Electronic Supplementary Information

Achieving Efficient and Stable Blue Thermally Activated Delayed Fluorescence Organic Light-Emitting Diodes Based on Four-Coordinate Fluoroboron Emitters by Simple Substitution Molecular Engineering

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Experimental Details

Materials and Reagents. 3,6-Di-*tert*-butylcarbazole (DTC) and 9,9-dimethyl-9,10-dihydroacridine (DMAC) were purchased from *AK Scientific, Inc*. Pyridine hydrochloride (py•HCl) and boron trifluoride diethyl etherate (BF_3•OEt_2) were obtained from *Sigma-Aldrich*. 3,6-Difluoro-9*H*-carbazole (DFC) was prepared according to the literature method with slight modifications.[1] All solvents were purified and distilled using standard procedures before use. All other reagents were of analytical grade and were used without further purification. Tetra-*n*-butylammonium hexafluorophosphate (Aldrich, 98 %, $^{n}Bu_4NPF_6$) was recrystallized for no less than three times from hot absolute ethanol prior to use.

Physical Measurements and Instrumentation. ^{1}H NMR and $^{19}F\{^{1}H\}$ NMR spectroscopy were performed using a Bruker AV400 NMR spectrometer at 298 K with chemical shifts (δ, ppm) relative to tetramethylsilane (Me_4Si) for the ^{1}H NMR and trichlorofluoromethane ($CFCl_3$) for the $^{19}F\{^{1}H\}$ NMR spectra. $^{11}B\{^{1}H\}$ NMR spectroscopy was performed using a Bruker DRX 500 NMR spectrometer at 298 K with chemical shifts (δ, ppm) relative to BF_3•OEt_2. High resolution electron ionization (EI) and electrospray ionization (ESI) mass spectra were recorded on a Thermo Scientific DFS High Resolution Magnetic Sector Mass Spectrometer and Bruker maXis II high-resolution QTOF mass spectrometer, respectively. Elemental analyses (C, H and N) were carried out at the Institute of Chemistry, Chinese Academy of Sciences, Beijing, People's Republic of China, using a Carlo Erba 1106 elemental analyzer. Thermal analyses were performed on a TA instruments Q50 thermogravimetric analyzer (TGA) with a heating rate of 10 °C min^{-1} under nitrogen atmosphere, in which the decomposition temperature (T_d) is defined as the temperature at which the material showed a 5 % weight loss. The UV−vis absorption spectra were recorded on a Varian Cary 50 spectrophotometer equipped with a Xenon flash lamp. Steady-state emission spectra were recorded using an Edinburgh Instruments FS5 spectrofluorometer. Toluene solutions of **1**–**8** (10^{-5} M) were prepared for the absorption and

photoluminescence (PL) characteristics in the solution state. Solutions were degassed by using a high vacuum line in a two-compartment cell with four freeze-pump-thaw cycles. The optical dilute method developed by Demas and Crosby[2] was applied to determine the relative luminescence quantum yields (PLQYs) of solutions with the use of quinine sulfate in 0.5 M sulfuric acid (Φ_{em} = 0.546, λ_{ex} = 365 nm) at 298 K as the standard.[3] Excited-state lifetimes of solutions and thin films were measured on a Quantaurus-Tau C11367-34 fluorescence lifetime spectrometer with the light-emitting diode (LED) at 280 nm excitation source. Time-resolved PL spectra in toluene matrix at 77 K were recorded on an Edinburgh Instruments LP980 Spectrometer. Thin films of 5 wt% **1**–**8** doped into 1,3-bis(carbazol-9-yl)benzene (mCP) were prepared by spin-coating a 10 mg cm^{-3} chloroform solution onto quartz substrates at spinning speed of 2000 rpm. Absolute PLQYs of thin films were measured on Hamamatsu C9920-03 absolute PLQY measurement system under an excitation at 300 nm. The thin film was placed in a holder inside an Oxford Instrument OptistatDN2 cryostat and maintained at the desired temperature until equilibrium was reached before recording the decay curves at variable temperatures. Nanosecond transient absorption spectra were recorded on a LP920-KS laser flash photolysis spectrometer (Edinburgh Instruments Ltd., Livingston, U.K.) at ambient temperature. The excitation source was the 355-nm output (third harmonic) of a Nd:YAG laser (Spectra-Physics Quanta-Ray Lab-130 Pulsed Nd:YAG Laser), and the probe light source was a Xe900 450W xenon arc lamp. The transient absorption spectra were detected by an image intensified CCD camera (Andor) with PC plug-in controller, fully operated by L900 spectrometer software. The picosecond transient absorption spectra were recorded on a picosecond transient absorption spectroscopy system (UNISOKU Co., Ltd.) at ambient temperature. The excitation source was 355 nm (third harmonic) of a picosecond mode-locked Nd/YAG laser (EKSPLA PT403 tunable wavelength picosecond laser), and the probe light source was a picosecond supercontinuum light source. The absorption kinetics were detected by amplified photodiodes and recorded on a digital oscilloscope (200 MHz, 12 bit) with a PC plugin controller, fully operated using UNISPEC software. Cyclic

voltammetric (CV) measurements were performed by using a CH Instruments, Inc. model CHI 620A electrochemical analyzer. Electrochemical measurements were performed in dimethylformamide (DMF) or dichloromethane (CH_2Cl_2) solutions with 0.1 mol dm^{-3} $^{n}Bu_4NPF_6$ used as supporting electrolyte at room temperature. The reference electrode was a $Ag/AgNO_3$ (0.1 mol dm^{-3} in acetonitrile) electrode, and the working electrode was a glassy carbon electrode (CH Instruments, Inc.) with a platinum wire as the counter electrode. The ferrocenium/ferrocene couple (Fc^{+}/Fc) was used as the internal reference. All solutions for electrochemical studies were deaerated with prepurified argon gas prior to measurements.

Synthesis and Characterization

The precursors, 4-Br-2-Me-Ph(dppy)Me_2,[4] 4-Br-3-F-Ph(dppy)Me_2,[4] 4-Br-3-Me-Ph(dppy)Me_2,[4] ((5-Br-Ph)$_2$-Py)Me_2[5] and 4-Br-2,6-Me_2-Ph(dppy)Me_2[4] were prepared according to modifications of literature procedures. Standard Buchwald-Hartwig coupling reactions[6] of precursors with the corresponding diarylamines afforded the intermediates 4-DTC-(dppy)Me_2, 4-DTC-2-Me-Ph(dppy)Me_2, 4-DTC-3-Me-Ph(dppy)Me_2, 4-DTC-3-F-Ph(dppy)Me_2, 4-DFC-Ph(dppy)Me_2, ((5-DTC-Ph)$_2$-Py)Me_2, 4-DTDPA-Ph(dppy)Me_2, 4-DTDPA-2,6-Me_2-Ph(dppy)Me_2. Subsequent demethylation by Py•HCl and the coordination with BF_3•OEt_2 gave title compounds **1**–**8** with good yields.[6,7] (Note: Due to the limited solubilities of 4-DFC-Ph(dppy)H_2 in common organic solvents, it was not further purified and used directly in the subsequent Lewis acid-base reaction.)

4-Cl-(dppy)Me_2. This was synthesized according to modification of literature procedure for the Suzuki–Miyaura coupling.[8] A mixture of 2,4,6-trichloropyridine (1.00 g, 548 mmol), (2-methoxyphenyl)boronic acid (1.65 g, 10.98 mmol), K_2CO_3 (4.50 g, 3.29 mmol), $Pd(OAc)_2$ (185 mg, 82.20 mmol) and PPh_3 (650 mg, 246.60 mmol) in 1,4-dioxane−water (80 mL, 3:1, v/v) was stirred at 70 ℃ for 24 hours. After cooling to room temperature, water was added and the reaction mixture was extracted with ethyl acetate for at least three times. The combined organic layer was dried over anhydrous $MgSO_4$ and filtered. The solvent was evaporated to dryness under vacuum and the crude product was then purified by column chromatography on silica gel using hexane−dichloromethane (4:1, v/v) as the eluent to give a white solid. Yield: 964 mg (54%). ^{1}H NMR (400 MHz, $CDCl_3$, 298 K, relative to Me_4Si, δ/ppm): δ 7.95 (dd, *J* = 7.5, 1.7 Hz, 2H, methoxyphenyl), 7.84 (s, 2H, pyridyl), 7.38 (dt, *J* = 7.5, 1.7 Hz, 2H, methoxyphenyl), 7.08 (dt, *J* = 7.5, 1.7 Hz, 2H, methoxyphenyl), 7.01 (d, *J* = 7.5 Hz, 2H, methoxyphenyl), 3.91 (s, 6H, −OCH_3). HRMS (positive EI) calcd for $C_{19}H_{16}ClNO_2$: *m*/*z* = 325.0870 $[M]^+$; found 325.0856 $[M]^+$.

4-Br-2-Me-Ph(dppy)Me$_2$. Yield: 1.08 g (78%). ^{1}H NMR (400 MHz, $CDCl_3$, 298 K, relative to Me_4Si, δ/ppm): δ 7.98 (dd, *J* = 7.6, 1.6 Hz, 2H, methoxyphenyl), 7.73 (s, 2H, pyridyl), 7.49 (d, *J* = 1.6 Hz, 1H, phenyl), 7.43 (dd, *J* = 8.2, 1.6 Hz, 1H, phenyl), 7.38 (dt, *J* = 8.4, 1.6 Hz, 2H, methoxyphenyl), 7.21 (d, *J* = 8.2 Hz, 1H, phenyl), 7.10 (dt, *J* = 7.6, 1.6 Hz, 2H, methoxyphenyl), 7.01 (d, *J* = 8.4 Hz, 2H, methoxyphenyl), 3.87 (s, 6H, −OCH_3), 2.41 (s, 3H, −CH_3). HRMS (positive EI) calcd for $C_{26}H_{22}BrNO_2$: *m*/*z* = 459.0834 $[M]^+$; found 459.0820 $[M]^+$.

4-Br-3-Me-Ph(dppy)Me$_2$. Yield: 1.32 g (95%). ^{1}H NMR (500 MHz, $CDCl_3$, 298 K, relative to Me_4Si, δ/ppm): δ 7.94 (d, *J* = 7.5 Hz, 2H, methoxyphenyl), 7.93 (s, 2H, pyridyl), 7.65 (d, *J* = 8.0 Hz, 1H, phenyl), 7.56 (s, 1H, phenyl), 7.37–7.40 (m, 3H, phenyl and methoxyphenyl), 7.11 (t, *J* = 7.5 Hz, 2H, methoxyphenyl), 7.03 (d, *J* = 7.5 Hz, 2H, methoxyphenyl), 3.90 (s, 6H, –OCH_3), 2.49 (s, 3H, –CH_3). HRMS (positive EI) calcd for $C_{26}H_{22}BrNO_2$: *m*/*z* = 459.0834 $[M]^+$; found 459.0817 $[M]^+$.

4-Br-3-F-Ph(dppy)Me$_2$. Yield: 774 mg (56%). ^{1}H NMR (500 MHz, $CDCl_3$, 298 K, relative to Me_4Si, δ/ppm): δ 7.96 (d, *J* = 8.0 Hz, 2H, methoxyphenyl), 7.94 (s, 2H, pyridyl), 7.67 (t, *J* = 8.0 Hz, 1H, phenyl), 7.47 (d, *J* = 8.0 Hz, 1H, phenyl), 7.37–7.41 (m, 3H, phenyl and methoxyphenyl), 7.11 (t, *J* = 8.0 Hz, 2H, methoxyphenyl), 7.03 (t, *J* = 8.0 Hz, 2H, methoxyphenyl), 3.90 (s, 6H, –CH_3). ^{19}F{^{1}H} NMR (376.4 MHz, $CDCl_3$, 298 K, relative to $CFCl_3$, δ/ppm): δ –106.62. HRMS (positive EI) calcd for $C_{25}H_{19}BrFNO_2$: *m*/*z* = 463.0583 $[M]^+$; found 463.0571 $[M]^+$.

4-Br-2,6-Me$_2$-Ph(dppy)Me$_2$. Yield: 576 mg (42%). ^{1}H NMR (500 MHz, $CDCl_3$, 298 K, relative to Me_4Si, δ/ppm): δ 8.05 (d, *J* = 7.5 Hz, 2H, methoxyphenyl), 7.59 (s, 2H, pyridyl), 7.38 (t, *J* = 7.5 Hz, 2H, methoxyphenyl), 7.32 (s, 2H, phenyl), 7.12 (t, *J* = 7.5 Hz, 2H, methoxyphenyl), 7.01 (d, *J* = 7.5 Hz, 2H, methoxyphenyl), 3.84 (s, 6H, –OCH_3), 2.16 (s, 6H, –CH_3). HRMS (positive EI) calcd for $C_{27}H_{24}BrNO_2$: *m*/*z* = 473.0990 $[M]^+$; found 473.0974 $[M]^+$.

4-DTC-(dppy)Me$_2$. Yield: 1.50 g (89%). ^{1}H NMR (400 MHz, $CDCl_3$, 298 K, relative to Me_4Si, δ/ppm): δ 8.16 (d, *J* = 1.6 Hz, 2H, carbazolyl), 8.10−8.12 (m, 4H, pyridyl and methoxyphenyl), 7.79 (d, *J* = 8.6 Hz, 2H, carbazolyl), 7.52 (dd, *J* = 8.6, 1.6 Hz, 2H, carbazolyl), 7.41 (dt, *J* = 8.3, 1.8 Hz, 2H, methoxyphenyl), 7.14 (dt, *J* = 8.3, 1.8 Hz, 2H, methoxyphenyl), 7.04 (d, *J* = 8.3 Hz, 2H, methoxyphenyl), 3.94 (s, 6H, −OCH_3), 1.49 (s, 18H, −CH_3). HRMS (positive EI) calcd for $C_{39}H_{40}N_2O_2$: *m*/*z* = 568.3090 $[M]^+$; found 568.3083 $[M]^+$.

4-DTC-2-Me-Ph(dppy)Me$_2$. Yield: 1.02 g (66%). ^{1}H NMR (400 MHz, $CDCl_3$, 298 K, relative to Me_4Si, δ/ppm): δ 8.15 (d, *J* = 1.2 Hz, 2H, carbazolyl), 8.03 (dd, *J* = 7.6, 1.7 Hz, 2H, methoxyphenyl), 7.88 (s, 2H, pyridyl), 7.45−7.56 (m, 7H, carbazolyl, phenyl and methoxyphenyl), 7.40 (dt, *J* = 7.6, 1.7 Hz, 2H, methoxyphenyl), 7.13 (td, *J* = 7.6, 1.7 Hz, 2H, methoxyphenyl), 7.04 (d, *J* = 7.6 Hz, 2H, methoxyphenyl), 3.92 (s, 6H, −OCH_3), 2.54 (s, 3H, −CH_3), 1.48 (s, 18H, −CH_3). HRMS (positive EI) calcd for $C_{46}H_{46}N_2O_2$: *m*/*z* = 658.3559 $[M]^+$; found 658.3566 $[M]^+$.

4-DTC-3-Me-Ph(dppy)Me$_2$. Yield: 1.57 g (85%). ^{1}H NMR (500 MHz, $CDCl_3$, 298 K, relative to Me_4Si, δ/ppm): δ 8.17 (s, 2H, carbazolyl), 8.08 (s, 2H, pyridyl), 7.98 (d, *J* = 7.5 Hz, 2H, methoxyphenyl), 7.79 (s, 1H, phenyl), 7.71 (d, *J* = 8.0 Hz, 1H, phenyl), 7.44–7.47 (m, 3H, phenyl and carbazolyl), 7.40 (t, *J* = 7.5 Hz, 2H, methoxyphenyl), 7.13 (t, *J* = 7.5 Hz, 2H, methoxyphenyl), 7.03–7.07 (m, 4H, methoxyphenyl and carbazolyl), 3.94 (s, 6H, –OCH_3), 2.11 (s, 3H, –CH_3), 1.48 (s, 18H, –CH_3). HRMS (positive EI) calcd for $C_{46}H_{46}N_2O_2$: *m*/*z* = 658.3559 $[M]^+$; found 658.3560 $[M]^+$.

4-DTC-3-F-Ph(dppy)Me$_2$. Yield: 754 mg (68%). ^{1}H NMR (500 MHz, $CDCl_3$, 298 K, relative to Me_4Si, δ/ppm): δ 8.17 (s, 2H, carbazolyl), 8.09 (s, 2H, pyridyl), 8.02 (d, *J* = 8.0 Hz, 2H, methoxyphenyl), 7.67–7.75 (m, 3H, phenyl), 7.50 (d, *J* = 7.5 Hz, 2H, carbazolyl), 7.42 (t, *J* = 8.0 Hz, 2H, methoxyphenyl), 7.25 (d, *J* = 7.5 Hz, 2H,

carbazolyl), 7.14 (t, *J* = 8.0 Hz, 2H, methoxyphenyl), 7.07 (d, *J* = 8.0 Hz, 2H, methoxyphenyl), 3.96 (s, 6H, –CH_3), 1.49 (s, 18H, –CH_3). $^{19}F\{^1H\}$ NMR (376.4 MHz, $CDCl_3$, 298 K, relative to $CFCl_3$, δ/ppm): δ –117.39. HRMS (positive ESI) calcd for $C_{45}H_{44}FN_2O_2$: *m*/*z* = 663.3387 $[M+H]^+$; found 663.3388 $[M+H]^+$.

4-DFC-Ph(dppy)Me$_2$. Yield: 653 mg (70%). ^1H NMR (400 MHz, $CDCl_3$, 298 K, relative to Me_4Si, δ/ppm): δ 8.09 (s, 2H, pyridyl), 8.00 (d, *J* = 8.0 Hz, 2H, methoxyphenyl), 7.95 (d, *J* = 8.5 Hz, 2H, phenyl), 7.75 (d, *J* = 8.6 Hz, 2H, carbazolyl), 7.67 (d, *J* = 8.5 Hz, 2H, phenyl), 7.39–7.44 (m, 4H, phenyl and carbazolyl), 7.19 (t, *J* = 8.6 Hz, 2H, carbazolyl), 7.13 (t, *J* = 8.0 Hz, 2H, methoxyphenyl), 7.06 (d, *J* = 8.0 Hz, 2H, methoxyphenyl), 3.94 (s, 6H, –OCH_3). $^{19}F\{^1H\}$ NMR (376.4 MHz, $CDCl_3$, 298 K, relative to $CFCl_3$, δ/ppm): δ –123.25. HRMS (positive EI) calcd for $C_{37}H_{26}F_2N_2O_2$: *m*/*z* = 568.1962 $[M]^+$; found 568.1938 $[M]^+$.

((5-DTC-Ph)$_2$-Py)Me$_2$. Yield: 1.73 g (78%). ^1H NMR (400 MHz, $CDCl_3$, 298 K, relative to Me_4Si, δ/ppm): δ 8.09 (s, 4H, carbazolyl), 7.98 (s, 2H, methoxyphenyl), 7.80–7.82 (m, 3H, pyridyl), 7.49 (d, *J* = 8.7 Hz, 2H, methoxyphenyl), 7.31–7.40 (m, 8H, carbazolyl), 7.15 (d, *J* = 8.7 Hz, 2H, methoxyphenyl), 3.91 (s, 6H, –OCH_3), 1.41 (s, 36H, –CH_3). HRMS (positive ESI) calcd for $C_{59}H_{64}N_3O_2$: *m*/*z* = 846.4999 $[M+H]^+$; found 846.4972 $[M+H]^+$.

4-DTDPA-Ph(dppy)Me$_2$. Yield: 730 g (69%). ^1H NMR (400 MHz, $CDCl_3$, 298 K, relative to Me_4Si, δ/ppm): δ 8.00−8.03 (m, 4H, pyridyl and methoxyphenyl), 7.64 (d, *J* = 8.6 Hz, 2H, phenyl), 7.41 (dt, *J* = 8.6, 1.7 Hz, 2H, phenyl), 7.35 (d, *J* = 8.6 Hz, 4H, phenyl), 7.20 (d, *J* = 8.6 Hz, 2H, phenyl), 7.13−7.16 (m, 6H, phenyl and methoxyphenyl), 7.06 (d, *J* = 8.2 Hz, 2H, methoxyphenyl), 3.92 (s, 6H, −OCH_3), 1.39 (s, 18H, −CH_3). HRMS (positive EI) calcd for $C_{45}H_{46}N_2O_2$: *m*/*z* = 646.3559 $[M]^+$; found 646.3546 $[M]^+$.

4-DTDPA-2,6-Me_2-Ph(dppy)Me_2. Yield: 493 mg (60%). ^{1}H NMR (500 MHz, acetone-d_6, 298 K, relative to Me_4Si, δ/ppm): δ 8.03 (d, *J* = 7.5 Hz, 2H, methoxyphenyl), 7.69 (s, 2H, pyridyl), 7.41 (t, *J* = 7.5 Hz, 2H, methoxyphenyl), 7.36 (d, *J* = 8.0 Hz, 4H, phenyl), 7.15 (d, *J* = 7.5 Hz, 2H, methoxyphenyl), 7.10 (t, *J* = 7.5 Hz, 2H, methoxyphenyl), 7.04 (d, *J* = 8.0 Hz, 4H, phenyl), 6.83 (s, 2H, phenyl), 3.90 (s, 6H, –OCH_3), 2.81 (s, 6H, –CH_3), 1.32 (s, 18H, –CH_3). HRMS (positive ESI) calcd for $C_{47}H_{50}N_2O_2$: *m*/*z* = 674.3872 $[M]^+$; found 674.3860 $[M]^+$.

4-DTC-(dppy)H_2. Yield: 642 mg (45%). ^{1}H NMR (400 MHz, $CDCl_3$, 298 K, relative to Me_4Si, δ/ppm): δ 10.17 (br, 2H, −OH), 8.16 (d, *J* = 1.7 Hz, 2H, carbazolyl), 7.99 (s, 2H, pyridyl), 7.70 (dd, *J* = 7.8, 1.5 Hz, 2H, hydroxyphenyl), 7.65 (d, *J* = 8.6 Hz, 2H, carbazolyl), 7.55 (dd, *J* = 8.6, 1.7 Hz, 2H, carbazolyl), 7.38 (dt, *J* = 8.3, 1.6 Hz, 2H, hydroxyphenyl), 7.09 (dd, *J* = 8.3, 1.6 Hz, 2H, hydroxyphenyl), 7.04 (dt, *J* = 7.8, 1.5 Hz, 2H, hydroxyphenyl), 1.49 (s, 18H, −CH_3). HRMS (positive EI) calcd for $C_{37}H_{36}N_2O_2$: *m*/*z* = 540.2777 $[M]^+$; found 540.2766 $[M]^+$.

4-DTC-2-Me-Ph(dppy)H_2. Yield: 800 mg (82%). ^{1}H NMR (400 MHz, $CDCl_3$, 298 K, relative to Me_4Si, δ/ppm): δ 8.20 (d, *J* = 1.4 Hz, 2H, carbazolyl), 7.84 (s, 2H, pyridyl), 7.79 (dd, *J* = 8.2, 1.4 Hz, 2H, hydroxyphenyl), 7.47−7.61 (m, 7H, carbazolyl and phenyl), 7.40 (td, *J* = 8.5, 1.4 Hz, 2H, hydroxyphenyl), 7.13 (dd, *J* = 8.5, 1.4 Hz, 2H, hydroxyphenyl), 7.05 (td, *J* = 8.2, 1.4 Hz, 2H, hydroxyphenyl), 2.51 (s, 3H, −CH_3), 1.52 (s, 18H, −CH_3). HRMS (positive EI) calcd for $C_{44}H_{42}N_2O_2$: *m*/*z* = 630.3246 $[M]^+$; found 630.3241 $[M]^+$.

4-DTC-3-Me-Ph(dppy)H_2. Yield: 1.04 g (69%). ^{1}H NMR (500 MHz, $CDCl_3$, 298 K, relative to Me_4Si, δ/ppm): δ 10.22 (br, 2H, –OH), 8.18 (s, 2H, carbazolyl), 8.00 (s, 2H, pyridyl), 7.82–7.84 (m, 3H, phenyl and hydroxyphenyl), 7.75 (d, *J* = 8.0 Hz, 1H, phenyl), 7.52 (d, *J* = 8.0 Hz, 1H. phenyl), 7.46 (d, *J* = 8.0 Hz, 2H, carbazolyl), 7.40 (t, *J* = 8.5 Hz, 2H, hydroxyphenyl), 7.10 (d, *J* = 8.0 Hz, 2H, hydroxyphenyl), 7.06 (t, *J* =

8.0 Hz, 2H, hydroxyphenyl), 7.02 (d, *J* = 8.5Hz, 2H, hydroxyphenyl), 2.17 (s, 3H, –CH_3), 1.48 (18H, –CH_3). HRMS (positive EI) calcd for $C_{44}H_{42}N_2O_2$: *m*/*z* = 630.3246 $[M]^+$; found 630.3235 $[M]^+$.

4-DTC-3-F-Ph(dppy)H$_2$. Yield: 375 mg (52%). ^{1}H NMR (500 MHz, $CDCl_3$, 298 K, relative to Me_4Si, δ/ppm): δ 8.16 (s, 2H, carbazolyl), 7.97 (s, 2H, pyridyl), 7.81 (d, *J* = 8.0 Hz, 2H, hydroxyphenyl), 7.70–7.76 (m, 3H, phenyl), 7.50 (d, *J* = 8.5 Hz, 2H, carbazolyl), 7.38 (t, *J* = 8.0 Hz, 2H, hydroxyphenyl), 7.24 (d, *J* = 8.5 Hz, 2H, carbazolyl), 7.09 (d, *J* = 8.0 Hz, 2H, hydroxyphenyl), 7.04 (t, *J* = 8.0 Hz, 2H, hydroxyphenyl), 1.48 (s, 18H, –CH_3). ^{19}F{^{1}H} NMR (376.4 MHz, $CDCl_3$, 298 K, relative to $CFCl_3$, δ/ppm): δ –116.13. HRMS (positive ESI) calcd for $C_{43}H_{40}FN_2O_2$: *m*/*z* = 635.3074 $[M+H]^+$; found 635.3064 $[M+H]^+$.

((5-DTC-Ph)$_2$-Py)H$_2$. Yield: 1.17 g (70%). ^{1}H NMR (400 MHz, $CDCl_3$, 298 K, relative to Me_4Si, δ/ppm): δ 10.50 (br, 2H, –OH), 8.18 (s, 4H, carbazolyl), 7.96 (t, *J* = 8.0 Hz, 1H, pyridyl), 7.86 (s, 2H, hydroxyphenyl), 7.69 (d, *J* = 8.0 Hz, 2H, pyridyl), 7.55 (d, *J* = 8.8 Hz, 2H, hydroxyphenyl), 7.50 (d, *J* = 8.4 Hz, 4H, carbazolyl), 7.34 (d, *J* = 8.4 Hz, 4H, carbazolyl), 7.31 (d, *J* = 8.8 Hz, 2H, hydroxyphenyl), 1.49 (s, 36H, –CH_3). HRMS (positive ESI) calcd for $C_{57}H_{60}N_3O_2$: *m*/*z* = 818.4686 $[M+H]^+$; found 818.4600 $[M+H]^+$.

4-DTDPA-Ph(dppy)H$_2$. Yield: 349 mg (50%). ^{1}H NMR (400 MHz, acetone-d_6, 298 K, relative to Me_4Si, δ/ppm): δ 8.24 (s, 2H, pyridyl), 8.01 (dd, *J* = 7.8, 1.6 Hz, 2H, hydroxyphenyl), 7.88 (d, *J* = 8.7 Hz, 2H, phenyl), 7.43 (d, *J* = 8.7 Hz, 4H, phenyl), 7.34 (dt, *J* = 8.8, 1.7 Hz, 2H, hydroxyphenyl), 7.08 −7.13 (m, 6H, phenyl), 6.98 −7.05 (m, 4H, hydroxyphenyl), 2.85 (br, 2H, −OH), 1.34 (s, 18H, −CH_3). HRMS (positive ESI) calcd for $C_{43}H_{43}N_2O_2$: *m*/*z* = 619.3280 $[M+H]^+$; found 619.3349 $[M+H]^+$.

4-DTDPA-2,6-Me$_2$-Ph(dppy)H$_2$. Yield: 425 mg (90%). ^{1}H NMR (500 MHz, $CDCl_3$, 298 K, relative to Me_4Si, δ/ppm): δ 10.28 (br, 2H, –OH), 7.68 (d, *J* = 8.0 Hz, 2H,

hydroxyphenyl), 7.59 (s, 2H, pyridyl), 7.36 (t, *J* = 8.0 Hz, 2H, hydroxyphenyl), 7.29 (d, *J* = 8.5 Hz, 4H, phenyl), 7.06–7.08 (m, 6H, phenyl and hydroxyphenyl), 6.99 (t, *J* = 8.0 Hz, 2H, hydroxyphenyl), 6.85 (s, 2H, phenyl), 2.04 (s, 6H, –CH_3), 1.33 (s, 18H, –CH_3). HRMS (positive ESI) calcd for $C_{45}H_{47}N_2O_2$: *m*/*z* = 647.3638 $[M+H]^+$; found 647.3623 $[M+H]^+$.

4-DTC-(dppy)BF (**1**). Yield: 378 mg (56%). ^{1}H NMR (400 MHz, CD_2Cl_2, 298 K, relative to Me_4Si, δ/ppm): δ 8.22 (s, 2H, pyridyl), 8.20 (d, *J* = 1.6 Hz, 2H, carbazolyl), 7.87 (dd, *J* = 8.3, 1.5 Hz, 2H, phenoxyl), 7.73 (d, *J* = 8.7 Hz, 2H, carbazolyl), 7.59 (dd, *J* = 8.7, 1.6 Hz, 2H, carbazoly), 7.54 (dt, *J* = 8.3, 1.5 Hz, 2H, phenoxyl), 7.21 (dd, *J* = 8.3, 1.5 Hz, 2H, phenoxyl), 7.09 (dt, *J* = 8.3, 1.5 Hz, 2H, phenoxyl), 1.49 (s, 18H, −CH_3). ^{19}F{^{1}H} NMR (376.4 MHz, CD_2Cl_2, 298 K, relative to CF_3Cl, δ/ppm): δ −139.60. ^{11}B{^{1}H} NMR (160.5 MHz, CD_2Cl_2, 298 K, relative to BF_3•OEt_2, δ/ppm): δ 1.60. HRMS (positive EI) calcd for $C_{37}H_{34}BFN_2O_2$: *m*/*z* = 568.2697 $[M]^+$; found 568.2690 $[M]^+$. Elemental analyses: Found (%): C, 78.55; H, 6.42; N, 4.61. Calcd for $C_{37}H_{34}BFN_2O_2$: C, 78.17; H, 6.03; N, 4.93.

