Electronic Supplementary Material (ESI) for Chemical Communications.

Supplementary Information

Incorporation of H_2O and CO_2 into a BN-embedded 3aH-3a^{1}H-acephenanthrylene derivative

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. ^{1}H, ^{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. Electrospray ionization (ESI) mass spectra were obtained at the Agilent Q-TOF6510 or Waters Q-Tof Premier Mass Spectrometers. Fourier transform infrared (FT-IR) spectra were recorded on a Bruker ALPHA II FTIR spectrometer. Melting points were measured on a X4 Melting Point apparatus (Beijing Tech, CN) in sealed capillaries and are uncorrected. $H_2O{\cdot}B(C_6F_5)_3$[S1] were synthesized according to literature procedures.

Synthesis of compounds 2-5 and their spectral data

Compound 2: 0.428 g (0.5 mmol) **1** were dissolved in toluene (10 mL) and a toluene solution of $H_2O{\cdot}B(C_6F_5)_3$ (0.265 g, 0.5 mmol) was added dropwise at –60 °C. The solution turned from yellow to colourless immediately. The solvents were removed under vacuum at low temperature and the residue was washed with n-hexane to afford a pale yellow powder. The resulting solid was re-dissolved with toluene and co-product IPr_2Me_2-$B(C_6F_5)_3$ was present as yellow oil at the bottom of reaction flask after an addition of n-hexane. The upper clear solution was collected and vacuumed and the residue was extracted with hot n-hexane to afford a white powder of **2** in 90 % yield (0.311 g).

Mp: 122.1 °C (dec); ^{1}H NMR (500 MHz, $CDCl_3$)**:** δ = 7.38 (t, *J* = 7.5 Hz, 1H, Ar-*H*), 7.26 (t, *J* = 7.5 Hz, 1H, Ar-*H*), 7.17 (d, *J* = 7.1 Hz, 1H, Ar-*H*), 7.12 (d, *J* = 7.5 Hz, 1H, Ar-*H*), 7.01 (d,

J = 7.3 Hz, 1H, Ar-*H*), 6.97 (s, 2H, Ar-*H*), 6.92 (s, 1H, Ar-*H*), 6.83 (s, 2H, Ar-*H*), 6.80 (s, 1H, Ar-*H*), 6.76 (d, *J* = 7.4 Hz, 1H, Ar-*H*), 6.08 (s, 1H, Ar-*H*), 5.29 (s, 1H, C-*H*), 2.71 (s, 1H, O-*H*), 2.34 (s, 3H, CH_3), 2.30 (s, 3H, CH_3), 2.23 (s, 3H, CH_3), 2.20 (s, 3H, CH_3), 1.99 (s, 3H, CH_3), 1.98 (s, 4H, CH_3 + C*H*), 1.93 (s, 3H, CH_3), 1.90 (s, 3H, CH_3), 1.89 (s, 3H, CH_3), 1.75 (s, 3H, CH_3), 1.50 (s, 3H, CH_3), 1.42 (s, 1H, N-*H*), 0.69 (s, 3H, CH_3); ^{13}C NMR (126 MHz, $CDCl_3$): δ = 145.5 (C^q), 145.1 (C^q), 144.0 (C^q), 143.9 (C^q), 140.4 (C^q), 140.1 (C^q), 139.2 (C^q), 137.2 (C^q), 137.2 (C^q), 136.8 (C^q), 136.7 (C^q), 136.7 (C^q), 136.25 (C^q), 135.6 (C^q), 135.4 (C^q), 135.2 (C^q), 135.0 (C^q), 129.91 (C^q), 129.0 (*C*H), 129.0 (*C*H), 128.9 (*C*H), 128.6 (*C*H), 128.5 (*C*H), 128.5 (*C*H), 128.1 (*C*H), 128.0 (*C*H), 128.0 (*C*H), 127.9 (*C*H), 126.8 (*C*H), 123.8 (C^q), 121.2 (*C*H), 60.0 (N-C^q), 48.2 (B-*C*H), 30.9 (*C*H_3), 24.1 (*C*H_3), 22.1 (*C*H_3), 21.3 (*C*H_3), 21.1 (*C*H_3), 21.0 (*C*H_3), 21.0 (*C*H_3), 21.0 (*C*H_3), 21.0 (*C*H_3), 19.9 (*C*H_3), B-*C* was not observed; ^{11}B NMR (160 MHz, $CDCl_3$): δ = 39.3 (br), 24.4 (br); HRMS (ESI): m/z calcd for $C_{48}H_{53}B_2N_2O$: 695.4344 $[(M + H)]^+$; found: 695.4371.

Compound 3: 0.428 g (0.5 mmol) **1** were dissolved in toluene (30 mL) and a toluene solution of $H_2O{\cdot}B(C_6F_5)_3$ (0.265 g, 0.5 mmol) was added at room temperature. The mixture was stirred for 3.5 h and all volatiles were removed under vacuum. The residue was washed by cold toluene to afford a white solid of **3** (0.212g, 35 %).

Mp: 156.2 ºC (dec); ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.45–7.38 (m, 2H, Ar-*H*), 7.26 (d, 2H, Ar-*H*), 7.20 (d, 1H, Ar-*H*), 6.99 (s, 1H, Ar-*H*), 6.86 (s, 2H, Ar-*H*), 6.78 (d, 1H, Ar-*H*), 6.76 (s, 1H, Ar-*H*), 6.71 (m, J = 6.6 Hz, 2H, Ar-*H*), 6.48 (s, 1H, Ar-*H*), 5.87 (s, 1H, Ar-*H*), 5.49 (s, 1H, C-*H*), 3.77– 3.63 (m, 2H, C*H*(CH_3)$_2$), 2.30 (s, 3H, CH_3), 2.25 (s, 3H, CH_3), 2.24 (s, 3H, CH_3), 2.23 (s, 6H, CH_3), 2.21 (s, 3H, CH_3), 1.94 (s, 3H, CH_3), 1.90 (s, 1H, C-*H*), 1.88 (s, 3H,

CH_3), 1.84 (s, 3H, CH_3), 1.79 (s, 3H, CH_3), 1.74 (s, 1H, N-*H*), 1.65 (s, 3H, CH_3), 1.63 (s, 3H, CH_3), 1.59 (s, 3H, CH_3), 1.27 (d, J = 6.8 Hz, 3H, CH_3), 1.05 (d, J = 7.0 Hz, 3H, CH_3), 0.81 (d, J = 6.8 Hz, 3H, CH_3), 0.79 (s, 3H, CH_3), 0.44 (d, J = 6.9 Hz, 3H, CH_3); ^{13}C NMR (126 MHz, $CDCl_3$): δ = 145.5 (C^q), 145.4 (C^q), 144.3 (C^q), 141.3 (C^q), 140.2 (C^q), 139.1 (C^q), 138.9 (C^q), 138.0 (C^q), 137.4 (C^q), 136.9 (C^q), 136.2 (C^q), 136.2 (C^q), 136.2 (C^q), 135.8 (C^q), 135.4 (C^q), 134.9 (C^q), 134.3 (C^q), 130.8 (*C*H), 129.8 (*C*H), 129.6 (*C*H), 129.4 (*C*H), 129.2 (*C*H), 129.1 (*C*H), 129.0 (*C*H), 129.0 (C^q), 128.3 (*C*H), 128.2 (*C*H), 127.7 (C^q), 127.2 (*C*H), 127.1 (C^q), 126.8 (C^q), 121.3 (*C*H), 64.3 (N-C^q), 54.4 (*C*H(CH_3)$_2$), 53.5 (*C*H(CH_3)$_2$), 29.2 (*C*H_3), 24.5 (*C*H_3), 22.9 (*C*H_3), 21.9 (*C*H_3), 21.9 (*C*H_3), 21.7 (*C*H_3), 21.4 (*C*H_3), 21.3 (*C*H_3), 21.2 (*C*H_3), 21.1 (*C*H_3), 20.9 (*C*H_3), 20.7 (*C*H_3), 20.6 (*C*H_3), 20.5 (*C*H_3), 19.5 (*C*H_3), 10.7 (*C*H_3), 10.4 (*C*H_3), B-*C*H was not observed; ^{11}B NMR (160 MHz, $CDCl_3$): δ = 44.6 (br), 26.5 (br), −3.8 (s); ^{19}F NMR (471 MHz, $CDCl_3$): δ = –135.42 (d, *J* = 21.8 Hz), –163.12 (t, *J* = 20.3 Hz), –166.43 (m); HRMS (ESI): m/z calcd for $C_{59}H_{71}B_2N_4$: 857.5865 $[(M)]^+$; found: 857.5861.

Compound 4: 0.428 g (0.5 mmol) **1** were dissolved in toluene (10 mL) and 2 mL of a 1 M THF solution (2 mmol) of H_2O were added at room temperature. The mixture was stirred overnight and all volatiles were removed under vacuum. The residue was washed by n-hexane to afford a white solid of **4** (0.323 g, 72 %). All the NMR data were same as the reported literature.[S2]

^{1}H NMR (500 MHz, C_6D_6): δ = 7.32 (t, *J* = 7.5 Hz, 2H, Ar-*H*), 7.05 (d, *J* = 7.5 Hz, 4H, Ar-*H*), 6.87 (s, 8H, Ar-*H*), 3.47 (sept, *J* = 6.8 Hz, 2H, C*H*(CH_3)$_2$), 2.33 (s, 12H, CH_3), 2.25 (s, 24H, CH_3), 1.31 (s, 6H, CH_3), 0.86 (d, *J* = 6.8 Hz, 12H, CH_3). ^{13}C NMR (126 MHz, C_6D_6): δ = 144.3 (C^q), 142.2 (C^q), 136.9 (C^q), 134.7 (C^q), 128.4 (N*C*HN), 127.9 (*C*H), 127.6 (*C*H), 126.8

(*C*H), 50.9 (N*C*H(CH_3)$_2$), 21.6 (*C*H_3), 21.5 (*C*H_3), 21.4 (*C*H_3), 7.7 (*C*H_3), B-*C* was not observed; ^{11}B NMR (160 MHz, C_6D_6): δ = 30.6 (br).

Compound 5: 0.428 g (0.5 mmol) **1** 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 n-hexane to afford a white solid of **5** in 72 % yield (0.260 g).

Mp: 154.8 ºC (dec); ^{1}H NMR (500 MHz, C_6D_6): δ = 7.24 – 7.17 (m, 3H, Ar-*H*), 7.09 (dd, *J* = 7.5, 0.8 Hz, 1H, Ar-*H*), 7.04 – 7.01 (m, 1H, Ar-*H*), 6.88 (m, 1H, Ar-*H*), 6.85 (s, 1H, Ar-*H*), 6.79 (s, 1H, Ar-*H*), 6.67 (m, 3H, Ar-*H*), 6.57 (s, 1H, Ar-*H*), 4.99 (s, 1H, C-*H*), 2.45 (s, 1H, C-*H*), 2.38 (s, 3H, C*H*$_3$), 2.20 (s, 3H, C*H*$_3$), 2.18 (s, 3H, C*H*$_3$), 2.15 (s, 3H, C*H*$_3$), 2.13 (s, 3H, C*H*$_3$), 2.09 (s, 3H, C*H*$_3$), 2.06 (s, 3H, C*H*$_3$), 2.02 (s, 3H, C*H*$_3$), 1.80 (s, 3H, C*H*$_3$), 1.73 (s, 3H, C*H*$_3$), 1.62 (s, 3H, C*H*$_3$), 1.13 (s, 3H, C*H*$_3$); ^{13}C NMR (126 MHz, C_6D_6): δ = 151.7 (*C*O), 146.4 (*C*^{q}), 145.2 (*C*^{q}), 144.4 (*C*^{q}), 144.2 (*C*^{q}), 139.1 (*C*^{q}), 139.0 (*C*^{q}), 138.8 (*C*^{q}), 138.6 (*C*^{q}), 137.0 (*C*^{q}), 136.9 (*C*^{q}), 136.8 (*C*^{q}), 136.6 (*C*^{q}), 136.2 (*C*^{q}), 135.7 (*C*^{q}), 135.4 (*C*^{q}), 135.0 (*C*^{q}), 131.6 (*C*^{q}), 131.1 (*C*H), 129.9 (*C*H), 129.6 (*C* H), 129.1 (*C*H), 129.0 (*C*H), 128.7 (*C*H), 128.7 (*C*H), 128.6 (*C*H), 128.5 (*C*H), 128.4 (*C*H), 128.0 (*C*H), 127.9 (*C*H), 126.5 (*C*^{q}), 122.9 (*C*H), 59.0 (*C*^{q}), 56.4 (B-*C*H), 29.8 (*C*H_3), 26.0 (*C*H_3), 22.8 (*C*H_3), 22.1 (*C*H_3), 21.5 (*C*H_3), 21.2 (*C*H_3), 21.1 (*C*H_3), 21.0 (*C*H_3), 20.9 (*C*H_3), 20.8 (*C*H_3), 20.7 (*C*H_3), 19.1 (*C*H_3), B-*C* was not observed; ^{11}B NMR (160 MHz, C_6D_6): δ = 48.9 (br), 32.6 (br); HRMS (ESI): m/z calcd for $C_{49}H_{51}B_2N_2O_2$: 721.4137 $[(M + H)]^+$; found: 721.4127.

