1. Synthesis of compound **1**

Synthesis of 2,2''-bis(dimesitylboranyl)-1,1':4',1''-terphenyl (1):

Under anaerobic and anhydrous conditions, ^{n}BuLi (8.2 mL, 13.1 mmol, 1.6 M in hexanes) was added dropwise to a stirred THF solution of 2,2''-dibromo-1,1':4',1''-terphenyl (2.48 g, 6.4 mmol) at -78 ^{o}C for 2 h, then Mes_2BF (3.43 g, 12.8 mmol) in THF (15 mL) was slowly added. Subsequently, the reaction mixture was slowly warmed up to room temperature and stirred overnight. After the addition of water, the solution was then extracted with dichloromethane. The crude product was then purified by column chromatography (CH_2Cl_2:hexane = 10:1) to afford **1** in 68 % yield (3.18 g). M. p.: 280-282 ^{o}C. UV-vis-NIR (THF): λ_{max} = 311, 253 and 233 nm; ^{1}H NMR (400 MHz, $CDCl_3$, ppm, 293 K) δ 7.47 (td, J = 8.0 Hz, J = 1.6 Hz, 2H, Ar-*H*), 7.37 (d, J = 8.0 Hz, 2H, Ar-*H*), 7.30 (d, J = 8.0 Hz, 2H, Ar-*H*), 7.07 (d, J = 8.0 Hz, 2H, Ar-*H*), 6.68 (s, 4H, Ar-*H*), 6.57 (s, 8H, Ar-*H*), 2.18 (s, 12H, -CH_3), 1.90 (s, 24H, -CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, ppm, 293 K) δ 148.90, 147.05, 142.91, 141.67, 140.27, 138.30, 135.28, 130.71, 129.30, 128.05, 127.00, 126.76, 23.29, 21.20; ^{11}B NMR (128.3 MHz, $CDCl_3$, 293 K): δ 72.6 ppm. MS (ESI): $[M]^+$ m/z 726.46. Elemental analysis: Calcd. for $C_{54}H_{56}B_2$: C 89.26, H 7.77 %; Found: C 88.95, H 7.63 %. IR (KBr, cm^{-1}): 2935 (br), 1604 (s), 1555 (s), 1462 (s), 1436 (s), 1370 (s), 1284 (m), 1246 (s), 1208 (s), 1208 (s), 1174 (m), 1152 (s), 1028 (m), 848 (s), 758 (s), 733 (m), 692 (m).

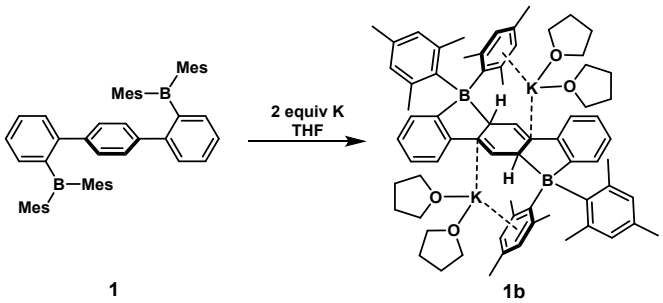


Scheme S2. Synthesis of complex **{[K(THF)$_2$(18-C-6)]$^+$}$_2$·1^{2-}**

Synthesis of {[K(THF)$_2$(18-C-6)]$^+$}$_2$·1^{2-} (1a):

Under anaerobic and anhydrous conditions, a mixture of **1** (0.145 g, 0.200 mmol), 18-crown-6 (0.106 g, 0.400 mmol) and excess potassium (0.039 g, 1.00 mmol) in THF (≈ 40 mL) was stirred

at room temperature for 1 day. The resultant blue solution was filtered to remove the excess K. The filtrate stored at room temperature to afford X-ray-quality colorless crystals of **1a** salts. Yield: 68.9 mg (21 %). M. p. 270 °C (dec.); ^{1}H NMR (400 MHz, CD_3CN, ppm, 293 K) δ 7.28 (s, 2H, Ar-*H*), 7.09 (d, *J* = 8.0 Hz, 2H, Ar-*H*), 6.67 (t, *J* = 4.0 Hz, 2H, Ar-*H*), 6.60 (t, *J* = 4.0 Hz, 2H, Ar-*H*), 6.51 (s, 4H, Ar-*H*), 6.29 (s, 4H, Ar-*H*), 5.93 (s, 2H, -C*H*=C), 3.64 (m, 4H, O-CH_2, THF), 3.54 (s, 48H, O-CH_2, 18-C-6), 2.98 (br, 2H, B-C*H*), 2.15-2.00 (m, 36H, -CH_3), 1.80 (m, 4H, O-CH$_2$-CH_2, THF); The lack of THF may be due to vacuum treatment of sample. ^{13}C NMR (150 MHz, CD_3CN, ppm, 293 K) δ 146.7, 134.0, 130.2, 129.8, 128.5, 123.9, 122.8, 120.8; 70.0 (18-C-6); 68.3 (THF); 26.3 (THF); 20.9, 20.8 (-*C*H$_3$); Two signals for the carbon atoms bound to the boron atom were not observed due to the quadrupolar relaxation.^{11}B NMR (128.3 MHz, CD_3CN, ppm, 293 K) δ -4.64. MS (ESI): [(**1**$^{2-}$)-(H$^-$)]$^-$ m/z 725.44. Elemental analysis: Calcd. for $C_{94}H_{136}B_2K_2O_{16}$: C 69.61, H 8.45 %; Found: C 68.96, H 8.03 %. IR (KBr, cm^{-1}): 3448 (br), 2910 (s), 1655 (m), 1462 (s), 1351 (s), 1278 (m), 1246 (m), 1099 (s), 959 (m), 833 (m), 750 (m).

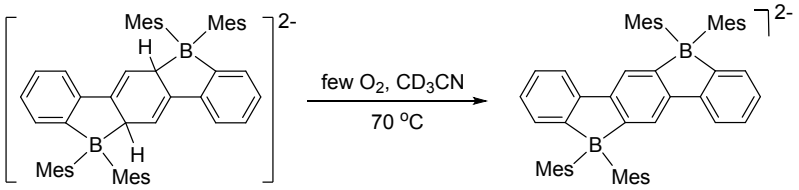


Scheme S3. Synthesis of complex **{[K(THF)$_2$]$^+$}$_2$·1^{2-}**

Synthesis of {[K(THF)$_2$]$^+$}$_2$·1^{2-} (1b):

Under anaerobic and anhydrous conditions, a mixture of **1** (0.145 g, 0.200 mmol) and excess potassium (0.039 g, 1.00 mmol) in THF (≈ 40 mL) was stirred at room temperature for 1 day. The resultant blue solution was filtered to remove the excess K. The filtrate stored at room temperature to afford colorless solid of **1b**. X-ray-quality colorless crystals of **1b** were collected by vapor diffusion of hexane to its saturated THF solution. Yield: 41.9 mg (19 %). ^{1}H NMR (400 MHz, CD_3CN, ppm, 293 K) δ 7.26 (s, 2H, Ar-*H*), 7.09 (d, *J* = 8.0 Hz, 2H, Ar-*H*), 6.68 (t, *J* = 4.0 Hz, 2H, Ar-*H*), 6.61 (t, *J* = 4.0 Hz, 2H, Ar-*H*), 6.51 (s, 4H, Ar-*H*), 6.31 (s, 4H, Ar-*H*), 5.94 (s, 2H, -C*H*=C), 3.64 (m, 16H, O-CH_2, THF), 2.98 (br, 2H, B-C*H*), 2.15-2.01 (m, 36H, -CH_3),, 1.80 (m, 16H, O-CH$_2$-CH_2, THF); The lack of THF may be due to vacuum treatment of sample. ^{13}C NMR (150

MHz, CD_3CN, ppm, 293 K) δ 146.8, 133.4, 130.2, 129.8, 129.1, 128.5, 124.0, 123.0, 120.8; 68.3 (THF); 26.2 (THF); 20.9, 20.7 (-*C*H_3); Two signals for the carbon atoms bound to the boron atom were not observed due to the quadrupolar relaxation. ^{11}B NMR (128.3 MHz, CD_3CN, ppm, 293 K) δ -4.64. MS (ESI): [(**1**$^{2-}$)-(H^-)]$^-$ m/z 725.44. Elemental analysis: Calcd. for $C_{72}H_{94}B_2K_2O_4$: C 76.90, H 8.11 %; Found: C 76.12, H 7.83 %. IR (KBr, cm^{-1}): 3455 (br), 2960 (m), 1659 (m), 1610 (m), 1424 (s), 1267 (s), 1204 (m), 1092 (s), 1022 (s), 805 (s), 763 (m), 666 (m).



Scheme S4. Synthesis of complex **{[K(THF)$_2$(18-C-6)]$_2$}$^{2+}$·2^{2-}**

Synthesis of [K(THF)$_2$(18-C-6)]$_2^{2+}$·2^{2-} (2a):

Under anaerobic and anhydrous conditions, the CD_3CN solution of **1a** (6.0 mg, 3.40×10^{-3} mmol) with trace amount of O_2 was heated at 70 °C for 4 hours, then continued to react for two days at room temperature. Subsequently, this CD_3CN solution was used directly for the NMR measurement that shows product **2a** was synthesized with 90 % NMR yield. Then, the solvent was removed under vacuum to afford a white solid. The obtained solid was further purified through recrystallization in THF. In the purification process, X-ray-quality colorless crystals of **2a** were also obtained. Although these crystals were used for the ^{1}H and ^{13}C NMR characterization, the result ^{1}H NMR spectrum is still slightly complex. ^{1}H NMR (400 MHz, CD_3CN, ppm, 293 K) δ 7.03 (d, *J* = 8.0 Hz, 2H Ar-*H*), 6.93 (s, 2H, Ar-*H*9), 6.82 (m, 3H, Ar-*H*), 6.72 (m, 3H, Ar-*H*), 6.37 (s, 8H, Mes-*H*), 3.55 (m, 8H, O-CH_2, THF), 3.47 (s, 48H, O-CH_2, 18-C-6), 2.05 (s, 12H, -CH_3), 1.77 (s, 24H, -CH_3), 1.71 (m, 16H, O-CH$_2$-CH_2, THF); ^{13}C NMR (150 MHz, CD_3CN, ppm, 293 K) δ 147.2, 142.7, 137.9, 131.7, 129.2, 128.7, 125.1, 123.3; 70.9 (18-C-6); 68.3 (THF); 27.0 (THF); 26.3, 26.0 (-*C*H_3); ^{11}B NMR (128.3 MHz, CD_3CN, ppm, 293 K) δ -0.26.

[S1] A. Velian, S. Lin, A. J. M. Miller, M. W. Day, T. Agapie, *J. Am. Chem. Soc.* **2010**, *132*, 6296–6297.

[S2] (1) *CrysAlisPro*, version 171.34.44; Oxford Diffraction Ltd.: Oxfordshire, U.K., **2010**. (2) Clark, R. C. & Reid, J. S. (**1995**). Acta Cryst. A51, 887–897.

[S3] (1) Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (**2009**), J. Appl. Cryst. 42, 339-341. (2) Sheldrick, G. M. (**2008**). Acta Cryst. A64, 112-122. (3) Sheldrick, G. M. (**2015**). Acta Cryst. C71, 3-8.