4-DTC-2-Me-Ph(dppy)BF (**2**). Yield: 501 mg (60%). ^{1}H NMR (400 MHz, CD_2Cl_2, 298 K, relative to Me_4Si, δ/ppm): δ 8.19 (d, *J* = 1.8 Hz, 2H, carbazolyl), 8.05 (s, 2H, pyridyl), 7.95 (dd, *J* = 8.2, 1.1 Hz, 2H, phenoxyl), 7.47−7.65 (m, 9H, carbazolyl, phenyl and phenoxyl), 7.21 (dd, *J* = 8.2, 1.1 Hz, 2H, phenoxyl), 7.12 (dt, *J* = 8.2, 1.1 Hz, 2H, phenoxyl), 2.50 (s, 3H, −CH_3), 1.49 (s, 18H, −CH_3). ^{19}F{^{1}H} NMR (376.4 MHz, CD_2Cl_2, 298 K, relative to CF_3Cl, δ/ppm): δ −140.09. ^{11}B{^{1}H} NMR (160.5 MHz, CD_2Cl_2, 298 K, relative to BF_3•OEt_2, δ/ppm): δ 1.53. HRMS (positive EI) calcd for $C_{44}H_{40}BFN_2O_2$: *m*/*z* = 658.3167 $[M]^+$; found 658.3175 $[M]^+$. Elemental analyses: Found (%): C, 79.72; H, 6.25; N, 4.42. Calcd for $C_{44}H_{40}BFN_2O_2$: C, 80.24; H, 6.12; N, 4.25.

4-DTC-3-Me-Ph(dppy)BF_2 (**3**). Yield: 815 mg (75%). ^{1}H NMR (500 MHz, $CDCl_3$, 298 K, relative to Me_4Si, δ/ppm): δ 8.19 (s, 2H, carbazolyl), 8.18 (s, 2H, pyridyl), 7.99 (d, *J* = 8.0 Hz, 2H, phenoxyl), 7.87 (s, 1H, phenyl), 7.79 (d, *J* = 8.0 Hz, 1H, phenyl), 7.58 (d, *J* = 8.0 Hz, 1H, phenyl), 7.52 (t, *J* = 8.0, 2H, phenoxyl), 7.47 (d, *J* = 8.5 Hz, 2H, carbazolyl), 7.27 (d, *J* = 8.0 Hz, 2H, phenoxyl), 7.10 (t, *J* = 8.0 Hz, 2H, phenoxyl), 7.02 (d, *J* = 8.5 Hz, 2H, carbazolyl), 2.20 (s, 3H, –CH_3), 1.48 (s, 18H, –CH_3). $^{19}F\{^1H\}$ NMR (376.4 MHz, CD_2Cl_2, 298 K, relative to $CFCl_3$, δ/ppm): δ –139.49. $^{11}B\{^1H\}$ NMR (160.5 MHz, CD_2Cl_2, 298 K, relative to BF_3•OEt_2, δ/ppm): δ 1.72. HRMS (positive ESI) calcd for $C_{44}H_{40}BFN_2O_2$: *m*/*z* = 658.3167 $[M]^+$; found 658.3165 $[M]^+$. Elemental analyses: Found (%): C, 76.39; H, 5.89; N, 4.11. Calcd for $C_{44}H_{40}BFN_2O_2$•$2H_2O$: C, 76.08; H, 6.38; N, 4.03.

4-DTC-3-F-Ph(dppy)BF_2 (**4**). Yield: 266 mg (68%). ^{1}H NMR (500 MHz, CD_2Cl_2, 298 K, relative to Me_4Si, δ/ppm): δ 8.21 (s, 2H, pyridyl), 8.19 (s, 2H, carbazolyl), 8.03 (d, *J* = 8.0 Hz, 2H, phenoxyl), 7.83–7.89 (m, 3H, phenyl), 7.53–7.57 (m, 4H, carbazolyl and phenoxyl), 7.27 (d, *J* = 8.5 Hz, 2H, carbazolyl), 7.21 (d, *J* = 8.0 Hz, 2H, phenoxyl), 7.14 (t, *J* = 8.0 Hz, 2H, phenoxyl), 1.48 (s, 18H, –CH_3). $^{19}F\{^1H\}$ NMR (376.4 MHz, CD_2Cl_2, 298 K, relative to $CFCl_3$, δ/ppm): δ –116.64, –139.32. $^{11}B\{^1H\}$ NMR (160.5 MHz, CD_2Cl_2, 298 K, relative to BF_3•OEt_2, δ/ppm): δ 1.67. HRMS (positive ESI) calcd for $C_{43}H_{37}BF_2N_2NaO_2$: *m*/*z* = 685.2814 $[M+Na]^+$; found 685.2824 $[M+Na]^+$. Elemental analyses: Found (%): C, 75.39; H, 5.31; N, 4.24. Calcd for $C_{43}H_{37}BF_2N_2O_2$•H_2O: C, 75.88; H, 5.78; N, 4.12.

4-DFC-Ph(dppy)BF_2 (**5**). Yield: 392 mg (60%) ^{1}H NMR (500 MHz, CD_2Cl_2, 298 K, relative to Me_4Si, δ/ppm): δ 8.25 (s, 2H, pyridyl), 8.10 (d, *J* = 8.5 Hz, 2H, phenoxyl), 8.05 (d, *J* = 8.0 Hz, 2H, carbazolyl), 7.84 (d, *J* = 8.5 Hz, 2H, phenyl), 7.80 (d, *J* = 8.5 Hz, 2H, phenyl), 7.56 (t, *J* = 8.5 Hz, 2H, phenoxyl), 7.49 (d, *J* = 8.0 Hz, 2H, carbazolyl), 7.26 (t, *J* = 8.0 Hz, 2H, carbazolyl), 7.22 (d, *J* = 8.5 Hz, 2H, phenoxyl), 7.16 (t, *J* = 8.5 Hz, 2H, phenoxyl). $^{19}F\{^1H\}$ NMR (376.4 MHz, CD_2Cl_2, 298 K, relative to $CFCl_3$,

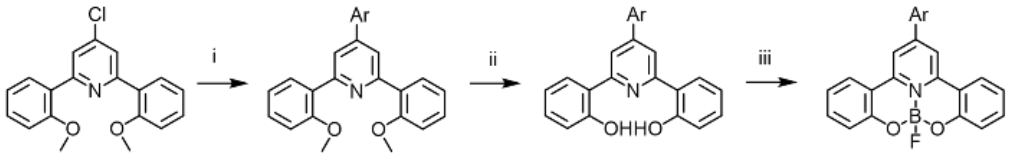
δ/ppm): δ −123.49. $^{11}B\{^{1}H\}$ NMR (160.5 MHz, CD_2Cl_2, 298 K, relative to BF_3•OEt_2, δ/ppm): δ 1.46. HRMS (positive ESI) calcd for $C_{35}H_{20}BF_3N_2NaO_2$: *m*/*z* = 591.1468 $[M+Na]^+$; found 591.1459 $[M+Na]^+$. Elemental analyses: Found (%): C, 73.69; H, 3.56; N, 4.77. Calcd for $C_{35}H_{20}BF_3N_2O_2$: C, 73.96; H, 3.55; N, 4.93.

((5-DTC-Ph)$_2$-Py)BF (**6**). Yield: 702 mg (58%). ^{1}H NMR (500 MHz, $CDCl_3$, 298 K, relative to Me_4Si, δ/ppm): δ 8.17 (s, 4H, carbazolyl), 8.13 (t, *J* = 8.0 Hz, 1H, pyridyl), 8.01 (s, 2H, phenoxyl), 7.90 (d, *J* = 8.0 Hz, 2H, pyridyl), 7.69 (d, *J* = 8.8 Hz, 2H, phenoxyl), 7.46–7.50 (m, 6H, phenoxyl and carbazolyl), 7.32 (d, *J* = 8.5 Hz, 4H, carbazolyl), 1.48 (s, 36H, $-CH_3$). $^{19}F\{^{1}H\}$ NMR (376.4 MHz, $CDCl_3$, 298 K, relative to $CFCl_3$, δ/ppm): δ −137.76. $^{11}B\{^{1}H\}$ NMR (160.5 MHz, $CDCl_3$, 298 K, relative to BF_3•OEt_2, δ/ppm): δ 1.85. HRMS (positive ESI) calcd for $C_{57}H_{57}BFN_3O_2$: *m*/*z* = 845.4528 $[M]^+$; found 845.4576 $[M]^+$. Elemental analyses: Found (%): C, 80.46; H, 7.09; N, 4.55. Calcd for $C_{57}H_{57}BFN_3O_2$: C, 80.36; H, 6.82; N, 4.93.

4-DTDPA-Ph(dppy)BF (**7**). Yield: 226 mg (62%). ^{1}H NMR (400 MHz, $CDCl_3$, 298 K, relative to Me_4Si, δ/ppm): δ 8.01 (s, 2H, pyridyl), 7.88 (dd, *J* = 8.0, 1.5 Hz, 2H, phenoxyl), 7.64 (d, *J* = 8.6 Hz, 2H, phenyl), 7.47 (dt, *J* = 8.6, 1.5 Hz, 2H, phenyl), 7.35 (d, *J* = 8.6 Hz, 4H, phenyl), 7.22 (d, *J* = 8.6 Hz, 2H, phenyl), 7.11−7.18 (m, 6H, phenyl and phenoxyl), 7.04 (dt, *J* = 8.0, 1.5 Hz, 2H, phenoxyl), 1.35 (s, 18H, $-CH_3$). $^{19}F\{^{1}H\}$ NMR (376.4 MHz, $CDCl_3$, 298 K, relative to CF_3Cl, δ/ppm): δ −139.86. $^{11}B\{^{1}H\}$ NMR (160.5 MHz, $CDCl_3$, 298 K, relative to BF_3•OEt_2, δ/ppm): δ 1.54. HRMS (positive EI) calcd for $C_{43}H_{40}BFN_2O_2$: *m*/*z* = 646.3167 $[M]^+$; found 646.3165 $[M]^+$. Elemental analyses: Found (%): C, 79.01; H, 6.04; N, 4.12. Calcd for $C_{43}H_{40}BFN_2O_2$: C, 79.87; H, 6.24; N, 4.33.

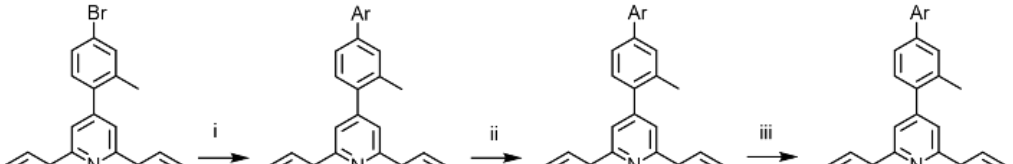
4-DTDPA-2,6-Me$_2$-Ph(dppy)BF (**8**). Yield: 310 mg (70%). ^{1}H NMR (500 MHz, $CDCl_3$, 298 K, relative to Me_4Si, δ/ppm): δ 7.80 (d, *J* = 8.0 Hz, 2H, phenoxyl), 7.78 (s, 2H, pyridyl), 7.49 (t, *J* = 8.0 Hz, 2H, phenoxyl), 7.31 (d, *J* = 7.5 Hz, 4H, phenyl), 7.24

(d, *J* = 8.0 Hz, 2H, phenoxyl), 7.08 (d, *J* = 7.5 Hz, 4H, phenyl), 7.03 (d, *J* = 8.0 Hz, 2H, phenoxyl), 6.84 (s, 1H, phenoxyl), 6.87 (s, 1H, phenoxyl), 2.11 (s, 3H, –CH_3), 1.97 (s, 3H, –CH_3), 1.34 (s, 18H, –CH_3). $^{19}F\{^1H\}$ NMR (376.4 MHz, $CDCl_3$, 298 K, relative to $CFCl_3$, δ/ppm): δ −139.78. $^{11}B\{^1H\}$ NMR (160.5 MHz, $CDCl_3$, 298 K, relative to BF_3•OEt_2, δ/ppm): δ 1.71. HRMS (positive ESI) calcd for $C_{45}H_{44}BFN_2NaO_2$: *m*/*z* = 697.3378 $[M+Na]^+$; found 697.3384 $[M+Na]^+$. Elemental analyses: Found (%): C, 79.81; H, 6.57; N, 4.17. Calcd for $C_{45}H_{44}BFN_2O_2$: C, 80.11; H, 6.57; N, 4.15.



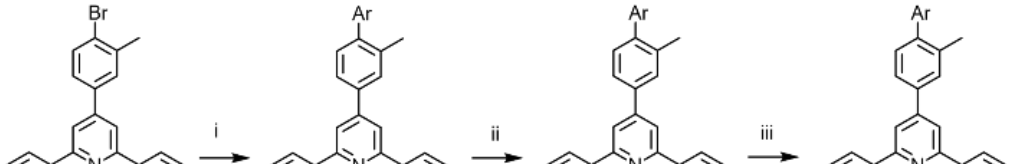
4-Cl-(dppy)Me_2 4-DTC-(dppy)Me_2 4-DTC-(dppy)H_2 4-DTC-(dppy)BF

(1)



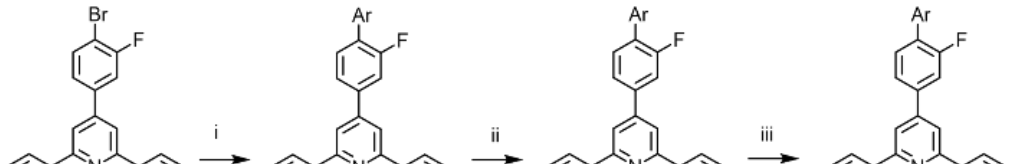
4-Br-2-Me-Ph(dppy)Me_2 4-DTC-2-Me-Ph(dppy)Me_2 4-DTC-2-Me-Ph(dppy)H_2 4-DTC-2-Me-Ph(dppy)BF

(2)



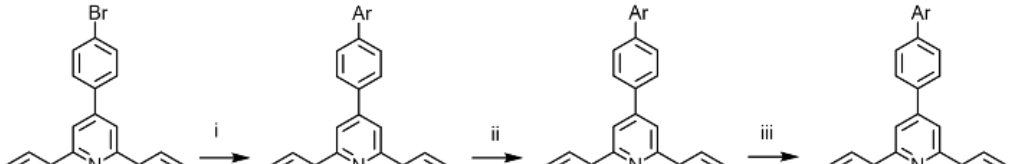
4-Br-3-Me-Ph(dppy)Me_2 4-DTC-3-Me-Ph(dppy)Me_2 4-DTC-3-Me-Ph(dppy)H_2 4-DTC-3-Me-Ph(dppy)BF

(3)



4-Br-3-F-Ph(dppy)Me_2 4-DTC-3-F-Ph(dppy)Me_2 4-DTC-3-F-Ph(dppy)H_2 4-DTC-3-F-Ph(dppy)BF

(4)



4-Br-Ph(dppy)Me_2 4-DFC-Ph(dppy)Me_2 4-DFC-Ph(dppy)H_2 4-DFC-Ph(dppy)BF

(5)

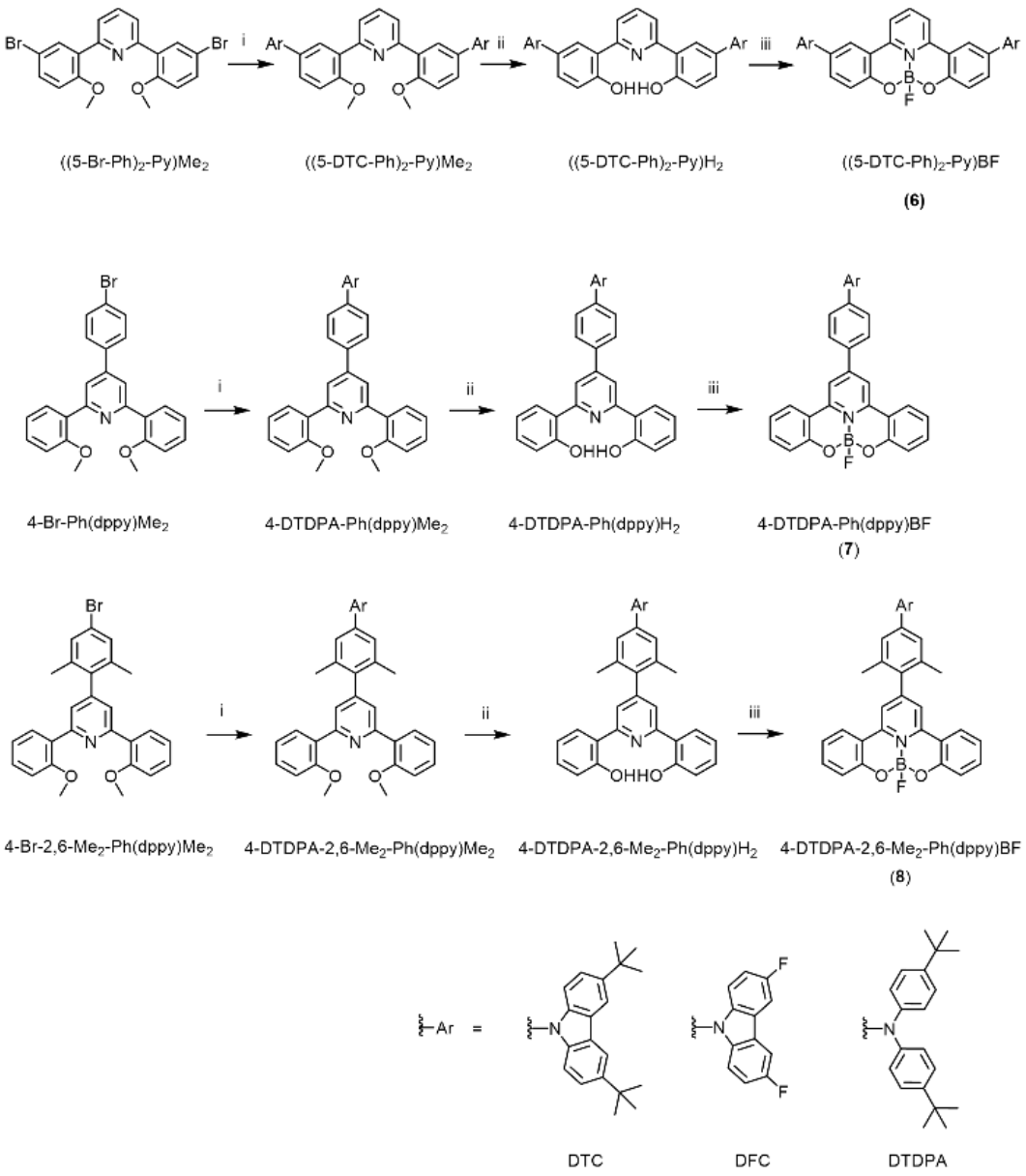


Fig. S1 Synthetic routes of **1**–**8**.

Thermogravimetric Analysis

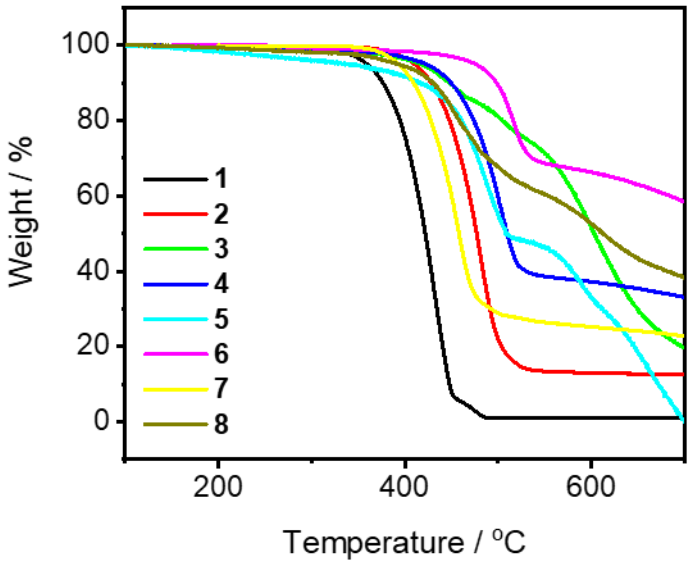


Fig. S2 TGA curves of compounds **1**–**8**.

Table S1 Thermal properties.

Compound	T_d / °C[a]
1	359
2	410
3	417
4	422
5	340
6	475
7	393
8	392

[a] T_d was determined at 5 % weight loss.

Photophysical Properties

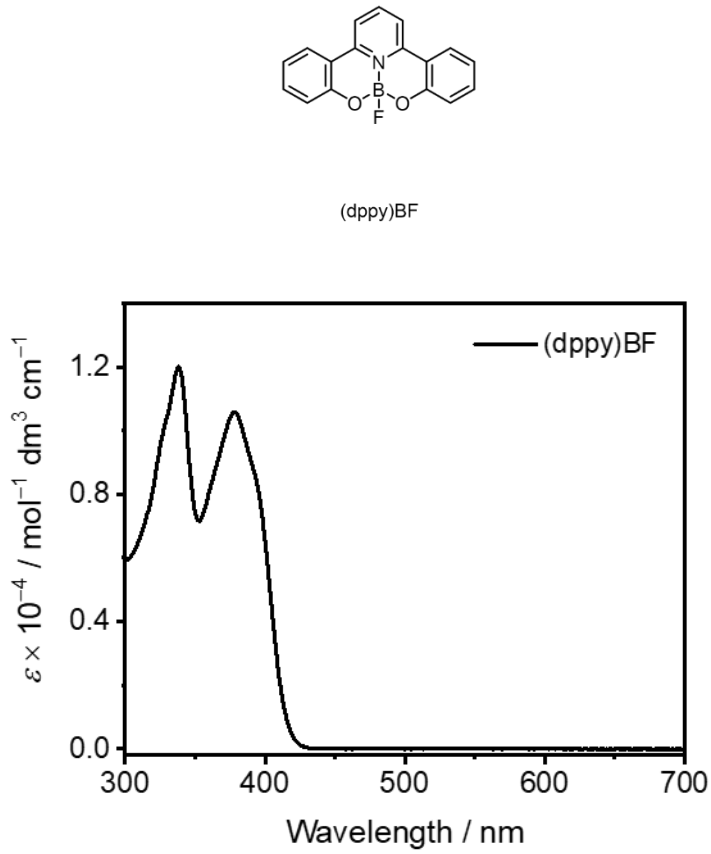


Fig. S3 Chemical structure and the electronic absorption spectrum of (dppy)BF.

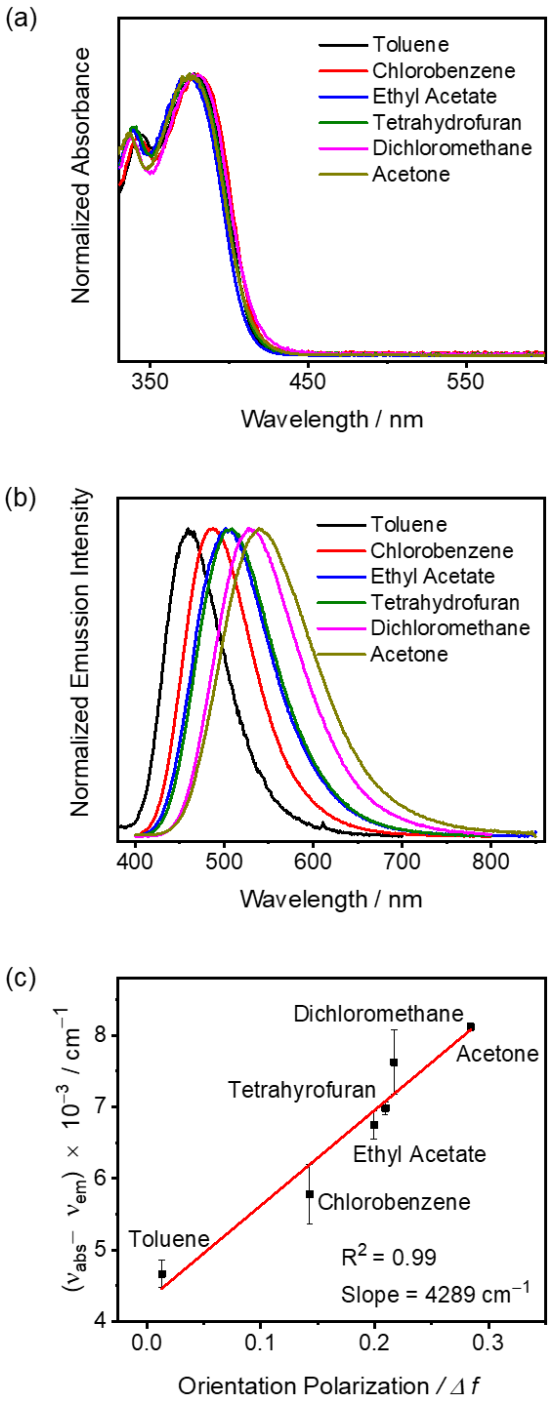


Fig. S4 (a) UV–Vis absorption spectra, (b) emission spectra and (c) Lippert–Mataga plot (ν_{abs}–ν_{em} against orientation polarizability of solvent) of **1** in different solvents at room temperature.

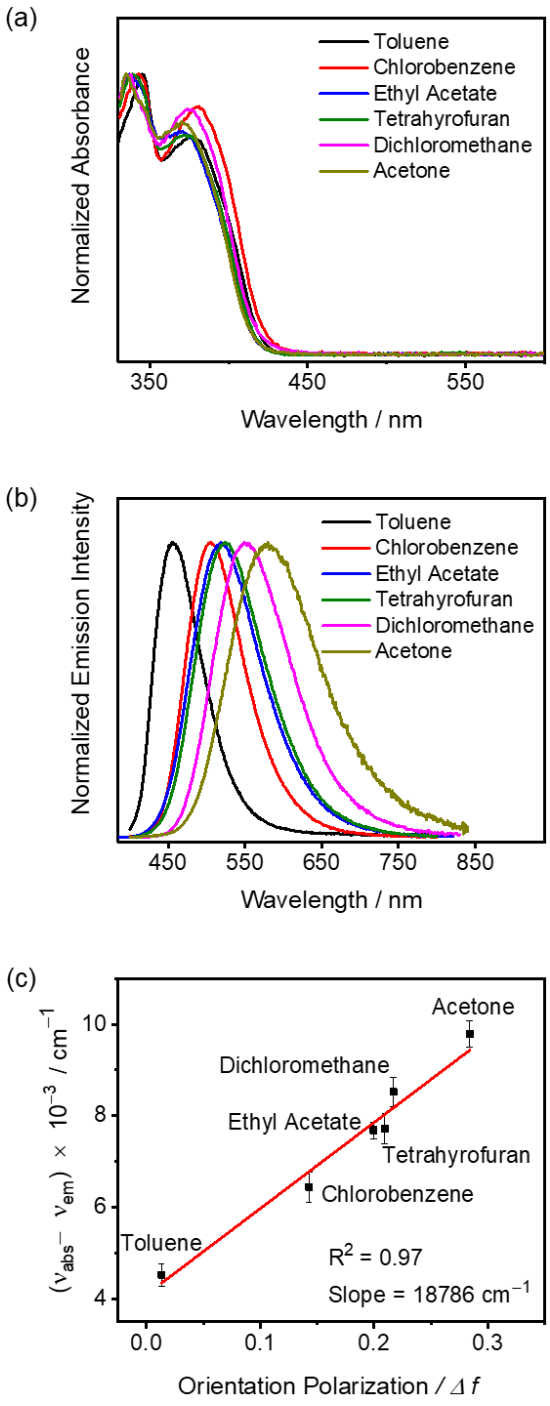


Fig. S5 (a) UV–Vis absorption spectra, (b) emission spectra and (c) Lippert–Mataga plot (ν_{abs}–ν_{em} against orientation polarizability of solvent) of **2** in different solvents at room temperature

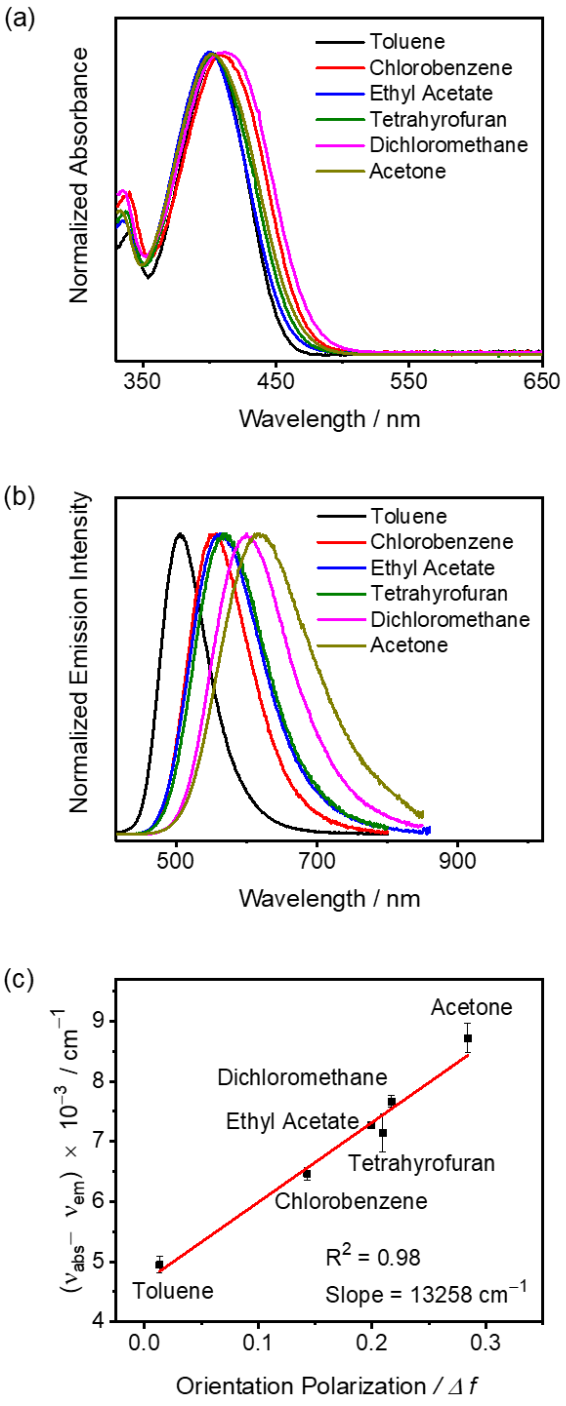


Fig. S6 (a) UV–Vis absorption spectra, (b) emission spectra and (c) Lippert–Mataga plot (ν_{abs}–ν_{em} against orientation polarizability of solvent) of **7** in different solvents at room temperature.

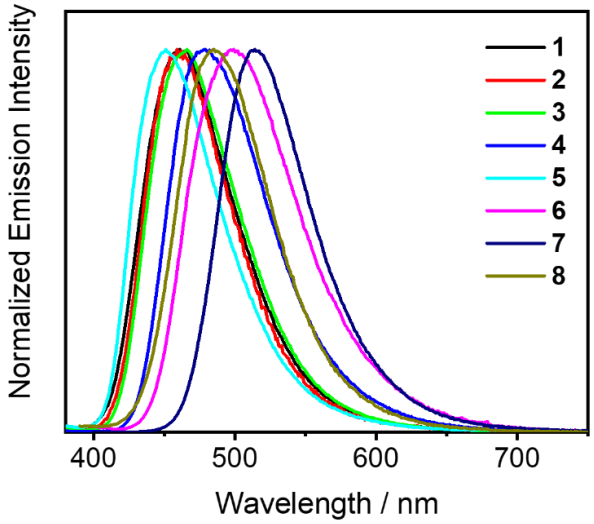


Fig. S7 Normalized emission spectra of 5 wt% **1**–**8** doped mCP thin films.