Fig. S1 ^{1}H NMR spectrum of **2**. (*n-hexane)

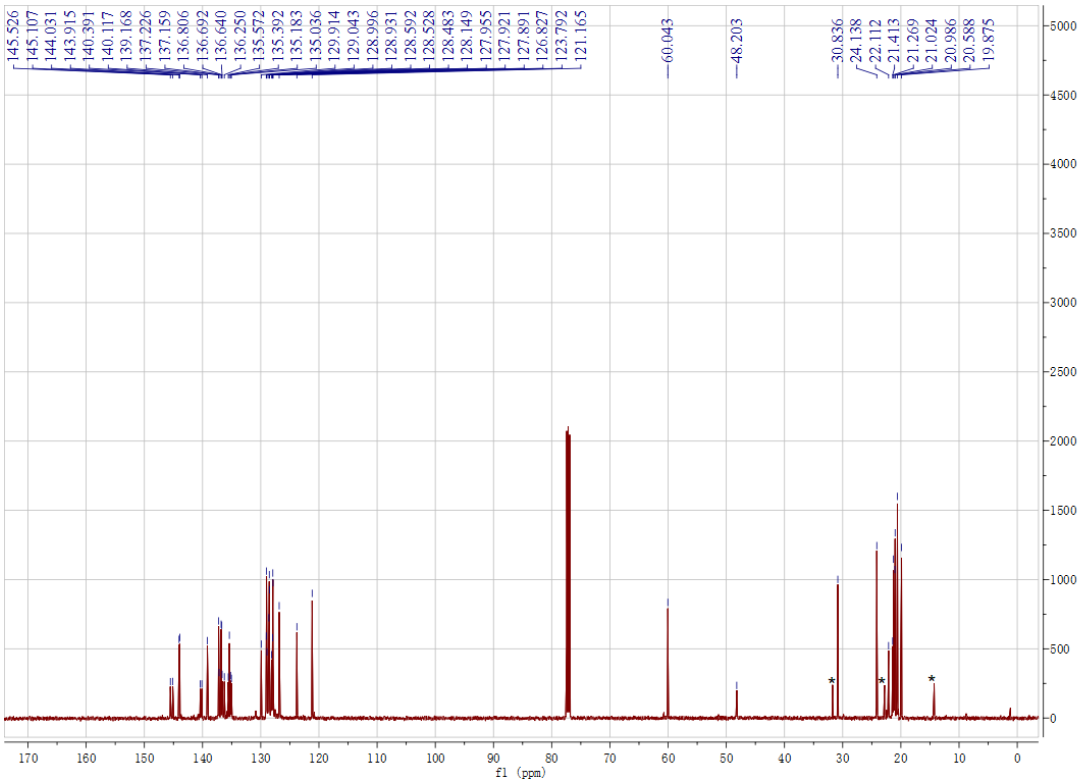


Fig. S2 ^{13}C NMR spectrum of **2**. (*n-hexane)

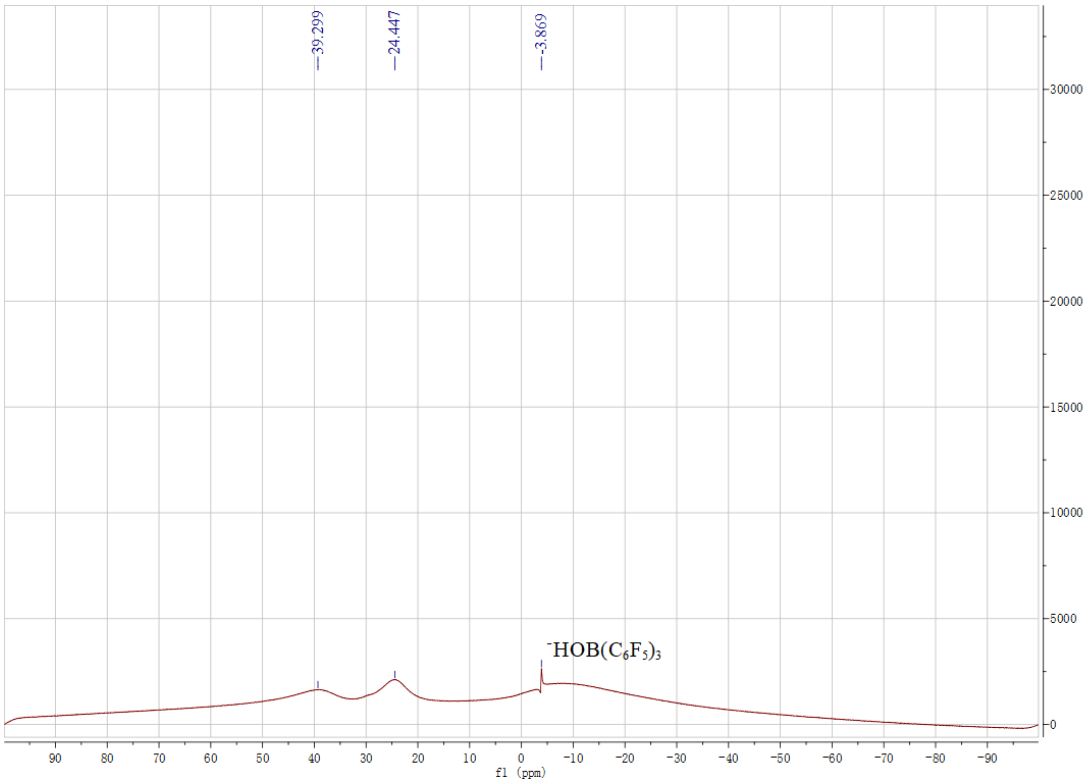


Fig. S3 ^{11}B NMR spectrum of **2**.

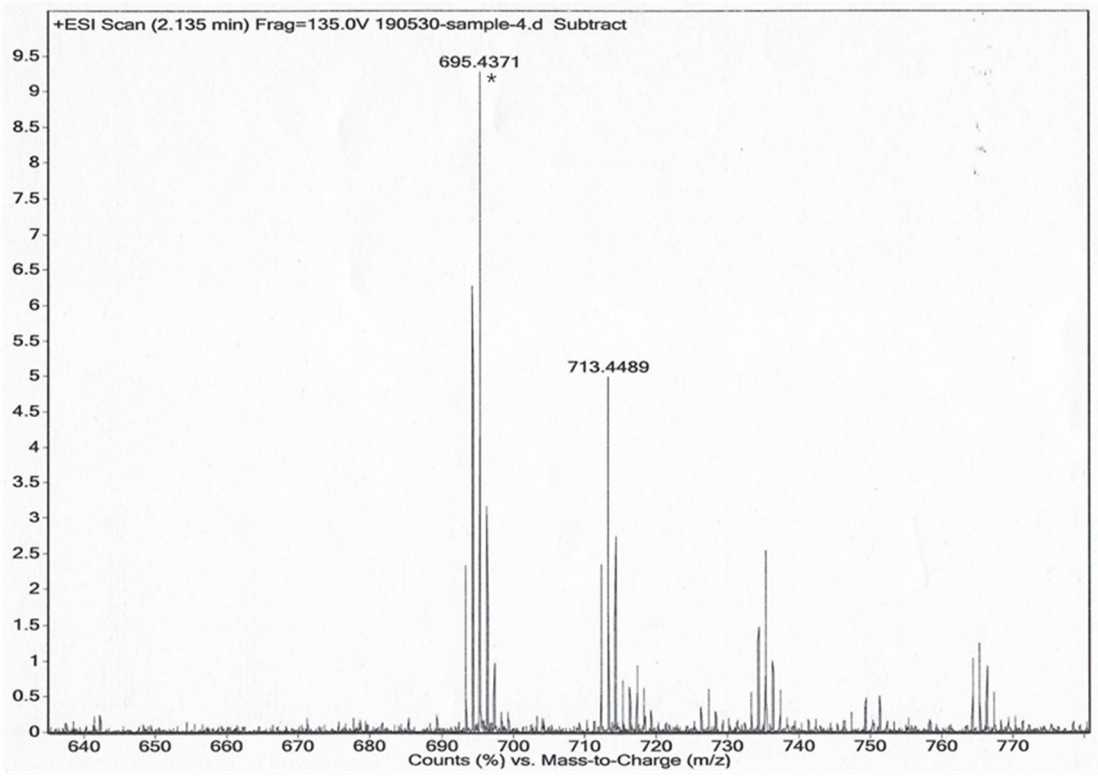


Fig. S4 HRMS spectrum of **2**.

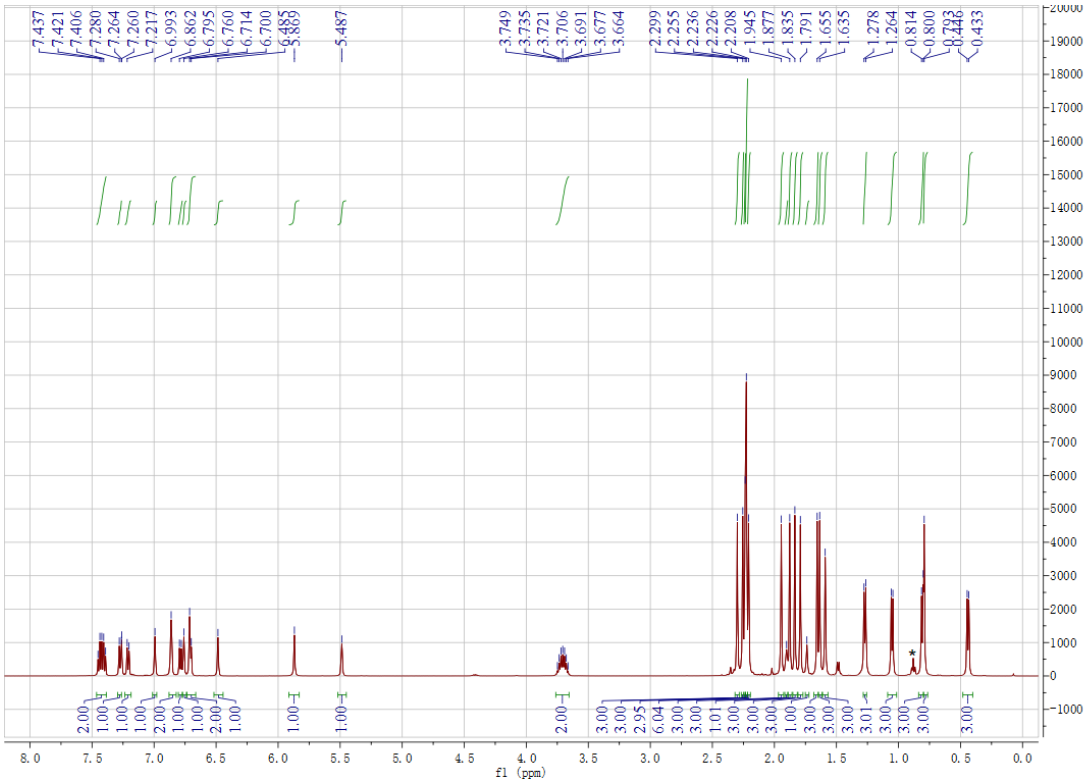


Fig. S5 ^{1}H NMR spectrum of **3**. (*n-hexane)

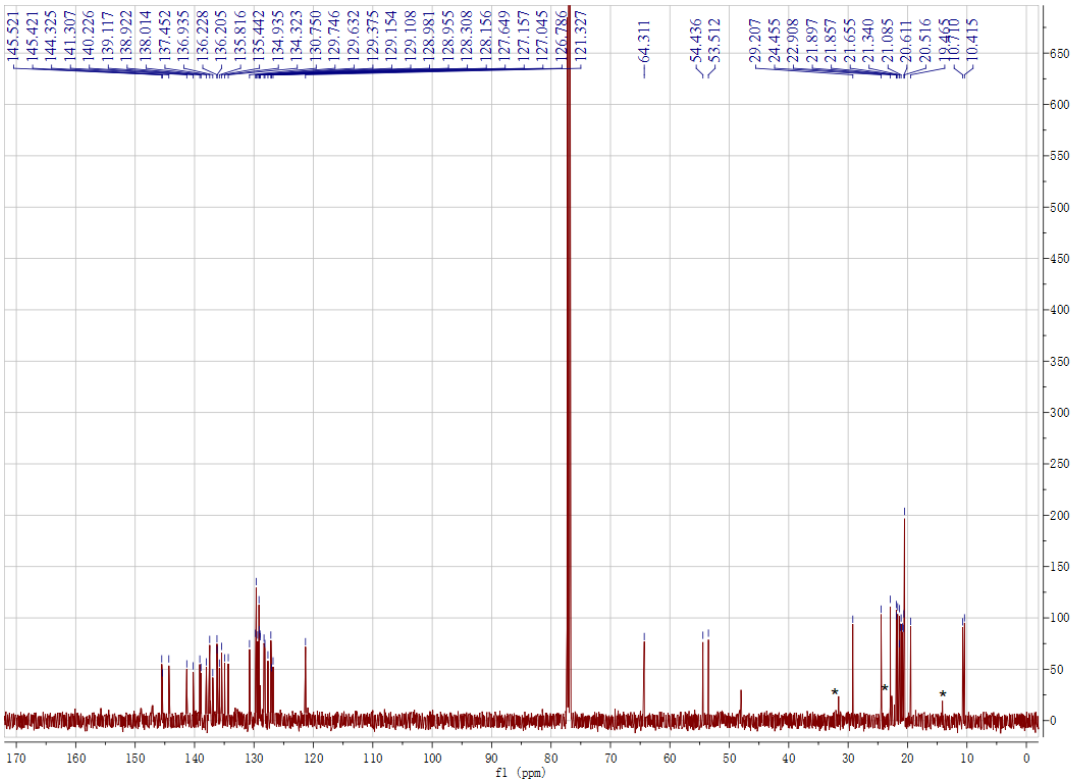


Fig. S6 ^{13}C NMR spectrum of **3**. (*n-hexane)