Table S1. Crystal data and structure refinement.

	1·CHCl$_3$	**1a·2THF**	**1b·2THF**	**2a·2THF**
Formula	$C_{56}H_{58}B_2Cl_6$	$C_{102}H_{152}B_2K_2O_{18}$	$C_{78}H_{104}B_2K_2O_6$	$C_{94}H_{134}B_2K_2O_{16}$
Mr [g mol^{-1}]	965.34	1766.05	1237.43	1619.82
Crystal system	*Monoclinic*	*Triclinic*	*Triclinic*	*Triclinic*
Space group	*P21/n*	P-*1*	P-*1*	P-*1*
Z	2	1	1	1
μ (mm^{-1})	0.375	0.157	0.187	0.171
a (Å)	15.3919(7)	12.8138(5)	12.2166(9)	12.0148(10)
b (Å)	8.1281(4)	13.8501(6)	12.8705(12)	12.4531(11)
c (Å)	20.3055(13)	16.3243(7)	13.0567(12)	15.4631(15)
α (°)		104.712(4)	72.277(8)	95.007(8)
β (°)	92.736(5)	107.141(4)	70.112(7)	105.069(8)
γ (°)		103.546(4)	67.341(8)	93.255(7)
V [Å^3]	2537.4(2)	2523.5(2)	1745.6(3)	2217.9(4)
F(000)	1012	956	668	874
Index ranges	-17 ≤ h ≤ 20, -10 ≤ k ≤ 9, -18 ≤ l ≤ 27	-15 ≤ h ≤ 15, -16 ≤ k ≤ 17, -20 ≤ l ≤ 19	-14 ≤ h ≤ 15, -15 ≤ k ≤ 14, -15 ≤ l ≤ 16	-14 ≤ h ≤ 9, -14 ≤ k ≤ 14, -17 ≤ l ≤ 18
Reflections collected	10772	18549	12129	12982
Independent reflections	5767 [R_{int} = 0.0394, R_{sigma} = 0.0703]	9906 [R_{int} = 0.0352, R_{sigma} = 0.0713]	6847 [R_{int} = 0.0471, R_{sigma} = 0.1001]	7780 [R_{int} = 0.0998, R_{sigma} = 0.2432]
Data/rest./para.	5767/0/295	9906/60/610	6847/0/407	7780/0/523
GOF	1.034	1.045	1.025	0.995
Final R indexes [I≥2σ (I)]	R_1 = 0.0602, wR_2 = 0.1290	R_1 = 0.0894, wR_2 = 0.2362	R_1 = 0.0673, wR_2 = 0.1448	R_1 = 0.0926, wR_2 = 0.1500
Final R indexes [all data]	R_1 = 0.0957, wR_2 = 0.1554	R_1 = 0.1337, wR_2 = 0.2779	R_1 = 0.1273, wR_2 = 0.1830	R_1 = 0.2134, wR_2 = 0.2156
CCDC Number	1544754	1544755	1544756	1544757

Table S2. Experimental structural parameters for **1, 1a, 1b** and **2a**.

	1	**1a**	**1b**	**2a**
B1-C1	1.579(4)	1.662(5)	1.661(4)	1.678(8)
B1-C10	1.586(4)	1.681(5)	1.668(5)	1.657(8)
B1-C19	1.582(4)	1.655(5)	1.670(4)	1.661(8)
B1-C8	3.282[a]	1.710(5)	1.728(4)	1.635(8)
C6-C7	1.481(3)	1.477(4)	1.478(4)	1.467(7)
C7-C8	1.398(3)	1.510(5)	1.513(4)	1.422(8)
C7-C9	1.395(3)	1.329(4)	1.339(4)[b]	1.403(7)
C8-C9’	1.382(4)	1.504(4)	1.498(4)[c]	1.400(6)
C1-C6	1.423(3)	1.413(5)	1.411(4)	1.406(7)
C1-C2	1.410(4)	1.410(5)	1.401(4)	1.405(7)
Hybridization mode of B1	sp^2	sp^3	sp^3	sp^2
∑ angles to C7 (°)	360	359.7	359.9	360
Hybridization mode of C8	sp^2	sp^3	sp^3	sp^2

[a] The distance of B1 and C8. [b] The bond length of C7-C9’. [c] The bond length of C8-C9.

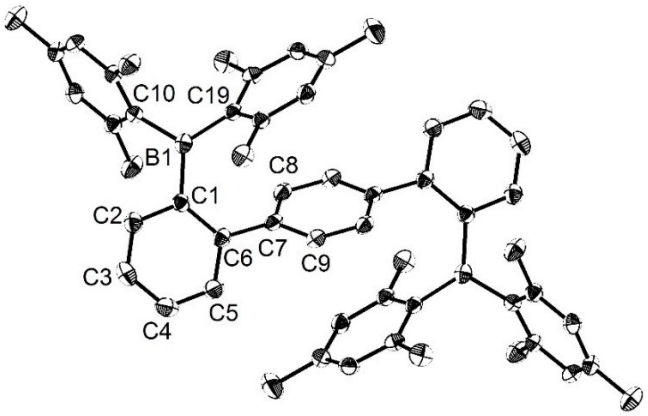


Fig. S1 Thermal ellipsoid (50%) drawings of **1**, all H atoms have been omitted for clarity. Selected bond lengths (Å) and angles (°): B1-C1 1.579(4), B1-C10 1.586(4), B1-C19 1.582(4), C6-C7 1.481(3), C7-C9 1.395(3), C7-C8 1.398(3), C8-C9’ 1.382(4), C1-C6 1.423(3), C1-B1-C10 118.3(2), C1-B1-C19, 122.7(2), C10-B1-C19 119.0(2).

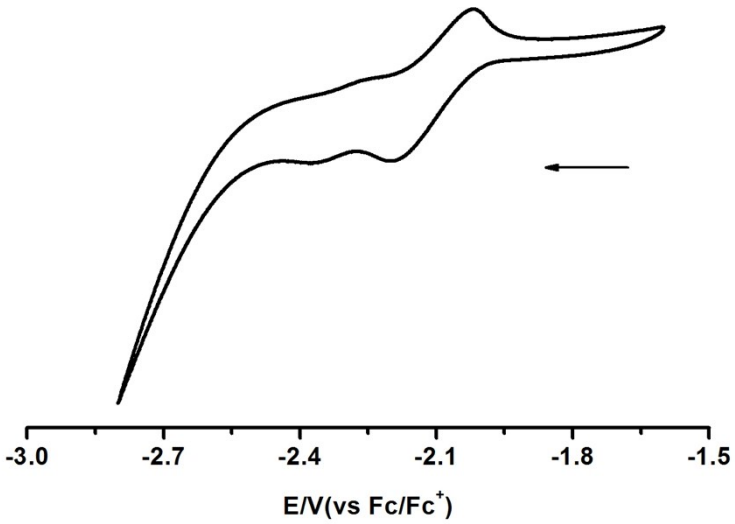


Fig. S2 Cyclic voltammogram of **1** (5×10^{-3} M) in THF, containing 0.1 M $^{n}Bu_4NPF_6$ measured at 100 mV s^{-1} at room temperature.

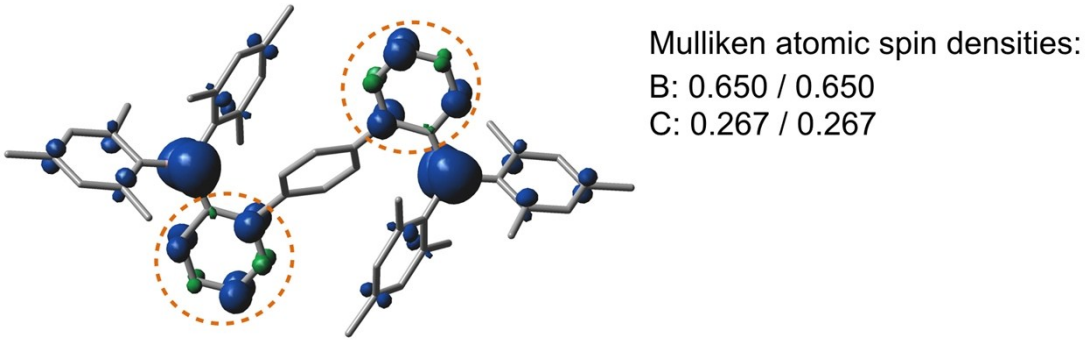


Fig. S3 Spin density distribution of triplet $[\mathbf{1}^{\cdot\cdot}]^{2-}$ (isovalue = 0.005 au), along with the Mulliken atomic spin densities for the two boron atoms and the carbon atoms of the adjacent benzene moiety (within dashed circle).

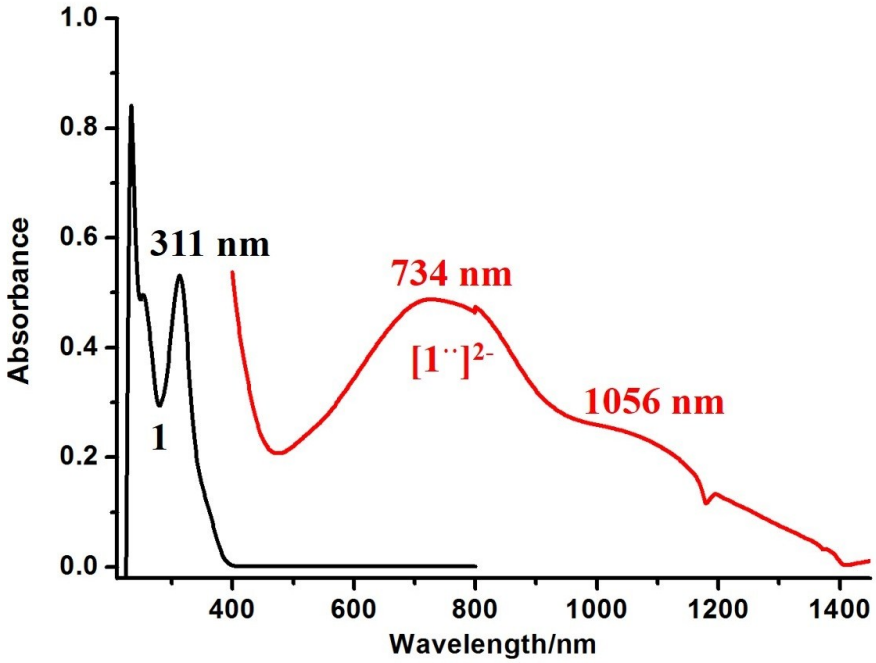


Fig. S4 UV-Vis spectra of **1** (black line) and **[1"]**$^{2-}$ (red line) measured in THF solution (5 × 10^{-4} M) at room temperature.