Table S2 Electronic absorption spectral data of **1**–**8** in toluene solution at 298 K.

Compound	λ_{abs} / nm (ε_{max} /dm^3 mol^{-1} cm^{-1})
1	343 (20630), 378 (26030)
2	345 (26840), 377 (20860)
3	344 (20780), 384 (13720)
4	341 (28260), 385 (25010)
5	349 (17180), 360 (17430)
6	336 (21280), 349 (22490), 401 (8050)
7	340 (20610), 405 (47280)
8	338 (33690), 380 (24430)

TADF Properties

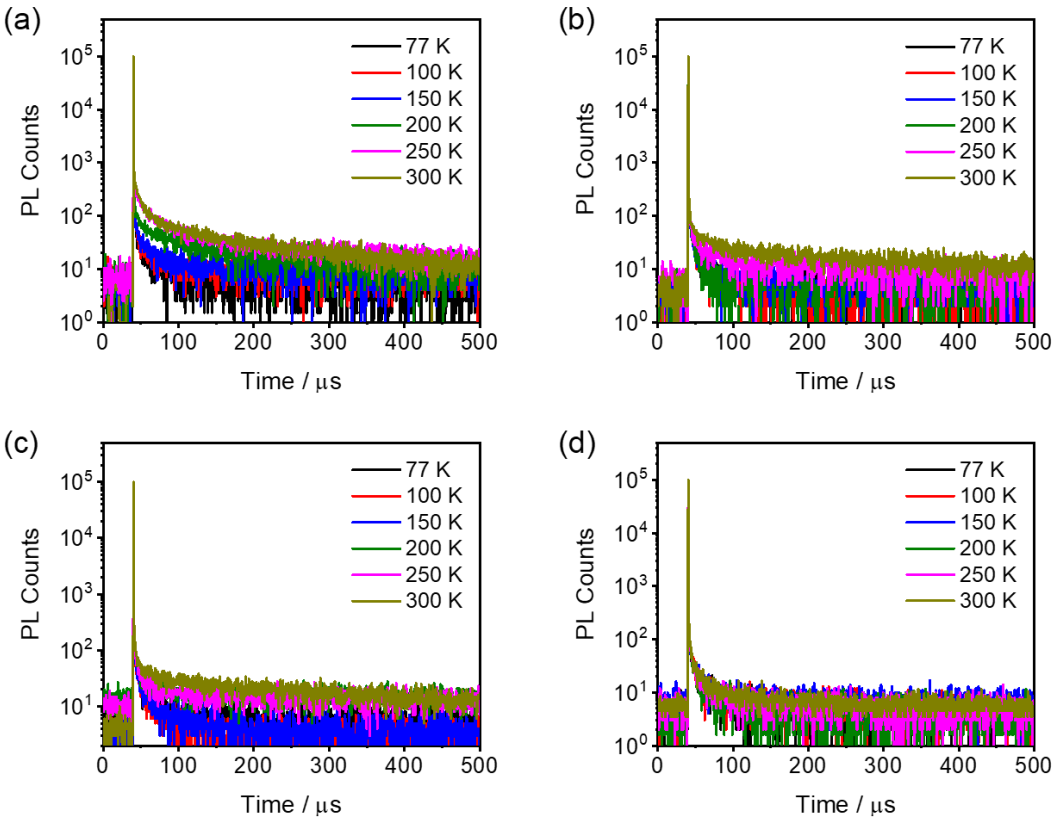


Fig. S8 Temperature-dependent PL decay curves of thin films of 5 wt% (a–d) **1**, **2**, **5** and **7** doped mCP thin films.

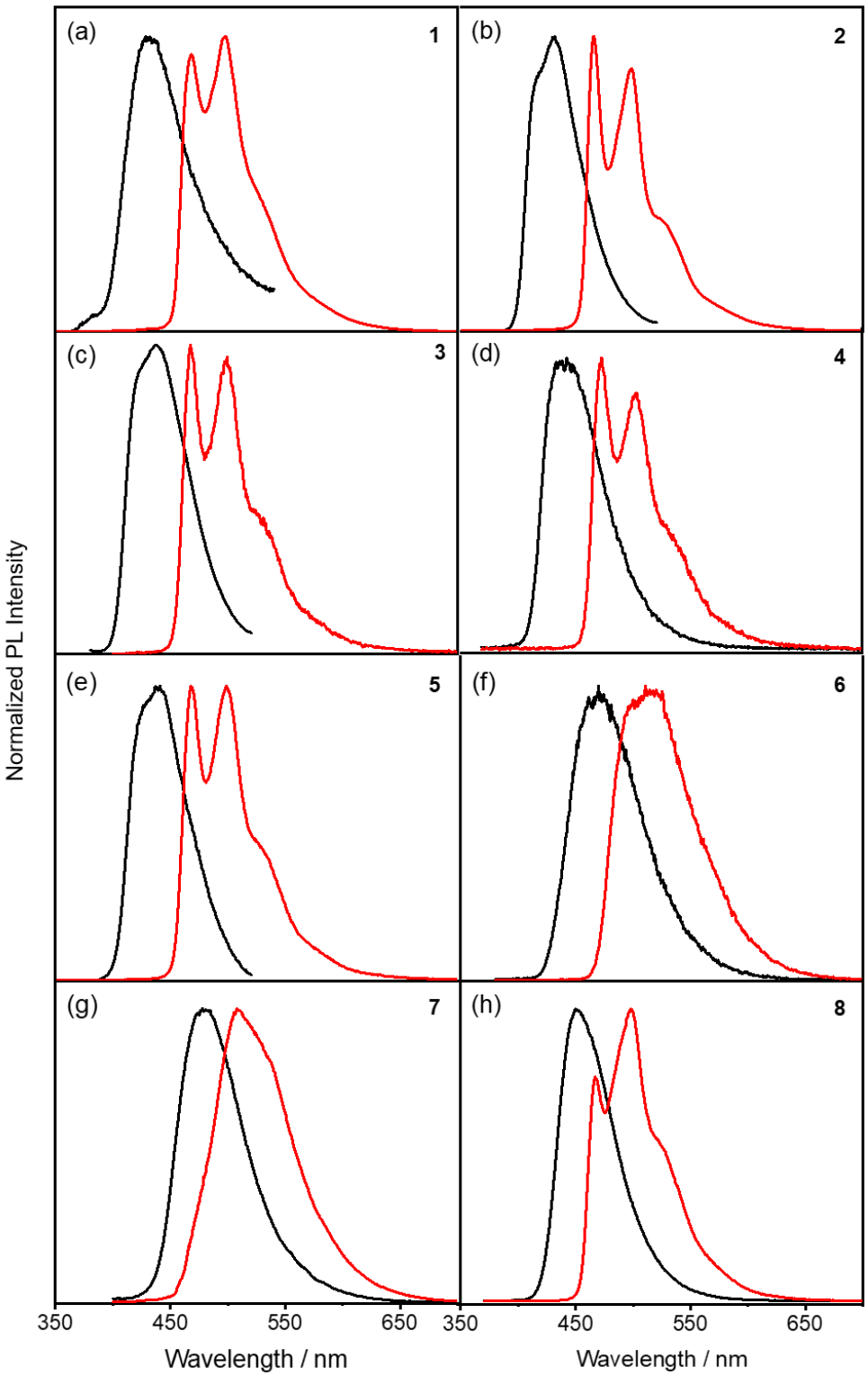


Fig. S9 Prompt fluorescence (black curve, delay time: 0 ns) and phosphorescence (red curve, gate time: 0.5–100 ms) spectra of (a–h) **1**–**8** measured in toluene matrix at 77 K.

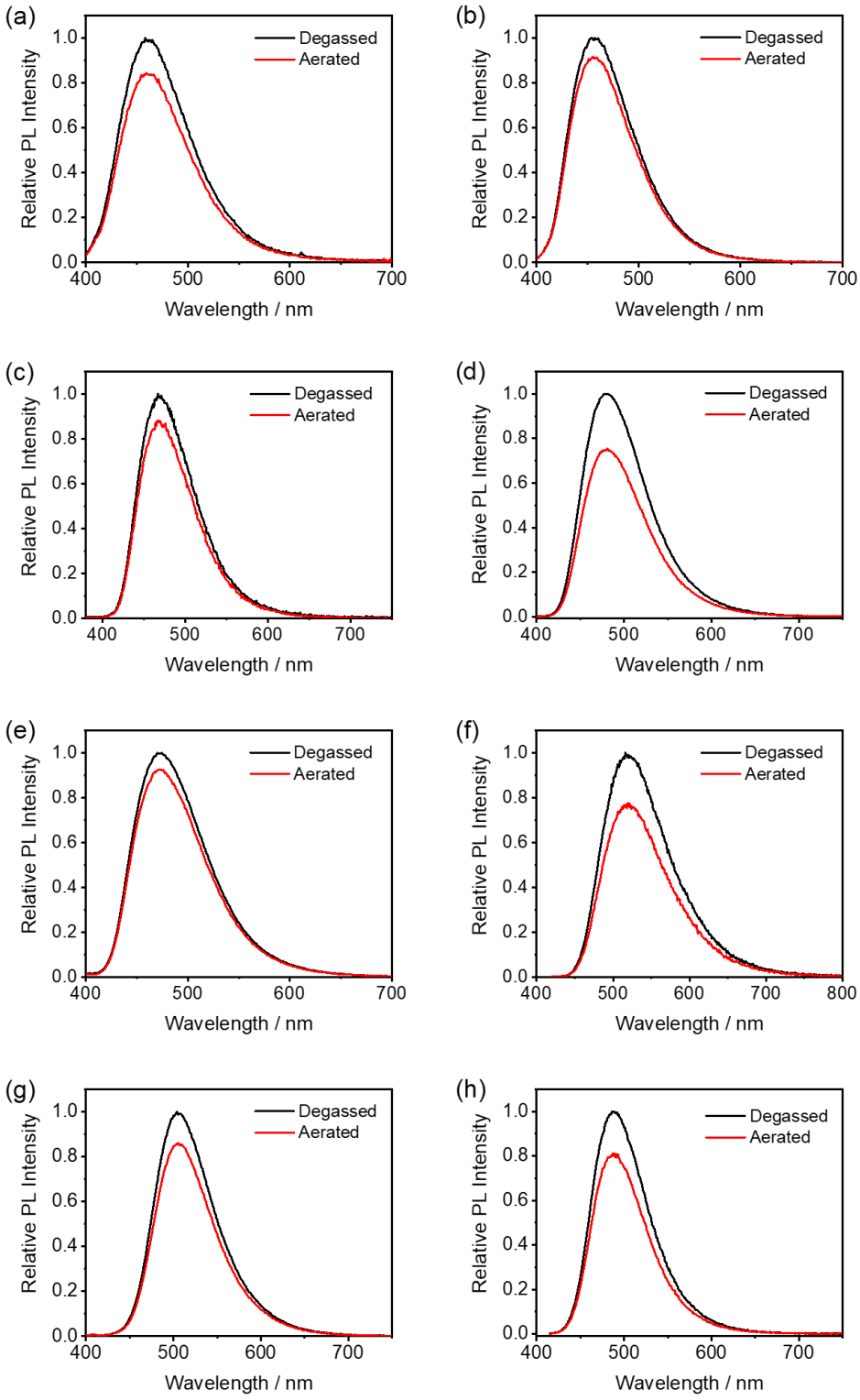


Fig. S10 Relative PL spectra of (a–h) **1**–**8** measured in aerated toluene solutions and in degassed toluene solutions (10^{-5} M) at room temperature, respectively.

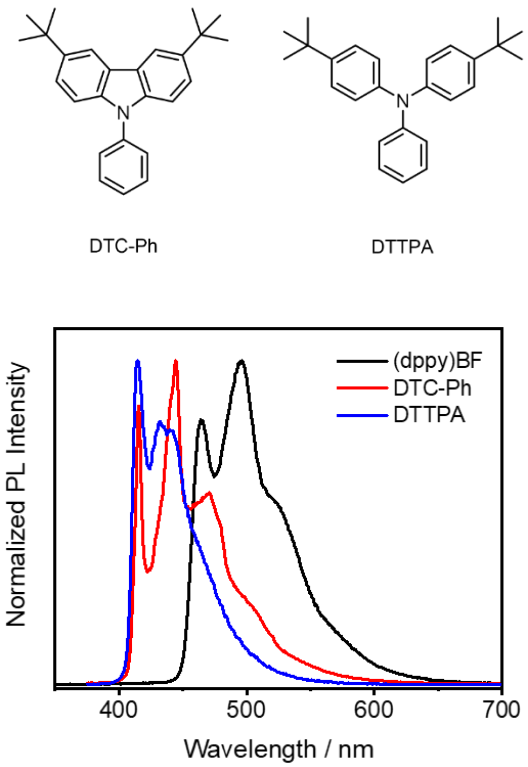


Fig. S11 Chemical structures and phosphorescence spectra of reference compounds (dppy)BF, DTC-Ph and DTTPA measured in toluene matrix at 77 K.

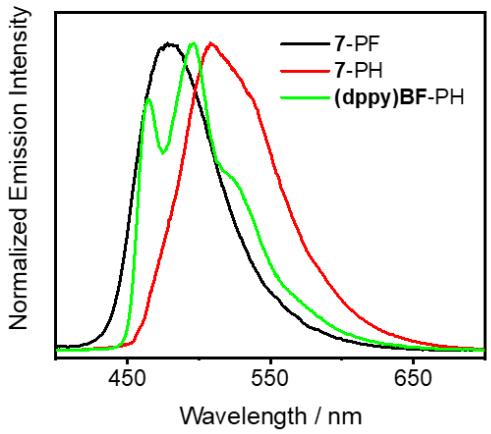


Fig. S12 Prompt fluorescence spectrum of **7** (**7**-PF), phosphorescence spectra of **7** (**7**-PH) and **(dppy)BF** (**(dppy)BF**-PF) measured in toluene matrix at 77 K.

Table S3 The S_1 and T_1 energies of **1**–**8**.

Compound	E_S[a] / eV	E_T[b] / eV	ΔE_{ST}[c] / eV
4-DTC-Ph(dppy)BF[6]	--		
1	3.17	2.75	0.42
2	3.12	2.74	0.38
3	3.10	2.74	0.36
4	3.02	2.71	0.31
5	3.10)	2.74	0.36
6	2.91	2.66	0.25
7	2.86	2.71	0.15
8	2.96	2.74	0.22

[a] Lowest energy excited singlet (E_S) energy estimated from the onset of the fluorescence spectrum in degassed toluene at 298 K to approach that of the most relaxed singlet state.

[b] E_T estimated from the onset of the phosphorescence spectrum in toluene matrix at 77 K.

[c] ΔE_{ST} determined from the energy difference between E_S measured at 298 K approaching that of the most relaxed singlet state energy and E_T measured at 77 K.

Transient Absorption Studies

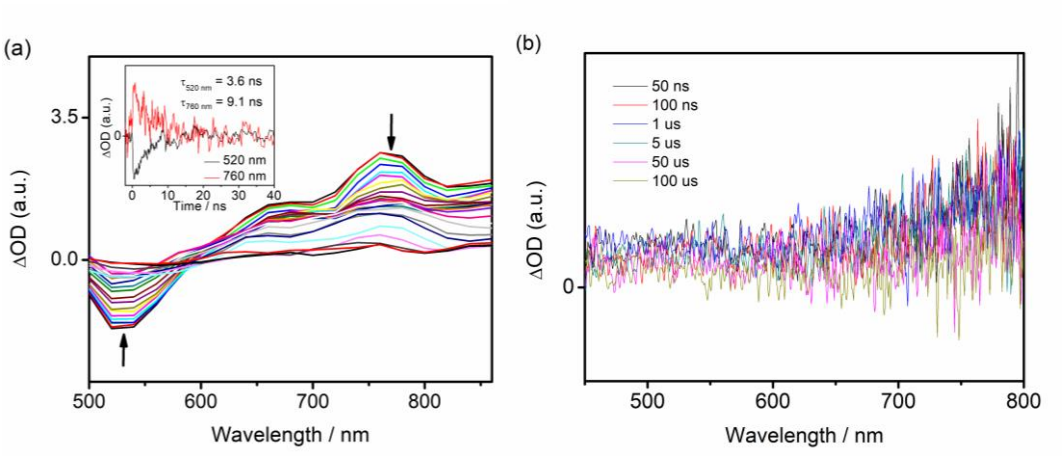


Fig. S13 (a) Picosecond transient absorption spectra of **7** in degassed toluene at 298 K and the decay trace monitored at 520 nm and 760 nm in the inset. (b) Nanosecond transient absorption spectra of **7** in degassed toluene at 298 K.

Electrochemical Studies

The electrochemical properties of **1**–**8** have been investigated by cyclic voltammetry in DMF solution. As no oxidative wave was observed in the potential window of DMF, the cyclic voltammogram of **5** was recorded in CH_2Cl_2 solution. All the cyclic voltammograms are shown in Fig. S14 and the corresponding electrochemical data are summarized in Table S4. Generally, all the compounds show one quasi-reversible oxidation couple from +0.94 to +1.46 V vs. saturated calomel electrode (SCE), which is assigned as one-electron oxidation of the respective *N*-donor moiety.[6] Comparing to 4-DTC-Ph(dppy)BF with one DTC donor moiety, it is found that the removal of the π-bridge in **1** and the introduction of one *ortho*-methyl substituent in **3** or one *ortho*-fluoro substituent in **4** with respect to the DTC donor have led to a considerable anodic shift in the potential for oxidation from +1.18 V vs. SCE for 4-DTC-Ph(dppy)BF to +1.40 V vs. SCE for **1**, +1.31 V vs. SCE for **3** and +1.36 V vs. SCE for **4**, whereas the presence of one methyl substituent *ortho* to the (dppy)BF acceptor in **2** gives rise to a relatively small anodic shift in the potential for oxidation (i.e. +1.24 V vs. SCE for **2**). Such anodic shift in the potential for oxidation is attributed to the reduced extent of π-conjugation and thus an interruption of the delocalization of π-electrons of the DTC moiety over the adjacent phenyl bridge (see computational studies). Unlike the anodic shift in the potential for oxidation of **1**–**4** as compared to 4-DTC-Ph(dppy)BF, the introduction of two methyl substituents *ortho* to the (dppy)BF acceptor moiety in **8** (+0.94 V vs. SCE) results in a clear cathodic shift as compared to **7** (+1.01 V vs. SCE). Indeed, the less rigid nature of the DTDPA moiety as compared to DTC moiety can render the compounds to adopt a relatively coplanar structure that facilitates the electron delocalization, and therefore the two extra electron-donating methyl substituents can destabilize the π orbitals. Also, the oxidation couple is observed to be sensitive to the electron-donating strength of the *N*-donor. Specifically, the potential for oxidation shifts to a less positive value from **5** with a weak DFC donor to **6** with two DTC donors to **7** and **8** with a strong DTDPA donor, in which +1.46 V vs. SCE for **5**, +1.20 V vs. SCE for **6**, +1.01 V vs. SCE for **7** and +0.94 V vs. SCE for **8** are determined respectively.

On the other hand, all the compounds show one quasi-reversible reduction couple from –1.30 V to –1.55 V vs. SCE, which is mainly assigned as one-electron reduction of the respective (dppy)BF moiety. Similar to our previous report,[6] the reduction couple is insensitive to the change of the *N*-donor strength when comparing DFC-based **5** (–1.41 V cs. SCE) with DTC-based 4-DTC-Ph(dppy)BF (–1.37 V vs. SCE). However, the reduction couples of **1**–**4** with one DTC donor moiety are recorded at –1.50 V, –1.46 V, –1.37 V and –1.30 V vs. SCE, respectively. The obvious cathodic shift in the reduction potential of **1** and **2** is reasonably attributed to a shortening of the molecular π-conjugation length in **1** and an increased dihedral angle between the (dppy)BF and its adjacent phenyl bridge in **2**, respectively. All these can restrict the delocalization of π-electrons of the respective (dppy)BF moiety and thus destabilize the π∗ orbitals. With an *ortho*-substitution with respect to the DTC donor moiety, i.e. methyl substituent in **3** and fluoro substituent in **4**, a comparable and an anodically shifted reduction potential in **3** (–1.37 V vs. SCE) and **4** (–1.30 V vs. SCE) was recorded, respectively. This is due to the fact the an *ortho*-substitution with respect to the DTC donor moiety has no influence on the dihedral angle between the (dppy)BF moiety and its adjacent phenyl bridge in **3**, while the negative inductive effect of the fluorine atom can stabilize the π∗ orbitals in **4**, respectively. In addition, the reduction potentials of **6**, which has two DTC moieties appended to the *para*- position of the phenolic hydroxy unit of (dppy)BF, and **7**, which has an acyclic and flexible DTDPA moiety, are also found to be shifted to more negative values (i.e. –1.46 V vs. SCE for **6** and –1.47 V vs. SCE for **7**). This observation can be ascribed to a more pronounced positive inductive effect of the two *para*-appended DTC moieties on the phenolic hydroxy units in **6**, and the relatively small dihedral angle between the acyclic DTDPA moiety and its adjacent phenyl bridge in **7**, both of which will destabilize π∗ orbitals. Again, the two methyl substituents *ortho* to the (dppy)BF in **8** restrict the delocalization of π-electrons of the (dppy)BF moiety over its adjacent phenyl bridge, and therefore resulting in a destabilization of π∗ orbitals and a further cathodically-shifted reduction potential, i.e. –1.55 V vs. SCE for **8**. These electrochemical properties have been further supported by computational studies.

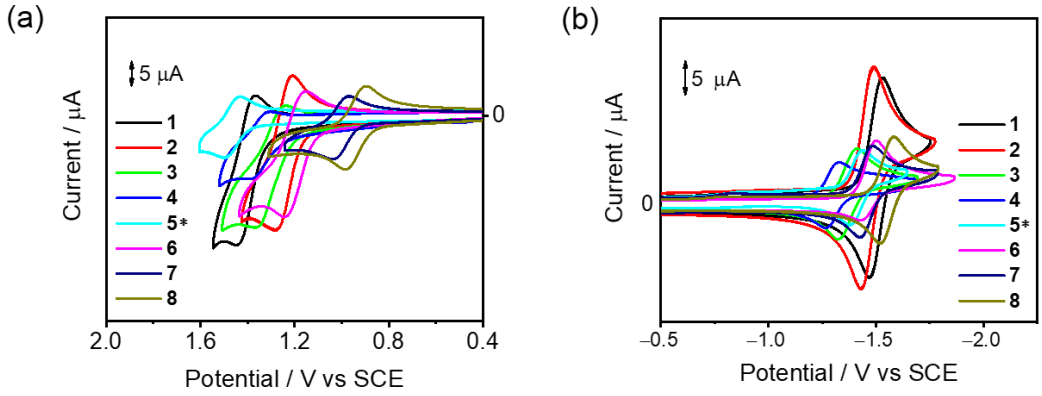


Fig. S14 Cyclic voltammograms of (a) oxidation scans and (b) reduction scans measured in DMF (*: measured in CH_2Cl_2).

Table S4 Electrochemical properties of **1**–**8**.[a]

Compound	Oxidation $E_{1/2}$ / V vs SCE[b] (ΔE_p / mV)[c]	Reduction $E_{1/2}$ / V vs SCE (ΔE_p / mV)[c]	HOMO / eV[e]	LUMO / eV[e]
1	+1.40 (73)	–1.50 (61)	–5.75	–2.85
2	+1.24 (72)	–1.46 (60)	–5.59	–2.89
3	+1.31 (72)	–1.37 (75)	–5.66	–2.98
4	+1.36 (68)	–1.30 (62)	–5.71	–3.05
5[d]	+1.46 (69)	–1.41 (60)	–5.80	–2.93
6	+1.20 (72)	–1.46 (61)	–5.55	–2.89
7	+1.01 (70)	–1.47 (73)	–5.36	–2.88
8	+0.94 (67)	–1.55 (79)	–5.29	–2.80

[a] Measured in DMF solution with 0.1 M ^{n}Bu$_4$NPF$_6$ (TBAH) as supporting electrolyte at 298 K; scan rate = 100 mV s^{-1}.

[b] $E_{1/2}$ = (E_{pa} + E_{pc})/2; E_{pa} and E_{pc} are the peak anodic and peak cathodic potentials, respectively.

[c] ΔE_p = (E_{pa} – E_{pc}).

[d] Measured in CH_2Cl_2 solution with 0.1 M ^{n}Bu$_4$NPF$_6$ (TBAH) as supporting electrolyte at 298 K; scan rate = 100 mV s^{-1}.

[e] E_{HOMO} and E_{LUMO} levels were calculated from electrochemical potentials, i.e. E_{HOMO} = −[$E_{1/2}^{ox}$ (vs Fc$^+$/Fc) + 4.80] eV; E_{LUMO} = −[$E_{1/2}^{red}$ (vs Fc$^+$/Fc) + 4.80] eV. E_o(Fc$^+$/Fc) = +0.45 V vs SCE in DMF (0.1 M ^{n}Bu$_4$NPF$_6$); E_o(Fc$^+$/Fc) = +0.46 V vs SCE in CH_2Cl_2 (0.1 M ^{n}Bu$_4$NPF$_6$).

Computational Studies

To gain more insights into the electronic structures, photophysical and electrochemical properties, density functional theory (DFT) and time-dependent DFT (TDDFT) calculations have been performed on **1**–**8**. All ground state geometries were optimized in toluene with the hybrid Perdew, Burke, and Ernzerhof (PBE0) functional and Pople 6-31G(d,p) basis set, in conjunction with the conductor-like polarizable continuum model (CPCM). TDDFT calculations at the same level were carried out to obtain the fully relaxed geometries for both S_1 and T_1 states. Vibrational frequency calculations were then performed on the stationary points to verify that each was a minimum (NIMAG = 0) on the potential energy surface (PES). To facilitate the numerical integration, a pruned (175,974) grid as implemented in Gaussian 09 package[9] was used for all the DFT and TDDFT calculations. For compounds **6**–**8**, spin-orbit coupling (SOC) effects were included to describe the interaction between excited S_1 and T_1/T_2 states by using the one-electron Breit Pauli Hamiltonian. The derivative coupling vector between excited T_1 and T_2 states were also computed to quantify the spin-vibronic effect in compounds **6**–**8**. The SOC and derivative coupling calculations were performed using Q-Chem 6.0.2 package.[10,11] We have used CPCM continuum solvation model to describe the solvation effect.

The first ten singlet excited states of **1**–**8** are summarized in Table S5, and the selected molecular orbitals involved in the transitions are shown in Fig. S15–S22. The low-energy absorption band of all complexes were computed to be the $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_2$ transitions, which were attributed to the HOMO → LUMO and HOMO–1 → LUMO excitations respectively. For **1**–**5** and **7**, the HOMO–1 was the π orbital localized on the (dppy)BF moiety and the HOMO was the π orbital localized on the *N*-donor moiety and the adjacent pyridyl ring of the (dppy)BF moiety, while the LUMO was the π* orbital localized on the (dppy)BF moiety. Therefore, the low-energy absorption band of **1**–**5** and **7** could be assigned as the ICT [π(*N*-donor) → π*((dppy)BF)] transition, mixed with the IL [π → π*((dppy)BF)] transition, in line with the experimental assignments. On the other hand, for **6** and **8**, both HOMO and HOMO–

1 are localized on the π orbital of the *N*-donor moieties, while the LUMO is the π* orbitals of the (dppy)BF moiety. The low-energy absorption band of **6** and **8** are thus assigned as ICT [π(*N*-donor) → π*((dppy)BF)] transition.

The orbital energy diagram showing the frontier molecular orbitals of **1**–**8** is given in Fig. S26. The introduction of methyl group at different position of the phenyl bridge (**2** and **3**) has insignificant effect on the energy of the frontier orbitals, while the introduction of electron-withdrawing fluoro group (**4**) slightly lowered both the HOMO and LUMO energies, owing to the limited contribution of the phenyl ring to these orbitals. As expected, introducing the electron-withdrawing group on the carbazolyl moiety (**5**) which has strong HOMO character will result in stabilization of the HOMO and thus widen the HOMO–LUMO energy gap. The electron-donating capability on the HOMO on the other hand is enhanced by introducing extra carbazolyl unit (**6**) and replacing the carbazolyl unit with a more electron-donating triphenylamine moiety (**7** and **8**). Such design leads to significant increases in the HOMO energy and narrowing of the HOMO–LUMO energy gap. The trend of the orbital energy is in good agreement with the results obtained by cyclic voltammetry.

The quantitative percentages of charge transfer (CT) character and locally excited (LE) state character of representative compounds **6**–**8** were evaluated by using interfragment charge transfer (IFCT) method as implemented in Multiwfn.[12] For **7** and **8**, three fragments were defined for each compound (Fig. S25). We have tried two fragmentation schemes for **6** (Schemes A and B in Fig. S25) considering that two phenyl rings of (dppy)BF in **6** contribute significantly to both HOMO and LUMO orbitals (Fig. S20). The electron/hole densities are partitioned with Hirshfeld scheme. Results from IFCT analysis for both T_1 and T_2 states were presented in Table S6. It should be noted that the CT and LE percentages for T_1 and T_2 states of **6** are highly dependent on the fragmentation scheme, possibly because they represent symmetric CT from two DTC donors to (dppy)BF acceptor. We believe the definition of fragments as shown in Scheme B of Fig. S25 is a better representation of the donor and acceptor fragments for **6**.

Table S5 The first ten singlet excited states (S_n) of **1**–**8** computed by TDDFT/CPCM using toluene as the solvent.