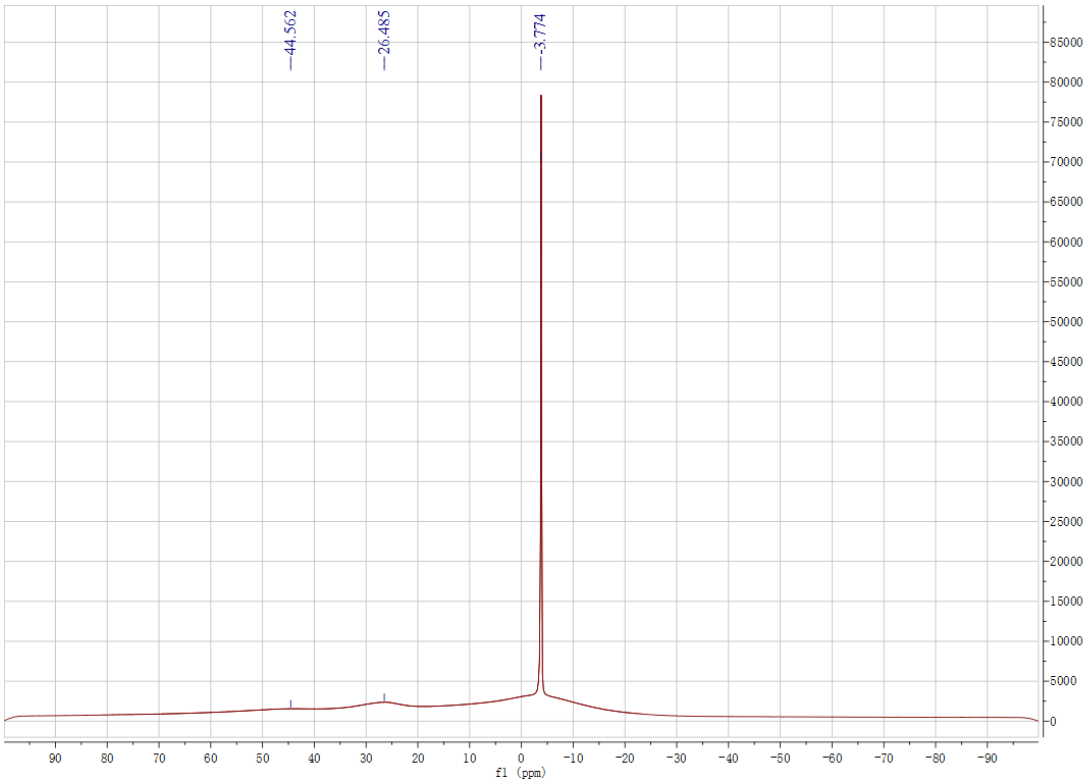


Fig. S7 ^{11}B NMR spectrum of **3**.

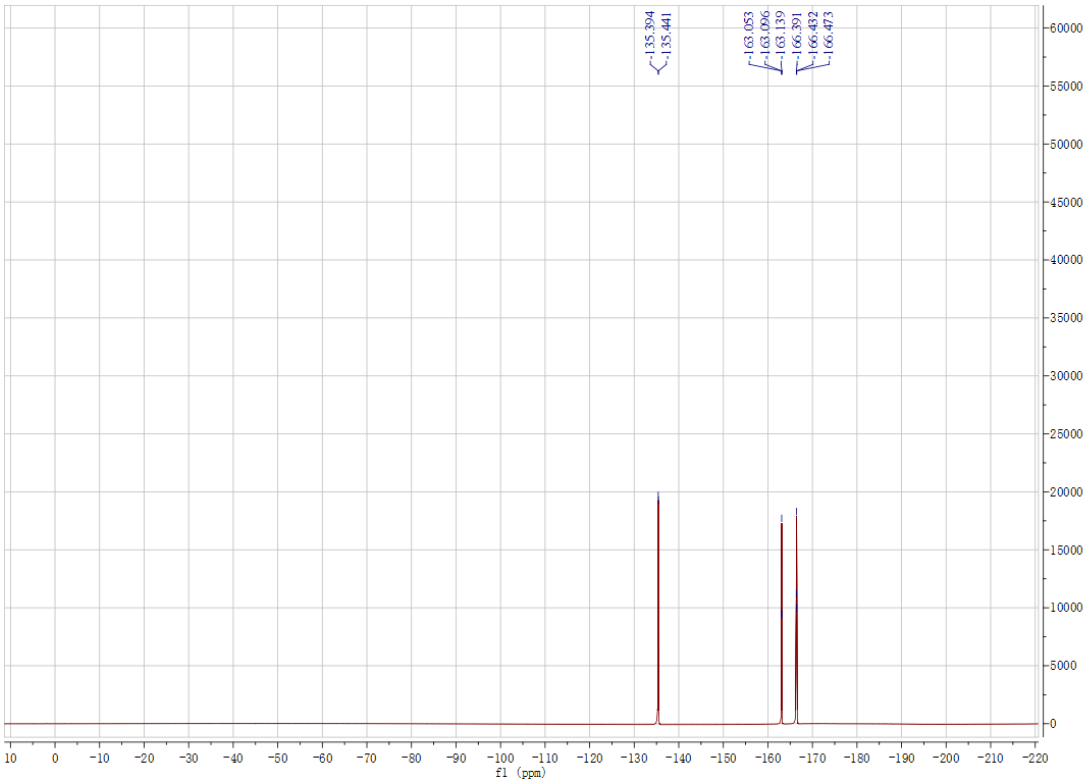


Fig. S8 ^{19}F NMR spectrum of **3**.

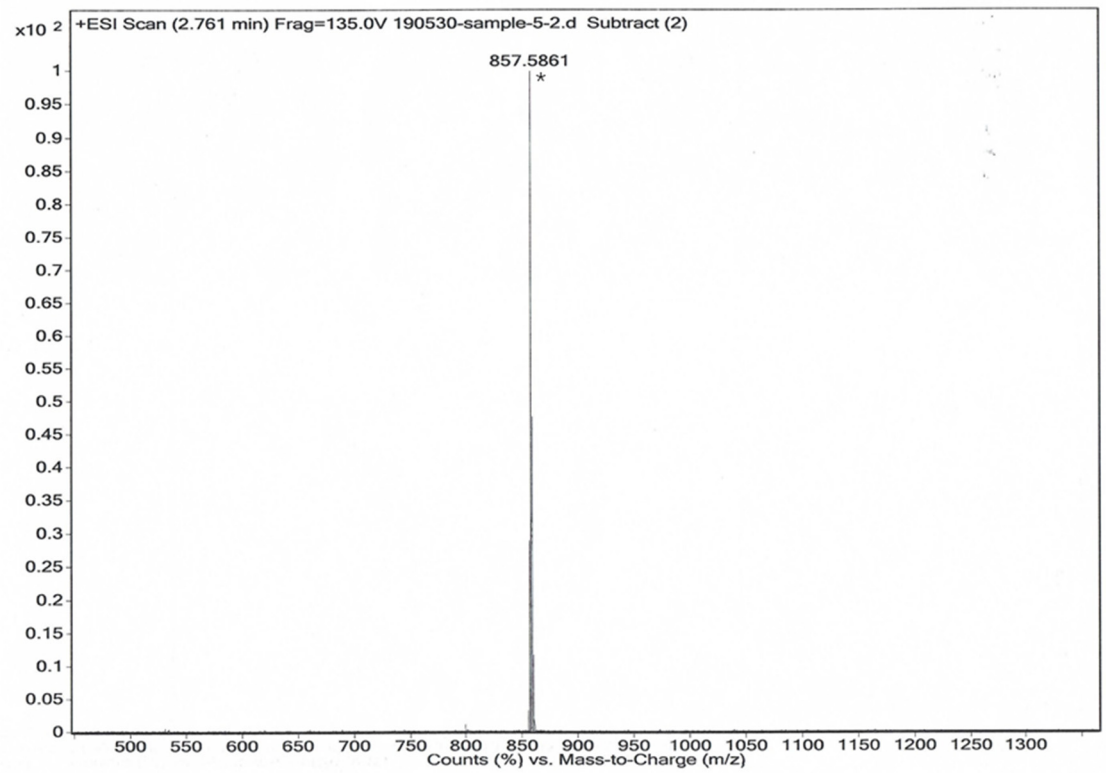


Fig. S9 HRMS spectrum of **3**.

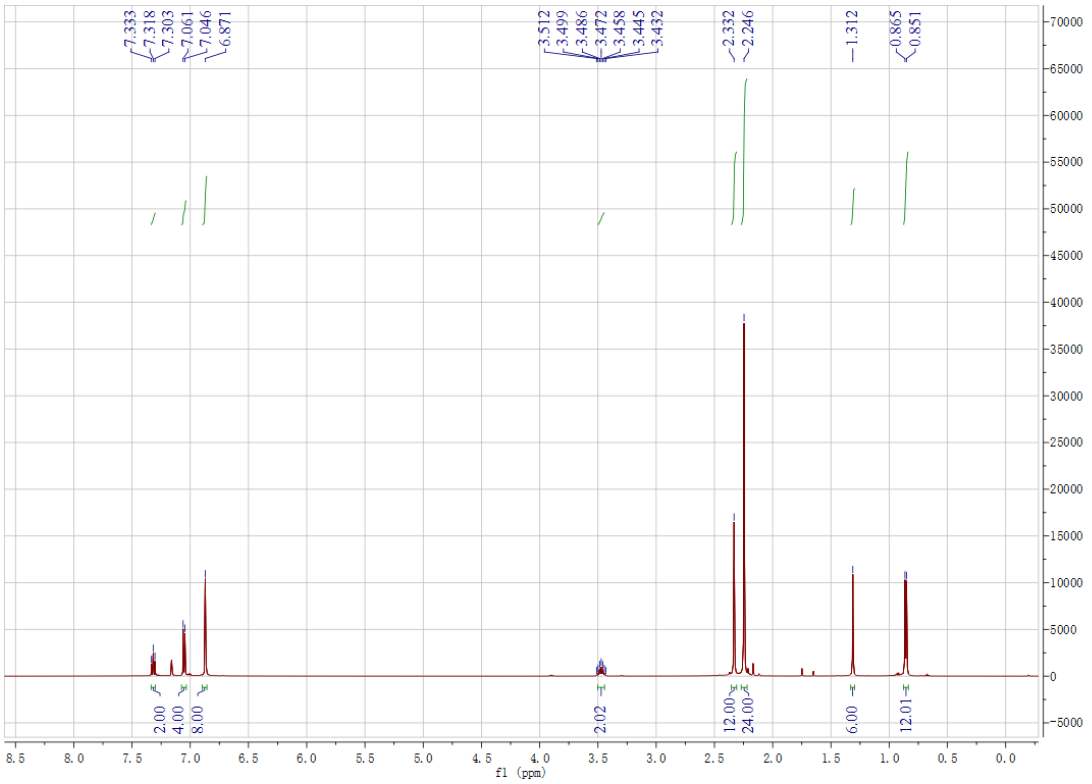


Fig. S10 ^{1}H NMR spectrum of **4**.

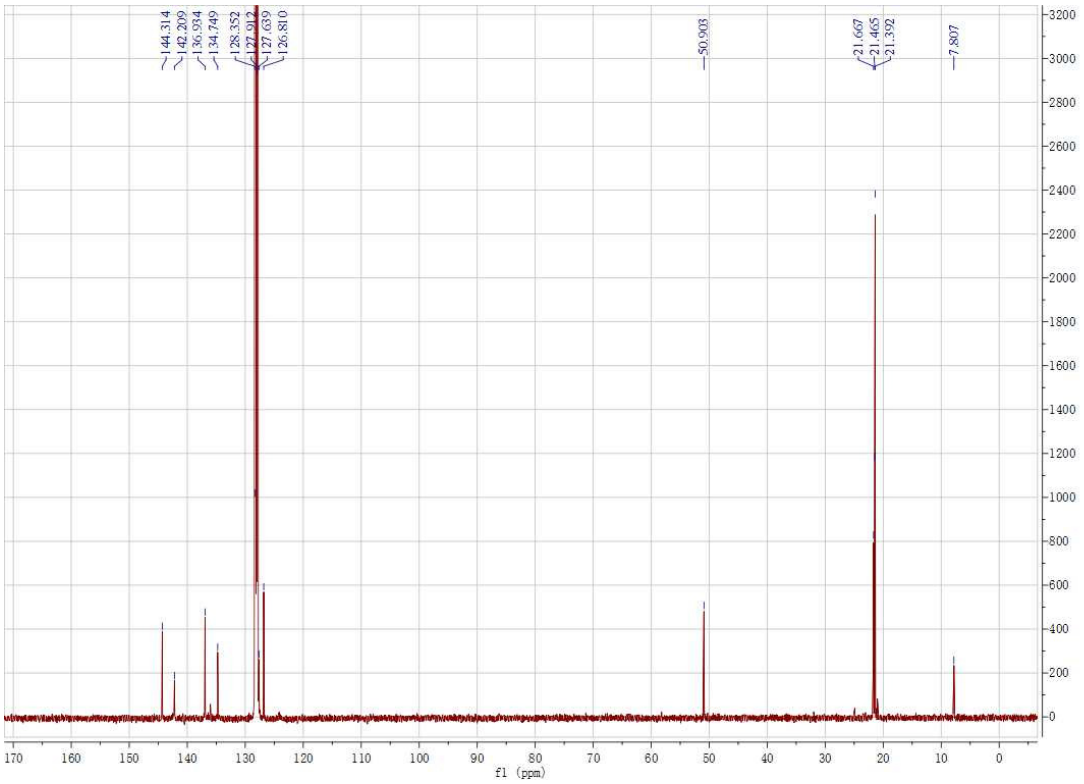


Fig. S11 ^{13}C NMR spectrum of **4**.