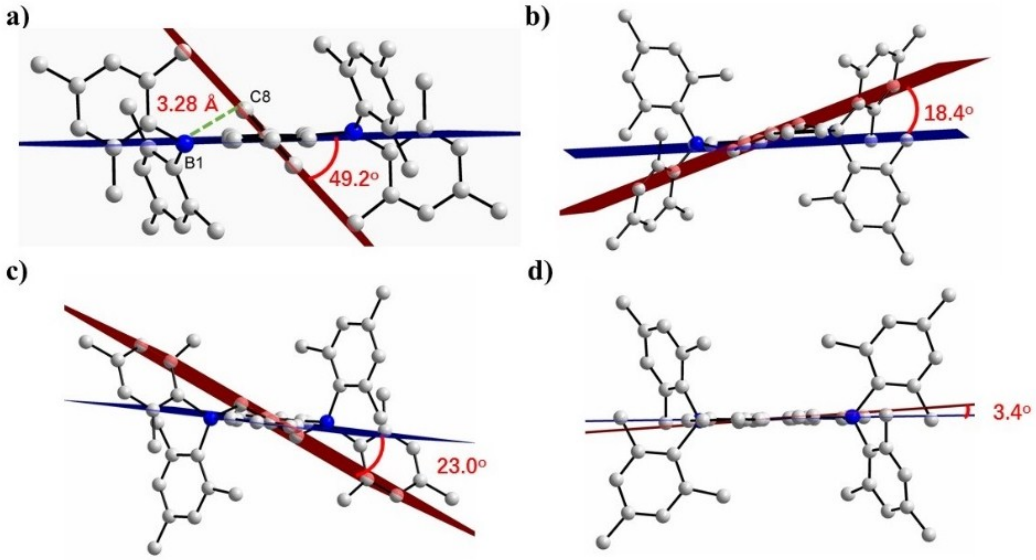


Fig. S5 The dihedral angles were measured between the benzene ring C1-C6 and the six-membered plane C7C8C9C7'C8'C9' in **1** (a), **1a** (b), **1b** (c) and **2a** (d), which came from the crystal data. The red and blue planes represent the six-membered ring C7C8C9C7'C8'C9' and benzene ring C1-C6, respectively.

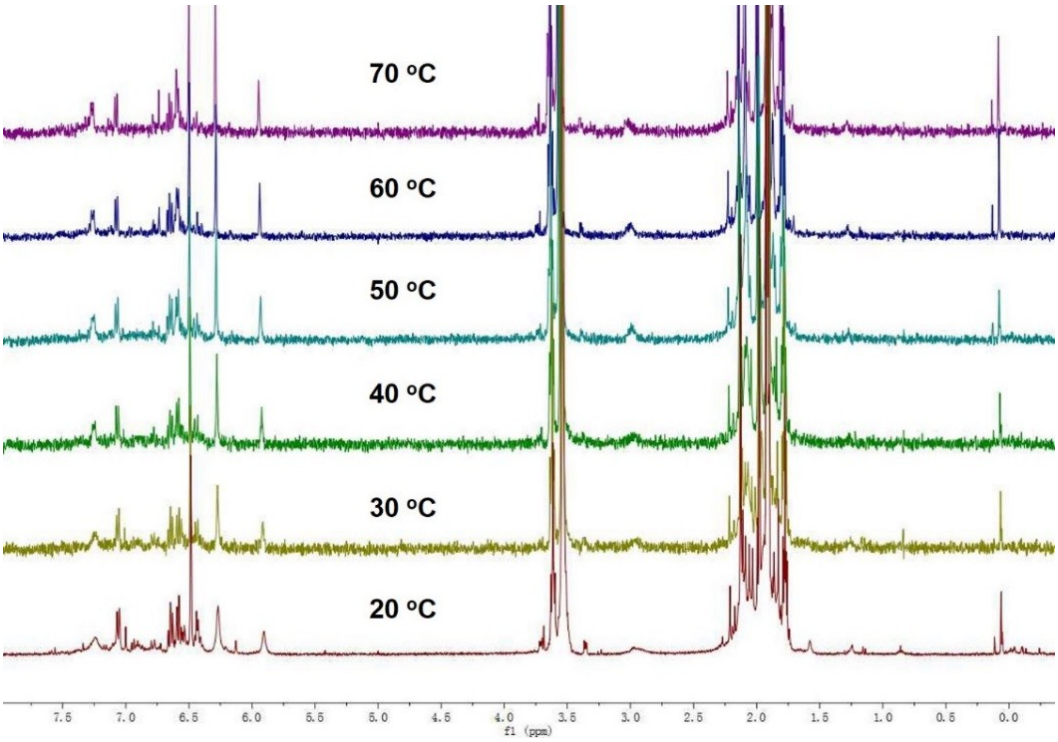


Fig. S6 The VT-NMR spectra of **1a** were measured from 20 °C to 70 °C in CD_3CN solution. The time interval for each collecting spectra of **1a** is 6 minutes.

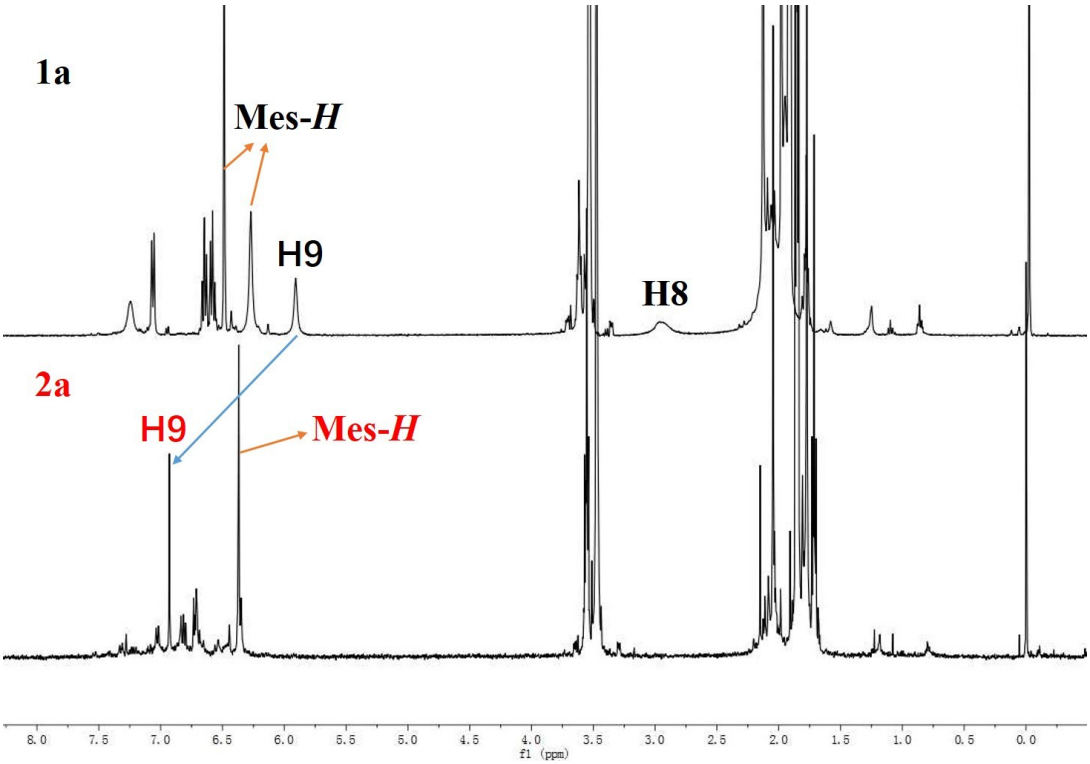


Fig. S7 The changes of characteristic hydrogen signals of **1a** and **2a** in ^1H NMR spectra. The peaks of H8 (or H8'), H9 (or H9') and Mes-*H* have obviously varied upon the dehydrogenation process was occurred.

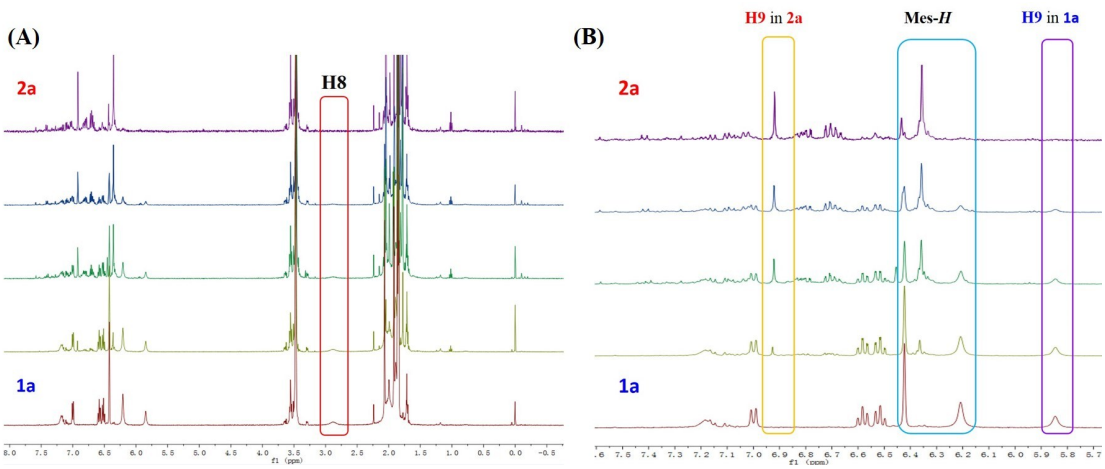


Fig. S8 The dehydrogenation process of **1a** was verified by monitoring its ^{1}H NMR spectra. A) The changes of ^{1}H NMR spectra of **1a** in CD_3CN solution with different reaction times. Reaction conditions: (a) The spectrum of **1a** in CD_3CN solution; (b) React for 12 hours at room temperature after heating 30 min; (c) React for 12 hours at room temperature after heating 30 min; (d) React for 12 hours at room temperature after heating 30 min; (e) React for 12 hours at room temperature after heating 30 min. B) The enlarged signals of aromatic region were displayed. The original signals of H8 (or H8') and H9 (or H9') gradually disappeared in **1a** and was gradually replaced by the new peak of H9 (or H9') at δ = 6.93 ppm in **2a**, indicating H8 and H8' atoms have left and aromatization of the 1,4–cyclohexadiene unit has occurred. Meanwhile, the signals of Mes-*H* also changed due to the changes of molecular geometry.

Computational Details

All the geometry optimizations were carried out at the (U)CAM-B3LYP/6-31G(d) level of theory. The obtained stationary points were characterized by frequency calculations. The broken-symmetry approach was applied for open-shell singlet calculations. The spin densities were calculated at the optimized geometries at the (U)CAM-B3LYP/6-311+G(d,p) level with the PCM solvent (THF) model. The NICS values were calculated at the (U)B3LYP/6-31+G(d) level with gauge independent atomic orbital (GIAO) method. The global ring centers for NICS(0), NICS(1) and $NICS(1)_{ZZ}$ values were designated at the non-weighted mean centers of and 1 Å above/below the central bridging benzenoid rings of $\mathbf{2}^{2-}$. Above/below plane NICS(1) or $NICS(1)_{ZZ}$ values were similar so the average values were reported. All calculations were performed with the Gaussian 09 program suite.[S4]

[S4] Gaussian 09, Revision B.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kieth, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; and Fox, D. J., Gaussian, Inc., Wallingford CT, 2010.