Compound	S_n	Excitation[a] (Coefficient)[b]	Vertical excitation wavelength (nm)	f[c]
1	S_1	H→L (0.70)	375	0.462
	S_2	H–1→L (0.68)	371	0.191
	S_3	H→L+1 (0.68)	346	0.006
	S_4	H–2→L (0.70)	331	0.000
	S_5	H–1→L+1 (0.69)	327	0.279
	S_6	H–3→L (0.70)	319	0.031
	S_7	H–2→L+1 (0.52)	304	0.004
		H–3→L+1 (–0.45)		
	S_8	H–2→L+1 (0.48)	304	0.004
		H–3→L+1 (0.50)		
	S_9	H→L+2 (0.68)	300	0.041
	S_{10}	H–4→L (0.68)	291	0.284
2	S_1	H→L (0.70)	406	0.344
	S_2	H–1→L (0.70)	384	0.195
	S_3	H→L+1 (0.70)	345	0.001
	S_4	H–2→L (0.70)	338	0.000
	S_5	H–3→L (0.70)	330	0.080
	S_6	H–1→L+1 (0.69)	323	0.346
	S_7	H→L+2 (0.69)	311	0.049
	S_8	H–4→L (0.55)	303	0.054
		H–3→L+1 (0.42)		
	S_9	H–3→L+1 (0.55)	298	0.204
		H–4→L (–0.43)		
	S_{10}	H–2→L+1 (0.71)	295	0.000
3	S_1	H→L (0.70)	414	0.181
	S_2	H−1→L (0.70)	390	0.184
	S_3	H−2→L (0.70)	349	0.000
	S_4	H→L+1 (0.70)	340	0.000
	S_5	H−3→L (0.70)	336	0.103
	S_6	H−1→L+1 (0.69)	324	0.359
	S_7	H→L+2 (0.68)	308	0.067
	S_8	H−4→L (0.65)	306	0.112
	S_9	H−3→L+1 (0.65)	300	0.131
	S_{10}	H−2→L+1 (0.71)	297	0.000

4	S_1	H→L (0.70)	420	0.360
	S_2	H−1→L (0.70)	396	0.176
	S_3	H−2→L (0.70)	355	0.001
	S_4	H→L+1 (0.70)	342	0.000
	S_5	H−3→L (0.70)	340	0.069
	S_6	H−1→L+1 (0.69)	326	0.338
	S_7	H−4→L (0.67)	310	0.130
	S_8	H→L+2 (0.39)	305	0.054
		H→L+3 (0.57)		
	S_9	H−3→L+1 (0.67)	302	0.112
	S_{10}	H−2→L+1 (0.71)	298	0.000
5	S_1	H→L (0.68)	395	0.417
	S_2	H−1→L 0.68)	393	0.192
	S_3	H−3→L (0.70)	338	0.053
	S_4	H→L+1 (0.69)	327	0.007
	S_5	H−1→L+1 (0.68)	325	0.329
	S_6	H−2→L (0.70)	324	0.000
	S_7	H→L+2 (0.69)	320	0.043
	S_8	H−4→L (0.65)	308	0.116
	S_9	H−3→L+1 (0.65)	301	0.128
	S_{10}	H→L+4 (0.68)	286	0.003
6	S_1	H→L (0.68)	449	0.061
	S_2	H−1→L (0.67)	437	0.017
	S_3	H→L+1 (0.67)	400	0.015
	S_4	H−1→L+1 (0.68)	397	0.004
	S_5	H−2→L (0.66)	355	0.006
	S_6	H−3→L (0.66)	355	0.000
	S_7	H−4→L (0.68)	351	0.386
	S_8	H−2→L+1 (0.68)	328	0.000
	S_9	H−3→L+1 (0.68)	328	0.000
	S_{10}	H−1→L+3 (0.47)	315	0.101
		H→L+2 (0.50)		
7	S_1	H→L (0.70)	430	0.785
	S_2	H–1→L (0.68)	383	0.185
	S_3	H→L+1 (0.68)	364	0.008
	S_4	H–2→L (0.70)	328	0.045
	S_5	H–1→L+1 (0.69)	322	0.327
	S_6	H→L+3 (0.69)	312	0.019
	S_7	H–3→L (0.58)	301	0.065
		H–2→L+1 (–0.37)		

	S_8	H→L+4 (0.70)	297	0.329
	S_9	H–2→L+1 (0.58) H–3→L (0.38)	296	0.196
	S_{10}	H→L+2 (0.67)	295	0.230
8	S_1	H→L (0.70)	440	0.110
	S_2	H→L+1 (0.70)	391	0.002
	S_3	H−1→L (0.70)	371	0.223
	S_4	H−1→L+1 (0.65)	324	0.604
	S_5	H−2→L (0.68)	319	0.056
	S_6	H→L+3 (0.69)	313	0.031
	S_7	H→L+2 (0.64)	308	0.267
	S_8	H→L+4 (0.70)	300	0.344
	S_9	H−2→L+1 (0.64)	300	0.000
	S_{10}	H−4→L (0.46)	291	0.260

[a] Orbitals involved in the major excitation (H = HOMO and L = LUMO).

[b] The coefficients in the configuration interaction (CI) expansion.

[c] Oscillator strengths.

Table S6 The percentages of charge transfer (CT) and locally excited state (LE) character of T_1 and T_2 states for **6**–**8**.

Compound	State	CT / %	LE / %
6	Scheme A		
	T_1	42	58
	T_2	38	62
	Scheme B		
	T_1	80	20
	T_2	78	22
7	T_1	73	27
	T_2	12	88
8	T_1	80	20
	T_2	12	88

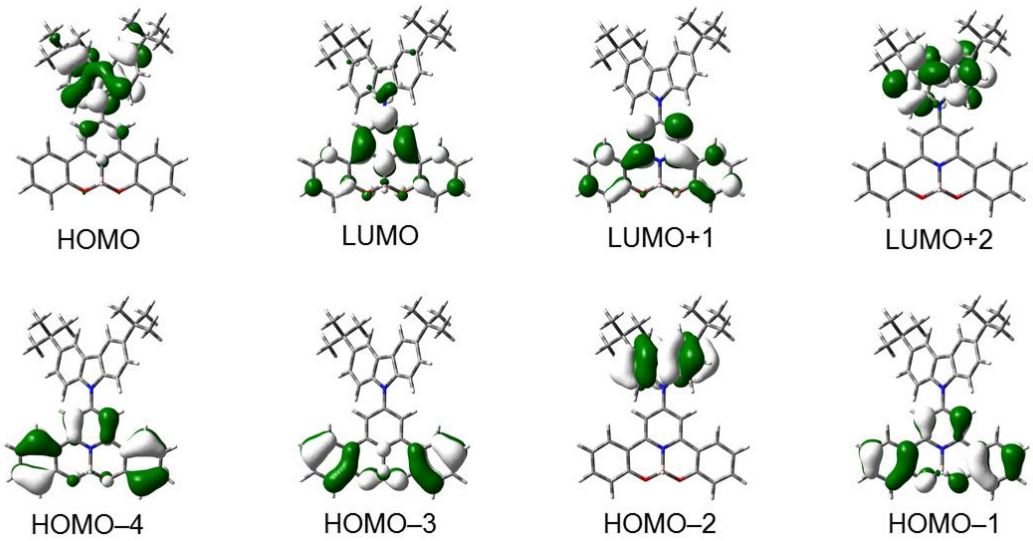


Fig. S15 Spatial plots (isovalue = 0.03) of selected molecular orbitals of **1** at the optimized ground-state (S_0) geometry.

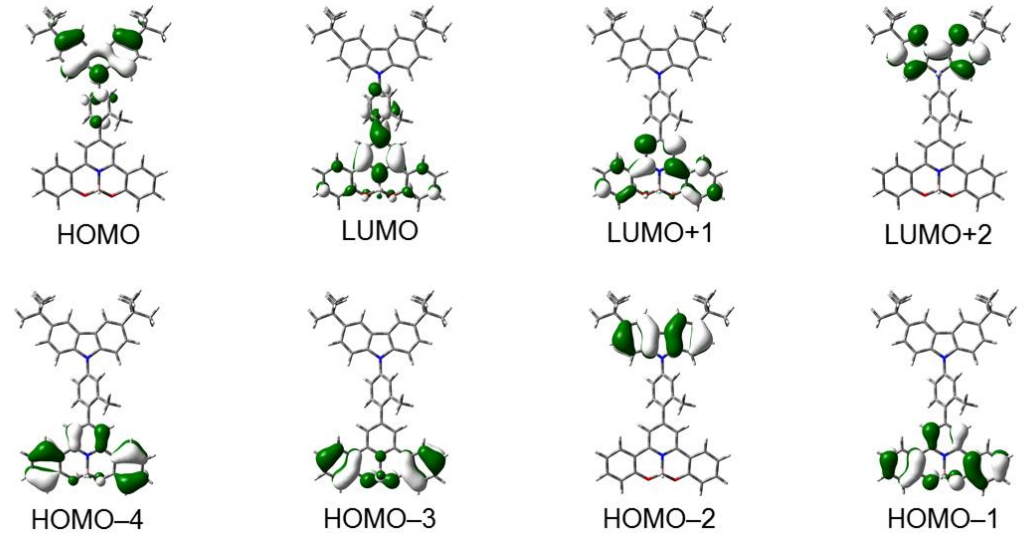


Fig. S16 Spatial plots (isovalue = 0.03) of selected molecular orbitals of **2** at the optimized ground-state (S_0) geometry.

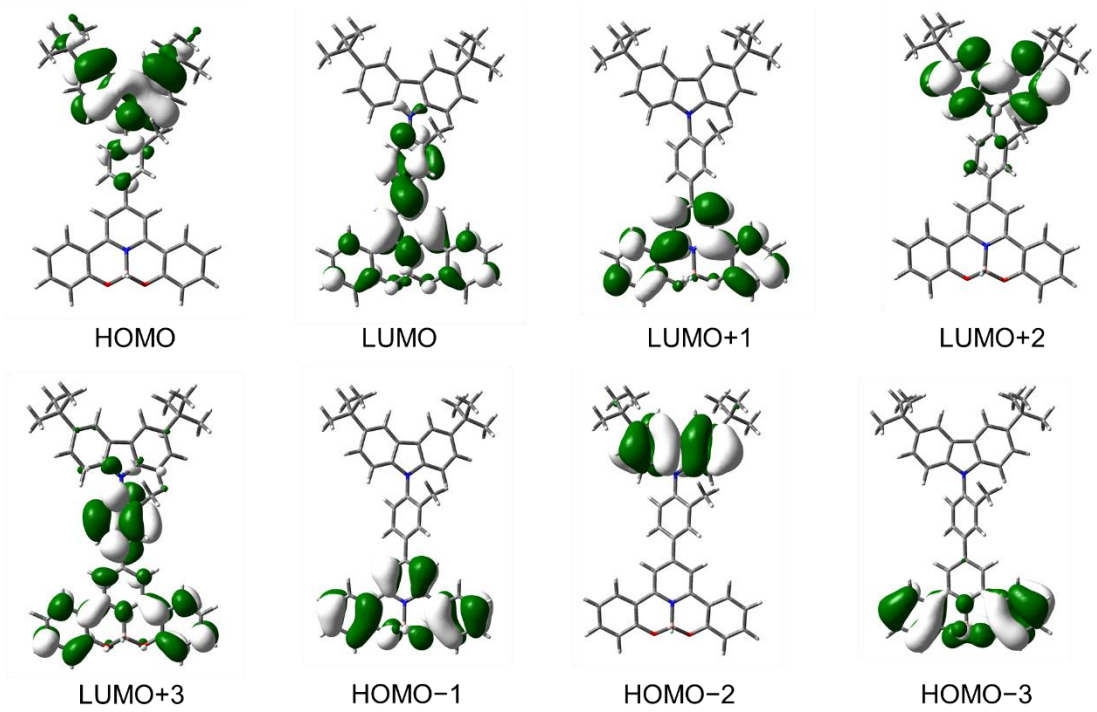


Fig. S17 Spatial plots (isovalue = 0.03) of selected molecular orbitals of **3** at the optimized ground-state geometry.

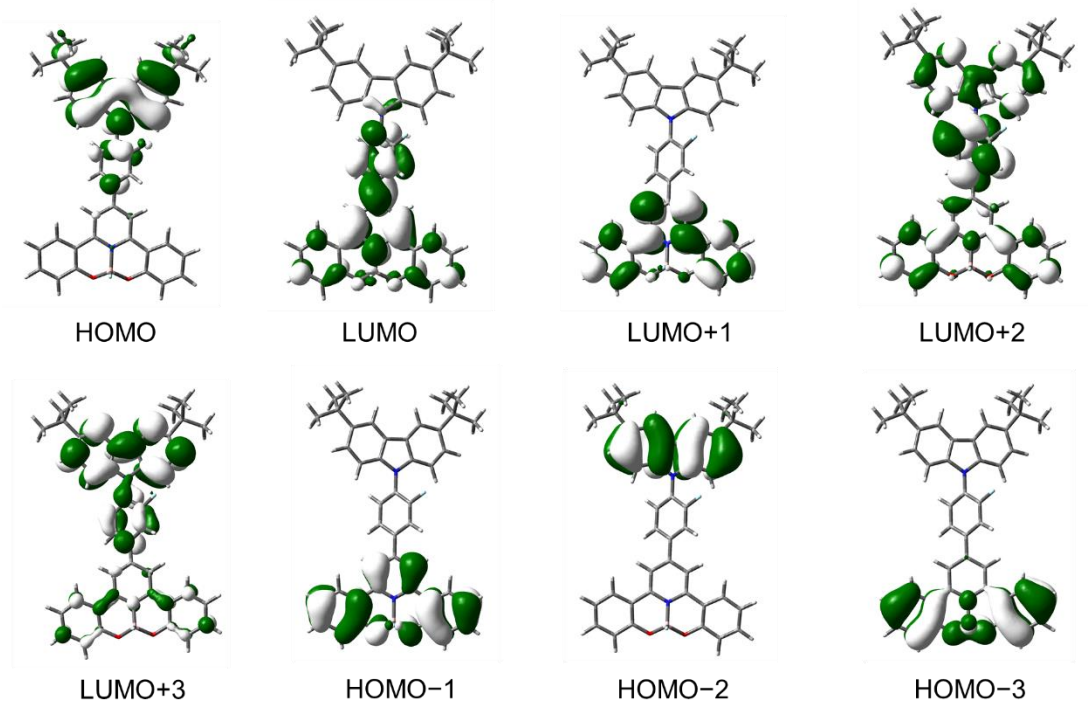


Fig. S18 Spatial plots (isovalue = 0.03) of selected molecular orbitals of **4** at the optimized ground-state geometry.

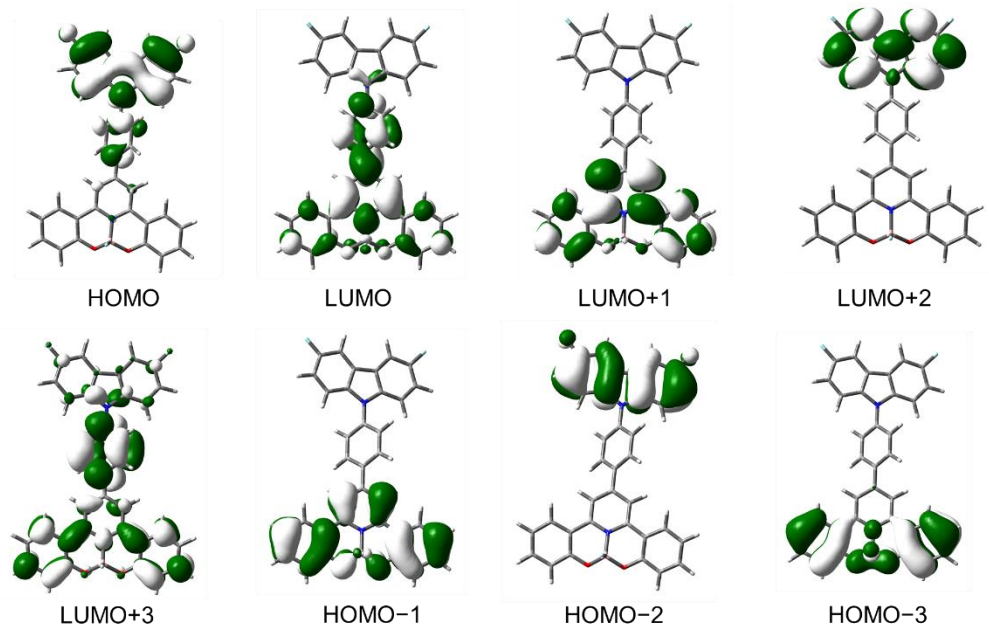


Fig. S19 Spatial plots (isovalue = 0.03) of selected molecular orbitals of **5** at the optimized ground-state geometry.

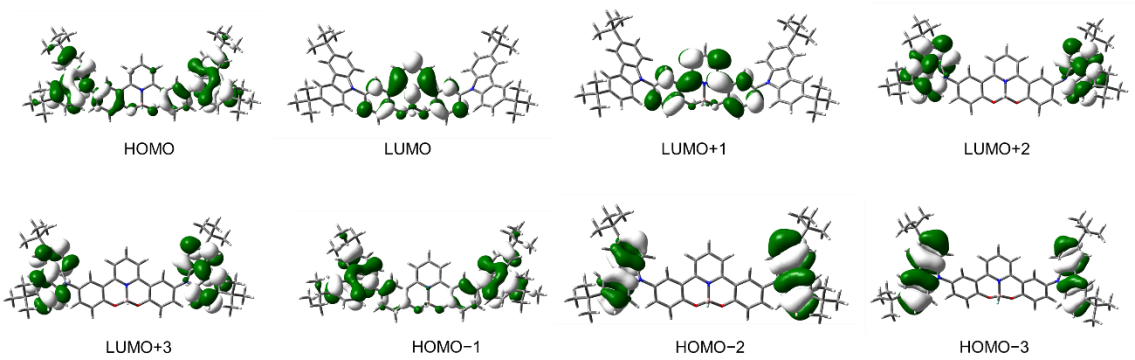


Fig. S20 Spatial plots (isovalue = 0.03) of selected molecular orbitals of **6** at the optimized ground-state geometry.

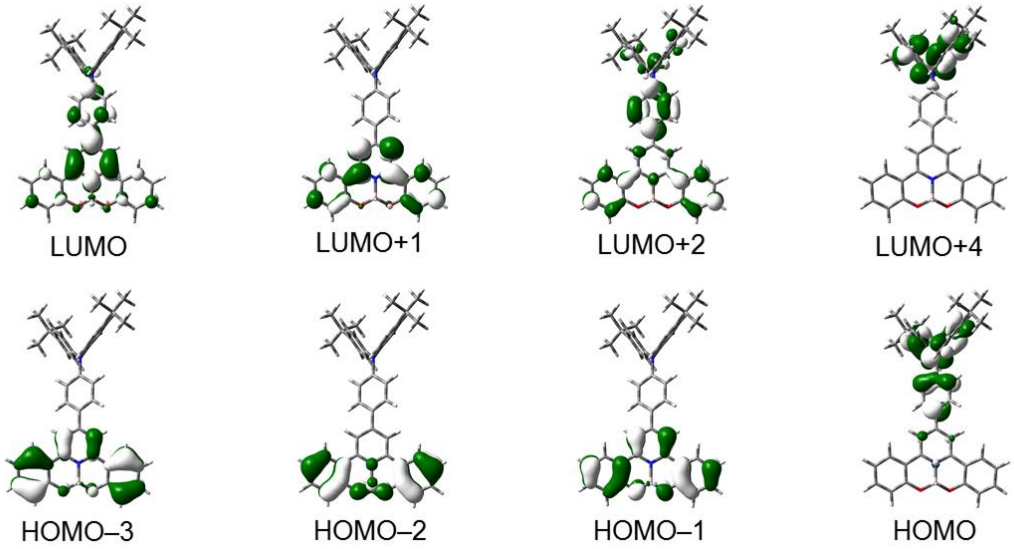


Fig. S21 Spatial plots (isovalue = 0.03) of selected molecular orbitals of **7** at the optimized ground-state (S_0) geometry.

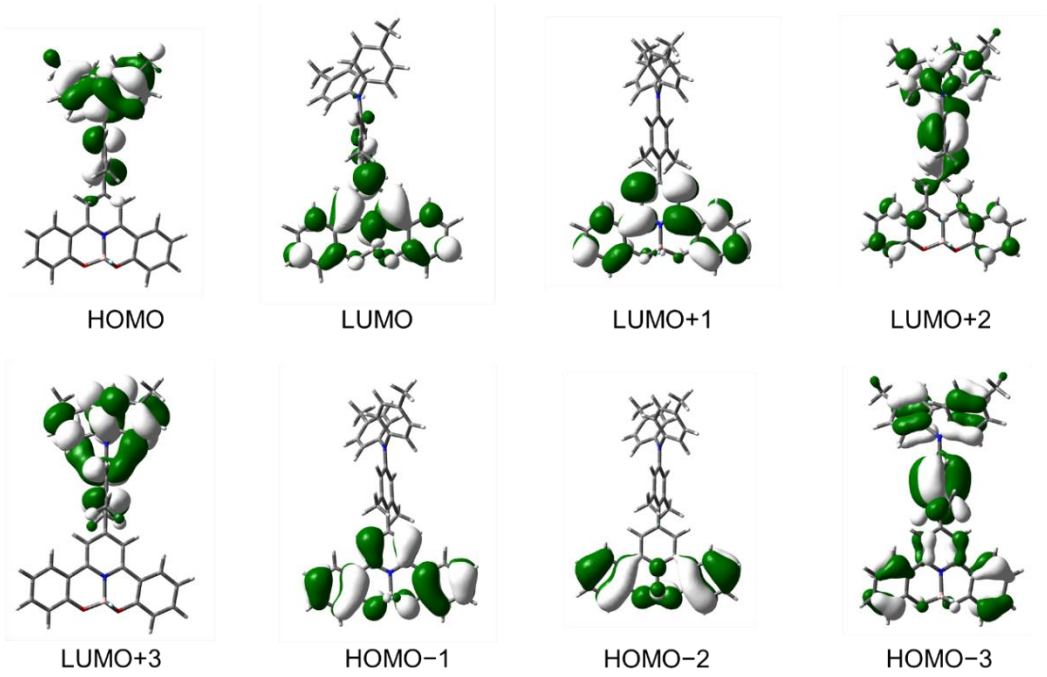


Fig. S22 Spatial plots (isovalue = 0.03) of selected molecular orbitals of **8** at the optimized ground-state (S_0) geometry.

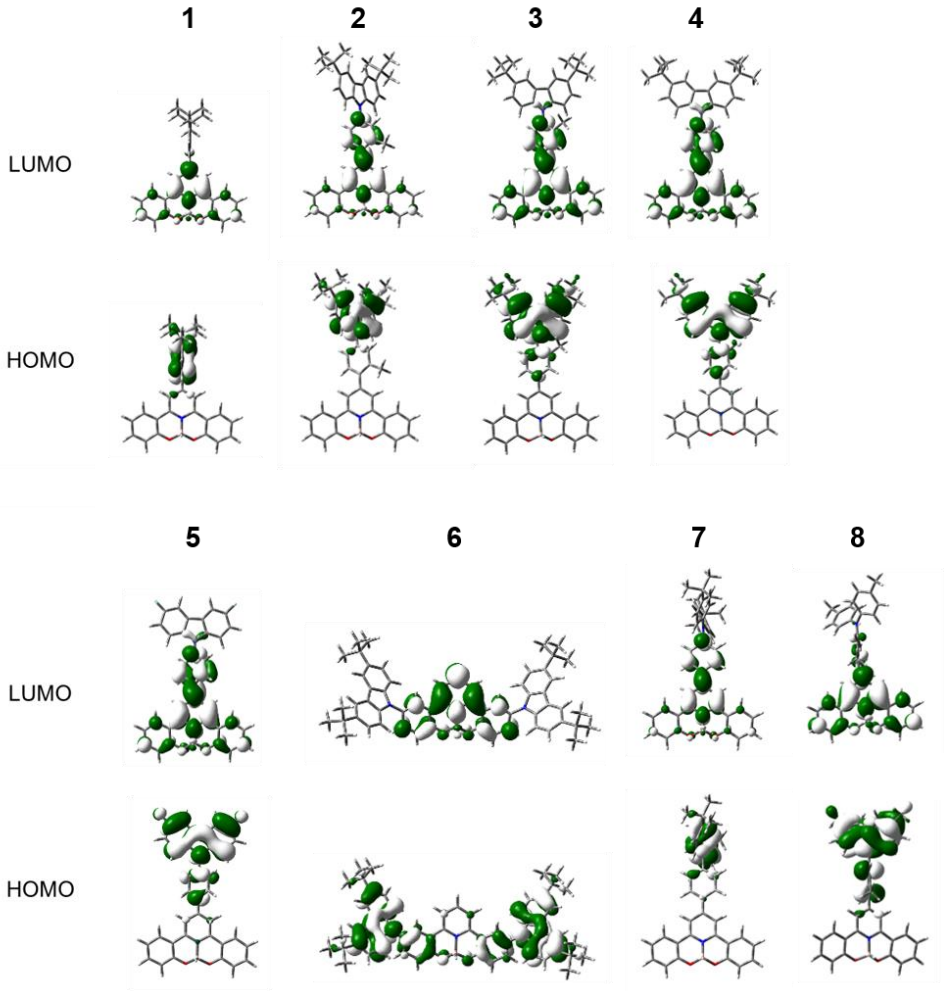


Fig. S23 The orbital transitions of **1**–**8** that contributed to the optimized S_1 geometry.

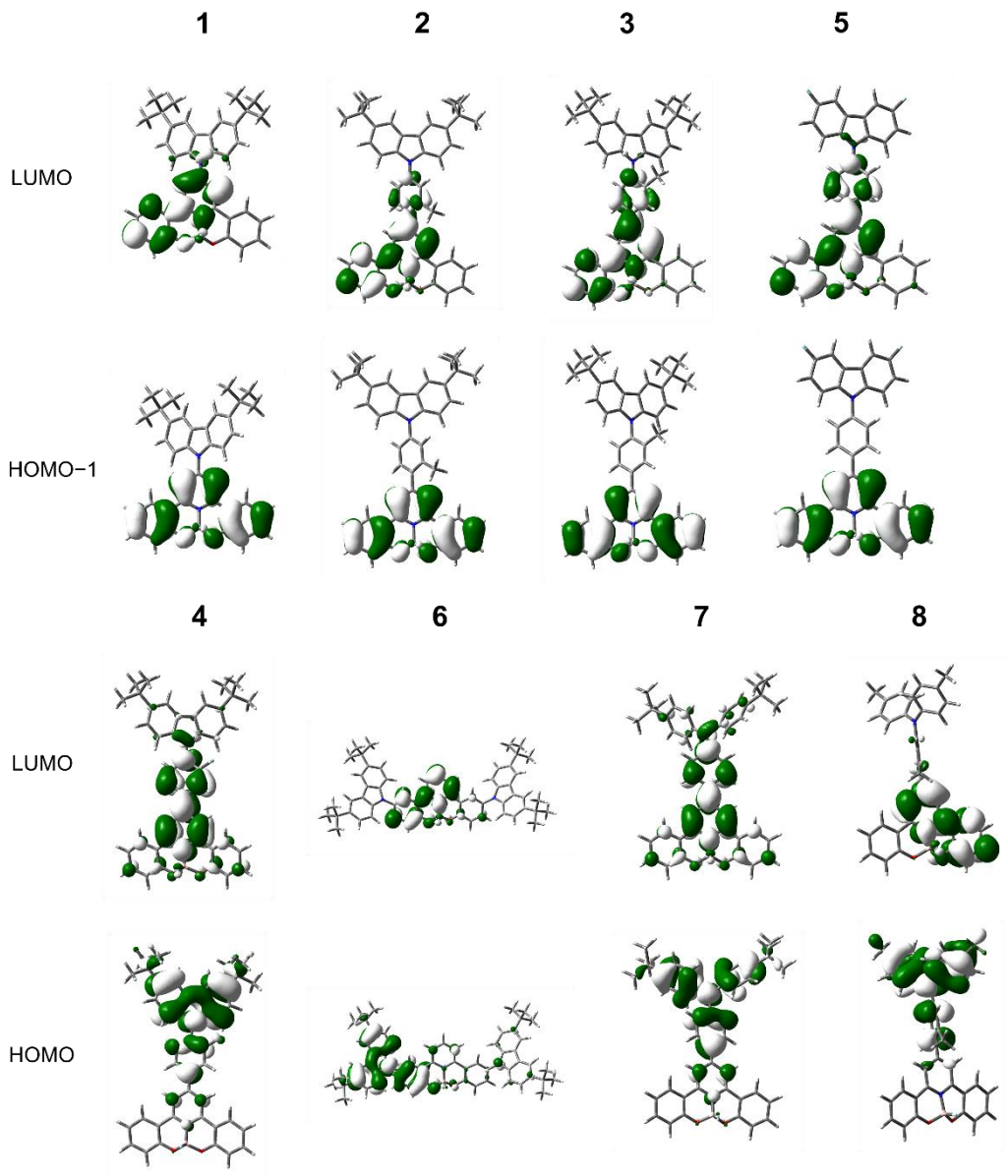


Fig. S24 The orbital transitions of **1–8** that contributed to the optimized T_1 geometry.

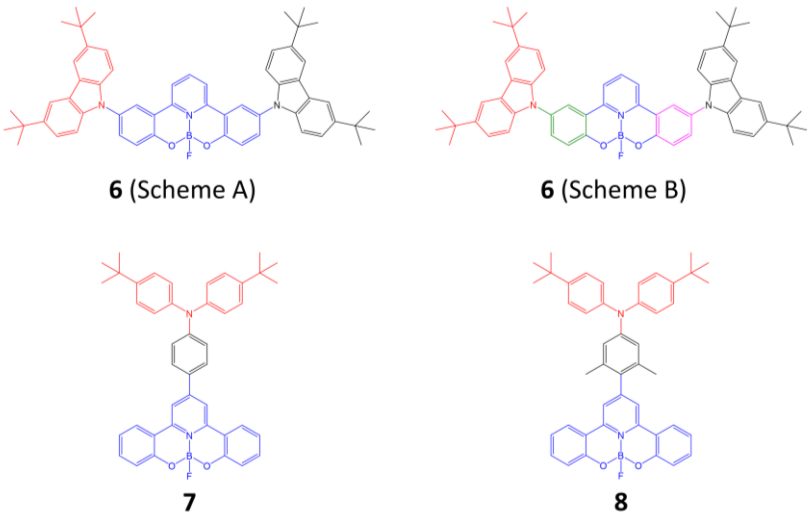


Fig. S25 Molecular fragments of compounds **6–8** defined for IFCT analysis.

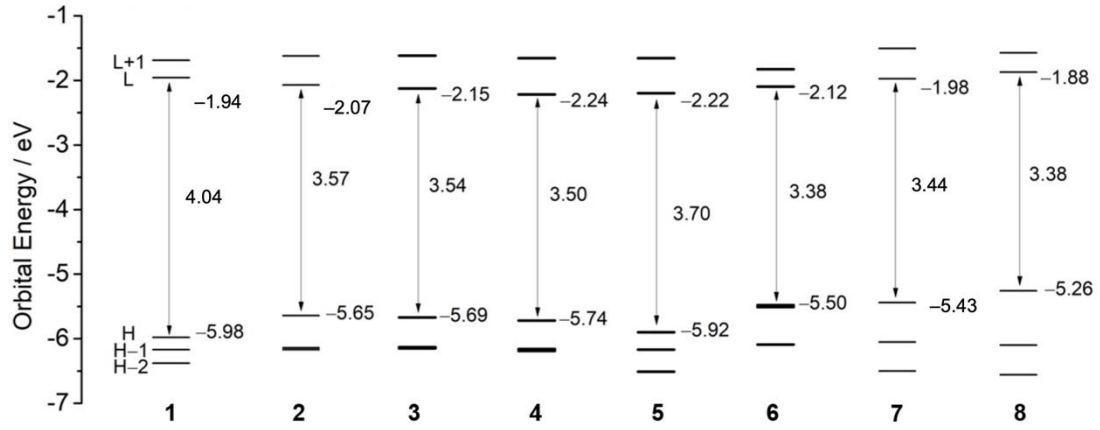


Fig. S26 Orbital energy diagram of **1**–**8**.