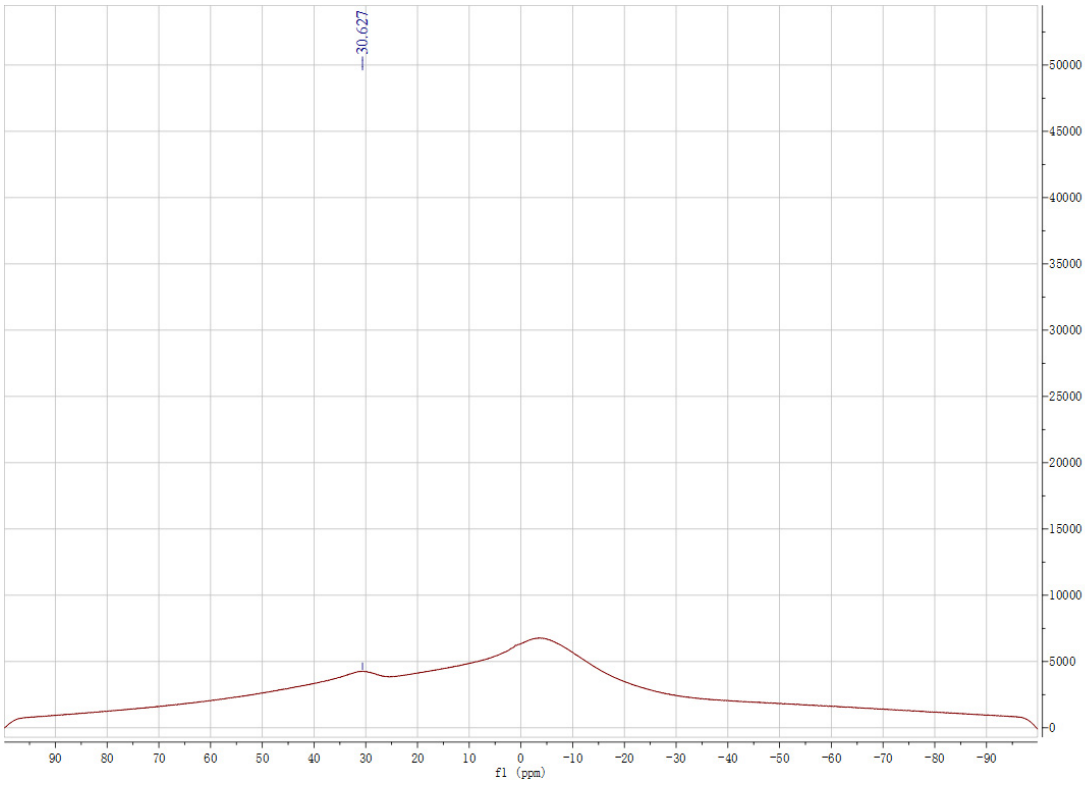


Fig. S12 ^{11}B NMR spectrum of **4**.

Fig. S13 ^{1}H NMR spectrum of **5**. (*n-hexane)

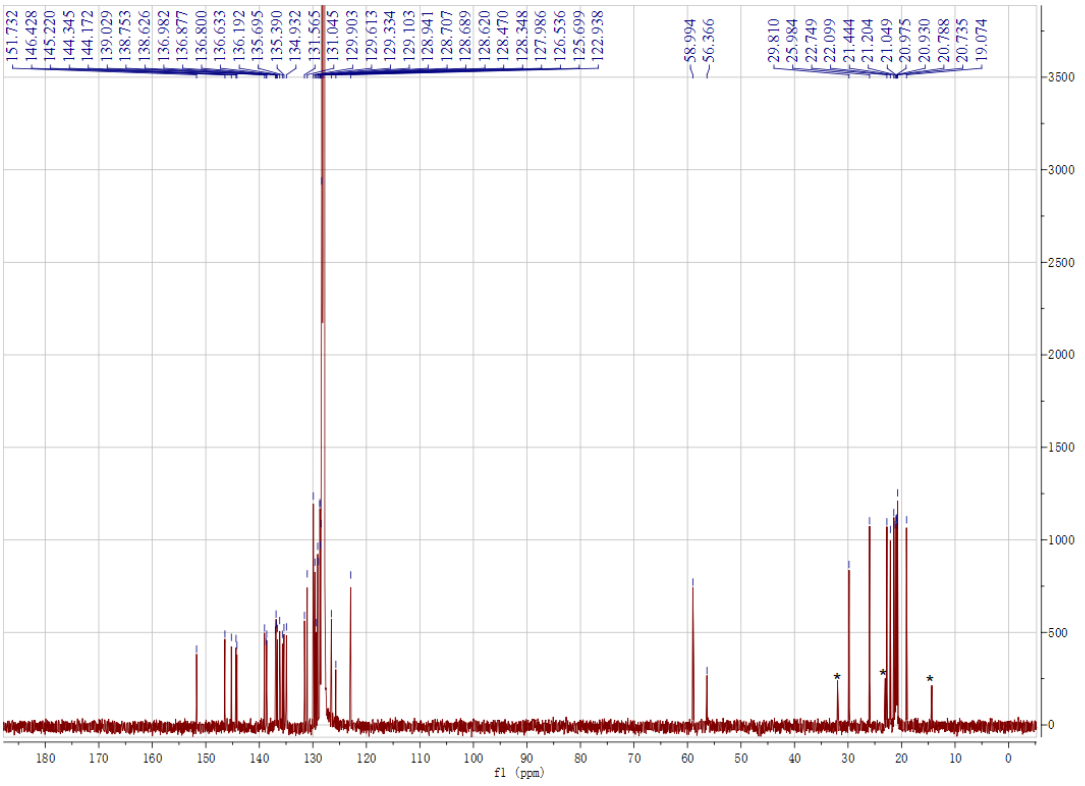


Fig. S14 ^{13}C NMR spectrum of **5**. (*n-hexane)

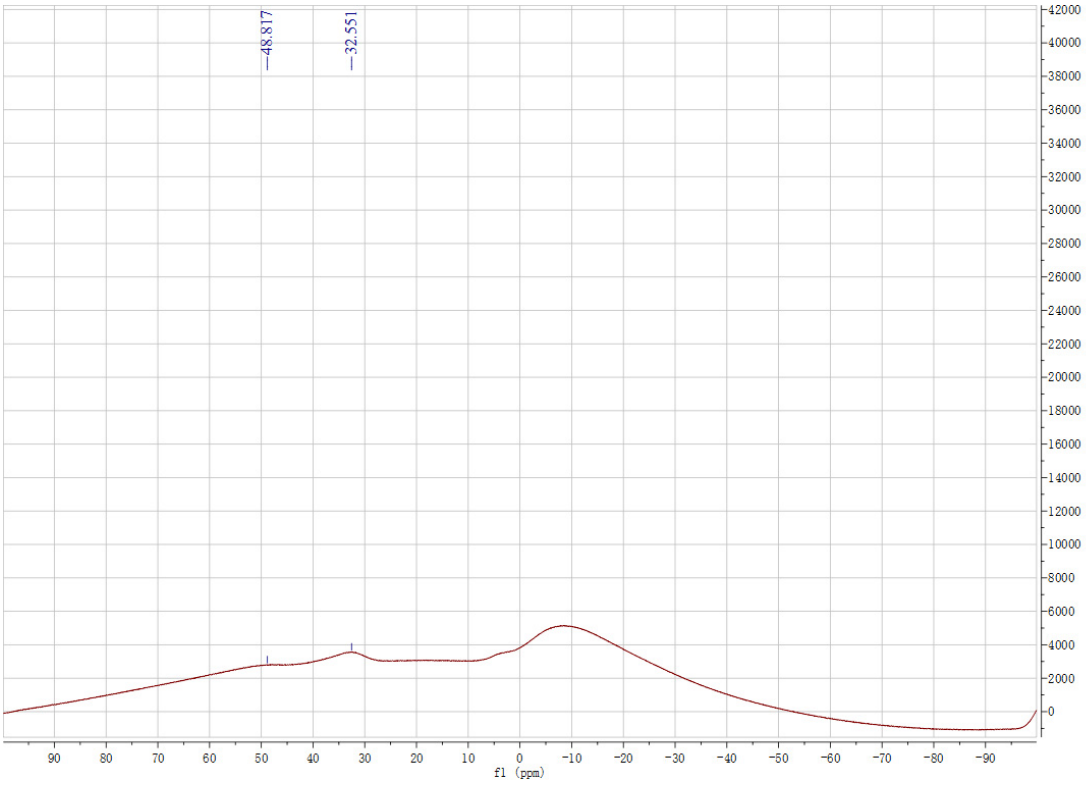
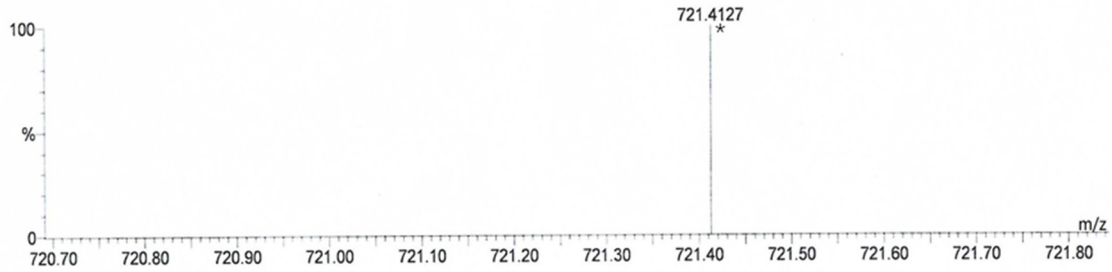


Fig. S15 ^{11}B NMR spectrum of **5**.

Elemental Composition Report

Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -5.0, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
66 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 49-59 H: 51-71 B: 1-6 N: 2-4 O: 2-2 Si: 0-4
C49H51B2N2O2
LW4A 15 (0.332)



Minimum:				-5.0			
Maximum:		5.0	10.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
721.4127	721.4137	-1.0	-1.4	26.5	9.8	0.0	C49 H51 B2 N2 O2

Fig. S16 HRMS spectrum of **5**.

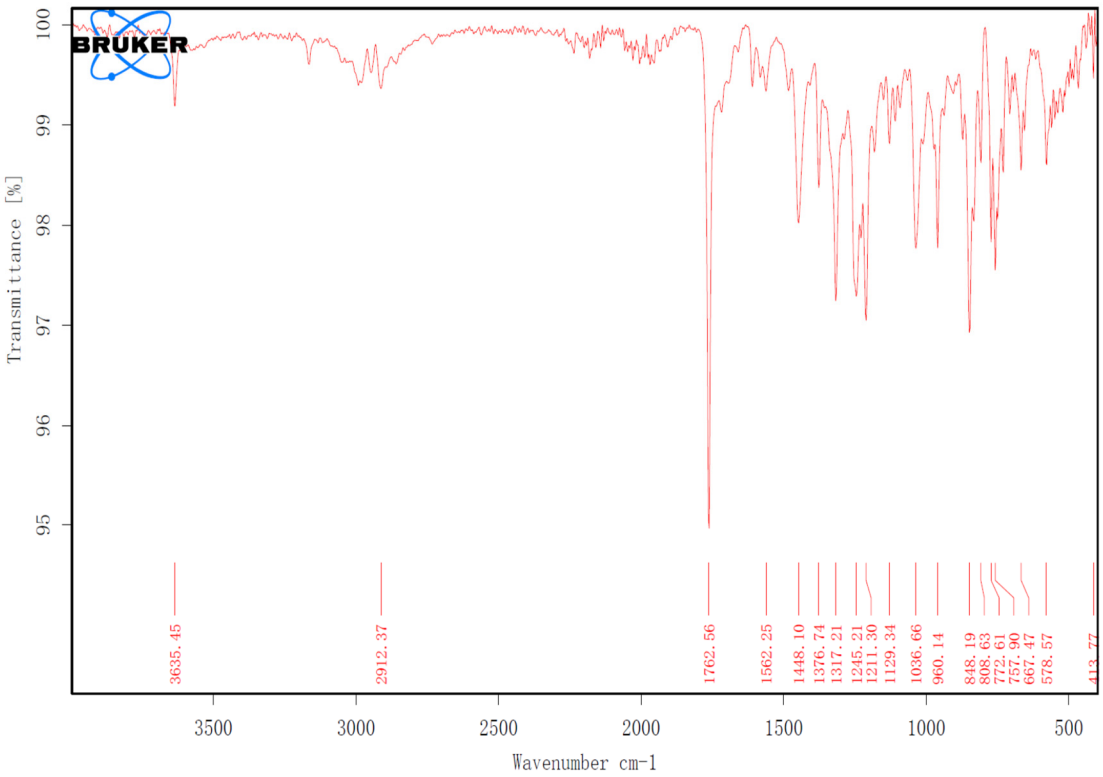


Fig. S17 IR spectrum of **5**.