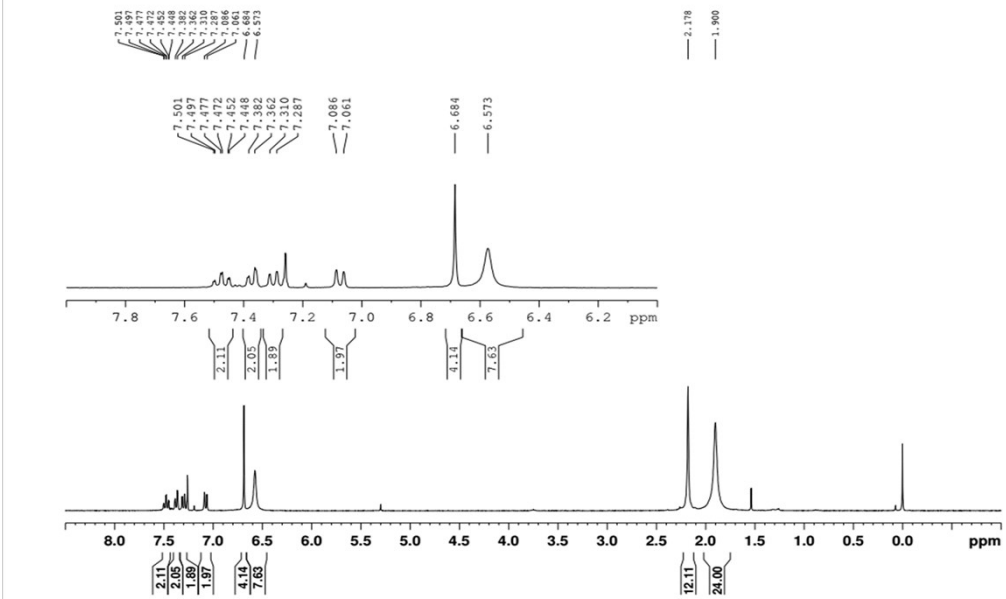


Fig. S9 The ^{1}H NMR spectrum of **1** in $CDCl_3$.

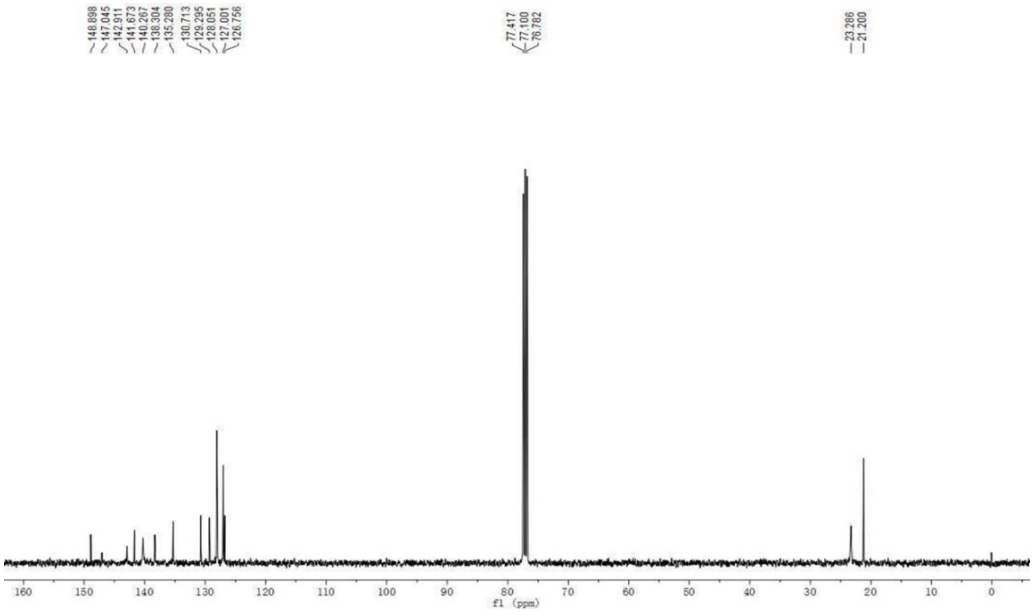


Fig. S10 The ^{13}C NMR spectrum of **1** in $CDCl_3$.

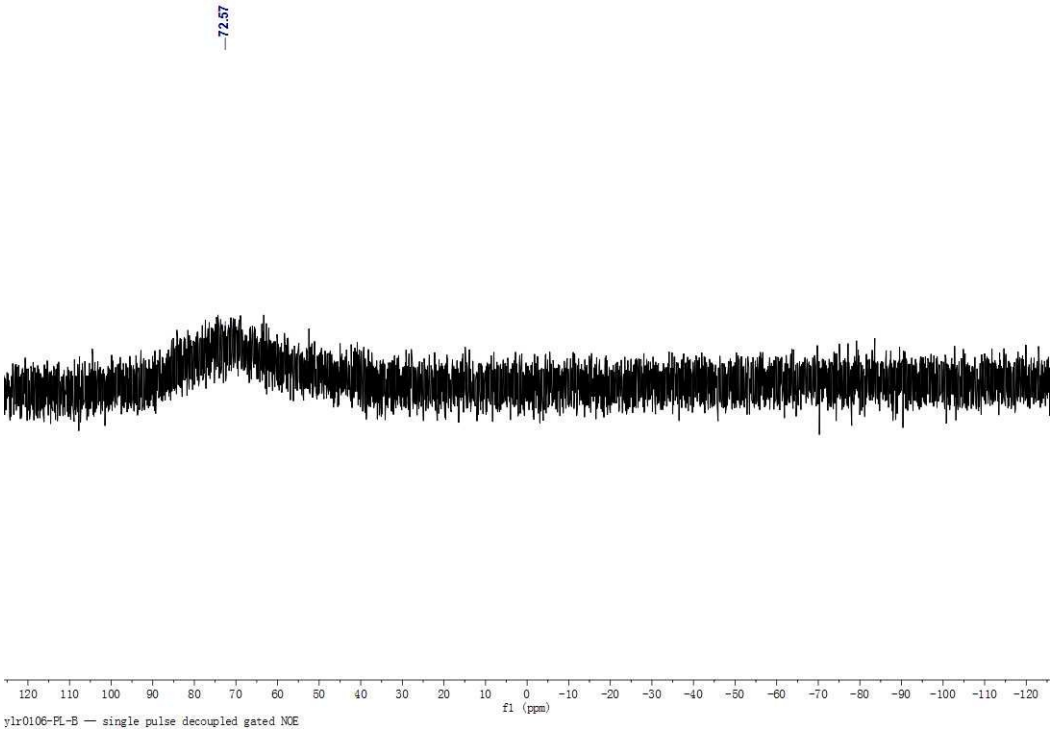


Fig. S11 The ^{11}B NMR spectrum of **1** in $CDCl_3$.

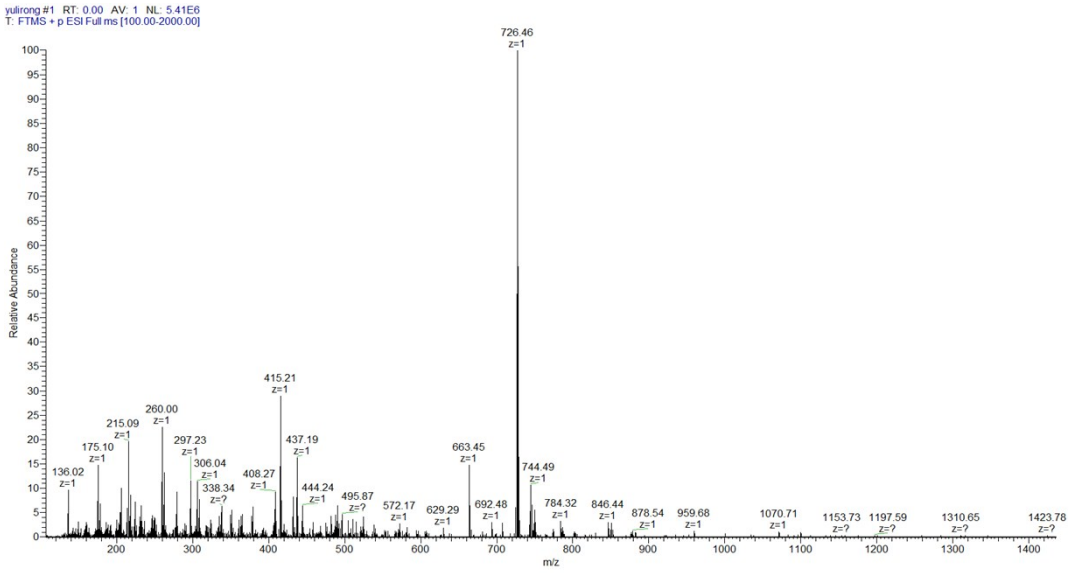


Fig. S12 ESI mass spectrum of **1** ($[M]^+$: m/z = 726.46) was recorded in $CHCl_3$.

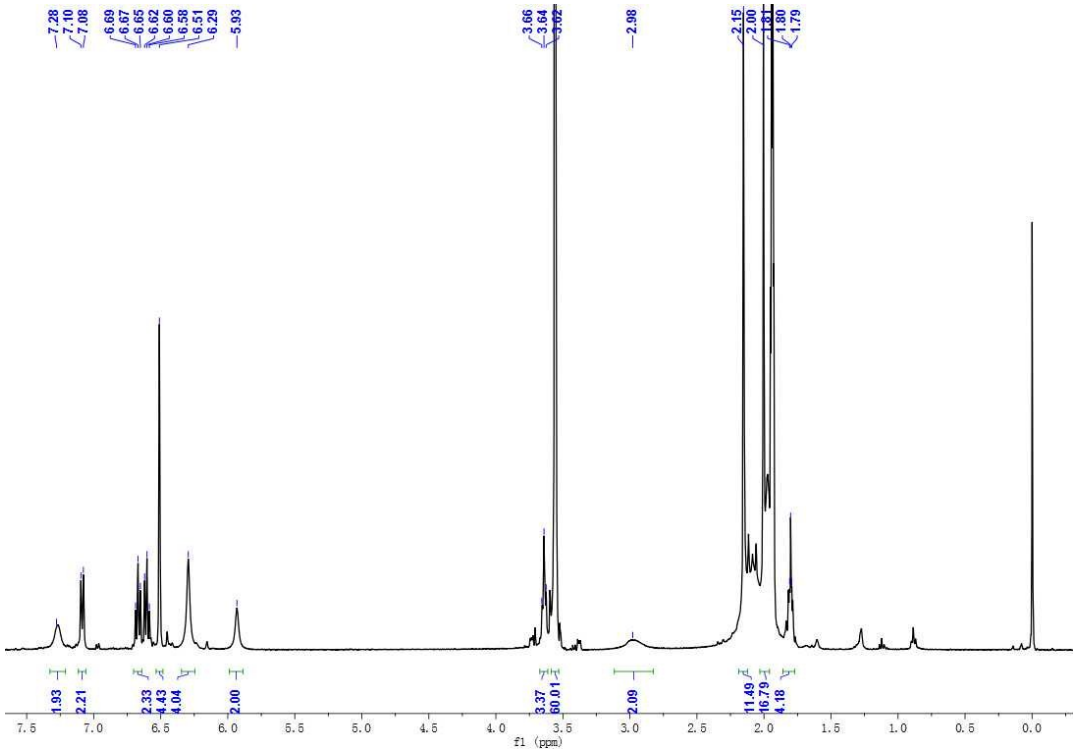


Fig. S13 The ^{1}H NMR spectrum of **1a** in CD_3CN. The lack of THF may be caused by vacuum treatment of sample **1a**.