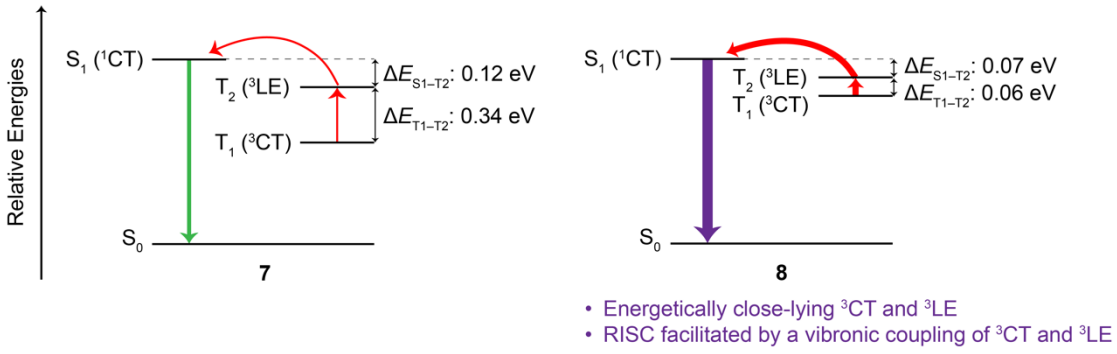


Fig. S27 A schematic illustration of an efficient RISC process facilitated by a spin-vibronic coupling mechanism in **8** as compared to that in **7**.

OLED Fabrication and Characterization

Vacuum-deposited OLEDs were fabricated with the configuration of indium tin oxide (ITO)/*N*,*N*′-bis(naphthalene-1-yl)-*N*,*N*′-bis(phenyl)-2,2'-dimethylbenzidine (α-NPD; 40 nm)/4,4′,4″-tris(carbazol-9-yl)triphenylamine (TCTA; 5 nm)/*x* % **1**, **2**, **7** and **8**:3,3′-di(9*H*-carbazol-9-yl)biphenyl (*m*-CBP; 20 nm)/1,3,5-tris(6-(3-(pyridin-3-yl)phenyl)pyridine-2-yl)benzene (Tm3PyP26PyB; 50 nm)/LiF (1 nm)/Al (150 nm) (device A) or ITO/α-NPD (40 nm)/*x* % 4-DTC-Ph(dppy)BF, **3**–**6** and **8**:*m*-CBP (20 nm)/diphenyl[4-(triphenylsilyl)phenyl]phosphine oxide (TSPO1; 5 nm)/Tm3PyP26PyB (35 nm)/LiF (1 nm)/Al (150 nm) (device B), in which the four-coordinate boron emitter was simultaneously co-evaporated with the *m*-CBP host at different concentrations, i.e. *x* = 2, 5, 8, 11 or 14 % v/v. Notably, 3,3′-di(9*H*-carbazol-9-yl)biphenyl (*m*-CBP) has been used as host material due to its higher thermal stability than mCP, favoring for higher operational stability of OLEDs, while the PLQYs in thin films are almost the same as those in mCP (Figure S29 and Table S7). The ITO coated glass substrates were cleaned with Decon 90, rinsed with deionized water, dried in an oven, and finally treated in an ultraviolet-ozone chamber. Then, the hole-transporting layer α-NPD, the electron-blocking layer TCTA, the emissive layer, the electron-transporting layer Tm3PyP26PyB, LiF and aluminum; or the hole-transporting layer α-NPD, the emissive layer, the hole-blocking layer TSPO1, the electron-transporting layer Tm3PyP26PyB, LiF and aluminum were sequentially thermally evaporated onto the ITO substrate. All organic materials and metals were thermally evaporated by a Trovato vacuum deposition system in vacuum under a base pressure of 10^{-6} Torr. High-purity α-NPD, TCTA, TSPO1, Tm3PyP26PyB and *m*-CBP (> 99.5 % HPLC) were purchased from Luminescence Technology Corporation and were used as received without further purification. All films were sequentially deposited at a rate of 0.1−0.2 nm s^{-1} without vacuum break. A shadow mask was used to define the cathode and to make four 0.1 cm^2 devices on each substrate. Current density−voltage−luminance characteristics and electroluminescence (EL) spectra were measured simultaneously with a programmable Keithley model 2420 power source and a Photoresearch PR-655

spectrometer. All the devices were measured under ambient conditions without encapsulation. For operational stability testing, vacuum-deposited devices with the configuration of ITO/dipyrazino[2,3-*f*:2′,3′-h]quinoxaline-2,3,6,7,10,11-hexacarbonitrile (HAT-CN; 10 nm)/α-NPD (40 nm)/9,9′,9″-triphenyl-9H,9′H,9″H-3,3′:6′,3″-tercarbazole (Tris-PCz; 10 nm)/11 v/v% **2**, **3**, **4**, **6**, **7** and **8**:*m*-CBP (25 nm)/2,4,6-tris[3-(diphenylphosphinyl)phenyl]-1,3,5-triazine (T2T; 10 nm)/2,7-di(2,2′-bipyridin-5-yl)triphenylene (BPy-TP2; 40 nm)/LiF (1 nm)/Al (150 nm) had been fabricated and encapsulated in a glovebox under nitrogen. The initial brightness of the encapsulated device was measured by a Keithley 2400 power source and a Photoresearch PR-655 spectrometer; while the operational lifetime of the encapsulated device was measured by a McScience OLED lifetime system by accelerated lifetime testing under a constant driving current density of 20 mA cm^{-2}.

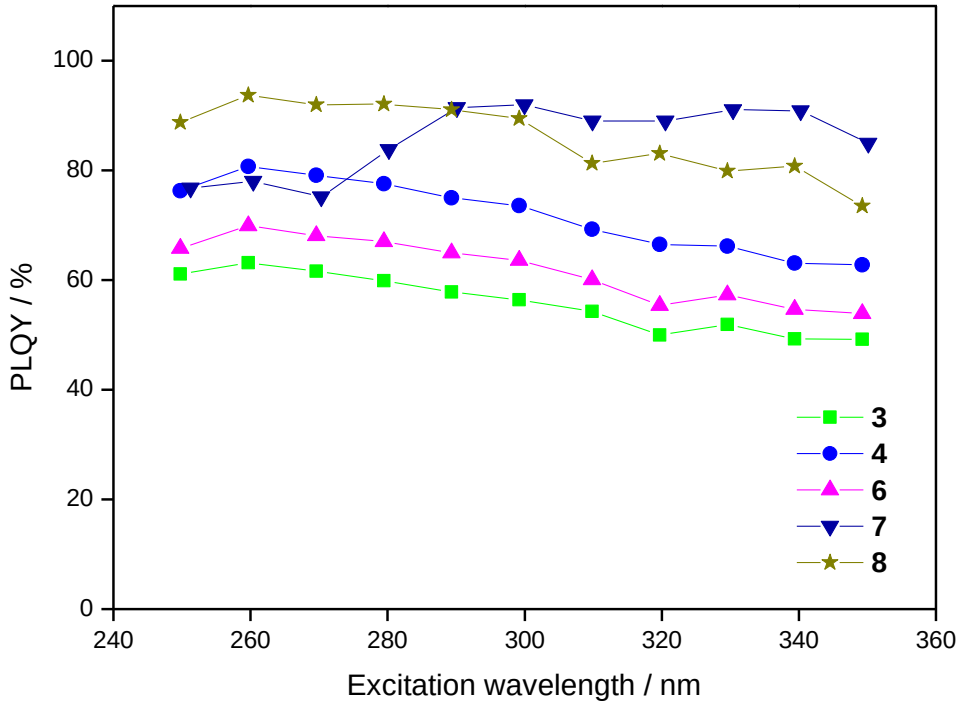


Fig. S28. Absolute PLQYs of the fluoroboron compounds **3**, **4**, **6**, **7** and **8** doped in *m*-CBP thin films.

Table S7. Absolute PLQY of the compounds doped in *m*-CBP thin films.[a]

Compound	PLQY / %[b]
3[c]	56
4[c]	74
6[c]	64
7[d]	92
8[c]	90

[a] The doped films in *m*-CBP were prepared by vacuum deposition.
[b] Measured under excitation wavelength of 300 nm.
[c] Measured in 5 v/v% doped *m*-CBP thin films.
[d] Measured in 8 v/v% doped *m*-CBP thin films.

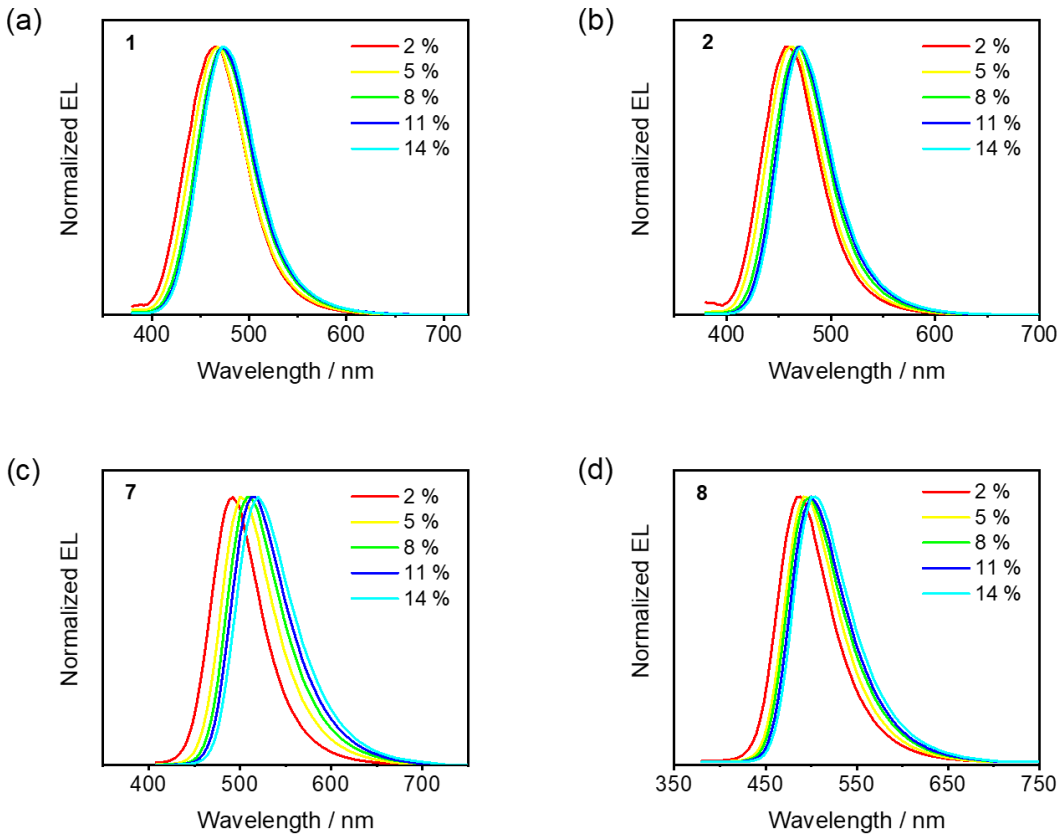


Fig. S29. Normalized EL spectra of the vacuum-deposited OLEDs (device A) based on (a) **1**, (b) **2**, (c) **7** and (d) **8**.

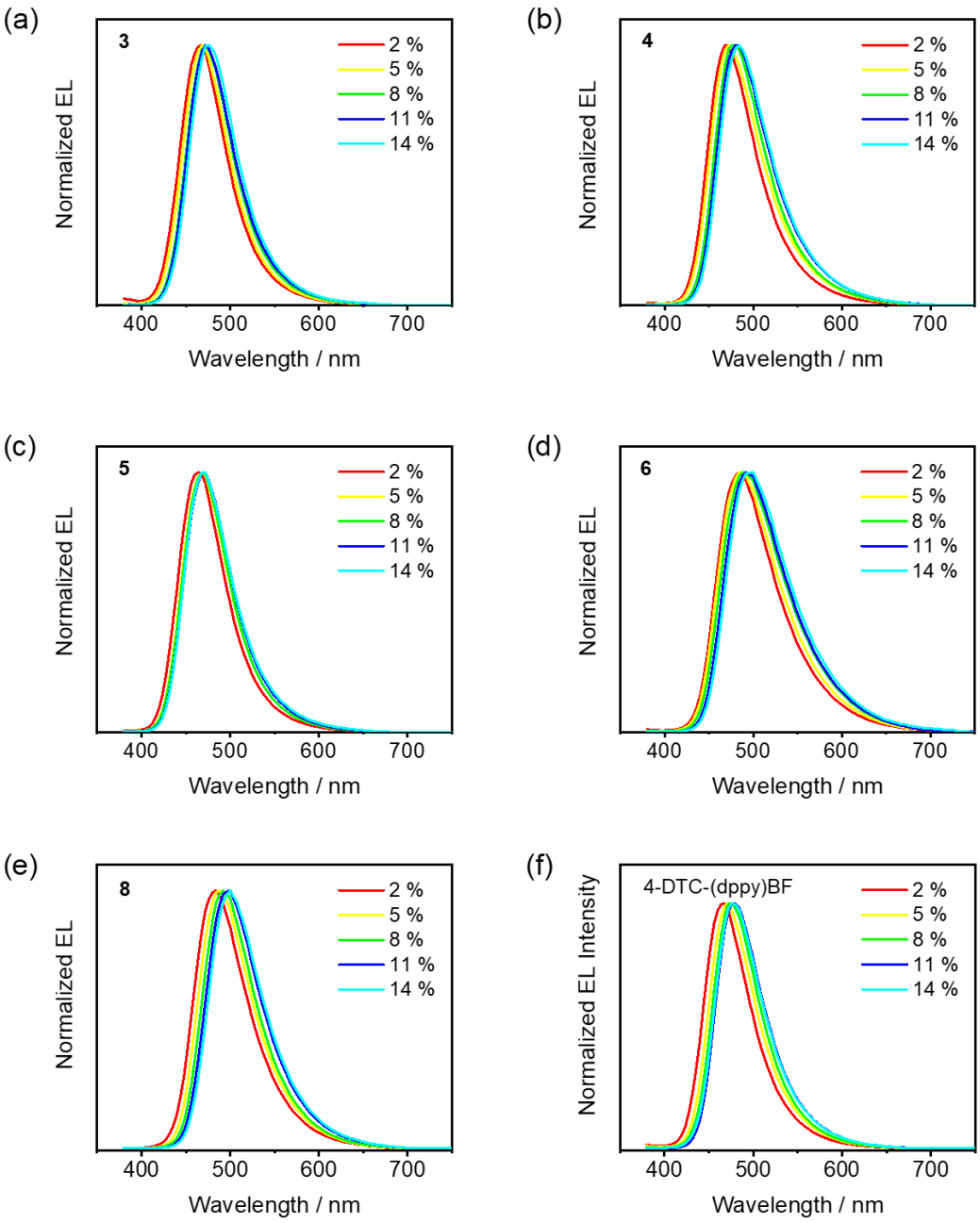


Fig. S30. Normalized EL spectra of the vacuum-deposited OLEDs (device B) based on (a) **3**, (b) **4**, (c) **5**, (d) **6**, (e) **8** and (f) 4-DTC-(dppy)BF.

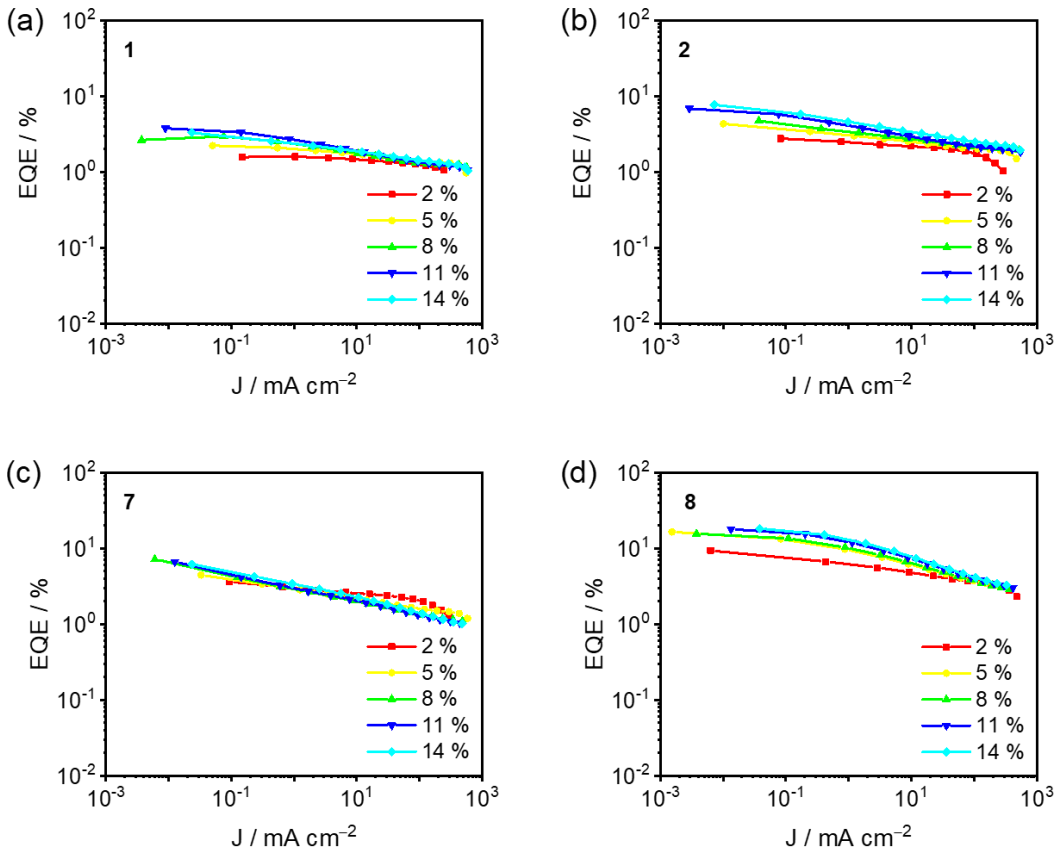


Fig. S31. EQE–current density (J) plots of the vacuum-deposited OLEDs (device A) based on (a) **1**, (b) **2**, (c) **7** and (d) **8**.

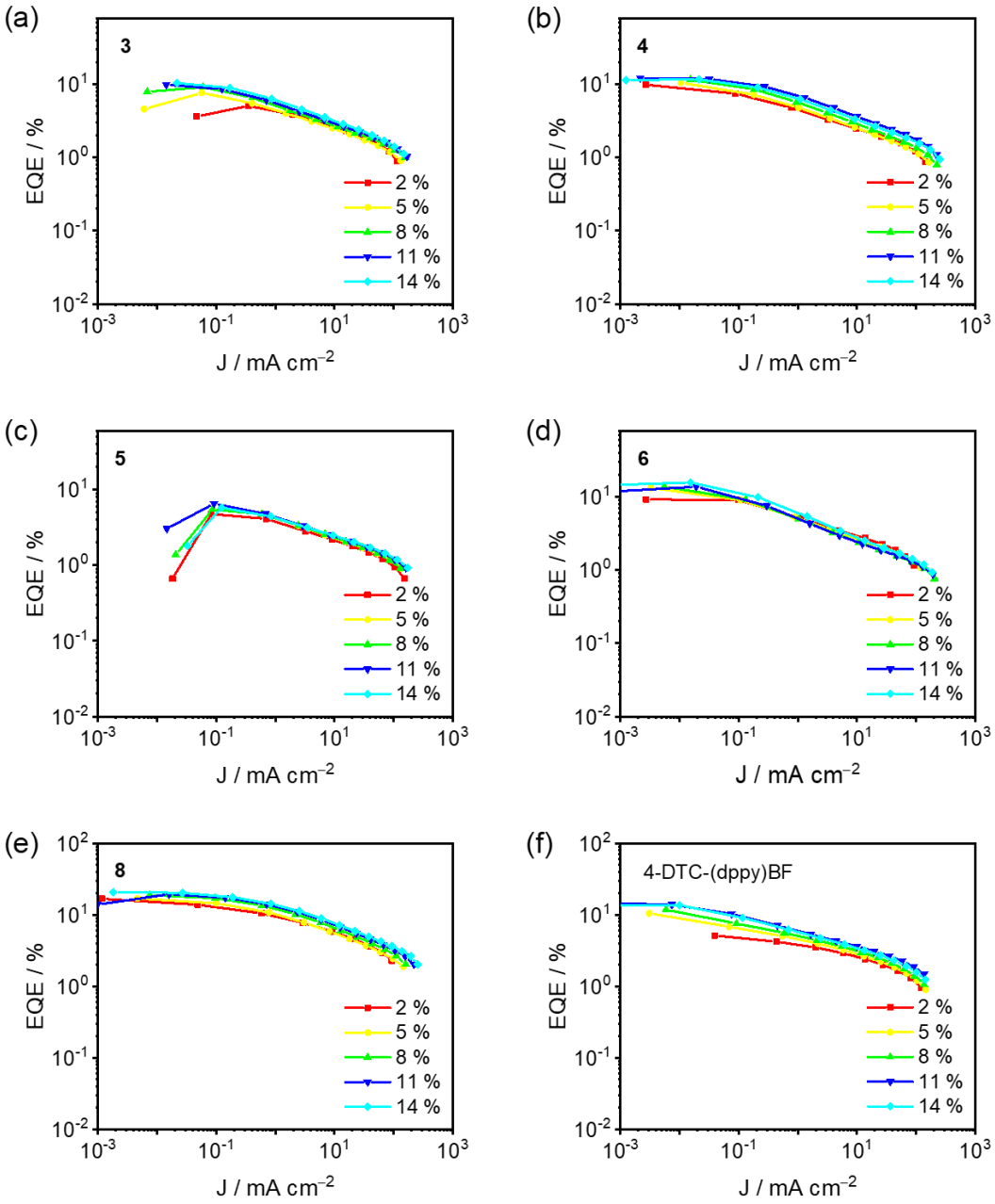


Fig. S32. EQE–current density (J) plots of the vacuum-deposited OLEDs (device B) based on (a) **3**, (b) **4**, (c) **5**, (d) **6**, (e) **8** and (f) 4-DTC-(dppy)BF.

Table S8 Key characteristics of vacuum-deposited devices made with 4-DTC-Ph(dppy)BF and **1**–**8**.

Compd.	Dopant conc. / v/v%	CE / cd A^{-1} [a]	PE / lm W^{-1} [b]	EQE / % [c]	L /cd m^{-2} [d]	λ_{max} / nm [e]	FWHM / nm (cm^{-1})
1 [f]	2	1.8	1.5	1.6	18.8	464 (0.14,0.14)	72 (3,335)
	5	3.0	2.7	2.2	1.5	468 (0.14,0.15)	67 (3,055)
	8	4.5	4.5	2.9	3.4	472 (0.14,0.19)	67 (2,991)
	11	6.2	6.5	3.8	0.6	472 (0.14,0.20)	66 (2,915)
	14	5.4	5.7	3.3	1.3	472 (0.14,0.21)	67 (2,941)
2 [f]	2	2.6	2.1	2.7	2.2	460 (0.14,0.11)	63 (2,972)
	5	5.2	4.7	4.3	0.6	464 (0.14,0.13)	62 (2,868)
	8	6.5	5.8	4.7	2.4	468 (0.14,0.16)	61 (2,755)
	11	11.7	12.3	6.8	0.4	470 (0.14,0.18)	60 (2,681)
	14	13.3	14.0	7.7	1.0	472 (0.14,0.20)	60 (2,658)
3 [g]	2	6.8	4.8	5.1	23.9	468 (0.15,0.16)	61 (1,972)
	5	11.4	9.0	7.7	6.5	468 (0.15,0.18)	61 (1,897)
	8	14.9	11.7	9.2	8.9	472 (0.15,0.21)	61 (1,865)
	11	17.0	15.3	9.9	2.4	472 (0.15,0.23)	61 (1,857)
	14	18.6	16.7	10.4	4.0	476 (0.15,0.25)	63 (1,922)
4 [g]	2	16.4	14.7	9.9	0.4	468 (0.15,0.22)	64 (2,825)
	5	19.6	17.6	10.5	2.1	472 (0.16,0.26)	67 (2,904)
	8	23.3	20.9	11.6	3.5	476 (0.16,0.30)	67 (2,844)
	11	25.4	26.4	11.7	5.3	480 (0.18,0.33)	69 (2,882)
	14	26.6	27.0	12.2	0.6	484 (0.18,0.35)	69 (2,823)
5 [g]	2	6.7	5.2	4.8	5.5	464 (0.15,0.15)	61 (2,831)
	5	7.2	5.0	4.9	42.1	468 (0.15,0.18)	61 (2,783)
	8	8.5	6.7	5.5	7.3	468 (0.15,0.19)	61 (2,732)
	11	10.8	8.5	6.5	9.9	468 (0.15,0.21)	62 (2,748)
	14	9.9	7.8	5.8	12.1	468 (0.15,0.21)	63 (2,787)
6 [g]	2	21.0	18.9	9.2	0.6	484 (0.19,0.35)	77 (3,181)
	5	31.3	28.1	13.3	1.0	484 (0.20, 0.37)	80 (3,308)

	8	35.3	31.7	13.8	1.9	492 (0.21, 0.41)	84 (3,357)
	11	36.2	32.5	13.8	6.9	492 (0.22, 0.43)	82 (3,250)
	14	43.2	40.6	15.8	6.5	500 (0.23, 0.45)	82 (3,244)
7[f]	2	8.5	6.6	3.6	7.7	492 (0.16,0.38)	64 (2,612)
	5	13.1	11.8	4.4	4.3	500 (0.21,0.52)	67 (2,592)
	8	22.9	24.0	7.2	1.4	508 (0.24,0.57)	69 (2,631)
	11	22.0	23.0	6.6	2.8	516 (0.26,0.59)	72 (2,645)
	14	21.1	22.1	6.2	5.0	520 (0.29,0.60)	73 (2,626)
8[f]	2	21.3	19.2	9.3	1.4	488 (0.17,0.35)	67 (2,764)
	5	41.4	43.3	16.5	0.6	492 (0.18,0.44)	68 (2,676)
	8	41.9	43.9	15.6	1.6	500 (0.20,0.47)	70 (2,792)
	11	50.7	53.1	17.9	6.8	500 (0.22,0.50)	71 (2,748)
	14	53.6	56.2	18.3	20.6	504 (0.23,0.53)	72 (2,749)
8[g]	2	32.8	29.5	16.8	0.4	484 (0.17,0.32)	69 (2,930)
	5	39.1	35.1	17.0	1.8	488 (0.18,0.38)	69 (2,859)
	8	46.6	41.8	18.9	3.5	492 (0.18,0.42)	69 (2,814)
	11	51.8	46.5	19.4	0.4	500 (0.20,0.47)	71 (2,838)
	14	57.9	60.6	20.8	1.0	500 (0.21,0.49)	71 (2,770)
4-DTC-Ph(dppy)BF[g]	2	7.5	5.9	5.1	2.9	468 (0.15,0.18)	61 (2,755)
	5	17.2	15.5	10.5	0.5	472 (0.15,0.22)	61 (2,675)
	8	21.4	19.2	11.8	1.3	476 (0.15,0.25)	62 (2,631)
	11	27.7	27.6	14.6	0.1	476 (0.16,0.29)	63 (2,684)
	14	27.8	29.1	13.8	0.1	476 (0.16, 0.29)	63 (2,673)

[a] Maximum current efficiency

[b] Maximum power efficiency

[c] Maximum EQE

[d] Luminance taken at the maximum EQE value

[e] CIE coordinates in parentheses, measured at 100 cd m^{-2}

[f] Device structure: ITO/ α-NPD/TCTA/*x* % emitter:*m*-CBP/Tm3PyP26PyB/LiF/Al

[g] Device structure: ITO/α-NPD /*x* % emitter:*m*-CBP/TSPO1/Tm3PyP26PyB/LiF/Al

Table S9 Summary of the state-of-the-art blue emitting TADF-OLEDs.

Compound	λ_{max}[a]	EQE_{max}/%	LT_x @ L_o[b]/h	Ref.
8	**492**	**18.9**	**LT_{50}: 9,113 @ 100 cd m^{-2}** **LT_{80}: 100 @ 500 cd m^{-2}** **LT_{50}: 590 @ 500 cd m^{-2}**	**this work**
4-DTC-Ph(dppy)BF (tetra-coordination)	480	8.8	LT_{50}: 2354 @ 100 cd m^{-2}	6
NOBF2-DPCz (tetra-coordination)	491	13.4	LT_{50}: 54 @ 500 cd m^{-2}	13
Cz-5-BF (tetra-coordination)	481	10.4	--[c]	14
TDBA-DI (tri-coordination)	(0.15, 0.28)[a]	38.15	LT_{50}: 2 @ 500 cd m^{-2}	15
v-DABNA (multi-resonance)	469	34.4	LT_{50}: 31 @ 100 cd m^{-2}	16
DDCzTrz	476	18.9	LT_{80}: 52 @ 500 cd m^{-2}	17
BCz-TRZ	486	20.5	LT_{50}: 32 @ 500 cd m^{-2}	18
5CzCN	476 to 495	19.7	LT_{80}: 100 @ 500 cd m^{-2}	19
5CzBN	(0.19, 0.41)[a]	18.0	LT_{97}: 3 @ 1000 cd m^{-2}	20
4TCzBN	(0.16, 0.22)[a]	16.2	LT_{50}: 167 @ 500 cd m^{-2}	21

[a] CIE coordinates.

[b] LT_x (L) = LT (L_0) × $(L_0/L)^n$, where LT is lifetime, L_0 is initial luminance, L is the specific initial luminance and n is a constant, i.e. 1.70.[20]

[c] Not available.

Cartesian coordinates of the optimized geometries of **1**–**8**.