Control experiments

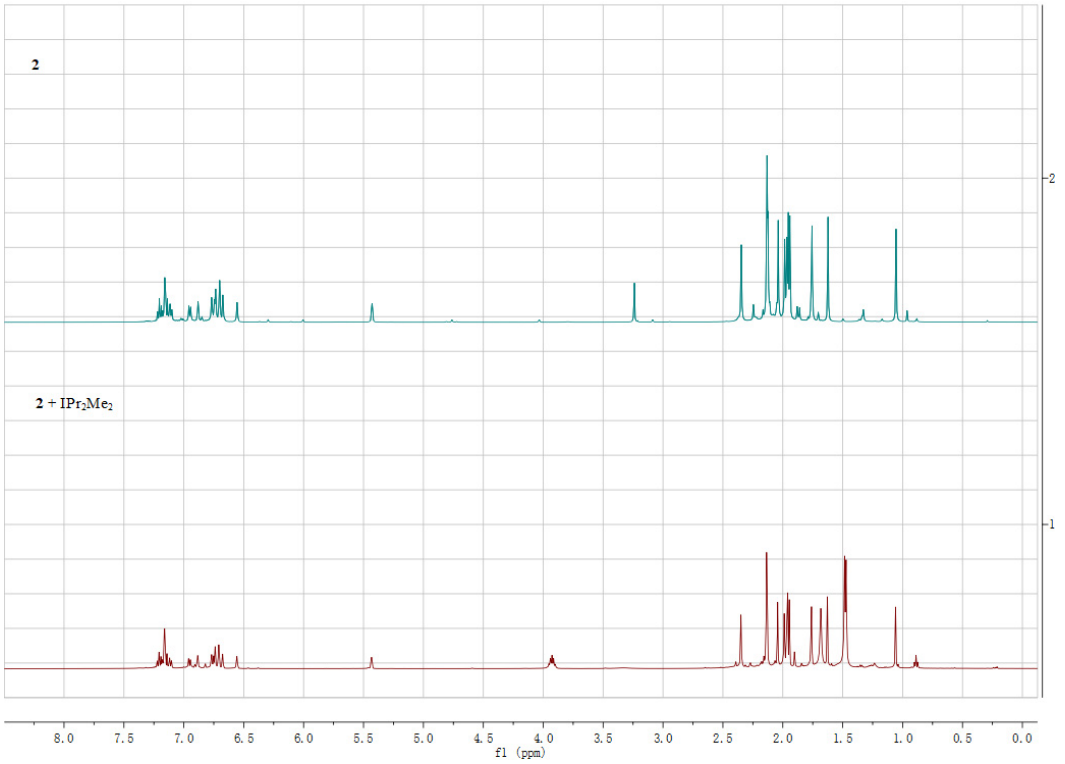


Fig. S18 Control experiment between **2** and IPr_2Me_2.

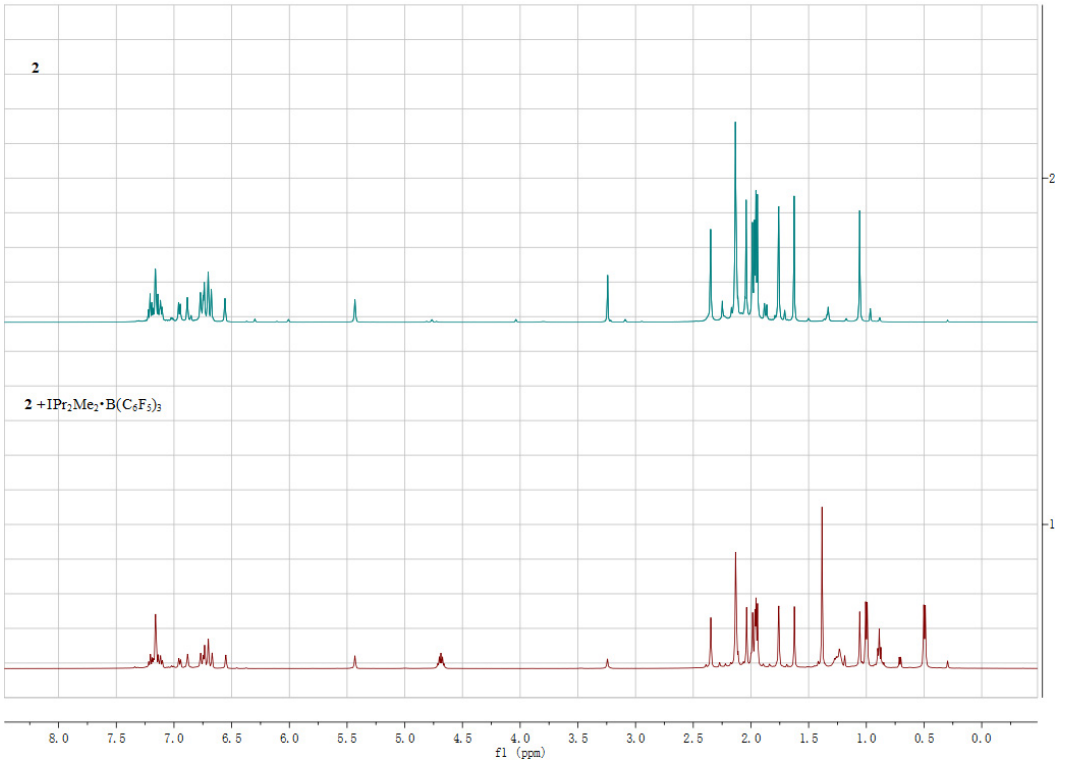


Fig. S19 Control experiment between **2** and $IPr_2Me_2{\cdot}B(C_6F_5)_3$.

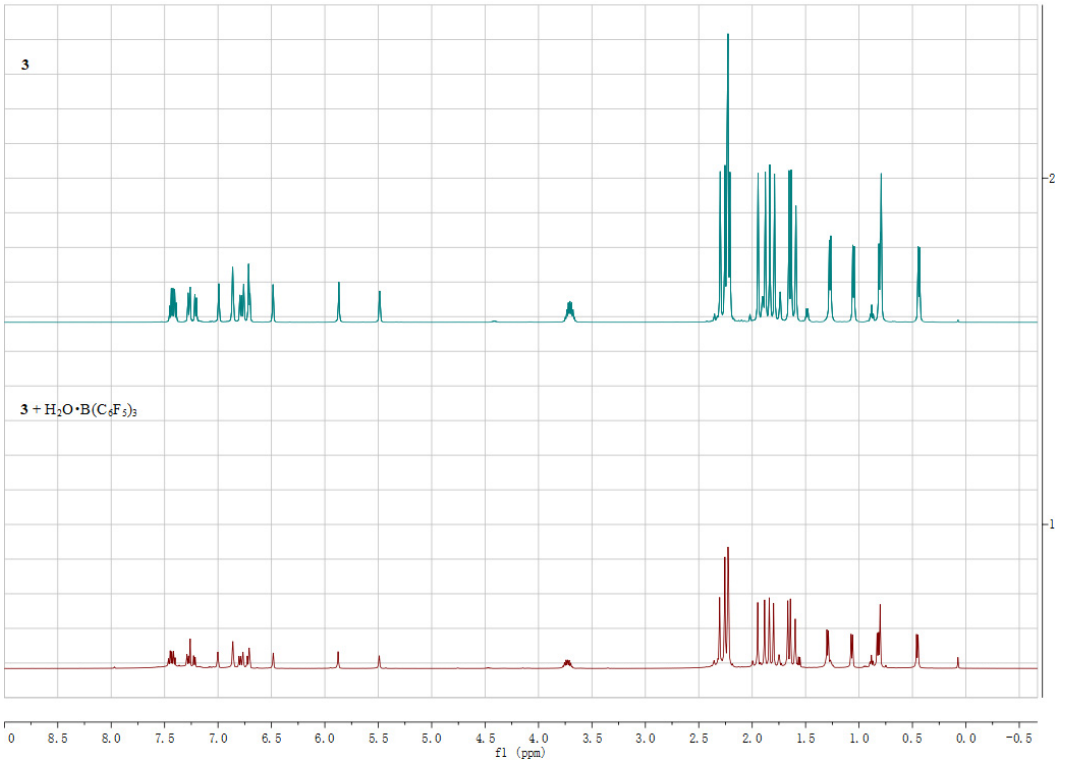


Fig. S20 Control experiment between **3** and $H_2O{\cdot}B(C_6F_5)_3$.

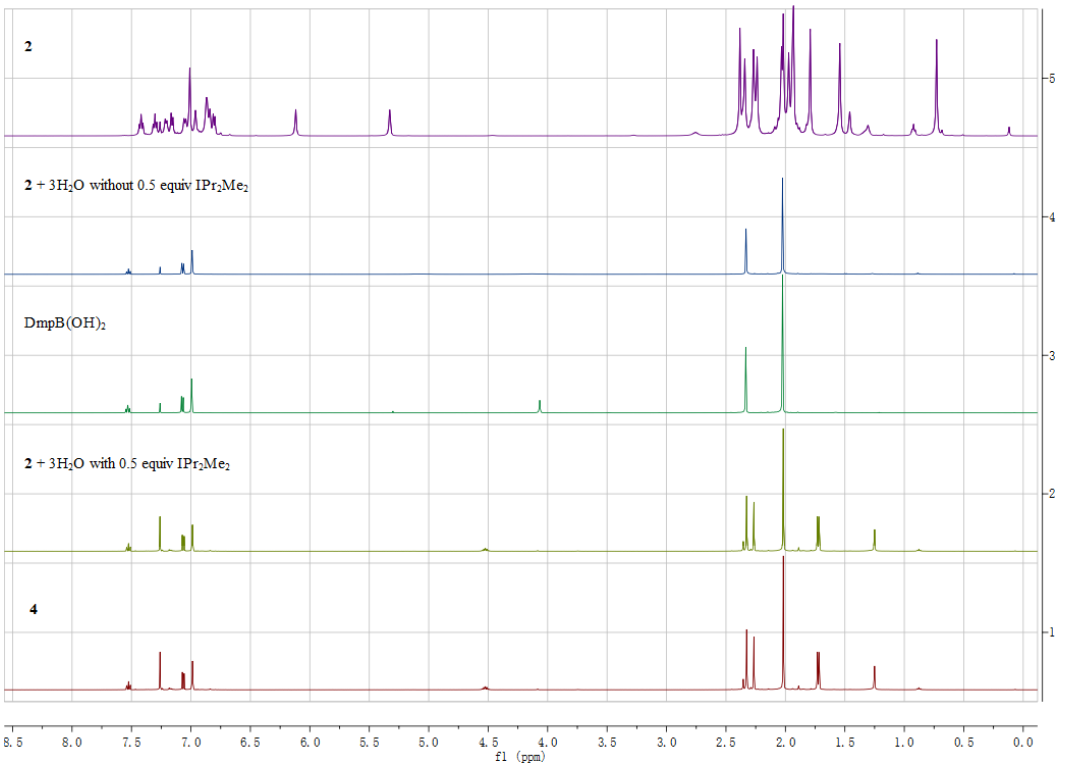


Fig. S21 Control experiments between **2** with 3 equiv of H_2O with or without IPr_2Me_2 (0.5 equiv).

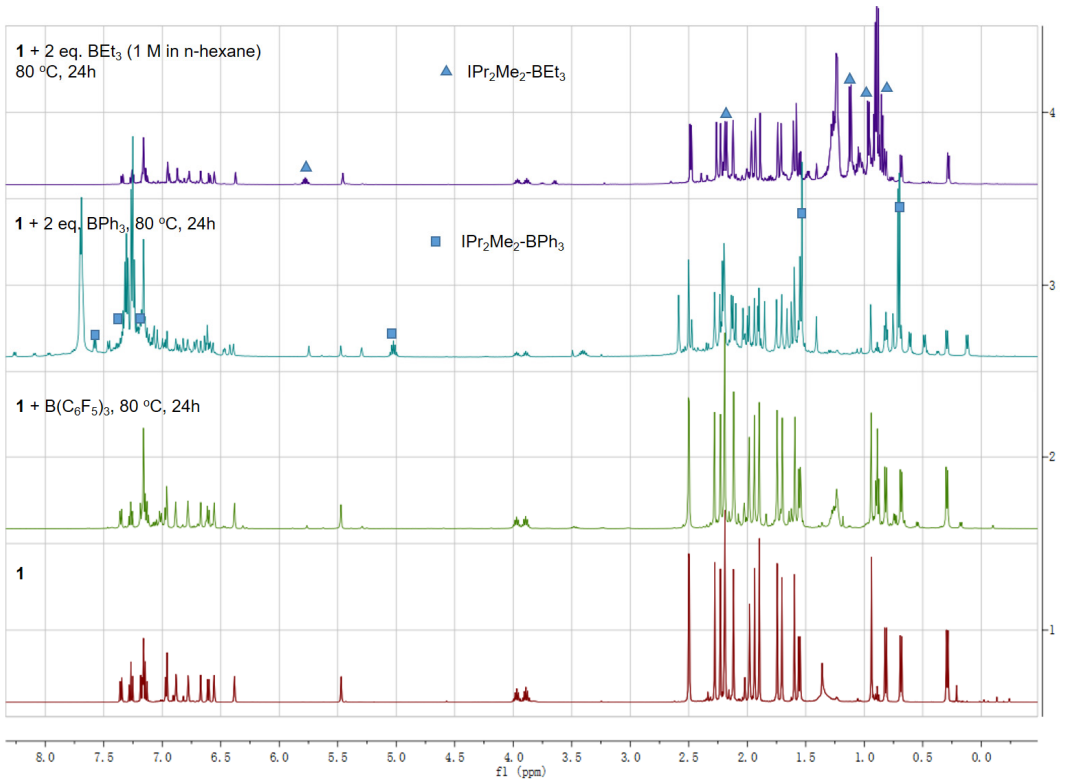


Fig. S22 Control experiments between **1** and Lewis acids.