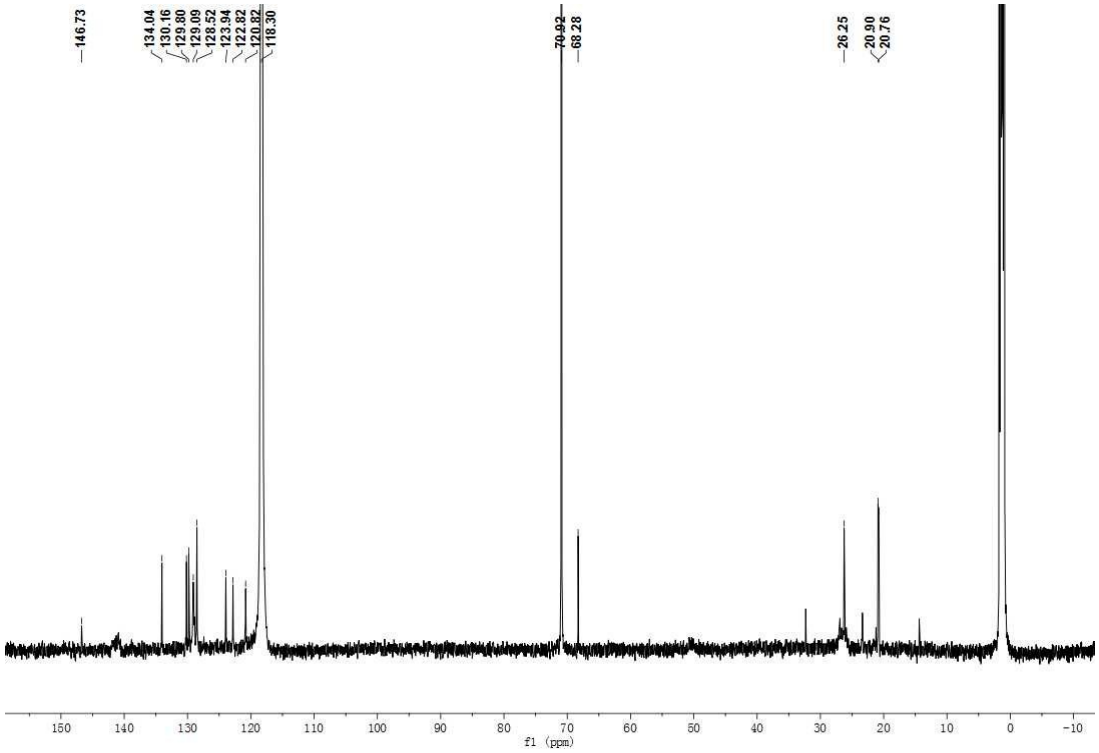


Fig. S14 The ^{13}C NMR spectrum of **1a** in CD_3CN.

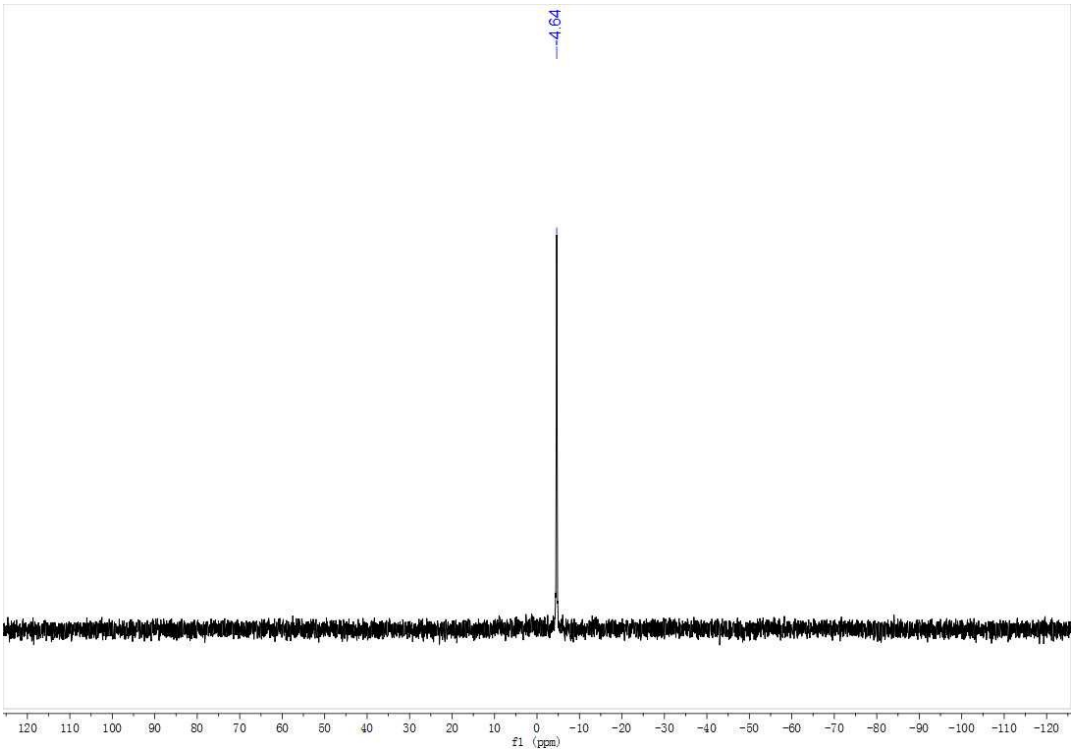


Fig. S15 The ^{11}B NMR spectrum of **1a** in CD_3CN.

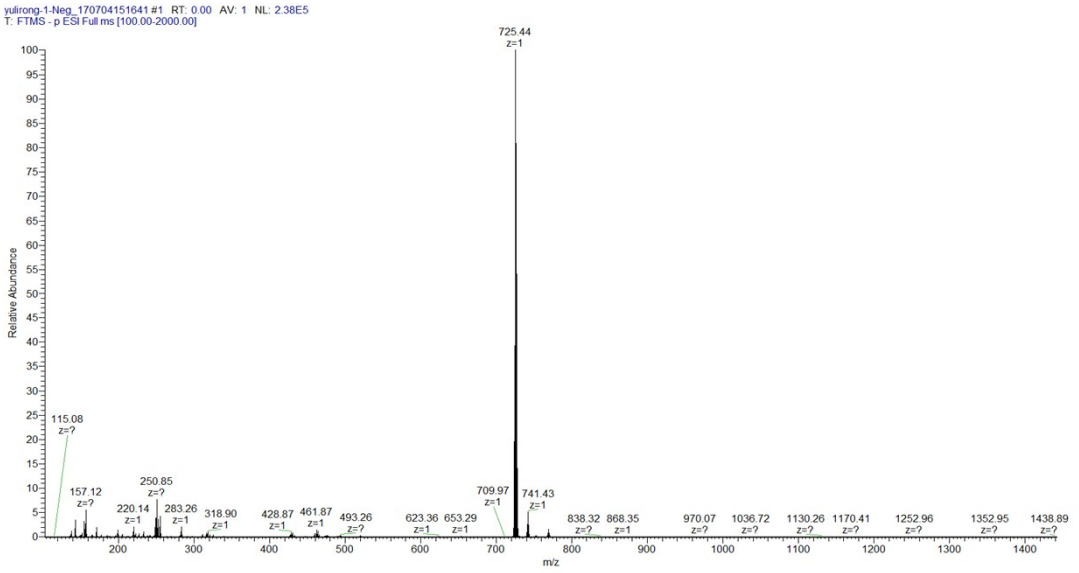


Fig. S16 Negative ion mass spectrum (ESI) of **1a** ($[(\mathbf{1}^{2-})\text{-}(H^-)]^-$: m/z = 725.44) was recorded in CD_3CN.

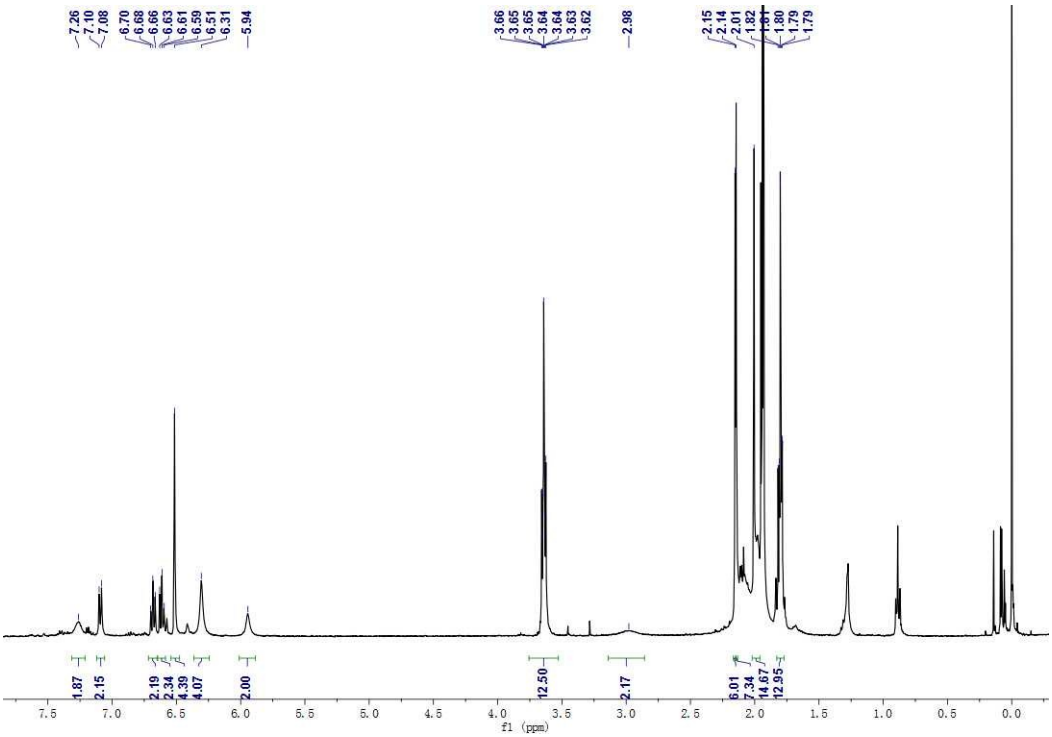


Fig. S17 The ^{1}H NMR spectrum of **1b** in CD_3CN.