1 (S_0)

B	4.852667	-0.112372	-0.159423
N	3.269615	-0.053299	-0.072473
C	2.598596	-1.116069	0.445244
C	2.616251	1.024489	-0.581074
C	1.209944	-1.106025	0.477933
C	1.227186	1.053733	-0.577342
C	0.512567	-0.019571	-0.048414
H	0.672128	-1.905722	0.966671
H	0.700345	1.900618	-0.991877
O	5.361839	-0.858031	0.965590
O	5.384290	1.223996	-0.057282
C	4.754140	-1.999760	1.283275
C	5.487984	-2.993778	1.940504
C	3.387012	-2.209517	1.002428
C	4.889179	-4.195713	2.274997
H	6.531844	-2.795765	2.159079
C	2.809232	-3.445996	1.334534
C	3.547053	-4.434344	1.959243
H	5.473512	-4.964058	2.772504
H	1.772011	-3.640704	1.081615
H	3.086886	-5.386663	2.199704
C	4.793103	2.190072	-0.757934
C	3.423810	2.126289	-1.094771
C	5.548810	3.307596	-1.130531
C	2.864810	3.169447	-1.851716
C	4.969207	4.329108	-1.862051
H	6.593964	3.334294	-0.841466
C	3.623773	4.258075	-2.239349
H	1.825012	3.117425	-2.157405
H	5.570330	5.184359	-2.156152
H	3.176776	5.048506	-2.832573
F	5.159035	-0.711738	-1.371387
C	-1.714457	-1.083760	-0.324162
C	-1.680139	1.103464	0.299349
C	-1.405576	-2.365140	-0.763971
C	-3.056279	-0.670082	-0.193683
C	-1.330533	2.377011	0.731867
C	-3.034451	0.720227	0.207727
C	-2.460164	-3.234892	-1.028254
H	-0.382426	-2.688926	-0.918101

C	-4.088936	-1.561196	-0.466665
C	-2.357602	3.269553	1.027042
H	-0.297001	2.679178	0.857235
C	-4.038648	1.633640	0.511194
C	-3.807092	-2.865376	-0.880554
H	-2.213344	-4.234574	-1.366425
H	-5.117825	-1.228561	-0.361556
C	-3.716082	2.930662	0.917706
H	-2.078647	4.262889	1.358865
H	-5.077245	1.323932	0.435743
N	-0.877175	0.000452	-0.024890
C	-4.837582	3.920611	1.237063
C	-4.301190	5.288145	1.663864
H	-3.693593	5.221258	2.572231
H	-3.696832	5.751119	0.876945
H	-5.139619	5.958914	1.875489
C	-5.697827	3.362654	2.380950
H	-6.510228	4.058178	2.618299
H	-6.147871	2.400795	2.117975
H	-5.096950	3.217146	3.284280
C	-5.711869	4.114625	-0.011042
H	-6.525443	4.816909	0.201110
H	-5.121560	4.515499	-0.841195
H	-6.160505	3.173127	-0.341551
C	-4.959166	-3.830131	-1.166564
C	-4.466006	-5.209642	-1.606754
H	-3.883196	-5.157026	-2.532145
H	-3.850079	-5.685635	-0.836743
H	-5.324986	-5.861504	-1.793577
C	-5.838849	-3.253643	-2.286231
H	-6.672958	-3.930960	-2.499743
H	-6.259709	-2.281887	-2.011569
H	-5.260724	-3.121907	-3.206367
C	-5.801766	-4.003692	0.106091
H	-5.197302	-4.417301	0.919641
H	-6.219496	-3.052127	0.448057
H	-6.636668	-4.687550	-0.082035

1 (S_1)

B	4.777620	-0.258830	0.000084
N	3.241352	-0.101564	0.000049
C	2.552738	-0.101430	1.210098
C	2.552769	-0.101640	-1.210017

C	1.178572	-0.089166	1.220832
C	1.178604	-0.089375	-1.220789
C	0.477110	-0.098420	0.000013
H	0.636497	-0.042464	2.156351
H	0.636554	-0.042832	-2.156330
O	5.348335	0.402185	1.162506
O	5.348368	0.401973	-1.162441
C	4.740096	0.224488	2.336710
C	5.498725	0.362060	3.505211
C	3.358768	-0.068172	2.426057
C	4.920326	0.185148	4.752170
H	6.551920	0.600570	3.396211
C	2.806868	-0.271956	3.701974
C	3.566631	-0.147066	4.853078
H	5.526788	0.288371	5.647278
H	1.760626	-0.548446	3.791259
H	3.111287	-0.313552	5.824234
C	4.740159	0.224071	-2.336629
C	3.358831	-0.068598	-2.425962
C	5.498818	0.361435	-3.505135
C	2.806963	-0.272604	-3.701857
C	4.920451	0.184306	-4.752078
H	6.552011	0.599960	-3.396149
C	3.566758	-0.147919	-4.852963
H	1.760722	-0.549104	-3.791121
H	5.526937	0.287370	-5.647189
H	3.111437	-0.314574	-5.824101
F	5.096039	-1.623179	0.000214
C	-1.784547	-1.130311	0.000062
C	-1.698402	1.107666	-0.000107
C	-1.445904	-2.482162	0.000169
C	-3.132369	-0.688415	0.000009
C	-1.256848	2.429533	-0.000201
C	-3.076143	0.770645	-0.000097
C	-2.490250	-3.399899	0.000222
H	-0.407429	-2.792985	0.000209
C	-4.145997	-1.617639	0.000061
C	-2.227751	3.424749	-0.000283
H	-0.197767	2.660411	-0.000209
C	-4.015395	1.774901	-0.000179
C	-3.836500	-3.002845	0.000166
H	-2.244659	-4.454085	0.000306
H	-5.181852	-1.294517	0.000027

C	-3.600476	3.132316	-0.000270
H	-1.901821	4.456925	-0.000357
H	-5.072878	1.531906	-0.000177
N	-0.946297	-0.042112	-0.000010
C	-4.665099	4.220658	-0.000369
C	-4.064392	5.626851	-0.000531
H	-3.452056	5.808579	0.888300
H	-3.452120	5.808404	-0.889441
H	-4.872510	6.363737	-0.000576
C	-5.538591	4.063620	1.256170
H	-6.311388	4.838750	1.265112
H	-6.041188	3.092748	1.290184
H	-4.938409	4.167908	2.165060
C	-5.538626	4.063343	-1.256848
H	-6.311446	4.838449	-1.265923
H	-4.938476	4.167462	-2.165779
H	-6.041195	3.092448	-1.290647
C	-4.981634	-4.006152	0.000230
C	-4.490755	-5.454355	0.000417
H	-3.894118	-5.682607	-0.888375
H	-3.894227	-5.682415	0.889331
H	-5.353042	-6.127046	0.000438
C	-5.840414	-3.782215	-1.256293
H	-6.670745	-4.495374	-1.265329
H	-6.266526	-2.775415	-1.290115
H	-5.250092	-3.932400	-2.165220
C	-5.840519	-3.781924	1.256630
H	-5.250282	-3.931928	2.165641
H	-6.266606	-2.775105	1.290195
H	-6.670869	-4.495059	1.265745

1 (T_1)

B	4.846467	-0.180516	-0.342013
N	3.305201	-0.047561	-0.070842
C	2.638126	-1.068448	0.461969
C	2.663882	1.091131	-0.543394
C	1.200602	-1.012239	0.566507
C	1.212438	1.075517	-0.623704
C	0.503944	0.046967	-0.048317
H	0.666781	-1.752658	1.142836
H	0.692858	1.859354	-1.155823
O	5.442860	-1.014983	0.684143
O	5.481390	1.111365	-0.238733

C	4.789954	-2.082136	1.112458
C	5.507707	-3.103011	1.746148
C	3.377678	-2.190444	0.975113
C	4.853904	-4.236906	2.192202
H	6.579959	-2.981312	1.853447
C	2.743010	-3.366975	1.431981
C	3.467126	-4.379247	2.023716
H	5.423330	-5.029956	2.667289
H	1.673841	-3.488334	1.299775
H	2.966324	-5.280365	2.360550
C	4.877899	2.192885	-0.723230
C	3.436434	2.201250	-0.913207
C	5.635241	3.321667	-1.002626
C	2.859164	3.410169	-1.423133
C	5.033595	4.478988	-1.488802
H	6.705480	3.265706	-0.834270
C	3.635939	4.506557	-1.700204
H	1.789962	3.466656	-1.588351
H	5.635767	5.352642	-1.713406
H	3.168672	5.407720	-2.085039
F	4.994570	-0.734091	-1.602844
C	-1.700887	-1.066578	-0.325056
C	-1.718421	1.130345	0.245263
C	-1.357365	-2.352869	-0.724490
C	-3.053768	-0.685157	-0.200641
C	-1.395598	2.427056	0.626861
C	-3.064878	0.714663	0.165607
C	-2.388059	-3.258539	-0.959235
H	-0.324220	-2.651009	-0.866710
C	-4.061821	-1.612848	-0.444728
C	-2.440991	3.305059	0.898628
H	-0.366778	2.755900	0.724290
C	-4.087945	1.616388	0.442545
C	-3.744850	-2.920252	-0.821023
H	-2.115403	-4.261375	-1.267134
H	-5.099572	-1.306678	-0.345434
C	-3.792538	2.931697	0.808094
H	-2.183837	4.316000	1.193076
H	-5.120132	1.283524	0.376584
N	-0.892167	0.040888	-0.051307
C	-4.934746	3.906526	1.100659
C	-4.427450	5.297279	1.486050
H	-3.815246	5.269616	2.393382

H	-3.836064	5.750684	0.683847
H	-5.279749	5.955368	1.681792
C	-5.780992	3.364700	2.262570
H	-6.608002	4.049114	2.481396
H	-6.210312	2.385886	2.029156
H	-5.175474	3.258857	3.168351
C	-5.815692	4.045558	-0.150048
H	-6.643939	4.736137	0.043348
H	-5.235652	4.434405	-0.993079
H	-6.244342	3.085296	-0.451830
C	-4.870959	-3.923539	-1.077739
C	-4.341422	-5.301506	-1.478812
H	-3.760206	-5.259683	-2.405754
H	-3.712763	-5.738647	-0.696127
H	-5.182690	-5.981241	-1.646220
C	-5.766497	-3.403802	-2.212470
H	-6.582435	-4.108928	-2.405597
H	-6.212797	-2.436010	-1.965371
H	-5.192412	-3.283086	-3.136654
C	-5.708507	-4.083612	0.199986
H	-5.092922	-4.457561	1.024367
H	-6.151240	-3.134148	0.515283
H	-6.525029	-4.794597	0.032457

2 (S_0)

B	-7.012786	0.100999	0.037308
N	-5.425378	0.056728	0.019630
C	-4.800191	-1.149006	0.030704
C	-4.730560	1.223268	0.053749
C	-3.410473	-1.200430	0.068115
C	-3.340257	1.189645	0.097668
C	-2.659660	-0.027052	0.117009
H	-2.912165	-2.157633	0.005742
H	-2.780802	2.115619	0.111316
O	-7.526709	-1.034686	-0.687897
O	-7.462072	1.283339	-0.654562
C	-6.976518	-2.225254	-0.453917
C	-7.746417	-3.375872	-0.656920
C	-5.631966	-2.345497	-0.042590
C	-7.207080	-4.626983	-0.412864
H	-8.770793	-3.251336	-0.991285
C	-5.115838	-3.625542	0.217511
C	-5.890357	-4.757556	0.041573

H	-7.819437	-5.511507	-0.560993
H	-4.099357	-3.731337	0.582472
H	-5.478120	-5.737499	0.256876
C	-6.842626	2.434074	-0.395644
C	-5.491549	2.467712	0.011040
C	-7.546135	3.631043	-0.569628
C	-4.901183	3.710775	0.292381
C	-6.934848	4.843778	-0.303087
H	-8.577505	3.572213	-0.900489
C	-5.610194	4.888764	0.144638
H	-3.878050	3.751781	0.651303
H	-7.496149	5.764875	-0.428910
H	-5.140589	5.838598	0.376740
F	-7.390596	0.091936	1.371093
C	-1.182746	-0.049970	0.128128
C	-0.502782	0.786237	-0.766865
C	-0.444013	-0.866407	1.008506
C	0.880335	0.808019	-0.833196
H	-1.077277	1.399694	-1.454680
C	0.947928	-0.810510	0.953379
C	1.616197	0.002327	0.037540
H	1.390373	1.425680	-1.564147
H	1.531447	-1.395244	1.658025
C	3.843359	-1.112359	-0.034987
C	3.827401	1.150244	-0.007025
C	3.515403	-2.462388	-0.087192
C	5.192228	-0.694063	-0.068196
C	3.482933	2.495272	0.064166
C	5.182115	0.751893	-0.047302
C	4.556609	-3.383830	-0.146436
H	2.483674	-2.796829	-0.090148
C	6.211043	-1.640623	-0.127928
C	4.512163	3.431949	0.067022
H	2.448251	2.814771	0.124281
C	6.188632	1.713332	-0.042372
C	5.909997	-3.004070	-0.161974
H	4.296316	-4.435452	-0.184318
H	7.244658	-1.306137	-0.152938
C	5.869837	3.072202	0.008872
H	4.238828	4.479612	0.119740
H	7.226874	1.394063	-0.073644
N	3.020300	0.012971	0.000981
C	7.048296	-4.024873	-0.220952

C	6.994490	4.109715	0.006569
C	6.463565	5.542980	0.070317
H	5.827887	5.779218	-0.789324
H	5.888736	5.723001	0.984671
H	7.303749	6.244408	0.063864
C	7.820445	3.960297	-1.279960
H	8.635923	4.691890	-1.296032
H	8.263538	2.963399	-1.362229
H	7.196011	4.124260	-2.164043
C	7.902525	3.879736	1.224056
H	8.717650	4.611799	1.234396
H	7.337208	3.983646	2.155708
H	8.350067	2.881525	1.212419
C	7.883831	-3.783782	-1.487226
H	8.316245	-2.778960	-1.501497
H	8.708022	-4.503619	-1.542000
H	7.269323	-3.897877	-2.385949
C	6.535959	-5.465927	-0.253497
H	5.952007	-5.709573	0.640116
H	5.914517	-5.656398	-1.134632
H	7.385515	-6.154910	-0.292291
C	7.942151	-3.860874	1.017524
H	7.370251	-4.032143	1.935136
H	8.767903	-4.580466	0.989116
H	8.374508	-2.857480	1.073860
C	-1.085863	-1.750896	2.042237
H	-2.030590	-1.341065	2.406467
H	-1.293951	-2.749923	1.642531
H	-0.416730	-1.881169	2.896133

2 (S_1)

B	-6.979543	-0.185033	0.049927
N	-5.431711	-0.108586	0.015749
C	-4.808254	0.887939	-0.703948
C	-4.672917	-1.068501	0.647945
C	-3.437315	0.932589	-0.794178
C	-3.302164	-1.029895	0.578545
C	-2.609884	-0.035556	-0.167782
H	-2.992015	1.786107	-1.282564
H	-2.740705	-1.798111	1.093868
O	-7.540481	1.15496	0.011582
O	-7.418526	-0.780115	1.300029
C	-7.016988	2.012349	-0.867722

C	-7.821217	3.0532	-1.34633
C	-5.675593	1.906673	-1.299088
C	-7.326229	3.962399	-2.268263
H	-8.841407	3.112704	-0.980803
C	-5.211464	2.820241	-2.257201
C	-6.017149	3.839475	-2.739859
H	-7.967292	4.758385	-2.636285
H	-4.201269	2.717215	-2.6421
H	-5.632393	4.530045	-3.483669
C	-6.762362	-1.858583	1.733266
C	-5.406192	-2.084839	1.408355
C	-7.441349	-2.766103	2.555118
C	-4.797866	-3.258897	1.876019
C	-6.806773	-3.904207	3.026917
H	-8.477663	-2.551709	2.795933
C	-5.479691	-4.162449	2.675776
H	-3.771994	-3.47435	1.593379
H	-7.351614	-4.602372	3.655997
H	-4.984453	-5.065159	3.019273
F	-7.418363	-0.939706	-1.043285
C	-1.165538	0.007486	-0.183653
C	-0.454315	-0.494492	0.940785
C	-0.386954	0.501358	-1.282171
C	0.921613	-0.498071	1.01769
H	-1.018133	-0.845587	1.798289
C	0.997391	0.491023	-1.1942
C	1.652847	0.007433	-0.059503
H	1.430835	-0.866437	1.902965
H	1.588567	0.841872	-2.036188
C	3.855392	1.053112	0.442661
C	3.894093	-1.016477	-0.415724
C	3.443409	2.287562	0.942658
C	5.225127	0.698656	0.338939
C	3.528127	-2.254336	-0.941895
C	5.250216	-0.64961	-0.219743
C	4.435045	3.174986	1.342869
H	2.390445	2.535099	1.012147
C	6.185756	1.596042	0.742337
C	4.552683	-3.132892	-1.273285
H	2.484557	-2.511416	-1.082387
C	6.244147	-1.538393	-0.556233
C	5.801085	2.861941	1.256134
H	4.132375	4.137882	1.733544

H	7.237045	1.338348	0.668885
C	5.906726	-2.80772	-1.093991
H	4.285881	-4.09854	-1.682857
H	7.285647	-1.271215	-0.411526
N	3.081556	0.014792	-0.013171
C	6.888398	3.832825	1.694394
C	7.029962	-3.769225	-1.455834
C	6.509223	-5.091344	-2.020672
H	5.881595	-5.623932	-1.299254
H	5.935534	-4.943871	-2.941098
H	7.356997	-5.738908	-2.261069
C	7.854992	-4.069305	-0.192485
H	8.669179	-4.757086	-0.44136
H	8.301541	-3.165924	0.232757
H	7.234727	-4.537385	0.57778
C	7.930614	-3.107644	-2.513119
H	8.745211	-3.788726	-2.778524
H	7.365032	-2.879812	-3.421609
H	8.379287	-2.178702	-2.149707
C	7.720259	3.178023	2.810685
H	8.201288	2.253593	2.47849
H	8.508471	3.866133	3.131776
H	7.095717	2.944065	3.678061
C	6.318672	5.149782	2.222834
H	5.737249	5.6777	1.460431
H	5.684648	4.996286	3.101732
H	7.142309	5.804412	2.521021
C	7.795396	4.141276	0.490637
H	7.225299	4.604539	-0.320236
H	8.584441	4.83601	0.794984
H	8.278083	3.242266	0.096775
C	-0.996515	0.9565	-2.579483
H	-1.865387	0.34749	-2.844783
H	-1.333993	1.998995	-2.544327
H	-0.264182	0.88442	-3.387947

2 (T_1)

B	-7.008115	0.096667	0.302319
N	-5.46853	0.044184	0.015102
C	-4.838901	-1.125584	-0.007927
C	-4.776188	1.259661	-0.052259
C	-3.405886	-1.168895	-0.09101
C	-3.331162	1.218616	0.017691

C	-2.647666	0.029417	0.003845
H	-2.910192	-2.113901	-0.254695
H	-2.781189	2.147498	0.094987
O	-7.64042	-1.076424	-0.275751
O	-7.599747	1.239451	-0.349658
C	-7.029404	-2.244695	-0.189201
C	-7.787858	-3.413801	-0.334888
C	-5.625253	-2.335128	0.01145
C	-7.181745	-4.650569	-0.226367
H	-8.853336	-3.311609	-0.50902
C	-5.040588	-3.614161	0.130086
C	-5.803939	-4.756558	0.022308
H	-7.782593	-5.549937	-0.322052
H	-3.978908	-3.704119	0.329472
H	-5.341378	-5.731999	0.125863
C	-6.956367	2.404581	-0.361345
C	-5.51184	2.4451	-0.187426
C	-7.67697	3.569399	-0.58427
C	-4.897175	3.740744	-0.225611
C	-7.038499	4.805596	-0.625895
H	-8.749919	3.479889	-0.71767
C	-5.638377	4.875172	-0.436415
H	-3.82647	3.830056	-0.087548
H	-7.612187	5.710805	-0.792238
H	-5.140966	5.839949	-0.459298
F	-7.172088	0.138758	1.677747
C	-1.171883	-0.001386	0.031812
C	-0.468707	0.843076	-0.836926
C	-0.452733	-0.839737	0.908798
C	0.916461	0.859021	-0.87397
H	-1.027802	1.470575	-1.524837
C	0.940012	-0.79735	0.878505
C	1.630422	0.029685	-0.008145
H	1.444926	1.488429	-1.581738
H	1.506747	-1.40207	1.580237
C	3.849835	-1.101133	-0.084712
C	3.852766	1.157429	0.027122
C	3.510345	-2.445356	-0.189519
C	5.203124	-0.695	-0.079692
C	3.51755	2.502055	0.139846
C	5.205006	0.749141	-0.005748
C	4.543766	-3.374268	-0.264013
H	2.475366	-2.768372	-0.219811

C	6.21394	-1.649122	-0.155749
C	4.553809	3.429244	0.193429
H	2.484086	2.826941	0.192651
C	6.21872	1.701572	0.05007
C	5.900848	-3.007391	-0.243683
H	4.274632	-4.421392	-0.343095
H	7.250968	-1.324333	-0.150549
C	5.909616	3.060266	0.144999
H	4.287967	4.476704	0.278793
H	7.254904	1.37514	0.023631
N	3.036539	0.028807	-0.020556
C	7.030499	-4.036732	-0.319397
C	7.042198	4.087822	0.197922
C	6.52152	5.522263	0.305009
H	5.901706	5.794598	-0.555537
H	5.933232	5.673917	1.215935
H	7.36711	6.216478	0.337365
C	7.887541	3.978088	-1.079993
H	8.708785	4.703059	-1.056964
H	8.324147	2.98113	-1.191178
H	7.27853	4.178749	-1.967269
C	7.929021	3.806883	1.420327
H	8.749571	4.531291	1.469789
H	7.349781	3.881964	2.346179
H	8.36889	2.806018	1.379754
C	7.8916	-3.758455	-1.560657
H	8.33355	-2.758149	-1.530537
H	8.70993	-4.484056	-1.626693
H	7.292745	-3.83371	-2.473931
C	6.505525	-5.470502	-0.41381
H	5.903526	-5.740869	0.459918
H	5.897998	-5.622311	-1.312001
H	7.349196	-6.166054	-0.463112
C	7.902973	-3.926984	0.940145
H	7.312645	-4.125698	1.840396
H	8.72241	-4.653279	0.900481
H	8.343426	-2.930622	1.040922
C	-1.127458	-1.730014	1.916142
H	-2.050668	-1.287263	2.298103
H	-1.384833	-2.705158	1.487332
H	-0.462687	-1.917651	2.762827

3 (S_0)

B	7.069027	0.061941	-0.101469
N	5.482629	0.047827	-0.030693
C	4.817962	-1.086344	-0.372813
C	4.825683	1.187652	0.307985
C	3.426967	-1.093387	-0.366475
C	3.434767	1.199942	0.314945
C	2.714753	0.057219	-0.030397
H	2.897834	-2.014611	-0.569682
H	2.911058	2.105307	0.590398
O	7.570239	-1.247789	0.234041
O	7.580133	0.976961	0.888452
C	6.973043	-2.304359	-0.315000
C	7.711007	-3.480520	-0.488750
C	5.612234	-2.269278	-0.687480
C	7.122938	-4.593528	-1.063851
H	8.749517	-3.481363	-0.175486
C	5.045720	-3.406469	-1.286395
C	5.787820	-4.556960	-1.480468
H	7.710467	-5.495734	-1.205798
H	4.014279	-3.379785	-1.622318
H	5.336051	-5.422095	-1.953771
C	6.990835	2.166069	1.004495
C	5.628835	2.347560	0.681953
C	7.739220	3.242943	1.492660
C	5.071427	3.631176	0.802632
C	7.160291	4.493559	1.619282
H	8.778481	3.066387	1.748410
C	5.823732	4.697527	1.259824
H	4.039003	3.799219	0.514394
H	7.755777	5.324192	1.986351
H	5.378521	5.683688	1.336231
F	7.400493	0.440107	-1.393284
C	-3.771910	-1.067515	0.295469
C	-3.773125	1.133237	-0.209360
C	-3.422776	-2.369627	0.632230
C	-5.125841	-0.667781	0.228028
C	-3.424976	2.439318	-0.529729
C	-5.126657	0.742558	-0.096266
C	-4.451604	-3.275320	0.873444
H	-2.383397	-2.671300	0.717682
C	-6.130990	-1.598284	0.477588
C	-4.455101	3.354612	-0.723973
H	-2.386546	2.739549	-0.626138
C	-6.133146	1.682992	-0.299344

C	-5.810107	-2.919799	0.798676
H	-4.178944	-4.291718	1.133571
H	-7.170024	-1.284322	0.424635
C	-5.813264	3.006067	-0.614315
H	-4.184068	4.374636	-0.971384
H	-7.171996	1.376278	-0.211774
N	-2.961366	0.026464	0.017938
C	-6.939308	4.019979	-0.829531
C	-6.409630	5.415201	-1.165783
H	-5.786980	5.818313	-0.360370
H	-5.821691	5.414820	-2.089469
H	-7.250875	6.100631	-1.308894
C	-7.782986	4.122842	0.450047
H	-8.599233	4.840520	0.311439
H	-8.226502	3.160020	0.720523
H	-7.170919	4.459224	1.293042
C	-7.830252	3.552818	-1.990437
H	-8.646340	4.265225	-2.154734
H	-7.252203	3.474865	-2.916818
H	-8.276190	2.574185	-1.789727
C	-6.935249	-3.922807	1.063603
C	-6.404081	-5.317397	1.400096
H	-5.808588	-5.733729	0.580966
H	-5.788448	-5.310195	2.305523
H	-7.244719	-5.995702	1.576730
C	-7.820473	-4.035633	-0.186739
H	-8.636723	-4.745556	-0.012784
H	-8.265825	-3.073052	-0.455064
H	-7.238256	-4.387023	-1.044646
C	-7.785065	-3.435077	2.246666
H	-7.176767	-3.349467	3.152764
H	-8.231078	-2.456040	2.048125
H	-8.599910	-4.139828	2.446309
C	1.240647	0.056274	-0.017685
C	0.531946	0.800361	0.932122
C	0.527649	-0.684811	-0.965657
C	-0.853753	0.775262	0.937721
H	1.063219	1.362557	1.693520
C	-0.865476	-0.704923	-0.995882
H	1.070968	-1.224877	-1.736366
C	-1.550261	0.025512	-0.010330
H	-1.414928	1.322642	1.688278
C	-1.603281	-1.446250	-2.069817
H	-2.038780	-2.377411	-1.692269

H	-2.431347	-0.845337	-2.456755
H	-0.934286	-1.694844	-2.896331

3 (S_1)

B	-7.048919	0.139623	0.057251
N	-5.498515	0.085252	0.005595
C	-4.795352	-0.528596	1.016208
C	-4.817932	0.700787	-1.020053
C	-3.422007	-0.538408	1.006793
C	-3.444882	0.694890	-1.050614
C	-2.670290	0.087092	-0.025476
H	-2.917844	-1.101097	1.780207
H	-2.958319	1.166784	-1.892807
O	-7.563287	-1.060701	0.693257
O	-7.587227	0.154318	-1.291235
C	-6.953064	-1.474195	1.805676
C	-7.689976	-2.218891	2.734463
C	-5.588778	-1.202150	2.049170
C	-7.103446	-2.661173	3.909492
H	-8.731313	-2.422956	2.506820
C	-5.029687	-1.634905	3.260183
C	-5.768182	-2.356629	4.184580
H	-7.692526	-3.229341	4.623784
H	-3.997744	-1.384996	3.486927
H	-5.310859	-2.675322	5.115889
C	-7.000478	0.962448	-2.176760
C	-5.635720	1.311155	-2.073243
C	-7.763044	1.446806	-3.246206
C	-5.101562	2.195418	-3.021580
C	-7.201315	2.295675	-4.186608
H	-8.804014	1.145022	-3.302287
C	-5.865427	2.686251	-4.068762
H	-4.069118	2.517210	-2.925502
H	-7.809950	2.670054	-5.004794
H	-5.426824	3.373078	-4.785667
F	-7.435273	1.283364	0.762793
C	3.795755	-1.015032	-0.491993
C	3.829228	1.074404	0.314211
C	3.385914	-2.259619	-0.967773
C	5.165309	-0.669142	-0.361622
C	3.459346	2.326586	0.802118
C	5.187014	0.692508	0.164296
C	4.379677	-3.166410	-1.316423
H	2.332556	-2.498995	-1.059009

C	6.128125	-1.585302	-0.714413
C	4.481690	3.204109	1.143407
H	2.414088	2.594738	0.905891
C	6.178751	1.580505	0.509134
C	5.745678	-2.861928	-1.202868
H	4.078764	-4.137533	-1.687643
H	7.179438	-1.334774	-0.619392
C	5.837327	2.863949	1.009729
H	4.211817	4.180735	1.523950
H	7.221590	1.301610	0.400635
N	3.017909	0.039934	-0.082991
C	6.958324	3.823341	1.384027
C	6.433444	5.161734	1.905024
H	5.831935	5.683924	1.154347
H	5.831875	5.039034	2.811175
H	7.279723	5.807115	2.156326
C	7.823158	4.089094	0.139793
H	8.636108	4.774821	0.398246
H	8.273533	3.172961	-0.252884
H	7.230412	4.546096	-0.658289
C	7.821092	3.176871	2.481539
H	8.633481	3.856630	2.756953
H	7.226601	2.973139	3.377218
H	8.272059	2.236691	2.151374
C	6.835385	-3.853579	-1.585182
C	6.267891	-5.180046	-2.091800
H	5.662032	-5.681640	-1.330648
H	5.658405	-5.045929	-2.991004
H	7.093108	-5.849549	-2.349937
C	7.707861	-4.135852	-0.349914
H	8.498443	-4.845136	-0.614105
H	8.187996	-3.230210	0.031675
H	7.112683	-4.571853	0.458057
C	7.701926	-3.237024	-2.696857
H	7.102300	-3.022286	-3.586507
H	8.182271	-2.307607	-2.377830
H	8.492129	-3.940218	-2.977912
C	-1.233125	0.080779	-0.043784
C	-0.489518	0.504030	-1.180583
C	-0.472876	-0.348356	1.080515
C	0.887401	0.488554	-1.187255
H	-1.001930	0.826074	-2.079558
C	0.908889	-0.373151	1.100695
H	-0.986629	-0.650017	1.987140

C	1.588522	0.052109	-0.057195
H	1.437635	0.805619	-2.068447
C	1.665377	-0.827299	2.315853
H	2.304615	-1.689373	2.094140
H	2.316505	-0.037070	2.706373
H	0.976836	-1.117510	3.111632

3 (T_1)

B	7.054668	0.145133	-0.348238
N	5.524786	0.028453	-0.036417
C	4.857320	-1.063488	-0.395179
C	4.871984	1.160306	0.470396
C	3.428974	-1.103574	-0.278682
C	3.429043	1.172818	0.454777
C	2.704788	0.064310	0.093834
H	2.909845	-2.038205	-0.432260
H	2.914743	2.087574	0.717709
O	7.665734	-1.167272	-0.227781
O	7.702816	0.985354	0.629796
C	7.015552	-2.222353	-0.685239
C	7.740558	-3.386753	-0.972558
C	5.604646	-2.209320	-0.856187
C	7.093648	-4.498639	-1.475669
H	8.812710	-3.372277	-0.810510
C	4.977704	-3.358118	-1.384135
C	5.707340	-4.484162	-1.698539
H	7.668136	-5.388916	-1.713203
H	3.909079	-3.352661	-1.565802
H	5.211969	-5.355422	-2.112860
C	7.097115	2.086939	1.065309
C	5.650292	2.213605	0.974300
C	7.862677	3.090368	1.644223
C	5.080587	3.428655	1.478864
C	7.267139	4.248939	2.131906
H	8.935685	2.938467	1.694939
C	5.864571	4.406957	2.034789
H	4.009544	3.581763	1.424650
H	7.874789	5.030601	2.574579
H	5.399714	5.314774	2.406884
F	7.181179	0.650400	-1.632329
C	-3.792289	-1.032422	0.387375
C	-3.780198	1.127639	-0.264769
C	-3.451211	-2.310586	0.812910