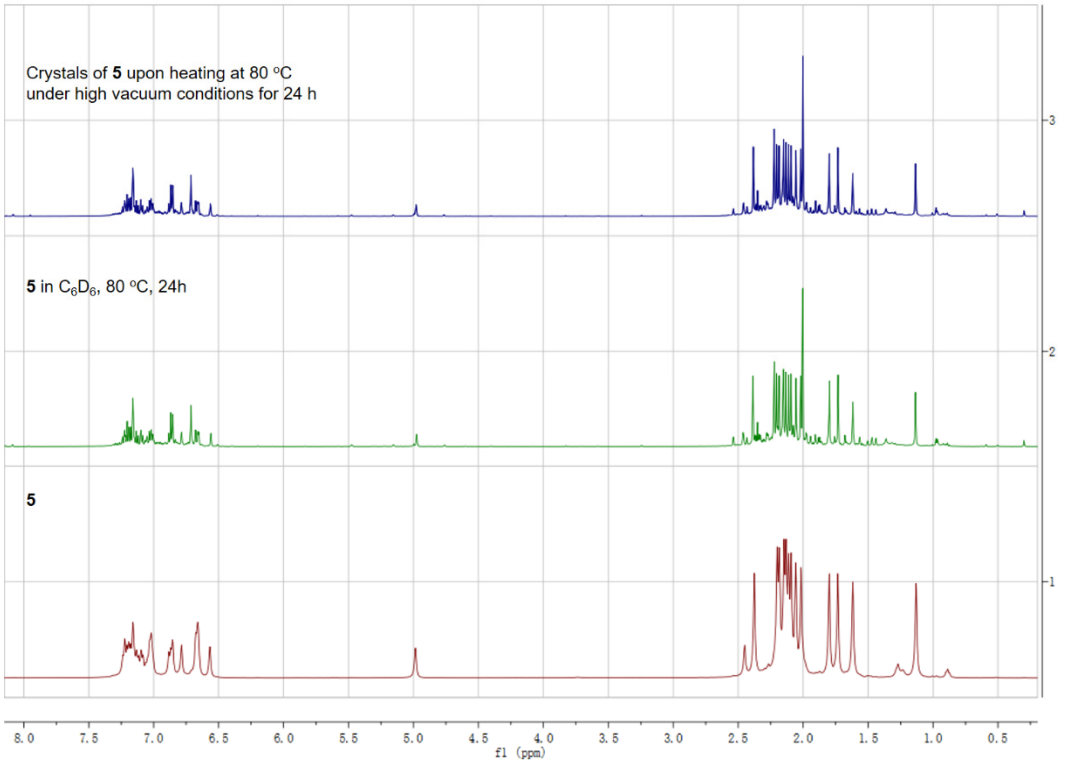


Fig. S23 Thermal stability of **5**.

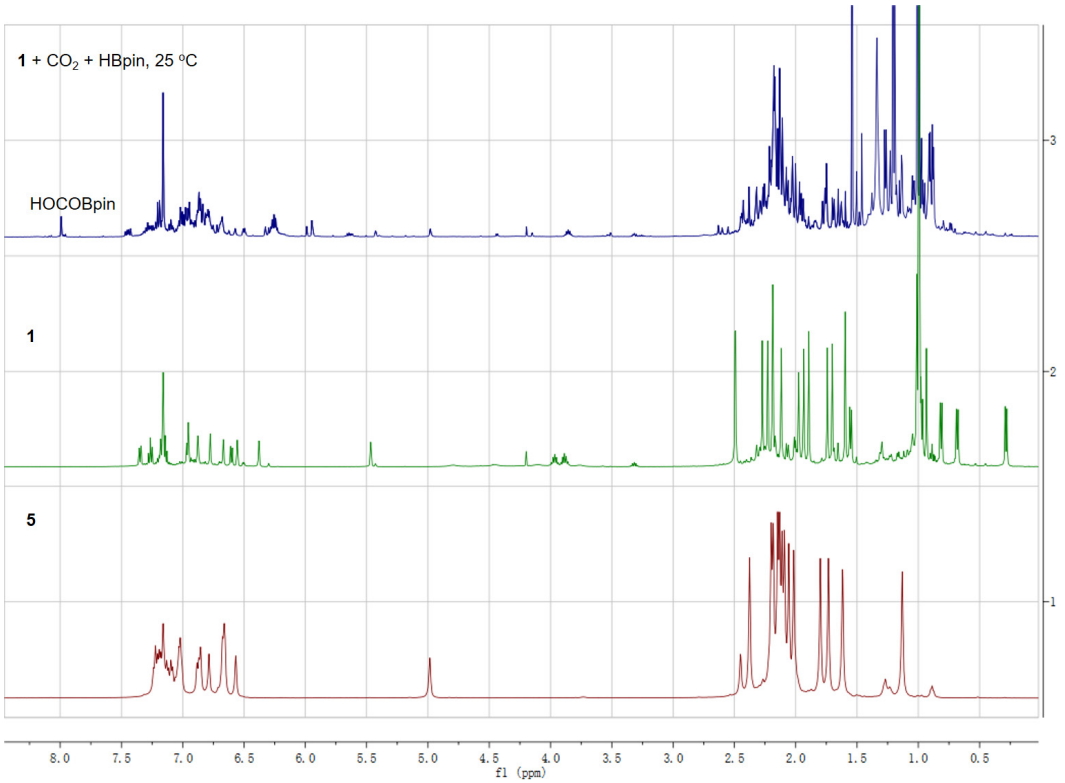


Fig. S24 Control experiment of **1** with CO_2 in the presence of HBpin.

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 Cu Kα radiation (λ = 1.54184 Å). 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.[S3] All structures were solved by intrinsic phasing (ShelXT-2015),[S4,S5] and refined to convergence by full-matrix least squares methods based on F^2 (SHELX-2018)[S6] embedded in the Olex2.[S7] All non-hydrogen atoms were refined with anisotropic displacement parameters (ADPs). Hydrogen atoms attached to carbon (CH) were placed in calculated positions and refined within a riding model, with U_{iso}(H) = 1.2 U_{eq} (C) of the carrier atom (U_{iso}(H) = 1.5 U_{eq} (C) for methyl groups). 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 *U*eq (N). Hydrogen atom bonded to oxygen (OH) was located and then fixed with U_{iso}(H) = 1.5 *U*eq (O). The threshold (I_{obs}-I_{calc})/σ(W)>10 was chosen for omitting these reflections.

Table S1. X-ray data for compounds **2**, **3** and **5**.

Compounds	**2•toluene**	**3**	**5•(0.5benzene)**
Formula	$C_{55}H_{60}B_2N_2O$	$C_{77}H_{72}B_3F_{15}N_4O$	$C_{52}H_{53}B_2N_2O_2$
Formula weight	786.67	1386.81	759.58
Temperature (K)	172.99(10)	173.00(10)	172.99(10)
Wavelength (Å)	1.54184	1.54184	1.54184
Crystal system	triclinic	triclinic	triclinic
Space group	P-1	P-1	P-1
a (Å)	11.6024(4)	11.1752(4)	8.1757(3)
b (Å)	12.4641(4)	14.7860(5)	13.4922(6)
c (Å)	17.0448(5)	21.3743(7)	19.8843(8)
α (°)	111.154(3)	81.940(3)	86.111(4)
β (°)	91.945(3)	77.947(3)	83.103(3)
γ (°)	97.305(3)	88.914(3)	72.919(4)
V (°)	2271.64(13)	3419.6(2)	2080.25(15)
Z	2	2	2
Density (calcd. g/cm^{-3})	1.150	1.347	1.213
Absorption coeff. (mm^{-1})	0.509	0.910	0.552
Reflections collected	22282	33871	19731
Independent reflections	7966	12111	7330
	[R_{int} = 0.0485]	[R_{int} = 0.0359]	[R_{int} = 0.0876]
Data/restraints/parameters	7966/1/555	12111/1/923	7330/0/535
R_1 [I>2sigma(I)]	0.0618	0.0420	0.0743
wR_2 [all data]	0.1601	0.1230	0.2211
GOF	1.074	1.075	1.040
CCDC No	2041862	2041863	2041864

Computational details

DFT calculations were carried out employing Gaussian 09 program package.[S8] Geometry optimizations and frequency calculations were calculated at M06-2X[S9] functional level combined with the def2-SVP basis set. Full optimization was applied in the reactants, intermediates, transition states, and the corresponding products of the research system. At the same level, the harmonic vibrational frequency calculations were implemented for all optimized geometries to verify the character of stationary points. Additionally, the solvent effects were taken into account in toluene using the SMD[S10] model (PhMe solvent, ε = 2.3741). NBO analysis was carried out using NBO 3.1 in Gaussian 09 package. All values in the square brackets of figures are the optimized bond distances in solution unless indicated. To refine the energetic accuracy of all the species, we recalculated the single point energies based on the optimized structures with M06-2X/def2-TZVP/SMD level of theory. In order to correct the overestimated entropies,[S11,S12] we used an empirical approach to correct the entropies: we estimated the total entropy in solution at 50%. [S13-S15]

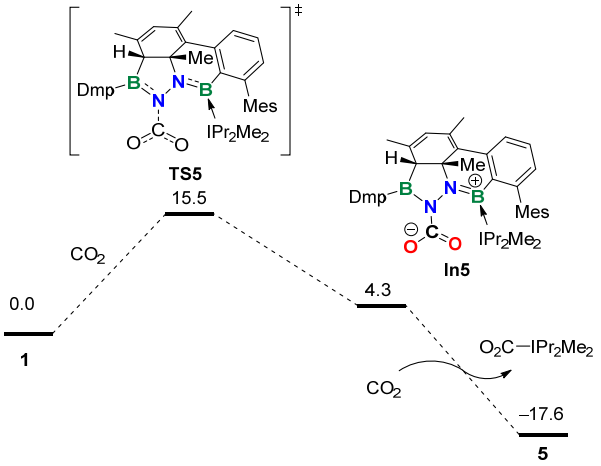
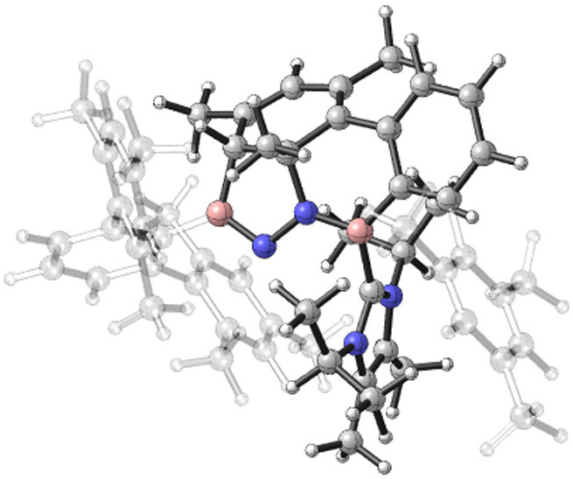


Fig. S25 Proposed reaction pathway for the generation of **5**.

Table S2. Calculated geometries (atom, x-, y-, z-positions in Å).

1



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C	-0.2890180	-0.7870120	3.9278580
C	-1.7365330	-0.5616140	3.8506320
C	-2.4744690	-0.8300720	2.7564790
H	-2.2195000	-0.1238020	4.7294210
N	-0.8559550	-0.0473120	-0.2366700
N	0.1338980	-0.4802120	0.6276800
C	1.8617330	-1.3436060	2.7518140
C	2.6415890	-1.9758860	3.7217910
C	2.4654160	-0.7349380	1.6090630
C	4.0289400	-2.0131270	3.5959200
H	2.1520120	-2.4564480	4.5710510
C	3.8657120	-0.8316230	1.4697420
C	4.6281650	-1.4543450	2.4739490
H	4.6386810	-2.5037740	4.3569220
H	5.7112760	-1.5213980	2.3455980
B	1.4390130	-0.0254910	0.6327170
H	-2.3239500	-2.4391940	1.4093780
C	1.2099230	3.4924980	-0.6756920
C	1.4207440	2.8460740	-1.8593740
C	0.8968840	2.8700210	1.7146020
H	1.1153390	3.9428870	1.7948730
C	1.8630660	0.4944920	-2.6045360
H	1.0783530	0.6985690	-3.3496650
N	1.3087690	2.5392550	0.3249360
N	1.6455140	1.5108880	-1.5485870

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C	5.2340610	0.8297050	0.0933820
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C	6.4439350	0.0588960	-1.8869760
H	6.0959850	-1.9991260	-2.4269520
H	6.5716030	2.0467240	-1.0740750
B	-2.0701940	-0.5788610	0.1437930
C	-3.4171420	-0.4952500	-0.7196100
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H	0.1505940	-1.0496430	6.0269640
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H	4.9025880	1.5795360	2.0958250
H	5.7131990	2.7275880	0.9981090
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C	-4.0063120	4.1117640	0.7083350
C	-2.3980180	4.0196590	-1.0561770
C	-3.0173590	4.7497220	-0.0368290
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C	-1.9903640	-3.0072250	-2.2735810
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H	-2.6211090	-1.6112430	-3.7989630
H	-1.4356310	-0.9612710	-2.6545870
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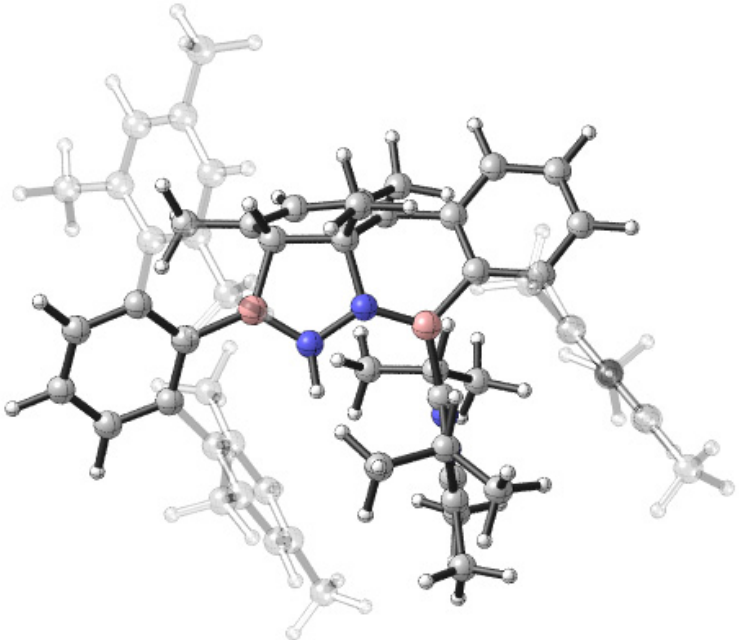
[1-H]$^+$