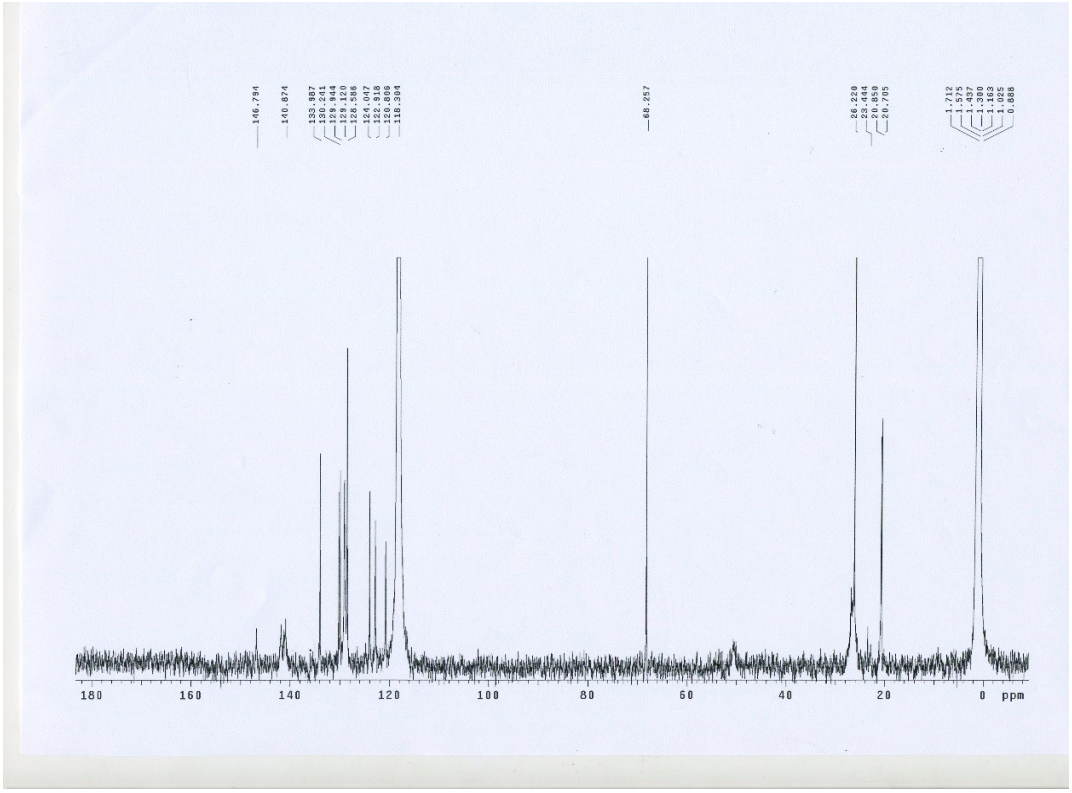


Fig. S18 The ^{13}C NMR spectrum of **1b** in CD_3CN.

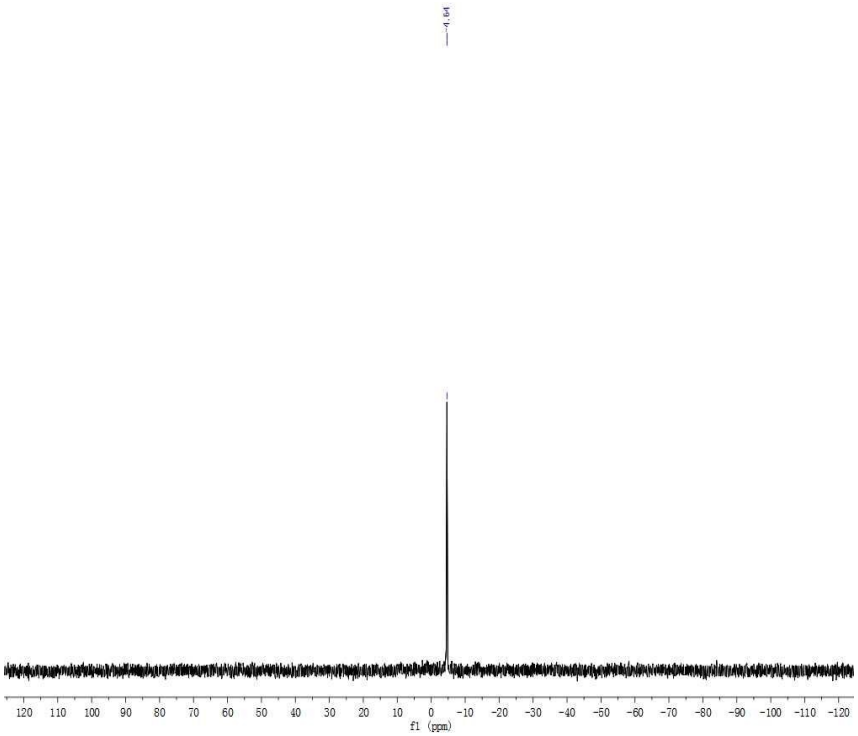


Fig. S19 The ^{11}B NMR spectrum of **1b** in CD_3CN.

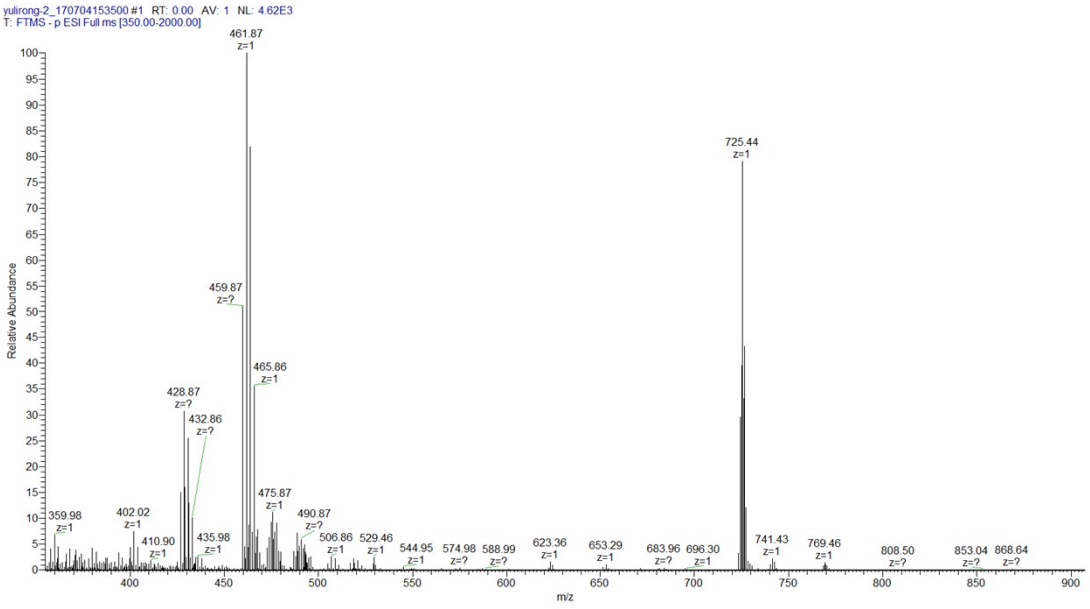


Fig. S20 Negative ion mass spectrum (ESI) of **1b** ($[(\mathbf{1}^{2-})\text{-}(H^-)]^{\cdot-}$: m/z = 725.44) was recorded in CD_3CN.

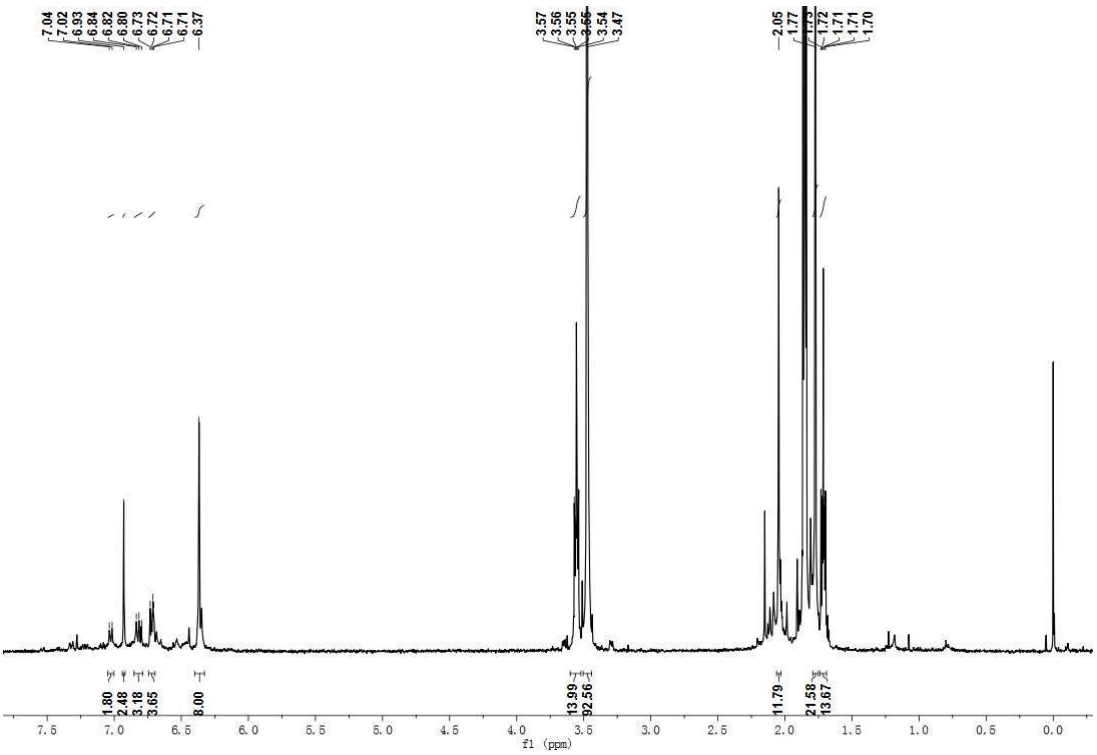


Fig. S21 The ^{1}H NMR spectrum of **2a** in CD_3CN.

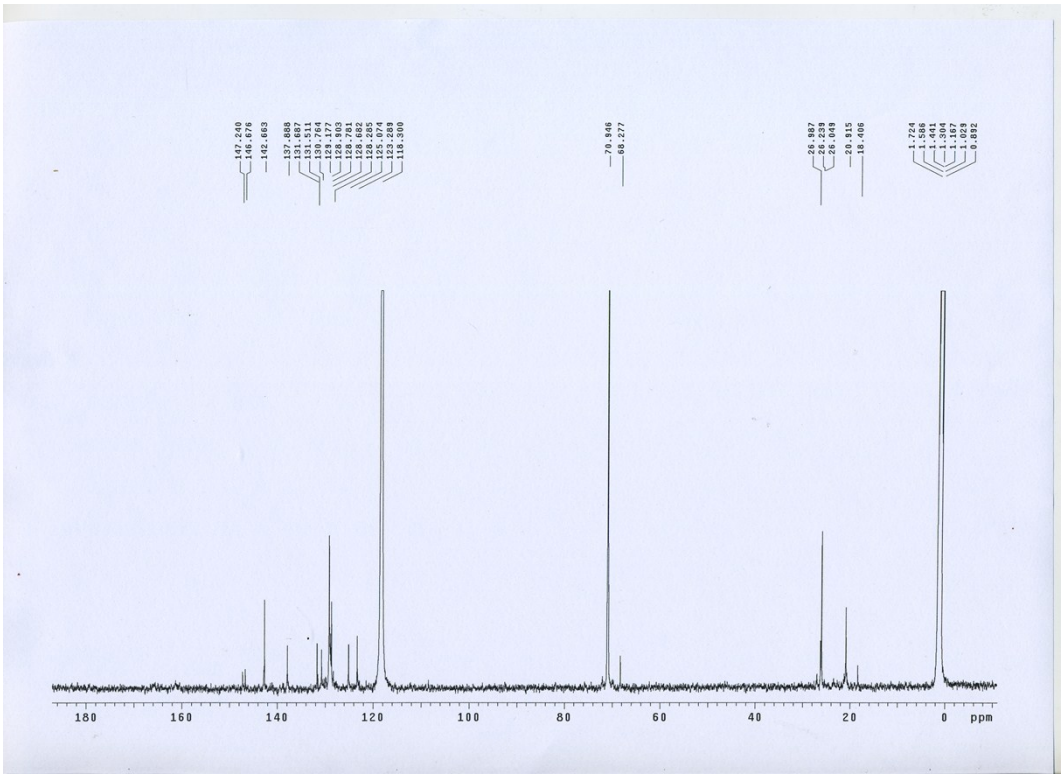


Fig. S22 The ^{13}C NMR spectrum of **2a** in CD_3CN.