C	-5.144545	-0.638973	0.265077
C	-3.422928	2.409085	-0.665066
C	-5.136797	0.746245	-0.153319
C	-4.485399	-3.199306	1.091088
H	-2.413637	-2.605450	0.936140
C	-6.155231	-1.552199	0.553468
C	-4.446907	3.309567	-0.942423
H	-2.381844	2.700881	-0.758911
C	-6.136952	1.671594	-0.440238
C	-5.841944	-2.849884	0.966173
H	-4.219039	-4.197042	1.420817
H	-7.192816	-1.243450	0.457869
C	-5.807886	2.969979	-0.837651
H	-4.168865	4.310397	-1.252590
H	-7.178109	1.372436	-0.353405
N	-2.975127	0.040101	0.055198
C	-6.927187	3.967709	-1.144511
C	-6.387874	5.336752	-1.563052
H	-5.781194	5.792841	-0.773874
H	-5.780791	5.273629	-2.472073
H	-7.224561	6.011530	-1.769626
C	-7.797403	4.157587	0.107046
H	-8.608675	4.865344	-0.096710
H	-8.249045	3.215702	0.432264
H	-7.202253	4.549145	0.938256
C	-7.794710	3.423874	-2.289675
H	-8.606191	4.123707	-2.518404
H	-7.197673	3.283841	-3.196515
H	-8.246037	2.460890	-2.033039
C	-6.973095	-3.834517	1.271630
C	-6.450094	-5.204256	1.708188
H	-5.838263	-5.672165	0.929950
H	-5.852990	-5.138297	2.623601
H	-7.294690	-5.870257	1.910988
C	-7.832283	-4.028428	0.013081
H	-8.652173	-4.726651	0.215204
H	-8.271716	-3.085531	-0.325644
H	-7.232408	-4.433426	-0.808256
C	-7.847244	-3.272415	2.402827
H	-7.258065	-3.128709	3.314204
H	-8.287816	-2.308186	2.132595
H	-8.666915	-3.963140	2.630010
C	1.233926	0.062040	0.088578

C	0.506500	0.843459	0.996137
C	0.530271	-0.721914	-0.833993
C	-0.878441	0.825857	0.975984
H	1.025294	1.432574	1.745806
C	-0.862429	-0.741758	-0.885290
H	1.081914	-1.299911	-1.570649
C	-1.562502	0.036104	0.050777
H	-1.450336	1.407407	1.692184
C	-1.585336	-1.537776	-1.930171
H	-2.038540	-2.441003	-1.507929
H	-2.398924	-0.953173	-2.369529
H	-0.902312	-1.840702	-2.726634

4 (S_0)

B	7.076936	0.048707	-0.100590
N	5.489808	0.040565	-0.036761
C	4.828731	-1.127254	-0.247350
C	4.830175	1.211328	0.162124
C	3.437488	-1.136197	-0.247732
C	3.438996	1.222138	0.159410
C	2.723398	0.044999	-0.052772
H	2.911680	-2.076597	-0.343567
H	2.912950	2.153052	0.321603
O	7.577096	-1.211578	0.389763
O	7.581661	1.074874	0.777157
C	6.984305	-2.326181	-0.035174
C	7.724267	-3.513448	-0.065639
C	5.625661	-2.337237	-0.417128
C	7.140542	-4.686815	-0.510229
H	8.760876	-3.476112	0.251615
C	5.063514	-3.537558	-0.882338
C	5.807864	-4.701457	-0.936225
H	7.729692	-5.598489	-0.542339
H	4.034162	-3.552117	-1.225331
H	5.359912	-5.616705	-1.307939
C	6.990181	2.268051	0.750777
C	5.629606	2.408223	0.402270
C	7.734456	3.395886	1.114358
C	5.069740	3.696194	0.370131
C	7.153160	4.651501	1.091600
H	8.772530	3.252339	1.394370
C	5.818174	4.809790	0.703976
H	4.038637	3.827844	0.059188
H	7.745564	5.520324	1.362653

H	5.371368	5.797312	0.662863
F	7.414128	0.272354	-1.426168
C	-3.785693	-1.093075	0.147006
C	-3.778557	1.151114	-0.162688
C	-3.448495	-2.422585	0.364149
C	-5.134372	-0.676386	0.139718
C	-3.434298	2.477788	-0.388298
C	-5.130256	0.756599	-0.061692
C	-4.484639	-3.332407	0.550749
H	-2.416033	-2.752492	0.390002
C	-6.148292	-1.611118	0.328619
C	-4.465214	3.407396	-0.491885
H	-2.399358	2.787594	-0.488147
C	-6.138075	1.710145	-0.171612
C	-5.839496	-2.957837	0.533378
H	-4.219527	-4.370275	0.716586
H	-7.183215	-1.280087	0.320740
C	-5.821437	3.054226	-0.384172
H	-4.194594	4.442518	-0.665798
H	-7.175532	1.396626	-0.093775
N	-2.967827	0.021340	-0.043619
C	-6.948276	4.083360	-0.495789
C	-6.420880	5.500266	-0.729007
H	-5.781239	5.836186	0.093745
H	-5.851483	5.573559	-1.661353
H	-7.262654	6.196211	-0.799579
C	-7.766559	4.083502	0.804269
H	-8.583086	4.811198	0.739804
H	-8.207748	3.102624	1.004533
H	-7.137442	4.349864	1.659651
C	-7.862574	3.711700	-1.672927
H	-8.679208	4.436468	-1.763585
H	-7.302770	3.707199	-2.613621
H	-8.307978	2.721021	-1.542531
C	-6.972040	-3.966884	0.734776
C	-6.452273	-5.390014	0.946216
H	-5.876967	-5.744424	0.084677
H	-5.820336	-5.463577	1.837346
H	-7.298022	-6.071179	1.082846
C	-7.878953	-3.966160	-0.505049
H	-8.700686	-4.679287	-0.375914
H	-8.316946	-2.979903	-0.684912
H	-7.315321	-4.251375	-1.399088
C	-7.795908	-3.568566	1.968580

H	-7.171713	-3.564054	2.867874
H	-8.233602	-2.571968	1.858615
H	-8.615633	-4.278726	2.124017
C	1.249630	0.044621	-0.046199
C	0.532843	0.898890	0.800692
C	0.542777	-0.817746	-0.890982
C	-0.853549	0.880638	0.814721
H	1.062535	1.548080	1.489910
C	-0.838564	-0.801747	-0.886249
H	1.051359	-1.468726	-1.593842
C	-1.568617	0.030403	-0.032468
H	-1.405472	1.516435	1.498788
F	-1.497934	-1.598143	-1.733092

4 (S_1)

B	-7.050300	0.130498	0.082808
N	-5.497779	0.077107	0.016527
C	-4.780341	-0.434859	1.070298
C	-4.835030	0.593886	-1.071444
C	-3.406844	-0.442385	1.043648
C	-3.462314	0.589962	-1.121115
C	-2.671752	0.084795	-0.053491
H	-2.890508	-0.922531	1.863084
H	-2.991260	0.976538	-2.013716
O	-7.548987	-1.004481	0.837890
O	-7.603837	0.013038	-1.253672
C	-6.922992	-1.305547	1.977198
C	-7.644349	-1.959164	2.983556
C	-5.557510	-1.006115	2.175299
C	-7.040303	-2.281628	4.188060
H	-8.687395	-2.188553	2.790778
C	-4.979970	-1.316478	3.414727
C	-5.703189	-1.946603	4.414843
H	-7.617173	-2.779442	4.962268
H	-3.946505	-1.042073	3.602524
H	-5.232655	-2.170979	5.366743
C	-7.032799	0.735153	-2.219877
C	-5.669348	1.098443	-2.167187
C	-7.810762	1.111401	-3.321297
C	-5.150914	1.890917	-3.201342
C	-7.264775	1.869748	-4.344408
H	-8.850501	0.800805	-3.335938
C	-5.929986	2.276574	-4.280667
H	-4.119426	2.225534	-3.148690

H	-7.885032	2.161778	-5.187008
H	-5.504220	2.894482	-5.064783
F	-7.429125	1.335937	0.679380
C	3.804978	-1.028995	-0.473238
C	3.834795	1.102417	0.220509
C	3.398248	-2.294434	-0.892931
C	5.172800	-0.685119	-0.325109
C	3.463856	2.382586	0.628658
C	5.192235	0.702659	0.126780
C	4.393666	-3.224907	-1.165852
H	2.346310	-2.533459	-0.999001
C	6.137513	-1.624913	-0.602039
C	4.484713	3.269803	0.947543
H	2.419252	2.664953	0.691969
C	6.182716	1.600529	0.448243
C	5.758360	-2.923748	-1.031501
H	4.095008	-4.212694	-1.492155
H	7.187792	-1.376426	-0.491579
C	5.840200	2.912489	0.868534
H	4.213893	4.267734	1.267191
H	7.225353	1.307896	0.382781
N	3.026979	0.054223	-0.145825
C	6.959724	3.881852	1.219681
C	6.434119	5.251243	1.651759
H	5.857774	5.735990	0.857478
H	5.807711	5.183702	2.546762
H	7.279665	5.902567	1.889826
C	7.860131	4.071343	-0.013320
H	8.672423	4.763543	0.229448
H	8.312027	3.131410	-0.342899
H	7.293503	4.488746	-0.851089
C	7.786241	3.289641	2.374375
H	8.597905	3.976600	2.633578
H	7.165905	3.141295	3.263338
H	8.236109	2.328568	2.109320
C	6.850130	-3.941397	-1.329391
C	6.286360	-5.289524	-1.779796
H	5.656197	-5.745614	-1.009820
H	5.702648	-5.200063	-2.701380
H	7.113106	-5.977076	-1.978820
C	7.685542	-4.162333	-0.056466
H	8.477422	-4.889946	-0.259974
H	8.162058	-3.240679	0.289636
H	7.064508	-4.550319	0.756461

C	7.752022	-3.390996	-2.447727
H	7.179354	-3.222232	-3.364639
H	8.229436	-2.448002	-2.166363
H	8.545081	-4.112667	-2.667138
C	-1.237912	0.083772	-0.086486
C	-0.504767	0.450494	-1.254091
C	-0.465992	-0.283547	1.056031
C	0.870352	0.445909	-1.288744
H	-1.032688	0.726302	-2.158804
C	0.902591	-0.281661	1.004365
H	-0.928903	-0.547347	1.998604
C	1.604902	0.075860	-0.151078
H	1.401122	0.721268	-2.194880
F	1.618939	-0.620670	2.090746

4 (T_1)

B	-7.079753	0.097007	0.074819
N	-5.508527	0.066706	0.032048
C	-4.839059	-1.012485	0.544422
C	-4.824296	1.140661	-0.471326
C	-3.460077	-1.033449	0.551930
C	-3.444958	1.141276	-0.483506
C	-2.694906	0.055193	0.047961
H	-2.969740	-1.928264	0.906243
H	-2.944669	1.988265	-0.928987
O	-7.590309	-1.248204	-0.067569
O	-7.576558	0.854495	-1.052174
C	-7.008043	-2.210407	0.649704
C	-7.762264	-3.335702	1.000655
C	-5.650928	-2.129108	1.029262
C	-7.196806	-4.351619	1.753027
H	-8.797377	-3.374129	0.677804
C	-5.110739	-3.160011	1.813466
C	-5.867779	-4.260511	2.176906
H	-7.797746	-5.213436	2.028192
H	-4.084870	-3.086798	2.160575
H	-5.431039	-5.041889	2.790028
C	-6.980320	2.014981	-1.329412
C	-5.621351	2.238503	-1.019914
C	-7.721229	3.013932	-1.970851
C	-5.065994	3.494794	-1.307480
C	-7.140879	4.235900	-2.267289
H	-8.758121	2.802415	-2.210192
C	-5.809901	4.487603	-1.921836

H	-4.038654	3.702922	-1.025578
H	-7.731543	5.006153	-2.754517
H	-5.361456	5.453946	-2.127552
F	-7.451541	0.667515	1.287930
C	3.813999	-1.070437	-0.317986
C	3.792851	1.090686	0.360854
C	3.476554	-2.336950	-0.779452
C	5.160865	-0.654199	-0.241950
C	3.430949	2.345056	0.839485
C	5.147773	0.732507	0.191407
C	4.515244	-3.198087	-1.119224
H	2.445356	-2.653749	-0.875254
C	6.174865	-1.528693	-0.593629
C	4.451723	3.256378	1.096488
H	2.395227	2.606896	1.023365
C	6.142785	1.654175	0.466250
C	5.866627	-2.827496	-1.030545
H	4.254751	-4.189066	-1.470779
H	7.208260	-1.199639	-0.540103
C	5.807863	2.943830	0.914298
H	4.173373	4.237097	1.462806
H	7.183900	1.371617	0.342744
N	2.986670	-0.005911	0.049893
C	6.924537	3.945032	1.201738
C	6.387243	5.296502	1.675187
H	5.741102	5.762836	0.924435
H	5.824417	5.206226	2.609848
H	7.224855	5.975996	1.858785
C	7.739151	4.171178	-0.081771
H	8.548982	4.883248	0.109076
H	8.189683	3.243810	-0.447413
H	7.107511	4.576785	-0.878287
C	7.841687	3.378161	2.296964
H	8.651163	4.084226	2.510266
H	7.283688	3.207310	3.222863
H	8.296996	2.429718	1.997304
C	7.002458	-3.777516	-1.404068
C	6.491755	-5.146907	-1.855004
H	5.919590	-5.647159	-1.067046
H	5.862095	-5.072963	-2.747527
H	7.342855	-5.787902	-2.103653
C	7.911451	-3.978909	-0.181314
H	8.735727	-4.654234	-0.434046
H	8.346112	-3.035894	0.162931

H	7.352963	-4.417158	0.651692
C	7.818083	-3.163209	-2.552699
H	7.191428	-3.008747	-3.436637
H	8.252662	-2.198722	-2.274172
H	8.640008	-3.832380	-2.828350
C	-1.272782	0.047578	0.059677
C	-0.489902	1.099305	-0.555314
C	-0.526023	-1.014813	0.691531
C	0.873315	1.080268	-0.552116
H	-0.988578	1.910488	-1.069787
C	0.832886	-1.018976	0.668075
H	-1.016491	-1.808820	1.238763
C	1.600374	0.008084	0.046503
H	1.430439	1.857702	-1.064370
F	1.496324	-1.988652	1.310091

5 (S_0)

B	5.790957	0.011858	-0.155784
N	4.204874	0.007476	-0.075572
C	3.542589	-1.173865	-0.180169
C	3.545620	1.190458	0.031363
C	2.151605	-1.183097	-0.164788
C	2.154733	1.200455	0.043061
C	1.436941	0.009822	-0.062013
H	1.626216	-2.128481	-0.175459
H	1.630150	2.141932	0.133476
O	6.298810	-1.203749	0.430191
O	6.302094	1.106684	0.630829
C	5.702267	-2.350093	0.107446
C	6.443385	-3.535531	0.168405
C	4.339300	-2.393706	-0.256270
C	5.856135	-4.742498	-0.168546
H	7.483568	-3.471151	0.469219
C	3.773529	-3.629214	-0.611884
C	4.518591	-4.793406	-0.576041
H	6.446082	-5.653424	-0.130433
H	2.740225	-3.672787	-0.940275
H	4.067476	-5.736923	-0.863832
C	5.709687	2.293603	0.509178
C	4.346165	2.403684	0.161535
C	6.455999	3.448166	0.770061
C	3.785192	3.684176	0.024371
C	5.873535	4.697340	0.645870
H	7.496437	3.329012	1.052742

C	4.535497	4.822149	0.256654
H	2.751689	3.788771	-0.289140
H	6.467430	5.586029	0.837681
H	4.087802	5.802650	0.135255
F	6.115127	0.127707	-1.498427
C	-5.056049	-1.115772	0.204572
C	-5.064086	1.112873	-0.174542
C	-4.698228	-2.436500	0.471784
C	-6.410725	-0.714289	0.151616
C	-4.716811	2.434854	-0.449341
C	-6.415869	0.706616	-0.092275
C	-5.716509	-3.361120	0.659136
H	-3.659889	-2.740417	0.541006
C	-7.428316	-1.651732	0.341839
C	-5.742173	3.355861	-0.614585
H	-3.681289	2.742461	-0.540827
C	-7.440651	1.640445	-0.260409
C	-7.051612	-2.957717	0.586019
H	-5.493460	-4.401631	0.867432
H	-8.478044	-1.381338	0.308537
C	-7.073947	2.947743	-0.512645
H	-5.527378	4.397175	-0.827492
H	-8.488442	1.366331	-0.204360
N	-4.245986	-0.000017	0.006244
C	-0.036191	0.008397	-0.041778
C	-0.744910	0.930693	0.738049
C	-0.758922	-0.917362	-0.804482
C	-2.131052	0.922402	0.766830
H	-0.206744	1.632965	1.367121
C	-2.145395	-0.914977	-0.801757
H	-0.231230	-1.618168	-1.444055
C	-2.840453	0.002469	-0.009629
H	-2.670574	1.610659	1.408725
H	-2.696611	-1.605962	-1.430653
F	-8.005707	-3.887066	0.770308
F	-8.035074	3.873730	-0.676150

5 (S_1)

B	5.772088	-0.026007	0.149147
N	4.219729	-0.017326	0.077958
C	3.525504	1.141734	0.332599
C	3.532630	-1.179660	-0.182191
C	2.151838	1.150693	0.322427
C	2.159153	-1.189598	-0.206178

C	1.392886	-0.023152	0.062769
H	1.653846	2.101857	0.450229
H	1.666682	-2.122210	-0.443577
O	6.290970	1.258357	-0.286113
O	6.301725	-1.017688	-0.768859
C	5.689652	2.352649	0.184651
C	6.433890	3.534454	0.282994
C	4.327169	2.349176	0.555695
C	5.856076	4.692936	0.776940
H	7.473639	3.504738	-0.026514
C	3.776704	3.527226	1.080646
C	4.522630	4.689663	1.193438
H	6.450662	5.598558	0.856296
H	2.746234	3.524983	1.422469
H	4.072634	5.586172	1.607828
C	5.707566	-2.212399	-0.792120
C	4.342544	-2.368925	-0.465921
C	6.462368	-3.326176	-1.179134
C	3.799506	-3.661793	-0.477245
C	5.892235	-4.588702	-1.209980
H	7.503926	-3.165870	-1.438402
C	4.555742	-4.763903	-0.843365
H	2.766604	-3.807129	-0.176151
H	6.494792	-5.443735	-1.502912
H	4.111055	-5.753942	-0.838215
F	6.157195	-0.302375	1.463863
C	-5.075576	0.458551	-1.042785
C	-5.110981	-0.452672	1.003782
C	-4.649668	1.001190	-2.258594
C	-6.447035	0.306439	-0.705594
C	-4.727431	-0.999328	2.231753
C	-6.470039	-0.286784	0.625507
C	-5.627594	1.399536	-3.155176
H	-3.593732	1.101443	-2.480120
C	-7.416834	0.703925	-1.599650
C	-5.735916	-1.387642	3.098454
H	-3.679712	-1.110149	2.484988
C	-7.470321	-0.674394	1.489853
C	-6.973116	1.246639	-2.815998
H	-5.373661	1.828631	-4.116756
H	-8.479432	0.616325	-1.405114
C	-7.068991	-1.221396	2.718904
H	-5.515387	-1.819055	4.067212
H	-8.525623	-0.576174	1.263237

N	-4.301396	-0.001085	-0.007656
C	-0.042767	-0.021293	0.046993
C	-0.796083	-1.128657	-0.441051
C	-0.798101	1.090287	0.522598
C	-2.173215	-1.126838	-0.461448
H	-0.284387	-1.998712	-0.835773
C	-2.175250	1.101716	0.508557
H	-0.286797	1.951054	0.937824
C	-2.871976	-0.008614	0.013136
H	-2.719270	-1.981297	-0.850301
H	-2.722893	1.959966	0.886682
F	-7.892048	1.634563	-3.688967
F	-8.017671	-1.600100	3.563706

5 (T_1)

B	-5.773968	-0.031597	-0.405633
N	-4.244942	0.011605	-0.073458
C	-3.581357	1.160367	-0.156715
C	-3.587416	-1.207356	0.143448
C	-2.153587	1.175837	-0.035874
C	-2.145983	-1.210687	0.126421
C	-1.424661	-0.045917	0.043954
H	-1.638584	2.122081	0.041595
H	-1.629713	-2.160835	0.160949
O	-6.390247	1.209799	0.029634
O	-6.419135	-1.086644	0.338691
C	-5.744075	2.346927	-0.155161
C	-6.473718	3.543575	-0.148824
C	-4.333229	2.381476	-0.323735
C	-5.831332	4.747056	-0.364249
H	-7.545699	3.485754	0.004361
C	-3.711025	3.626975	-0.554115
C	-4.444993	4.792877	-0.583388
H	-6.409295	5.666196	-0.376862
H	-2.642525	3.670354	-0.731048
H	-3.953223	5.740980	-0.771500
C	-5.809295	-2.258379	0.494768
C	-4.362376	-2.354657	0.376311
C	-6.571750	-3.374900	0.813232
C	-3.788959	-3.653518	0.571118
C	-5.972527	-4.614757	1.005437
H	-7.645166	-3.243000	0.898882
C	-4.569501	-4.740035	0.872963
H	-2.717488	-3.785769	0.481544

H	-6.577311	-5.482439	1.245298
H	-4.101596	-5.709520	1.013711
F	-5.899058	-0.210738	-1.773774
C	5.071562	1.079149	0.311038
C	5.079421	-1.093769	-0.305512
C	4.713320	2.362525	0.721708
C	6.426974	0.692886	0.192452
C	4.729620	-2.380908	-0.711708
C	6.431955	-0.693530	-0.202180
C	5.731066	3.267632	0.989274
H	3.674605	2.650668	0.837832
C	7.443982	1.611067	0.463946
C	5.753547	-3.275631	-0.990295
H	3.692677	-2.679741	-0.816188
C	7.455238	-1.601272	-0.484992
C	7.066381	2.881453	0.851791
H	5.508017	4.279207	1.309943
H	8.494133	1.352198	0.383918
C	7.086305	-2.875636	-0.868110
H	5.537284	-4.289582	-1.308085
H	8.503518	-1.331615	-0.416978
N	4.262069	-0.011487	0.007129
C	0.044859	-0.037493	0.040278
C	0.777295	-1.015665	0.728754
C	0.753667	0.955004	-0.651489
C	2.162879	-1.006564	0.725285
H	0.255637	-1.767440	1.313028
C	2.140458	0.959247	-0.676558
H	0.213847	1.708231	-1.217149
C	2.854765	-0.020135	0.016485
H	2.717858	-1.744957	1.294574
H	2.676539	1.707726	-1.250766
F	8.020136	3.791855	1.117714
F	8.046302	-3.776232	-1.144576

6 (S_0)

B	0.000182	-1.759259	-1.713978
N	-0.000087	-0.384378	-0.909692
C	1.188208	0.166414	-0.551633
C	-1.188473	0.166131	-0.551535
C	1.200028	1.342537	0.196767
C	-1.200499	1.342256	0.196881
C	-0.000292	1.922255	0.574873
H	2.141249	1.810026	0.453358

H	-2.141799	1.809515	0.453590
O	1.158913	-1.807121	-2.570818
O	-1.158910	-1.808102	-2.570202
C	2.329008	-1.434224	-2.058309
C	3.506050	-1.963837	-2.600176
C	2.406477	-0.490679	-1.013044
C	4.738290	-1.590649	-2.098963
H	3.420514	-2.667177	-3.421118
C	3.662148	-0.161881	-0.484722
C	4.822156	-0.699152	-1.019846
H	5.650353	-1.990786	-2.530102
H	3.745813	0.502973	0.367763
C	-2.329009	-1.435188	-2.057746
C	-2.406625	-0.491285	-1.012800
C	-3.505968	-1.965210	-2.599397
C	-3.662362	-0.162546	-0.484608
C	-4.738283	-1.592076	-2.098320
H	-3.420302	-2.668817	-3.420097
C	-4.822306	-0.700191	-1.019542
H	-3.746206	0.502615	0.367637
H	-5.650251	-1.992534	-2.529349
F	0.000868	-2.764749	-0.762896
C	7.046533	-1.229182	-0.027055
C	6.548174	0.954529	-0.316660
C	7.026442	-2.617407	0.042122
C	8.158657	-0.493389	0.441266
C	5.958739	2.169907	-0.645826
C	7.839256	0.905033	0.256874
C	8.144034	-3.257429	0.568773
H	6.168650	-3.189534	-0.295731
C	9.261327	-1.164622	0.963075
C	6.672905	3.333483	-0.376669
H	4.977436	2.216536	-1.106749
C	8.527119	2.087977	0.513922
C	9.274043	-2.559594	1.031525
H	8.126758	-4.340093	0.620362
H	10.111889	-0.590204	1.320344
C	7.953068	3.323446	0.205349
H	6.210908	4.279726	-0.634488
H	9.519047	2.039236	0.955235
N	6.076927	-0.343326	-0.486128
H	-0.000375	2.842763	1.149481
C	8.729197	4.608481	0.502348
C	9.025821	4.687759	2.007467

H	9.619205	3.834065	2.348011
H	9.587989	5.599681	2.237624
H	8.096790	4.703066	2.586416
C	10.052907	4.595892	-0.276954
H	9.868696	4.543371	-1.354759
H	10.625026	5.507397	-0.070971
H	10.676302	3.740272	-0.001090
C	7.951439	5.863555	0.102144
H	7.735288	5.882556	-0.971066
H	7.004819	5.945361	0.646401
H	8.546120	6.752211	0.336015
C	10.500239	-3.273069	1.605457
C	10.724713	-2.815044	3.054435
H	11.603672	-3.312535	3.479324
H	10.889120	-1.735210	3.116463
H	9.858436	-3.059178	3.677614
C	11.735155	-2.919470	0.763058
H	11.927130	-1.842400	0.759482
H	12.625185	-3.417192	1.163977
H	11.602030	-3.240153	-0.275138
C	10.341332	-4.794583	1.604817
H	9.491571	-5.114518	2.216668
H	10.205010	-5.188167	0.592221
H	11.242051	-5.256269	2.021492
C	-6.548027	0.953847	-0.317053
C	-7.046850	-1.229613	-0.026356
C	-5.958306	2.168877	-0.646953
C	-7.839118	0.904942	0.256479
C	-7.027119	-2.617802	0.043569
C	-8.158821	-0.493310	0.441571
C	-6.672193	3.332772	-0.378442
H	-4.977005	2.214944	-1.107967
C	-8.526696	2.088190	0.512885
C	-8.144879	-3.257278	0.570523
H	-6.169470	-3.190340	-0.293933
C	-9.261664	-1.164002	0.963705
C	-7.952347	3.323351	0.203622
H	-6.209991	4.278759	-0.636829
H	-9.518635	2.039947	0.954230
C	-9.274728	-2.558933	1.032890
H	-8.127853	-4.339919	0.622680
H	-10.112106	-0.589194	1.320631
N	-6.077020	-0.344193	-0.485795
C	-10.501178	-3.271809	1.607018

C	-10.342525	-4.793350	1.607413
H	-10.206027	-5.187632	0.595112
H	-9.492956	-5.113012	2.219674
H	-11.243422	-5.254618	2.024168
C	-10.725976	-2.812829	3.055635
H	-10.890252	-1.732934	3.116964
H	-11.605136	-3.309914	3.480582
H	-9.859920	-3.056709	3.679220
C	-11.735794	-2.918517	0.764041
H	-12.626042	-3.415804	1.165018
H	-11.927525	-1.841405	0.759729
H	-11.602425	-3.239888	-0.273911
C	-8.728133	4.608734	0.500013
C	-9.024428	4.688924	2.005155
H	-9.586304	5.601122	2.234927
H	-9.617964	3.835567	2.346273
H	-8.095271	4.704298	2.583898
C	-10.051996	4.596043	-0.279011
H	-10.675568	3.740740	-0.002568
H	-10.623842	5.507804	-0.073404
H	-9.868023	4.542896	-1.356827
C	-7.950152	5.863392	0.098933
H	-7.003395	5.945287	0.642940
H	-7.734223	5.881718	-0.974334
H	-8.544562	6.752329	0.332425

6 (S_1)

B	0.022059	-1.998942	-1.252497
N	0.022712	-0.608539	-0.612870
C	1.213904	-0.004510	-0.242262
C	-1.196758	-0.033160	-0.244884
C	1.212008	1.149076	0.496922
C	-1.194526	1.129200	0.510883
C	-0.006168	1.735831	0.907956
H	2.148731	1.635633	0.740266
H	-2.141943	1.588658	0.767563
O	1.206013	-2.155624	-2.131680
O	-1.118200	-2.170681	-2.119509
C	2.354171	-1.670411	-1.728518
C	3.530089	-2.201878	-2.298518
C	2.438783	-0.633684	-0.751221
C	4.775877	-1.782574	-1.890383
H	3.414394	-2.951730	-3.073284
C	3.702669	-0.241605	-0.336623

C	4.862918	-0.798336	-0.891498
H	5.674494	-2.167970	-2.358450
H	3.810523	0.471085	0.472396
C	-2.303436	-1.716884	-1.693300
C	-2.399376	-0.677851	-0.730981
C	-3.459021	-2.274535	-2.243400
C	-3.685209	-0.298221	-0.308885
C	-4.717722	-1.843163	-1.853407
H	-3.339476	-3.050357	-2.992392
C	-4.825694	-0.857546	-0.865648
H	-3.807329	0.438496	0.477339
H	-5.613042	-2.261071	-2.301137
F	0.077269	-2.983131	-0.265073
C	7.195911	-1.182879	-0.133422
C	6.477120	0.962955	-0.222369
C	7.283989	-2.571175	-0.123024
C	8.273846	-0.376249	0.294096
C	5.763920	2.132767	-0.467482
C	7.812256	1.001230	0.238332
C	8.492868	-3.137252	0.270213
H	6.442546	-3.197279	-0.394953
C	9.460057	-0.964825	0.689913
C	6.391270	3.341805	-0.183432
H	4.762527	2.114238	-0.881027
C	8.415237	2.216324	0.501905
C	9.594196	-2.365571	0.671319
H	8.567607	-4.217622	0.272173
H	10.283106	-0.341387	1.024839
C	7.703718	3.415336	0.307719
H	5.836042	4.253659	-0.364827
H	9.443118	2.241364	0.849935
N	6.111268	-0.363220	-0.441953
H	-0.013221	2.652515	1.483625
C	8.387818	4.743336	0.617922
C	8.799459	4.759406	2.098966
H	9.492824	3.948234	2.339537
H	9.297217	5.705211	2.336597
H	7.924378	4.660544	2.748656
C	9.639096	4.883489	-0.263912
H	9.372067	4.871674	-1.325143
H	10.142147	5.831690	-0.047972
H	10.357255	4.077656	-0.086511
C	7.475972	5.943121	0.357136
H	7.176387	6.006597	-0.693866