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H	4.5618350	0.7243390	-2.5001150
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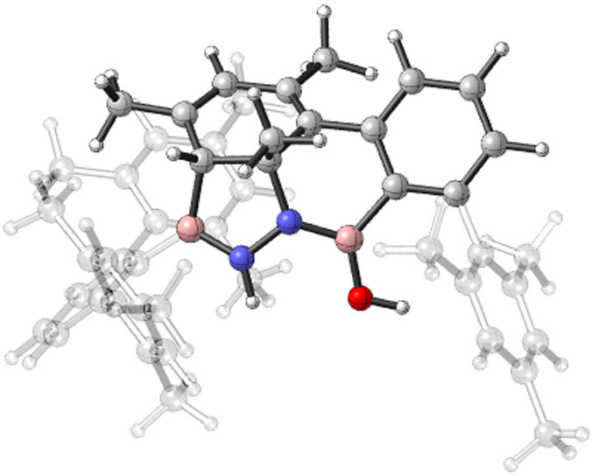
2



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C	4.8629910	2.1386760	1.5411750
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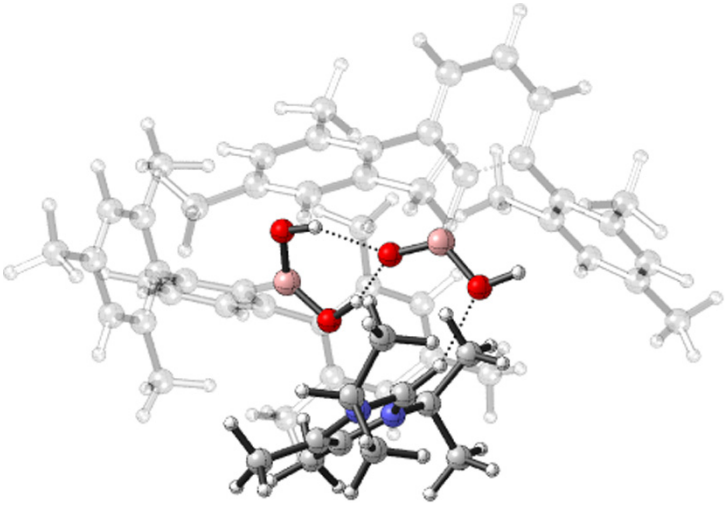
4



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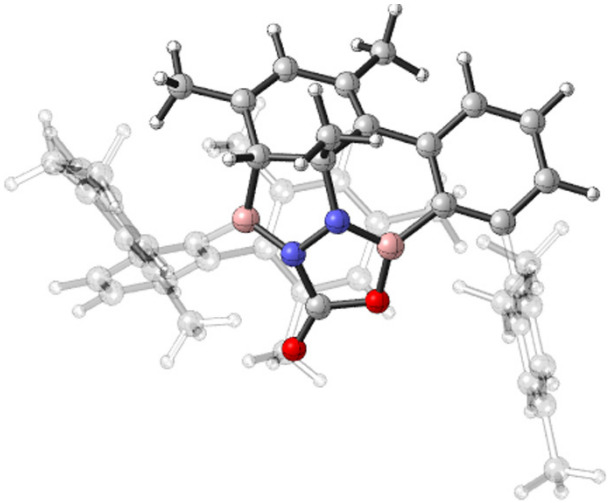

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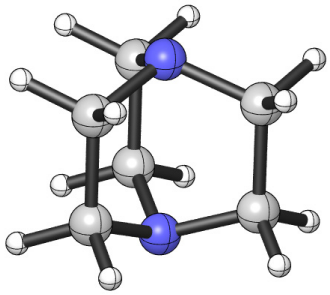

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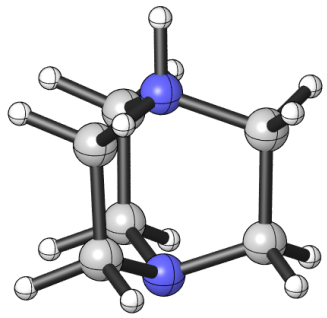
H	1.1828480	-0.6841020	-1.9717120
H	1.1876930	-1.3599210	1.5793820
H	1.1867240	-2.0834250	-0.0399310

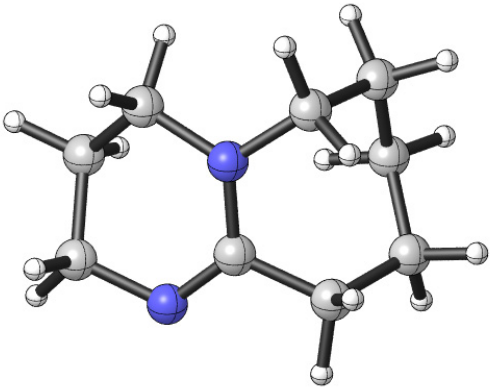
[DABCO-H]$^{+}$.



N	1.2798370	0.0123150	-0.0040990
C	0.8114050	0.8307800	1.1032510
C	0.8061410	0.5529800	-1.2684030

N	-1.2148030	-0.0118540	0.0037590
C	0.8297270	-1.3610440	0.1577980
C	-0.7205280	-1.4237950	0.1355380
C	-0.7457660	0.5866060	-1.2907300
C	-0.7401680	0.8173830	1.1618790
H	-2.2396990	-0.0231800	0.0071930
H	1.2297590	0.4415770	2.0401990
H	1.1798870	1.8560150	0.9708480
H	1.2097950	1.5648440	-1.4000020
H	1.1872560	-0.0701700	-2.0874870
H	1.2460340	-1.9739270	-0.6516130
H	1.2146570	-1.7543680	1.1071280
H	-1.1180430	-1.9826420	-0.7201630
H	-1.1518820	-1.8313120	1.0577250
H	-1.1559870	1.6025680	-1.3392240
H	-1.1808260	-0.0128050	-2.0995110
H	-1.1345050	0.3501560	2.0721830
H	-1.1865510	1.8125570	1.0491030

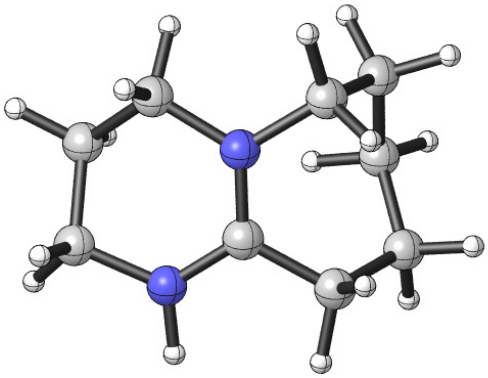
DBU



N	-0.2753860	-0.5573980	-0.5707810
C	-0.3285180	0.8085810	-0.3852190
N	-1.3679800	1.4725510	-0.0326630
C	-2.5935010	0.7291310	0.1795070
C	-2.3352700	-0.6623990	0.7476340
C	-1.3913270	-1.4087780	-0.1811820
C	0.9635570	-1.2158260	-0.9437820
C	1.9438920	-1.3651610	0.2278180
C	1.9855580	-0.1101420	1.0993760
C	2.1311560	1.2037490	0.3265840
C	0.9648880	1.5574030	-0.6337470
H	-3.2456930	1.3054950	0.8529410

H	-3.1426090	0.6372250	-0.7769590
H	-3.2690040	-1.2291870	0.8704890
H	-1.8726820	-0.5594660	1.7424570
H	-1.9347980	-1.7553930	-1.0791670
H	-0.9920000	-2.3063590	0.3186250
H	0.7093170	-2.1998020	-1.3647790
H	1.4427580	-0.6562210	-1.7588630
H	1.6604370	-2.2278980	0.8519970
H	2.9439630	-1.5869730	-0.1790140
H	1.0660730	-0.0642090	1.7050460
H	2.8143040	-0.1955100	1.8186850
H	3.0764490	1.1903560	-0.2394350
H	2.2296760	2.0128620	1.0645250
H	1.2666030	1.3908130	-1.6784970
H	0.7081620	2.6188620	-0.5458690

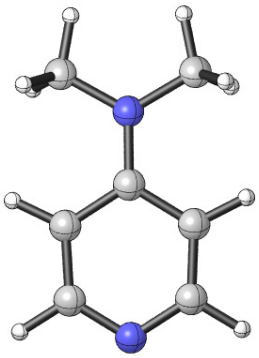
$[DBU-H]^+$



N	-0.2378980	-0.5803370	-0.5416120
C	-0.2695350	0.7334760	-0.4009640
N	-1.3774750	1.3588880	-0.0375640
C	-2.6429290	0.6830290	0.2277730
C	-2.3460520	-0.7217020	0.7232980
C	-1.4038360	-1.4224000	-0.2400710
C	1.0146800	-1.2517030	-0.9099120
C	1.9723720	-1.3631850	0.2783760
C	2.0301150	-0.0783310	1.1053190
C	2.1665330	1.2059450	0.2844140
C	0.9732730	1.5411180	-0.6537400
H	-1.3329950	2.3693510	0.0425760
H	-3.1881450	1.2656620	0.9796770
H	-3.2474440	0.6602180	-0.6919740
H	-3.2765470	-1.2959610	0.8112570

H	-1.8878210	-0.6693150	1.7222320
H	-1.9110800	-1.6719890	-1.1853250
H	-1.0274750	-2.3573850	0.1961790
H	0.7483070	-2.2385400	-1.3085210
H	1.4794520	-0.6943790	-1.7330950
H	1.6749110	-2.2013400	0.9262280
H	2.9679970	-1.6109000	-0.1194120
H	1.1299240	-0.0080690	1.7382570
H	2.8753620	-0.1388510	1.8049010
H	3.0826100	1.1620320	-0.3220790
H	2.2983440	2.0433960	0.9819170
H	1.2488430	1.3770550	-1.7054440
H	0.7056390	2.6016760	-0.5700950

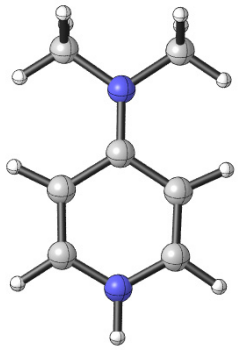
DMAP



C	0.5648320	1.1988270	0.0005710
C	1.9518820	1.1308550	0.0005890
N	2.6585070	0.0000030	0.0000000
C	1.9518910	-1.1308540	-0.0005850
C	0.5648410	-1.1988380	-0.0005710
C	-0.1872830	-0.0000070	-0.0000070
N	-1.5498720	-0.0000020	-0.0000230
C	-2.2686590	1.2545090	-0.0010160
C	-2.2686850	-1.2545000	0.0010290
H	0.0823590	2.1741980	0.0012490
H	2.5255820	2.0640300	0.0011480
H	2.5255990	-2.0640240	-0.0011390
H	0.0823790	-2.1742130	-0.0012370
H	-2.0364680	1.8596870	0.8915610
H	-2.0327940	1.8601350	-0.8922900
H	-3.3453210	1.0531540	-0.0034700
H	-2.0328650	-1.8600810	0.8923470
H	-3.3453420	-1.0531200	0.0034320

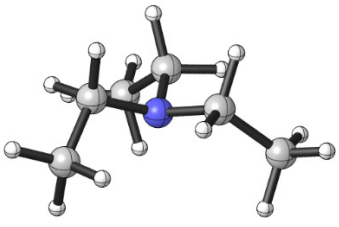
H	-2.0364780	-1.8597340	-0.8915040

[DMAP-H]$^+$



C	-0.5484480	1.2119500	0.0000000
C	-1.9136180	1.1727230	-0.0000080
N	-2.5820500	0.0000170	-0.0000050
C	-1.9136660	-1.1727100	0.0000040
C	-0.5484930	-1.2119960	0.0000100
C	0.2239660	-0.0000390	0.0000060
N	1.5590800	-0.0000140	0.0000110
C	2.3775350	1.2040060	0.0000030
C	2.3776400	-1.2039660	-0.0000130
H	-3.5990630	0.0000390	-0.0000030
H	-0.0900410	2.1959110	-0.0000020
H	-2.5167880	2.0799760	-0.0000170
H	-2.5168690	-2.0799420	0.0000060
H	-0.0901490	-2.1959850	0.0000160
H	1.7811360	2.1160120	-0.0000790
H	3.0203120	1.2064490	0.8919710
H	3.0204350	1.2063440	-0.8918770
H	1.7813410	-2.1160300	0.0001320
H	3.0203620	-1.2063700	-0.8920220
H	3.0206030	-1.2062290	0.8918220

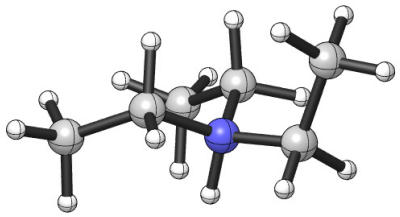
NEt_3



N	-0.0010460	0.0008760	-0.0338200

C	-2.2792370	0.8635480	0.4443420
C	-1.3971880	0.0048830	-0.4497400
C	0.3889870	-2.4035320	0.4424470
C	0.6948620	-1.2096180	-0.4497210
C	1.8943140	1.5331490	0.4409620
C	0.6990830	1.2107880	-0.4436090
H	-3.3273000	0.8217450	0.1135930
H	-2.2242280	0.5057610	1.4824500
H	-1.9725340	1.9197090	0.4351950
H	-1.4941910	0.3276350	-1.5101480
H	-1.7689100	-1.0295130	-0.4133590
H	0.9527850	-3.2894580	0.1155480
H	0.6644510	-2.1758980	1.4821590
H	-0.6786980	-2.6673180	0.4276970
H	0.4669670	-1.4538020	-1.5111140
H	1.7764100	-1.0149240	-0.4100090
H	2.3718250	2.4709500	0.1215640
H	1.5696740	1.6419060	1.4857260
H	2.6603530	0.7449160	0.4058610
H	1.0146670	1.1462460	-1.5088660
H	-0.0088830	2.0505990	-0.3876330

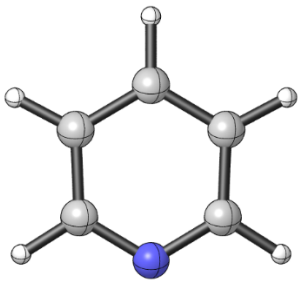
$[HNEt_3]^+$



N	-0.4471010	0.0649330	0.0000000
H	-1.2893400	-0.5267340	0.0000000
C	0.2969990	-1.7295570	1.6277650
C	0.2969990	-0.2557180	1.2706760
C	0.1542210	2.5172510	0.0000000
C	-0.9529240	1.4861920	0.0000000
C	0.2969990	-1.7295570	-1.6277650
C	0.2969990	-0.2557180	-1.2706760
H	0.6291040	-1.8296680	2.6693880
H	-0.7139830	-2.1579210	1.5620070
H	0.9758130	-2.3246390	1.0082870

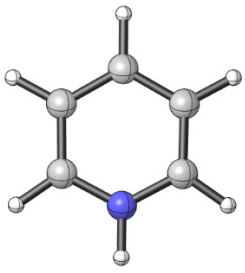
H	1.3131560	0.1427680	1.1559570
H	-0.2059840	0.3194110	2.0588190
H	-0.3070670	3.5135840	0.0000000
H	0.7864700	2.4495180	0.8955180
H	0.7864700	2.4495180	-0.8955180
H	-1.5894050	1.5811620	-0.8892240
H	-1.5894050	1.5811620	0.8892240
H	0.6291040	-1.8296680	-2.6693880
H	0.9758130	-2.3246390	-1.0082870
H	-0.7139830	-2.1579210	-1.5620070
H	-0.2059840	0.3194110	-2.0588190
H	1.3131560	0.1427680	-1.1559570

Py.