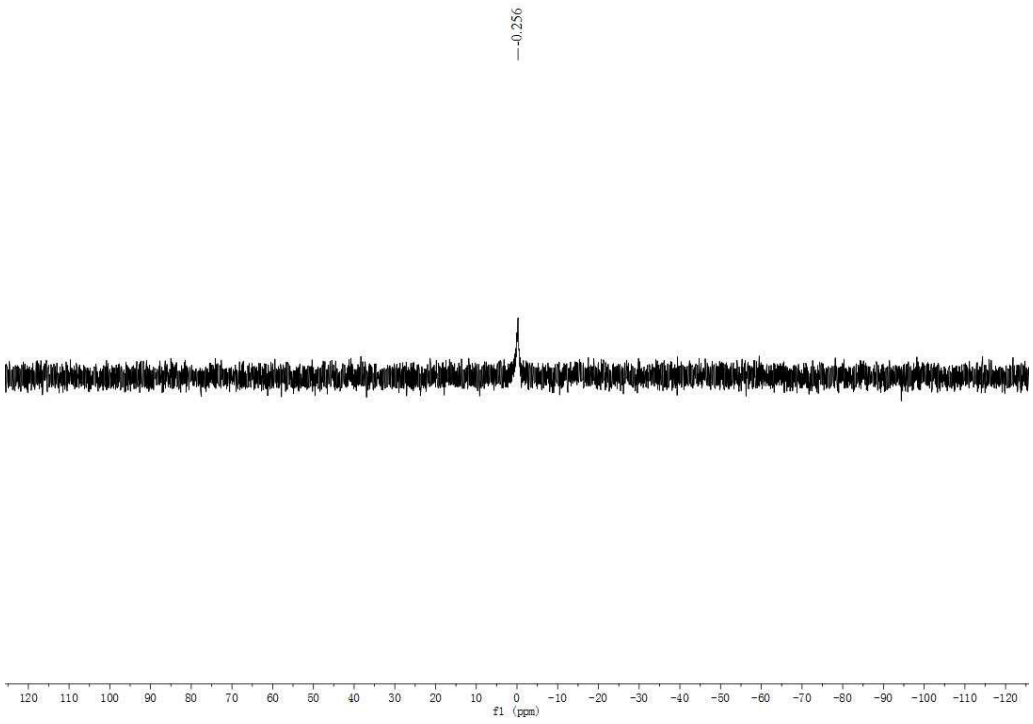


Fig. S23 The ^{11}B NMR spectrum of **2a** in CD_3CN.

Coordinates for calculated geometries

1

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C	-2.831742000	-2.207499000	1.431129000
C	-3.379338000	-3.303159000	2.120694000
H	-4.449862000	-3.320831000	2.301463000
C	-2.606411000	-4.371490000	2.556252000
H	-3.071368000	-5.207783000	3.069402000
C	-1.235388000	-4.352509000	2.339215000
H	-0.612136000	-5.172086000	2.684710000
C	-0.656424000	-3.265840000	1.696291000
H	0.421026000	-3.226088000	1.565237000
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C	0.182433000	-1.293893000	-0.453107000
H	0.317874000	-2.304583000	-0.827008000
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[1$^{\cdot\cdot}$**]**$^{2-}$-OS

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C	5.741697000	0.190746000	-0.030602000
C	6.756290000	-0.657311000	0.495783000
C	8.064530000	-0.612542000	0.018850000
H	8.808169000	-1.275378000	0.462394000
C	8.454879000	0.257924000	-0.994219000
C	7.473845000	1.086697000	-1.526597000
H	7.739141000	1.764921000	-2.338092000
C	6.155506000	1.068372000	-1.072531000
C	5.180633000	1.992012000	-1.761694000
H	5.597657000	2.365952000	-2.704197000

H	4.235452000	1.483290000	-1.973512000
H	4.922626000	2.853482000	-1.137518000
C	6.464418000	-1.625141000	1.618169000
H	5.920772000	-1.132127000	2.430037000
H	5.833488000	-2.456459000	1.291056000
H	7.394238000	-2.040157000	2.025533000
C	9.882630000	0.317524000	-1.474015000
H	10.362294000	-0.667404000	-1.434387000
H	9.941342000	0.675541000	-2.508079000
H	10.496877000	0.995870000	-0.865048000

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B	-4.233431000	0.124198000	0.492220000
C	-3.535763000	1.449912000	0.933790000
C	-4.367010000	2.519056000	1.372247000
H	-5.442055000	2.359743000	1.343278000
C	-3.894251000	3.722032000	1.862110000
H	-4.597543000	4.486703000	2.189544000
C	-2.519247000	3.944257000	1.950225000
H	-2.122206000	4.882436000	2.330354000
C	-1.662833000	2.940346000	1.514122000
H	-0.589073000	3.112781000	1.526188000
C	-2.127286000	1.722086000	1.004139000
C	-1.068766000	0.800450000	0.499780000
C	0.065747000	0.520561000	1.270910000
H	0.126531000	0.919159000	2.280427000
C	-1.105582000	0.259967000	-0.786634000
H	-1.964850000	0.464623000	-1.417253000
C	-3.527432000	-1.298706000	0.619696000
C	-2.895499000	-1.726027000	1.814986000
C	-2.261214000	-2.964696000	1.894332000
H	-1.780521000	-3.250565000	2.829588000
C	-2.214187000	-3.841758000	0.817924000
C	-2.864690000	-3.451513000	-0.347575000
H	-2.852549000	-4.119634000	-1.208723000
C	-3.508722000	-2.220830000	-0.457941000
C	-4.153655000	-1.893689000	-1.784531000
H	-3.871203000	-2.630374000	-2.545368000
H	-3.849188000	-0.903831000	-2.139139000
H	-5.246151000	-1.873900000	-1.720095000
C	-2.895874000	-0.870511000	3.058872000
H	-2.663264000	-1.473580000	3.944506000
H	-3.862662000	-0.381092000	3.209561000

H	-2.154186000	-0.068533000	2.996630000
C	-1.452014000	-5.139643000	0.893677000
H	-1.913345000	-5.915615000	0.271733000
H	-1.403039000	-5.516677000	1.921450000
H	-0.418943000	-5.015688000	0.544577000
C	-5.740851000	0.189276000	-0.030199000
C	-6.755695000	-0.662696000	0.490026000
C	-8.063280000	-0.616417000	0.011523000
H	-8.806963000	-1.282233000	0.450539000
C	-8.453205000	0.259224000	-0.997264000
C	-7.472005000	1.091587000	-1.523962000
H	-7.736694000	1.773670000	-2.332445000
C	-6.154332000	1.071943000	-1.068376000
C	-5.179156000	1.998990000	-1.752454000
H	-5.595212000	2.376614000	-2.693918000
H	-4.233567000	1.491348000	-1.965306000
H	-4.922090000	2.858031000	-1.124544000
C	-6.464875000	-1.636442000	1.607562000
H	-5.920544000	-1.148093000	2.421784000
H	-5.834964000	-2.467011000	1.276487000
H	-7.395204000	-2.052413000	2.012821000
C	-9.880391000	0.320473000	-1.478448000
H	-10.361167000	-0.663925000	-1.439193000
H	-9.937781000	0.678445000	-2.512633000
H	-10.494601000	0.999598000	-0.870254000
B	4.233431000	-0.124198000	-0.492220000
C	3.535763000	-1.449912000	-0.933790000
C	4.367010000	-2.519056000	-1.372247000
H	5.442055000	-2.359743000	-1.343278000
C	3.894251000	-3.722032000	-1.862110000
H	4.597543000	-4.486703000	-2.189544000
C	2.519247000	-3.944257000	-1.950225000
H	2.122206000	-4.882436000	-2.330354000
C	1.662833000	-2.940346000	-1.514122000
H	0.589073000	-3.112781000	-1.526188000
C	2.127286000	-1.722086000	-1.004139000
C	1.068766000	-0.800450000	-0.499780000
C	-0.065747000	-0.520561000	-1.270910000
H	-0.126531000	-0.919159000	-2.280427000
C	1.105582000	-0.259967000	0.786634000
H	1.964850000	-0.464623000	1.417253000
C	3.527432000	1.298706000	-0.619696000
C	2.895499000	1.726027000	-1.814986000
C	2.261214000	2.964696000	-1.894332000

H	1.780521000	3.250565000	-2.829588000
C	2.214187000	3.841758000	-0.817924000
C	2.864690000	3.451513000	0.347575000
H	2.852549000	4.119634000	1.208723000
C	3.508722000	2.220830000	0.457941000
C	4.153655000	1.893689000	1.784531000
H	3.871203000	2.630374000	2.545368000
H	3.849188000	0.903831000	2.139139000
H	5.246151000	1.873900000	1.720095000
C	2.895874000	0.870511000	-3.058872000
H	2.663264000	1.473580000	-3.944506000
H	3.862662000	0.381092000	-3.209561000
H	2.154186000	0.068533000	-2.996630000
C	1.452014000	5.139643000	-0.893677000
H	1.913345000	5.915615000	-0.271733000
H	1.403039000	5.516677000	-1.921450000
H	0.418943000	5.015688000	-0.544577000
C	5.740851000	-0.189276000	0.030199000
C	6.755695000	0.662696000	-0.490026000
C	8.063280000	0.616417000	-0.011523000
H	8.806963000	1.282233000	-0.450539000
C	8.453205000	-0.259224000	0.997264000
C	7.472005000	-1.091587000	1.523962000
H	7.736694000	-1.773670000	2.332445000
C	6.154332000	-1.071943000	1.068376000
C	5.179156000	-1.998990000	1.752454000
H	5.595212000	-2.376614000	2.693918000
H	4.233567000	-1.491348000	1.965306000
H	4.922090000	-2.858031000	1.124544000
C	6.464875000	1.636442000	-1.607562000
H	5.920544000	1.148093000	-2.421784000
H	5.834964000	2.467011000	-1.276487000
H	7.395204000	2.052413000	-2.012821000
C	9.880391000	-0.320473000	1.478448000
H	10.361167000	0.663925000	1.439193000
H	9.937781000	-0.678445000	2.512633000
H	10.494601000	-0.999598000	0.870254000

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B	0.475899000	0.076008000	-3.049992000
B	-0.475899000	-0.076008000	3.049992000
C	2.025836000	0.647887000	-2.829269000