C	-1.1979880	0.6697270	-0.0000040
C	-1.1404700	-0.7240360	-0.0000180
N	0.0010160	-1.4100650	0.0000110
C	1.1412630	-0.7229470	0.0000040
C	1.1970300	0.6714000	-0.0000050
C	-0.0007860	1.3816500	0.0000060
H	-2.1617430	1.1801220	0.0000100
H	-2.0639830	-1.3117270	0.0000240
H	2.0656590	-1.3092670	-0.0000130
H	2.1599970	1.1832930	-0.0000230
H	-0.0013370	2.4732720	0.0000250

$[PyH]^+$



C	0.7138220	-1.2103810	0.0000000

C	-0.6686300	-1.1828090	0.0000010
N	-1.3022390	0.0016440	-0.0000010
C	-0.6658710	1.1843630	-0.0000010
C	0.7169550	1.2086710	0.0000010
C	1.4121150	-0.0017140	0.0000010
H	-2.3241680	0.0027020	0.0000000
H	1.2323570	-2.1682020	-0.0000050
H	-1.2945470	-2.0750150	0.0000030
H	-1.2896060	2.0781450	-0.0000010
H	1.2379920	2.1651280	0.0000030
H	2.5033020	-0.0030420	-0.0000040

Table S3. The NPA charges of **1**.

			Natural Population			
		Natural	---			
Atom	No	Charge	Core	Valence	Rydberg	Total

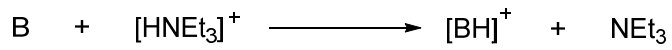
C	1	-0.61889	1.99914	4.59922	0.02053	6.61889
C	2	0.11931	1.99923	3.85806	0.02341	5.88069
C	3	-0.03360	1.99886	4.01376	0.02097	6.03360
C	4	0.00084	1.99898	3.98256	0.01762	5.99916
C	5	-0.29292	1.99895	4.27552	0.01845	6.29292
C	6	0.10554	1.99910	3.87798	0.01737	5.89446
H	7	0.20324	0.00000	0.79493	0.00182	0.79676
N	8	-0.80027	1.99926	5.76956	0.03146	7.80027
N	9	-0.53803	1.99925	5.51240	0.02638	7.53803
C	10	-0.01175	1.99905	3.99256	0.02014	6.01175
C	11	-0.22086	1.99911	4.20370	0.01805	6.22086
C	12	-0.40260	1.99891	4.37915	0.02454	6.40260
C	13	-0.20969	1.99921	4.19314	0.01734	6.20969
H	14	0.22142	0.00000	0.77713	0.00144	0.77858
C	15	-0.01810	1.99904	3.99663	0.02244	6.01810
C	16	-0.22709	1.99912	4.20986	0.01811	6.22709
H	17	0.22121	0.00000	0.77778	0.00102	0.77879
H	18	0.21920	0.00000	0.77951	0.00130	0.78080
B	19	0.91369	1.99854	2.06050	0.02727	4.08631
H	20	0.24504	0.00000	0.75234	0.00262	0.75496
C	21	0.13762	1.99894	3.84528	0.01815	5.86238
C	22	0.13440	1.99892	3.84877	0.01790	5.86560
C	23	-0.03016	1.99933	4.01603	0.01479	6.03016
H	24	0.20860	0.00000	0.78930	0.00210	0.79140
C	25	-0.02962	1.99934	4.01507	0.01520	6.02962
H	26	0.21251	0.00000	0.78528	0.00222	0.78749

N	27	-0.30852	1.99932	5.28456	0.02464	7.30852
N	28	-0.29866	1.99932	5.27390	0.02544	7.29866
C	29	0.18907	1.99895	3.78341	0.02856	5.81093
C	30	-0.06186	1.99891	4.04204	0.02091	6.06186
C	31	0.00729	1.99909	3.97480	0.01882	5.99271
C	32	-0.00019	1.99908	3.98263	0.01848	6.00019
C	33	-0.22974	1.99903	4.21414	0.01657	6.22974
C	34	-0.23050	1.99904	4.21503	0.01642	6.23050
C	35	-0.01489	1.99916	3.99847	0.01726	6.01489
H	36	0.21243	0.00000	0.78609	0.00148	0.78757
H	37	0.21109	0.00000	0.78740	0.00150	0.78891
B	38	0.88023	1.99897	2.08954	0.03126	4.11977
C	39	-0.34171	1.99888	4.31857	0.02426	6.34171
C	40	-0.02039	1.99905	4.00059	0.02076	6.02039
C	41	-0.01895	1.99906	3.99899	0.02090	6.01895
C	42	-0.22270	1.99911	4.20597	0.01762	6.22270
C	43	-0.22417	1.99910	4.20710	0.01798	6.22417
C	44	-0.22098	1.99920	4.20412	0.01766	6.22098
H	45	0.21664	0.00000	0.78203	0.00134	0.78336
H	46	0.21729	0.00000	0.78132	0.00139	0.78271
H	47	0.21881	0.00000	0.78015	0.00104	0.78119
C	48	-0.61145	1.99941	4.59798	0.01407	6.61145
H	49	0.21117	0.00000	0.78745	0.00138	0.78883
H	50	0.21560	0.00000	0.78342	0.00098	0.78440
H	51	0.23080	0.00000	0.76773	0.00146	0.76920
C	52	-0.64191	1.99944	4.63031	0.01216	6.64191
H	53	0.21666	0.00000	0.78213	0.00121	0.78334
H	54	0.22328	0.00000	0.77557	0.00115	0.77672
H	55	0.22559	0.00000	0.77346	0.00095	0.77441
C	56	-0.63472	1.99941	4.62258	0.01272	6.63472
H	57	0.23026	0.00000	0.76814	0.00159	0.76974
H	58	0.21658	0.00000	0.78201	0.00141	0.78342
H	59	0.21397	0.00000	0.78489	0.00114	0.78603
C	60	-0.63853	1.99944	4.62668	0.01241	6.63853
H	61	0.21866	0.00000	0.78047	0.00086	0.78134
H	62	0.23035	0.00000	0.76841	0.00123	0.76965
H	63	0.22819	0.00000	0.77050	0.00131	0.77181
C	64	-0.62807	1.99945	4.61705	0.01156	6.62807
H	65	0.22248	0.00000	0.77656	0.00096	0.77752
H	66	0.22153	0.00000	0.77732	0.00115	0.77847
H	67	0.21787	0.00000	0.78127	0.00086	0.78213
C	68	-0.63324	1.99944	4.62157	0.01224	6.63324
H	69	0.22020	0.00000	0.77842	0.00137	0.77980
H	70	0.22849	0.00000	0.77035	0.00116	0.77151

H	71	0.21968	0.00000	0.77940	0.00092	0.78032
C	72	-0.65108	1.99942	4.63896	0.01271	6.65108
H	73	0.23556	0.00000	0.76341	0.00103	0.76444
H	74	0.23732	0.00000	0.76180	0.00088	0.76268
H	75	0.23165	0.00000	0.76701	0.00135	0.76835
C	76	-0.65251	1.99942	4.64012	0.01298	6.65251
H	77	0.23723	0.00000	0.76189	0.00088	0.76277
H	78	0.23711	0.00000	0.76158	0.00131	0.76289
H	79	0.23199	0.00000	0.76682	0.00119	0.76801
C	80	-0.05533	1.99892	4.03620	0.02021	6.05533
C	81	0.00486	1.99909	3.97871	0.01734	5.99514
C	82	0.02689	1.99908	3.95643	0.01761	5.97311
C	83	-0.22798	1.99904	4.21300	0.01595	6.22798
C	84	-0.23866	1.99903	4.22267	0.01696	6.23866
C	85	-0.02481	1.99914	4.00848	0.01718	6.02481
H	86	0.20747	0.00000	0.79116	0.00137	0.79253
H	87	0.20234	0.00000	0.79522	0.00244	0.79766
C	88	-0.05725	1.99892	4.03758	0.02074	6.05725
C	89	0.01319	1.99908	3.96912	0.01861	5.98681
C	90	0.00104	1.99908	3.98127	0.01861	5.99896
C	91	-0.23050	1.99903	4.21547	0.01600	6.23050
C	92	-0.22883	1.99904	4.21301	0.01678	6.22883
C	93	-0.01561	1.99916	3.99945	0.01701	6.01561
H	94	0.20813	0.00000	0.79021	0.00166	0.79187
H	95	0.20929	0.00000	0.78921	0.00151	0.79071
C	96	-0.63571	1.99944	4.62414	0.01213	6.63571
H	97	0.22485	0.00000	0.77398	0.00117	0.77515
H	98	0.21776	0.00000	0.78138	0.00087	0.78224
H	99	0.22440	0.00000	0.77418	0.00141	0.77560
C	100	-0.62700	1.99945	4.61604	0.01150	6.62700
H	101	0.21624	0.00000	0.78291	0.00085	0.78376
H	102	0.21908	0.00000	0.77992	0.00100	0.78092
H	103	0.22194	0.00000	0.77691	0.00115	0.77806
C	104	-0.64509	1.99944	4.63314	0.01251	6.64509
H	105	0.21034	0.00000	0.78869	0.00097	0.78966
H	106	0.22492	0.00000	0.77390	0.00118	0.77508
H	107	0.24573	0.00000	0.75216	0.00211	0.75427
C	108	-0.64336	1.99945	4.63140	0.01251	6.64336
H	109	0.23009	0.00000	0.76907	0.00084	0.76991
H	110	0.22303	0.00000	0.77591	0.00106	0.77697
H	111	0.22222	0.00000	0.77671	0.00107	0.77778
C	112	-0.63079	1.99945	4.61954	0.01180	6.63079
H	113	0.21439	0.00000	0.78471	0.00090	0.78561
H	114	0.22398	0.00000	0.77504	0.00097	0.77602

H	115	0.21807	0.00000	0.78074	0.00119	0.78193
C	116	-0.66356	1.99943	4.65241	0.01172	6.66356
H	117	0.20092	0.00000	0.79755	0.00153	0.79908
H	118	0.27182	0.00000	0.72558	0.00260	0.72818
H	119	0.22212	0.00000	0.77617	0.00171	0.77788
C	120	-0.62738	1.99944	4.61433	0.01360	6.62738
H	121	0.22014	0.00000	0.77715	0.00271	0.77986
H	122	0.25828	0.00000	0.73896	0.00276	0.74172
H	123	0.22483	0.00000	0.77424	0.00094	0.77517
C	124	-0.62035	1.99945	4.60763	0.01327	6.62035
H	125	0.21976	0.00000	0.77941	0.00082	0.78024
H	126	0.21015	0.00000	0.78885	0.00100	0.78985
H	127	0.23265	0.00000	0.76590	0.00145	0.76735
C	128	-0.62349	1.99944	4.61071	0.01333	6.62349
H	129	0.23610	0.00000	0.76135	0.00256	0.76390
H	130	0.22314	0.00000	0.77572	0.00114	0.77686
H	131	0.22445	0.00000	0.77472	0.00083	0.77555
C	132	-0.62545	1.99944	4.61143	0.01458	6.62545
H	133	0.22982	0.00000	0.76878	0.00140	0.77018
H	134	0.24191	0.00000	0.75498	0.00311	0.75809
H	135	0.21544	0.00000	0.78371	0.00085	0.78456
==========						
* Total *		0.00000	129.94603	330.78940	1.26458	462.00000

Table S4. Comparison of the basicity of **1** with typical bases.



Species	Sum of electronic and thermal Enthalpies (Hartree)	ΔH (kcal/mol)
NEt_3	-291.823482	0
$[HNEt_3]^+$	-292.241923	
Py	-247.901192	7.4
$[Py\text{-}H]^+$	-248.307898	
DABCO	-344.729960	−0.4
$[DABCO\text{-}H]^+$	-345.149102	
DMAP	-381.639614	−3.5
$[DMAP\text{-}H]^+$	-382.063603	
DBU	-461.287903	−16.2
$[DBU\text{-}H]^+$	-461.732175	
1	-2555.114983	-37.4
$[1\text{-}H]^+$	-2555.593102	

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