C	2.976041000	1.127152000	-3.737534000
H	2.774129000	1.087102000	-4.805019000
C	4.191506000	1.666522000	-3.322784000
H	4.911248000	2.014446000	-4.062226000
C	4.486977000	1.763315000	-1.964956000
H	5.439111000	2.175906000	-1.636646000
C	3.550566000	1.337929000	-1.032290000
H	3.761939000	1.418026000	0.031639000
C	2.332614000	0.803767000	-1.458022000
C	1.220316000	0.382384000	-0.589114000
C	0.257363000	-0.423646000	-1.423059000
H	0.740808000	-1.413836000	-1.524408000
C	-1.016388000	-0.725031000	-0.690063000
H	-1.734594000	-1.373900000	-1.192127000
C	-0.282853000	1.379224000	-3.791750000
C	-0.215276000	1.528228000	-5.202226000
C	-0.769597000	2.635870000	-5.853732000
H	-0.688748000	2.697640000	-6.939512000
C	-1.414147000	3.653126000	-5.170437000
C	-1.463048000	3.537493000	-3.787798000
H	-1.939701000	4.327084000	-3.207328000
C	-0.912758000	2.451186000	-3.106511000
C	0.421674000	0.514602000	-6.135767000
H	1.285230000	0.014527000	-5.703065000
H	0.740348000	1.008922000	-7.061812000
H	-0.281865000	-0.279211000	-6.409940000
C	-2.037213000	4.823462000	-5.888234000
H	-1.655291000	4.910752000	-6.911503000
H	-1.831718000	5.769286000	-5.373161000
H	-3.129550000	4.729686000	-5.956383000
C	-1.011972000	2.499620000	-1.603067000
H	-1.513887000	1.622554000	-1.190249000
H	-1.562497000	3.390805000	-1.281709000
H	-0.024334000	2.529011000	-1.137670000
C	0.176731000	-1.339321000	-3.881077000
C	1.147448000	-2.340756000	-4.140489000
C	0.811021000	-3.542663000	-4.766686000
H	1.596921000	-4.276269000	-4.947337000
C	-0.488579000	-3.842068000	-5.150768000
C	-1.458577000	-2.895924000	-4.855108000
H	-2.498362000	-3.108712000	-5.104595000
C	-1.154074000	-1.680160000	-4.236832000
C	-2.336240000	-0.764835000	-3.987460000
H	-2.254915000	-0.228648000	-3.042835000

H	-3.264751000	-1.348052000	-3.969661000
H	-2.434852000	-0.004942000	-4.769641000
C	-0.828213000	-5.131382000	-5.854653000
H	-0.756301000	-5.036367000	-6.947065000
H	-1.850750000	-5.453214000	-5.627842000
H	-0.150221000	-5.939658000	-5.558293000
C	2.601768000	-2.188351000	-3.751320000
H	3.111965000	-1.419302000	-4.337827000
H	3.134618000	-3.134771000	-3.900597000
H	2.719073000	-1.894253000	-2.706153000
C	-2.025836000	-0.647887000	2.829269000
C	-2.976041000	-1.127152000	3.737534000
H	-2.774129000	-1.087102000	4.805019000
C	-4.191506000	-1.666522000	3.322784000
H	-4.911248000	-2.014446000	4.062226000
C	-4.486977000	-1.763315000	1.964956000
H	-5.439111000	-2.175906000	1.636646000
C	-3.550566000	-1.337929000	1.032290000
H	-3.761939000	-1.418026000	-0.031639000
C	-2.332614000	-0.803767000	1.458022000
C	-1.220316000	-0.382384000	0.589114000
C	-0.257363000	0.423646000	1.423059000
H	-0.740808000	1.413836000	1.524408000
C	1.016388000	0.725031000	0.690063000
H	1.734594000	1.373900000	1.192127000
C	0.282853000	-1.379224000	3.791750000
C	0.215276000	-1.528228000	5.202226000
C	0.769597000	-2.635870000	5.853732000
H	0.688748000	-2.697640000	6.939512000
C	1.414147000	-3.653126000	5.170437000
C	1.463048000	-3.537493000	3.787798000
H	1.939701000	-4.327084000	3.207328000
C	0.912758000	-2.451186000	3.106511000
C	-0.421674000	-0.514602000	6.135767000
H	-1.285230000	-0.014527000	5.703065000
H	-0.740348000	-1.008922000	7.061812000
H	0.281865000	0.279211000	6.409940000
C	2.037213000	-4.823462000	5.888234000
H	1.655291000	-4.910752000	6.911503000
H	1.831718000	-5.769286000	5.373161000
H	3.129550000	-4.729686000	5.956383000
C	1.011972000	-2.499620000	1.603067000
H	1.513887000	-1.622554000	1.190249000
H	1.562497000	-3.390805000	1.281709000

H	0.024334000	-2.529011000	1.137670000
C	-0.176731000	1.339321000	3.881077000
C	-1.147448000	2.340756000	4.140489000
C	-0.811021000	3.542663000	4.766686000
H	-1.596921000	4.276269000	4.947337000
C	0.488579000	3.842068000	5.150768000
C	1.458577000	2.895924000	4.855108000
H	2.498362000	3.108712000	5.104595000
C	1.154074000	1.680160000	4.236832000
C	2.336240000	0.764835000	3.987460000
H	2.254915000	0.228648000	3.042835000
H	3.264751000	1.348052000	3.969661000
H	2.434852000	0.004942000	4.769641000
C	0.828213000	5.131382000	5.854653000
H	0.756301000	5.036367000	6.947065000
H	1.850750000	5.453214000	5.627842000
H	0.150221000	5.939658000	5.558293000
C	-2.601768000	2.188351000	3.751320000
H	-3.111965000	1.419302000	4.337827000
H	-3.134618000	3.134771000	3.900597000
H	-2.719073000	1.894253000	2.706153000

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C	2.407268000	0.410688000	2.558117000
C	3.563471000	0.579249000	3.319331000
H	3.487670000	0.828058000	4.375294000
C	4.835864000	0.444932000	2.761037000
H	5.719099000	0.567747000	3.386017000
C	4.977166000	0.165551000	1.405303000
H	5.967850000	0.066422000	0.965435000
C	3.844390000	0.033123000	0.608169000
H	3.948823000	-0.159829000	-0.457065000
C	2.578077000	0.158494000	1.177710000
C	1.279970000	0.066312000	0.487486000
C	0.221445000	0.349946000	1.377837000
C	-1.067507000	0.254895000	0.856152000
H	-1.928968000	0.436818000	1.496362000
C	-0.011686000	-0.519105000	3.827453000
C	0.428576000	-1.855384000	4.009329000
C	-0.308012000	-2.770436000	4.762542000
H	0.077593000	-3.783625000	4.876077000
C	-1.522396000	-2.442980000	5.351003000

C	-1.997532000	-1.160694000	5.124765000
H	-2.968678000	-0.877217000	5.531318000
C	-1.281181000	-0.217919000	4.381577000
C	1.692384000	-2.387000000	3.372725000
H	1.693889000	-2.214803000	2.293665000
H	1.777763000	-3.466468000	3.543503000
H	2.593896000	-1.907791000	3.761926000
C	-2.288215000	-3.436553000	6.187272000
H	-1.926576000	-3.468431000	7.224460000
H	-2.198289000	-4.452742000	5.786657000
H	-3.354105000	-3.186266000	6.225396000
C	-1.960839000	1.128898000	4.225048000
H	-1.646431000	1.839808000	4.997125000
H	-3.047857000	1.009831000	4.306834000
H	-1.742234000	1.599060000	3.267775000
C	0.769966000	2.138020000	3.586006000
C	0.639711000	3.335431000	2.834035000
C	0.681883000	4.588523000	3.446796000
H	0.569681000	5.476206000	2.824519000
C	0.878104000	4.744885000	4.812855000
C	1.062525000	3.587053000	5.551111000
H	1.253755000	3.666897000	6.621832000
C	1.017542000	2.315224000	4.970798000
C	1.237676000	1.166178000	5.937045000
H	0.291498000	0.772324000	6.323882000
H	1.829675000	1.508125000	6.795068000
H	1.752503000	0.322253000	5.481168000
C	0.479654000	3.341212000	1.331110000
H	-0.444895000	2.859511000	1.006205000
H	1.289698000	2.798558000	0.838623000
H	0.481432000	4.369998000	0.953314000
C	0.889767000	6.107916000	5.457268000
H	1.411051000	6.844254000	4.834423000
H	1.388519000	6.082442000	6.432582000
H	-0.125539000	6.493225000	5.623098000
B	0.797653000	0.610278000	2.907523000
C	-2.407268000	-0.410688000	-2.558117000
C	-3.563471000	-0.579249000	-3.319331000
H	-3.487670000	-0.828058000	-4.375294000
C	-4.835864000	-0.444932000	-2.761037000
H	-5.719099000	-0.567747000	-3.386017000
C	-4.977166000	-0.165551000	-1.405303000
H	-5.967850000	-0.066422000	-0.965435000
C	-3.844390000	-0.033123000	-0.608169000

H	-3.948823000	0.159829000	0.457065000
C	-2.578077000	-0.158494000	-1.177710000
C	-1.279970000	-0.066312000	-0.487486000
C	-0.221445000	-0.349946000	-1.377837000
C	1.067507000	-0.254895000	-0.856152000
H	1.928968000	-0.436818000	-1.496362000
C	0.011686000	0.519105000	-3.827453000
C	-0.428576000	1.855384000	-4.009329000
C	0.308012000	2.770436000	-4.762542000
H	-0.077593000	3.783625000	-4.876077000
C	1.522396000	2.442980000	-5.351003000
C	1.997532000	1.160694000	-5.124765000
H	2.968678000	0.877217000	-5.531318000
C	1.281181000	0.217919000	-4.381577000
C	-1.692384000	2.387000000	-3.372725000
H	-1.693889000	2.214803000	-2.293665000
H	-1.777763000	3.466468000	-3.543503000
H	-2.593896000	1.907791000	-3.761926000
C	2.288215000	3.436553000	-6.187272000
H	1.926576000	3.468431000	-7.224460000
H	2.198289000	4.452742000	-5.786657000
H	3.354105000	3.186266000	-6.225396000
C	1.960839000	-1.128898000	-4.225048000
H	1.646431000	-1.839808000	-4.997125000
H	3.047857000	-1.009831000	-4.306834000
H	1.742234000	-1.599060000	-3.267775000
C	-0.769966000	-2.138020000	-3.586006000
C	-0.639711000	-3.335431000	-2.834035000
C	-0.681883000	-4.588523000	-3.446796000
H	-0.569681000	-5.476206000	-2.824519000
C	-0.878104000	-4.744885000	-4.812855000
C	-1.062525000	-3.587053000	-5.551111000
H	-1.253755000	-3.666897000	-6.621832000
C	-1.017542000	-2.315224000	-4.970798000
C	-1.237676000	-1.166178000	-5.937045000
H	-0.291498000	-0.772324000	-6.323882000
H	-1.829675000	-1.508125000	-6.795068000
H	-1.752503000	-0.322253000	-5.481168000
C	-0.479654000	-3.341212000	-1.331110000
H	0.444895000	-2.859511000	-1.006205000
H	-1.289698000	-2.798558000	-0.838623000
H	-0.481432000	-4.369998000	-0.953314000
C	-0.889767000	-6.107916000	-5.457268000
H	-1.411051000	-6.844254000	-4.834423000

H	-1.388519000	-6.082442000	-6.432582000
H	0.125539000	-6.493225000	-5.623098000
B	-0.797653000	-0.610278000	-2.907523000