H	6.572895	5.909773	0.974976
H	8.011136	6.864810	0.603484
C	10.917546	-2.990640	1.102969
C	11.214112	-2.587920	2.556515
H	12.163850	-3.027586	2.878208
H	11.293169	-1.503080	2.672552
H	10.427149	-2.943871	3.228529
C	12.038148	-2.471122	0.187890
H	12.135904	-1.382774	0.238764
H	12.996605	-2.906566	0.488830
H	11.849852	-2.745679	-0.854645
C	10.895119	-4.517581	1.019723
H	10.136931	-4.950663	1.679981
H	10.708206	-4.866801	-0.000845
H	11.867020	-4.911429	1.331048
C	-6.548011	0.890009	-0.415002
C	-7.116149	-1.241026	0.046270
C	-5.907644	2.056786	-0.819443
C	-7.872322	0.923560	0.081385
C	-7.134896	-2.617575	0.244953
C	-8.237114	-0.443984	0.376581
C	-6.605061	3.254883	-0.705155
H	-4.897790	2.035706	-1.215329
C	-8.542273	2.139668	0.183389
C	-8.295995	-3.184166	0.760362
H	-6.272002	-3.231560	0.009858
C	-9.383958	-1.042576	0.891027
C	-7.917825	3.327587	-0.204818
H	-6.102600	4.162414	-1.020307
H	-9.559343	2.154655	0.566415
C	-9.434107	-2.424790	1.087822
H	-8.308160	-4.257452	0.912756
H	-10.240114	-0.421646	1.141652
N	-6.100798	-0.424408	-0.432870
C	-10.708728	-3.058069	1.650098
C	-10.586753	-4.575437	1.801909
H	-10.400023	-5.065621	0.840840
H	-9.781976	-4.850954	2.491271
H	-11.521264	-4.979140	2.204463
C	-11.008191	-2.460904	3.033399
H	-11.149800	-1.377227	2.983672
H	-11.922497	-2.899727	3.448630
H	-10.186182	-2.660307	3.728337
C	-11.883206	-2.764007	0.704583

H	-12.807409	-3.204719	1.095200
H	-12.048044	-1.688772	0.587872
H	-11.696349	-3.184439	-0.288776
C	-8.675020	4.651292	-0.077361
C	-9.055124	4.881193	1.393179
H	-9.604898	5.822845	1.502820
H	-9.689348	4.076470	1.776664
H	-8.160391	4.931592	2.021987
C	-9.952120	4.592918	-0.929067
H	-10.612737	3.780816	-0.611412
H	-10.510652	5.531967	-0.844378
H	-9.707943	4.433421	-1.984212
C	-7.842545	5.845649	-0.547293
H	-6.926907	5.959001	0.042311
H	-7.564021	5.756173	-1.602393
H	-8.425846	6.765142	-0.434860

6 (T_1)

B	0.012701	-2.085532	-1.155592
N	0.012895	-0.664628	-0.536456
C	1.195361	-0.076019	-0.224750
C	-1.208171	-0.089767	-0.172489
C	1.224763	1.116371	0.484288
C	-1.179420	1.101592	0.594726
C	0.010269	1.695104	0.919760
H	2.166666	1.609534	0.680055
H	-2.112324	1.559963	0.898927
O	1.127098	-2.235966	-2.063828
O	-1.189264	-2.292699	-1.971904
C	2.307394	-1.762467	-1.670023
C	3.467959	-2.294072	-2.247005
C	2.410511	-0.731636	-0.711521
C	4.715111	-1.841477	-1.862159
H	3.356072	-3.066442	-3.000155
C	3.685121	-0.325964	-0.296070
C	4.829351	-0.864110	-0.864042
H	5.612876	-2.243865	-2.320443
H	3.797068	0.409368	0.492547
C	-2.348235	-1.817762	-1.570501
C	-2.401159	-0.702129	-0.626993
C	-3.517766	-2.383116	-2.086226
C	-3.685797	-0.275911	-0.241284
C	-4.766284	-1.938682	-1.695509
H	-3.407025	-3.177106	-2.816837

C	-4.835905	-0.870334	-0.752703
H	-3.800435	0.478494	0.525940
H	-5.669780	-2.321561	-2.151540
F	0.045357	-3.021069	-0.129711
C	7.132482	-1.229414	0.019463
C	6.532858	0.900754	-0.421824
C	7.170450	-2.606329	0.208560
C	8.245402	-0.419865	0.343367
C	5.874829	2.062266	-0.810939
C	7.860923	0.945295	0.061439
C	8.344198	-3.161202	0.708565
H	6.313908	-3.232200	-0.019113
C	9.405276	-1.006946	0.842344
C	6.559539	3.267793	-0.694500
H	4.862014	2.034775	-1.199374
C	8.517796	2.168598	0.166016
C	9.475434	-2.389285	1.029513
H	8.371658	-4.235133	0.853953
H	10.255612	-0.376371	1.088344
C	7.876130	3.351894	-0.206803
H	6.043686	4.171680	-0.998159
H	9.538312	2.192293	0.539087
N	6.101500	-0.420675	-0.444551
H	0.025071	2.616863	1.491024
C	8.619280	4.683443	-0.077227
C	9.011257	4.907018	1.391124
H	9.658764	4.107193	1.762473
H	9.551079	5.854165	1.502049
H	8.122428	4.942627	2.029252
C	9.888258	4.645758	-0.942076
H	9.635511	4.490709	-1.995862
H	10.436403	5.590724	-0.856393
H	10.561740	3.839561	-0.636611
C	7.768226	5.871204	-0.530275
H	7.480387	5.786265	-1.583263
H	6.857353	5.969968	0.069290
H	8.341912	6.796536	-0.416958
C	10.763673	-3.009756	1.575065
C	11.068969	-2.417524	2.959169
H	11.992741	-2.847357	3.362478
H	11.196608	-1.331862	2.915163
H	10.256579	-2.631814	3.660948
C	11.924633	-2.694522	0.619800
H	12.074965	-1.616556	0.508782

H	12.858063	-3.126070	0.998305
H	11.733335	-3.110790	-0.374467
C	10.662354	-4.529483	1.718120
H	9.868252	-4.819798	2.413779
H	10.472552	-5.016014	0.755781
H	11.605859	-4.923689	2.108755
C	-6.434806	0.941705	-0.170055
C	-7.203890	-1.196635	-0.088587
C	-5.704483	2.102341	-0.397019
C	-7.789534	1.005381	0.216843
C	-7.330380	-2.579882	-0.040922
C	-8.278914	-0.359135	0.272962
C	-6.336495	3.322524	-0.172151
H	-4.681930	2.073328	-0.753489
C	-8.396431	2.233975	0.428112
C	-8.571356	-3.106222	0.308264
H	-6.494946	-3.236873	-0.250875
C	-9.501086	-0.909619	0.627301
C	-7.671366	3.419767	0.249462
H	-5.761584	4.224970	-0.342187
H	-9.441191	2.268611	0.722431
C	-9.672338	-2.300544	0.636853
H	-8.670388	-4.184783	0.334783
H	-10.319869	-0.253934	0.908376
N	-6.079711	-0.402663	-0.361202
C	-11.030800	-2.884938	1.021325
C	-11.040196	-4.413754	0.975346
H	-10.812500	-4.791621	-0.026653
H	-10.323152	-4.846686	1.680315
H	-12.034391	-4.779551	1.249233
C	-11.386886	-2.442021	2.448918
H	-11.443033	-1.352914	2.535184
H	-12.361271	-2.850522	2.737406
H	-10.640402	-2.799159	3.165283
C	-12.096387	-2.365558	0.043671
H	-13.079068	-2.770237	0.308457
H	-12.168413	-1.274119	0.062973
H	-11.865951	-2.670222	-0.982052
C	-8.356871	4.762036	0.500524
C	-8.836884	4.816128	1.959189
H	-9.337386	5.770322	2.155531
H	-9.546424	4.014269	2.183594
H	-7.993589	4.723374	2.650776
C	-9.563737	4.898533	-0.440648

H	-10.296775	4.102358	-0.281035
H	-10.067825	5.855606	-0.269158
H	-9.247514	4.861090	-1.487822
C	-7.420974	5.947200	0.257678
H	-6.548337	5.917990	0.918206
H	-7.070243	5.983155	-0.778806
H	-7.956429	6.880213	0.457674

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B	6.767344	-0.130208	-0.107533
N	5.184439	-0.067528	-0.055758
C	4.516178	-0.904273	0.780782
C	4.524879	0.776063	-0.892366
C	3.127095	-0.893571	0.798034
C	3.135802	0.795215	-0.893407
C	2.407999	-0.047526	-0.049977
H	2.603257	-1.506766	1.518649
H	2.617072	1.471440	-1.559071
O	7.273132	-0.460243	1.202845
O	7.284667	1.173567	-0.444136
C	6.673552	-1.444250	1.871826
C	7.412008	-2.162041	2.819336
C	5.310793	-1.749017	1.668170
C	6.822554	-3.196780	3.524830
H	8.452296	-1.891595	2.965688
C	4.743237	-2.816445	2.382380
C	5.485540	-3.539874	3.298183
H	7.410613	-3.754801	4.247469
H	3.710002	-3.094283	2.201338
H	5.032092	-4.367322	3.833353
C	6.693598	1.843758	-1.432552
C	5.329279	1.653236	-1.739320
C	7.443751	2.780751	-2.152000
C	4.771640	2.371679	-2.809230
C	6.864320	3.489586	-3.190020
H	8.485023	2.916316	-1.879726
C	5.525362	3.276971	-3.534128
H	3.736940	2.203160	-3.089139
H	7.461307	4.204010	-3.749127
H	5.078892	3.814766	-4.363672
F	7.095980	-1.088449	-1.055284
C	0.939990	-0.029931	-0.037122
C	0.222484	1.139854	-0.324112

C	0.205740	-1.186101	0.262564
C	-1.160691	1.158984	-0.314064
H	0.754540	2.061423	-0.540421
C	-1.177525	-1.180006	0.275976
C	-1.889476	-0.003866	-0.013106
H	-1.689553	2.078724	-0.537711
H	-1.719429	-2.089709	0.509239
N	-3.283731	0.009156	-0.001562
H	0.725601	-2.116419	0.471224
C	-3.995076	1.193147	0.310976
C	-3.629548	1.979675	1.407838
C	-5.090291	1.581505	-0.459030
C	-4.339373	3.133001	1.705041
H	-2.786576	1.681340	2.023512
C	-5.804291	2.731242	-0.136892
H	-5.384876	0.975894	-1.310464
C	-5.445645	3.538536	0.945412
H	-4.028935	3.722185	2.563353
H	-6.650708	2.999410	-0.759322
C	-4.022269	-1.161266	-0.301638
C	-5.112254	-1.528469	0.485968
C	-3.689367	-1.955055	-1.403679
C	-5.853087	-2.664488	0.175933
H	-5.381691	-0.917128	1.341622
C	-4.425696	-3.094707	-1.688841
H	-2.850832	-1.673047	-2.032950
C	-5.527295	-3.478814	-0.911469
H	-6.694425	-2.916199	0.811978
H	-4.140223	-3.689932	-2.551643
C	-6.200525	4.812527	1.319909
C	-7.371262	5.088665	0.375141
H	-7.879508	6.008132	0.681675
H	-7.035538	5.223901	-0.658210
H	-8.108628	4.279541	0.395380
C	-6.752981	4.674333	2.746735
H	-5.954265	4.515373	3.477204
H	-7.292420	5.583627	3.033512
H	-7.445687	3.829530	2.815627
C	-5.237968	6.008304	1.259203
H	-4.832538	6.130683	0.249760
H	-5.762288	6.930754	1.531616
H	-4.396444	5.886369	1.947511
C	-6.312332	-4.738192	-1.273139

C	-5.372069	-5.952217	-1.227015
H	-5.918276	-6.864516	-1.490464
H	-4.539424	-5.846692	-1.928703
H	-4.953055	-6.082041	-0.224070
C	-7.472966	-4.991531	-0.309699
H	-8.194885	-4.168395	-0.318636
H	-8.003598	-5.901139	-0.607591
H	-7.123496	-5.132943	0.718253
C	-6.884701	-4.589857	-2.691074
H	-7.446062	-5.488679	-2.968643
H	-7.562021	-3.731890	-2.749452
H	-6.094842	-4.446553	-3.434301

7 (S_1)

B	6.658086	-0.179688	0.013263
N	5.107289	-0.094730	0.003414
C	4.413152	-0.063150	1.191054
C	4.421591	-0.117969	-1.189746
C	3.038527	-0.046818	1.195176
C	3.047116	-0.094960	-1.204433
C	2.285038	-0.073265	-0.007634
H	2.536750	0.062337	2.146932
H	2.551085	-0.095211	-2.165223
O	7.183336	0.544857	1.156958
O	7.195322	0.469796	-1.168541
C	6.578963	0.357740	2.331705
C	7.323052	0.543098	3.503015
C	5.212999	0.007516	2.416328
C	6.742227	0.349661	4.746140
H	8.365184	0.828064	3.400331
C	4.659466	-0.211764	3.686522
C	5.405308	-0.044731	4.842186
H	7.336751	0.487755	5.644718
H	3.626411	-0.536037	3.766324
H	4.952660	-0.225611	5.811923
C	6.599469	0.215297	-2.335104
C	5.231108	-0.128047	-2.410890
C	7.355668	0.323652	-3.508183
C	4.686717	-0.415837	-3.671431
C	6.784297	0.061960	-4.743177
H	8.399403	0.605180	-3.412521
C	5.444431	-0.324554	-4.827919
H	3.651185	-0.733828	-3.743480

H	7.387955	0.141232	-5.642768
H	4.998200	-0.557987	-5.789378
F	7.031459	-1.525801	0.059109
C	0.843753	-0.052184	-0.010167
C	0.096823	0.217737	-1.189423
C	0.091773	-0.304092	1.170059
C	-1.283148	0.241124	-1.190560
H	0.612737	0.449256	-2.114286
C	-1.288238	-0.286543	1.175076
C	-1.982889	-0.011315	-0.006656
H	-1.829790	0.464998	-2.102057
H	-1.838983	-0.495883	2.087554
N	-3.420960	0.011681	-0.004656
H	0.604645	-0.556181	2.091312
C	-4.061589	1.240661	-0.018495
C	-3.406128	2.376200	0.501569
C	-5.332194	1.399489	-0.607375
C	-4.035597	3.600818	0.479380
H	-2.419160	2.268647	0.934962
C	-5.936889	2.642920	-0.629783
H	-5.810574	0.555659	-1.091380
C	-5.316751	3.773670	-0.080575
H	-3.517761	4.452214	0.908314
H	-6.903539	2.733695	-1.110219
C	-4.100950	-1.195917	0.011296
C	-5.374351	-1.313438	0.603790
C	-3.484137	-2.352150	-0.510408
C	-6.019055	-2.536573	0.627963
H	-5.823713	-0.454533	1.089085
C	-4.152942	-3.555711	-0.486293
H	-2.495385	-2.276679	-0.946510
C	-5.437521	-3.686853	0.077126
H	-6.986792	-2.595894	1.111109
H	-3.664189	-4.423521	-0.916463
C	-5.958005	5.153506	-0.089230
C	-7.342270	5.146376	-0.739108
H	-7.760616	6.156475	-0.710272
H	-7.298186	4.837988	-1.788596
H	-8.036930	4.485712	-0.210337
C	-6.101579	5.643228	1.361678
H	-5.134607	5.714111	1.867515
H	-6.556977	6.638595	1.371097
H	-6.740117	4.969410	1.941218

C	-5.054312	6.121449	-0.870693
H	-4.932801	5.792632	-1.907281
H	-5.502858	7.119963	-0.878542
H	-4.060305	6.205729	-0.422672
C	-6.123261	-5.045127	0.087611
C	-5.249519	-6.041906	0.866878
H	-5.730312	-7.025285	0.876035
H	-4.259944	-6.158511	0.416299
H	-5.114693	-5.717156	1.903104
C	-7.504902	-4.993034	0.741016
H	-8.179098	-4.310200	0.213925
H	-7.955876	-5.989030	0.713351
H	-7.448181	-4.686228	1.790363
C	-6.286416	-5.529993	-1.362856
H	-6.773675	-6.510169	-1.370974
H	-6.904456	-4.835950	-1.940748
H	-5.323586	-5.631991	-1.871273

7 (T_1)

B	6.706254	-0.063998	-0.138893
N	5.140484	-0.039500	-0.070472
C	4.460646	-1.149274	0.360814
C	4.459759	1.072873	-0.493655
C	3.083158	-1.152138	0.389443
C	3.082196	1.089090	-0.483728
C	2.325032	-0.033464	-0.050951
H	2.587979	-2.033428	0.770271
H	2.585967	2.007857	-0.760939
O	7.223761	-0.904322	0.919654
O	7.221287	1.267998	0.096883
C	6.630391	-2.082308	1.119818
C	7.381423	-3.125464	1.673410
C	5.266426	-2.283651	0.816461
C	6.806351	-4.366831	1.889576
H	8.422227	-2.930739	1.910379
C	4.716732	-3.558438	1.020219
C	5.469989	-4.593318	1.548575
H	7.405007	-5.169991	2.309387
H	3.684653	-3.746043	0.741069
H	5.024091	-5.572345	1.690470
C	6.626670	2.280919	-0.535713
C	5.264173	2.226217	-0.901168
C	7.374956	3.431302	-0.810605

C	4.713555	3.313339	-1.596730
C	6.798787	4.501730	-1.474382
H	8.414645	3.446243	-0.500491
C	5.464148	4.440689	-1.884980
H	3.682810	3.264750	-1.933756
H	7.395445	5.383120	-1.690852
H	5.017692	5.265964	-2.430001
F	7.067094	-0.540024	-1.397084
C	0.896965	-0.027220	-0.039040
C	0.135919	1.047086	-0.625557
C	0.131687	-1.094413	0.554568
C	-1.229851	1.058470	-0.609822
H	0.649108	1.853846	-1.134132
C	-1.234228	-1.085219	0.564981
C	-1.959540	-0.006928	-0.013488
H	-1.772582	1.865087	-1.092728
H	-1.779469	-1.886334	1.054159
N	-3.353706	0.004348	0.001237
H	0.641132	-1.915443	1.043637
C	-4.040011	1.209638	0.215095
C	-3.523240	2.164039	1.105126
C	-5.228769	1.488601	-0.471040
C	-4.190689	3.360080	1.295500
H	-2.613444	1.943924	1.653397
C	-5.883026	2.693543	-0.263192
H	-5.621641	0.767340	-1.179826
C	-5.384988	3.659661	0.620125
H	-3.775619	4.074538	1.999700
H	-6.794474	2.883352	-0.818006
C	-4.064251	-1.189293	-0.198715
C	-5.242369	-1.449371	0.512640
C	-3.582856	-2.150803	-1.100783
C	-5.921182	-2.642798	0.317403
H	-5.607712	-0.722690	1.230567
C	-4.274279	-3.335168	-1.278241
H	-2.681531	-1.945042	-1.668298
C	-5.458686	-3.615653	-0.577747
H	-6.823573	-2.818122	0.891450
H	-3.886611	-4.055370	-1.992145
C	-6.081174	4.994411	0.866116
C	-7.359504	5.141444	0.039381
H	-7.819805	6.111166	0.250872
H	-7.155778	5.099488	-1.035517

H	-8.093395	4.366622	0.283891
C	-6.450142	5.102842	2.354151
H	-5.567350	5.048696	2.997707
H	-6.946598	6.059519	2.547772
H	-7.132160	4.298346	2.646833
C	-5.125251	6.137687	0.491030
H	-4.847729	6.083383	-0.566316
H	-5.609115	7.103896	0.668528
H	-4.206132	6.110796	1.083413
C	-6.182528	-4.938009	-0.810544
C	-5.238549	-6.097885	-0.456783
H	-5.742366	-7.055495	-0.625140
H	-4.331717	-6.085706	-1.068290
H	-4.938067	-6.049794	0.594573
C	-7.445605	-5.064440	0.042610
H	-8.171003	-4.276718	-0.185474
H	-7.926848	-6.025766	-0.160422
H	-7.218739	-5.027771	1.113057
C	-6.584317	-5.038036	-2.290642
H	-7.101058	-5.985793	-2.474818
H	-7.258392	-4.221564	-2.568170
H	-5.714368	-4.998145	-2.952478

8 (S_0)

C	3.439794	-1.002008	0.637950
C	3.442325	1.081459	-0.502321
C	2.050117	1.083413	-0.518427
C	1.335654	0.033780	0.052554
C	2.047846	-1.016966	0.624736
C	4.237739	-2.085533	1.202338
C	5.601942	-2.188954	0.856575
C	6.345157	-3.295079	1.282975
C	5.758058	-4.264488	2.077597
C	4.418941	-4.150246	2.465890
C	3.671840	-3.073178	2.025014
H	1.516106	1.895963	-0.993210
H	1.512730	-1.866094	1.029141
H	7.386607	-3.354699	0.985461
H	3.967581	-4.898227	3.108857
H	2.636806	-2.983700	2.338282
C	4.243197	2.139221	-1.110242
C	3.680223	3.364286	-1.503807
C	4.430292	4.313508	-2.173797
H	2.644892	3.582282	-1.263495

C	6.353890	2.853647	-2.083115
C	5.769816	4.045579	-2.475295
H	3.980743	5.258042	-2.460804
H	7.395376	2.632758	-2.290973
H	6.363609	4.782586	-3.007819
C	-0.147785	0.022749	0.031644
C	-0.831685	-0.211020	-1.174122
C	-0.864042	0.244752	1.220837
C	-2.222815	-0.216292	-1.176177
C	-2.254587	0.229722	1.189812
C	-2.950742	0.001737	-0.001860
H	-2.753345	-0.394036	-2.106113
H	-2.809847	0.398099	2.106966
C	5.607588	1.900873	-1.380898
H	6.349472	-5.111185	2.413290
O	6.200978	0.766420	-1.012153
O	6.197442	-1.268781	0.099004
F	6.006370	0.724676	1.330417
N	4.100409	0.040311	0.070290
C	-0.152464	0.501179	2.521114
H	0.373986	-0.390456	2.877885
H	0.599048	1.290177	2.416529
H	-0.859636	0.803427	3.296478
C	-0.086592	-0.460192	-2.456985
H	0.420630	0.442376	-2.813989
H	0.684719	-1.226135	-2.328728
H	-0.769294	-0.790887	-3.242632
N	-4.353650	-0.008800	-0.018621
C	-5.087304	0.834726	0.846284
C	-6.212186	0.349929	1.520060
C	-4.708329	2.166812	1.037666
C	-6.940025	1.184844	2.357802
H	-6.510337	-0.684622	1.381928
C	-5.433911	2.984370	1.894464
H	-3.838151	2.554073	0.517002
C	-6.566896	2.515761	2.565693
H	-7.810369	0.787799	2.874506
H	-5.119586	4.015802	2.033723
C	-5.054074	-0.864503	-0.898938
C	-4.649595	-2.190403	-1.080969
C	-6.171665	-0.398238	-1.597489
C	-5.343173	-3.019995	-1.952583
H	-3.784822	-2.563398	-0.541243
C	-6.867623	-1.245218	-2.450071

H	-6.489377	0.631442	-1.466759
C	-6.468758	-2.570083	-2.648598
H	-5.009294	-4.046290	-2.084080
H	-7.732812	-0.862522	-2.985898
C	-7.371487	3.417907	3.457106
H	-8.165602	3.923799	2.894913
H	-7.852144	2.856552	4.263290
H	-6.747183	4.194460	3.907609
C	-7.239302	-3.485587	-3.556323
H	-8.036448	-4.004668	-3.010681
H	-7.712275	-2.932379	-4.372616
H	-6.592826	-4.251631	-3.993345
B	5.686552	0.078779	0.145946

8 (S_1)

C	3.395639	1.032073	-0.617576
C	3.403435	-1.101093	0.501903
C	2.026215	-1.101547	0.510533
C	1.289942	-0.041703	-0.056581
C	2.019278	1.029354	-0.616211
C	4.193181	2.134281	-1.144183
C	5.572944	2.205225	-0.834623
C	6.323393	3.311643	-1.248245
C	5.740431	4.330543	-1.986590
C	4.389943	4.252099	-2.336820
C	3.637751	3.166059	-1.919989
H	1.501588	-1.929787	0.971278
H	1.488982	1.891266	-1.002833
H	7.374636	3.335571	-0.978872
H	3.930623	5.031345	-2.937169
H	2.593921	3.105961	-2.213166
C	4.208285	-2.159829	1.099343
C	3.661049	-3.388199	1.508822
C	4.422031	-4.346739	2.157842
H	2.616561	-3.599632	1.300752
C	6.348068	-2.908118	1.993162
C	5.773302	-4.098704	2.412680
H	3.968424	-5.286085	2.458767
H	7.399450	-2.695676	2.159731
H	6.380505	-4.840966	2.922707
C	-0.185385	-0.031126	-0.033936
C	-0.879702	0.030378	1.198828
C	-0.910701	-0.078281	-1.249603
C	-2.268831	0.034179	1.203470

C	-2.299171	-0.058640	-1.221401
C	-2.975113	-0.006569	-0.000507
H	-2.812615	0.061601	2.142990
H	-2.865729	-0.074371	-2.147622
C	5.588908	-1.940278	1.326505
H	6.341045	5.177643	-2.305199
O	6.194069	-0.812547	0.945623
O	6.185698	1.252258	-0.128634
F	5.965463	-0.716240	-1.389986
N	4.091059	-0.030798	-0.056991
C	-0.195977	-0.167897	-2.565691
H	0.278813	0.780830	-2.835091
H	0.606277	-0.909549	-2.514460
H	-0.885447	-0.440654	-3.368167
C	-0.134647	0.113203	2.498694
H	0.309036	-0.848374	2.775334
H	0.692721	0.823960	2.420208
H	-0.797604	0.423534	3.309863
N	-4.392404	0.006871	0.016867
C	-5.094164	-0.880184	-0.796954
C	-6.316786	-0.500352	-1.380028
C	-4.564754	-2.156626	-1.062743
C	-6.991720	-1.388174	-2.196206
H	-6.700890	0.500711	-1.217940
C	-5.258576	-3.028649	-1.878413
H	-3.628557	-2.452815	-0.603587
C	-6.483936	-2.668544	-2.459789
H	-7.923423	-1.078720	-2.659858
H	-4.850174	-4.017048	-2.065794
C	-5.056761	0.907631	0.846864
C	-4.496451	2.173730	1.098477
C	-6.271930	0.551771	1.459943
C	-5.153155	3.059404	1.930042
H	-3.566278	2.451618	0.616235
C	-6.909392	1.452839	2.291532
H	-6.679169	-0.441737	1.308155
C	-6.370678	2.723332	2.541413
H	-4.721263	4.039808	2.106418
H	-7.835278	1.161717	2.778142
C	-7.234790	-3.633769	-3.321960
H	-7.835240	-4.310369	-2.702020
H	-7.917157	-3.117879	-4.001177
H	-6.554523	-4.253475	-3.911650
C	-7.081853	3.703269	3.420457

H	-7.688349	4.387386	2.814802
H	-7.753500	3.200528	4.119939
H	-6.375844	4.313809	3.989018
B	5.626929	-0.090029	-0.181935

8 (T_1)

C	-3.421467	-1.105125	0.453219
C	-3.421870	1.041701	-0.583869
C	-2.044271	1.062588	-0.560996
C	-1.292905	-0.022526	-0.046813
C	-2.043759	-1.109316	0.466471
C	-4.224467	-2.185094	1.026722
C	-5.589874	-1.957719	1.307558
C	-6.337794	-2.941740	1.964301
C	-5.759707	-4.153110	2.307381
C	-4.422515	-4.409277	1.991547
C	-3.672556	-3.431808	1.359201
H	-1.532364	1.918126	-0.976717
H	-1.533717	-1.922376	0.963180
H	-7.379542	-2.727057	2.179257
H	-3.973543	-5.367210	2.233263
H	-2.639496	-3.643001	1.100644
C	-4.225254	2.146346	-1.108387
C	-3.671116	3.174647	-1.886490
C	-4.425571	4.263833	-2.289370
H	-2.632328	3.110562	-2.195139
C	-6.347965	3.334008	-1.166991
C	-5.769138	4.347128	-1.913755
H	-3.974342	5.042295	-2.896055
H	-7.393595	3.365605	-0.878566
H	-6.369312	5.199010	-2.220049
C	0.153633	-0.012831	-0.025069
C	0.885323	1.156303	0.419103
C	0.906191	-1.176586	-0.448613
C	2.258982	1.135987	0.434521
C	2.279537	-1.142892	-0.436524
C	2.988755	0.000689	0.004859
H	2.802439	2.010283	0.780007
H	2.838609	-2.012843	-0.767759
C	-5.595450	2.221496	-0.773488
H	-6.356587	-4.910667	2.806979
O	-6.194711	1.267793	-0.058096
O	-6.188146	-0.809289	0.986152
F	-6.015309	-0.684111	-1.353878

N	-4.104010	-0.033086	-0.068166
C	0.230207	-2.401600	-0.997785
H	-0.154159	-3.064162	-0.214829
H	-0.621322	-2.133146	-1.629805
H	0.936026	-2.983561	-1.595411
C	0.187810	2.372328	0.962298
H	-0.173792	3.044964	0.177226
H	-0.681530	2.093208	1.564588
H	0.873081	2.947979	1.589268
N	4.384385	0.008627	0.017123
C	5.096676	-0.605715	-1.023712
C	6.283813	-1.306578	-0.758794
C	4.606468	-0.548378	-2.337207
C	6.961836	-1.925812	-1.793949
H	6.647367	-1.379552	0.260649
C	5.299017	-1.177343	-3.358631
H	3.697060	0.006152	-2.542077
C	6.488340	-1.874216	-3.112875
H	7.871594	-2.478090	-1.575860
H	4.915254	-1.118144	-4.373135
C	5.071198	0.631266	1.070183
C	4.559418	0.567014	2.375053
C	6.253599	1.347330	0.825700
C	5.226296	1.204399	3.408301
H	3.653803	0.000797	2.564214
C	6.905843	1.974804	1.872399
H	6.633515	1.425402	-0.187382
C	6.410531	1.916636	3.183015
H	4.826070	1.139876	4.416091
H	7.812030	2.538797	1.669978
C	7.248259	-2.525577	-4.228532
H	8.018524	-1.849616	-4.618780
H	7.755174	-3.432802	-3.888977
H	6.590375	-2.787304	-5.060836
C	7.142708	2.577465	4.311585
H	7.915738	1.911927	4.714078
H	7.642514	3.491968	3.981115
H	6.467523	2.829277	5.133023
B	-5.663122	-0.076573	-0.148765

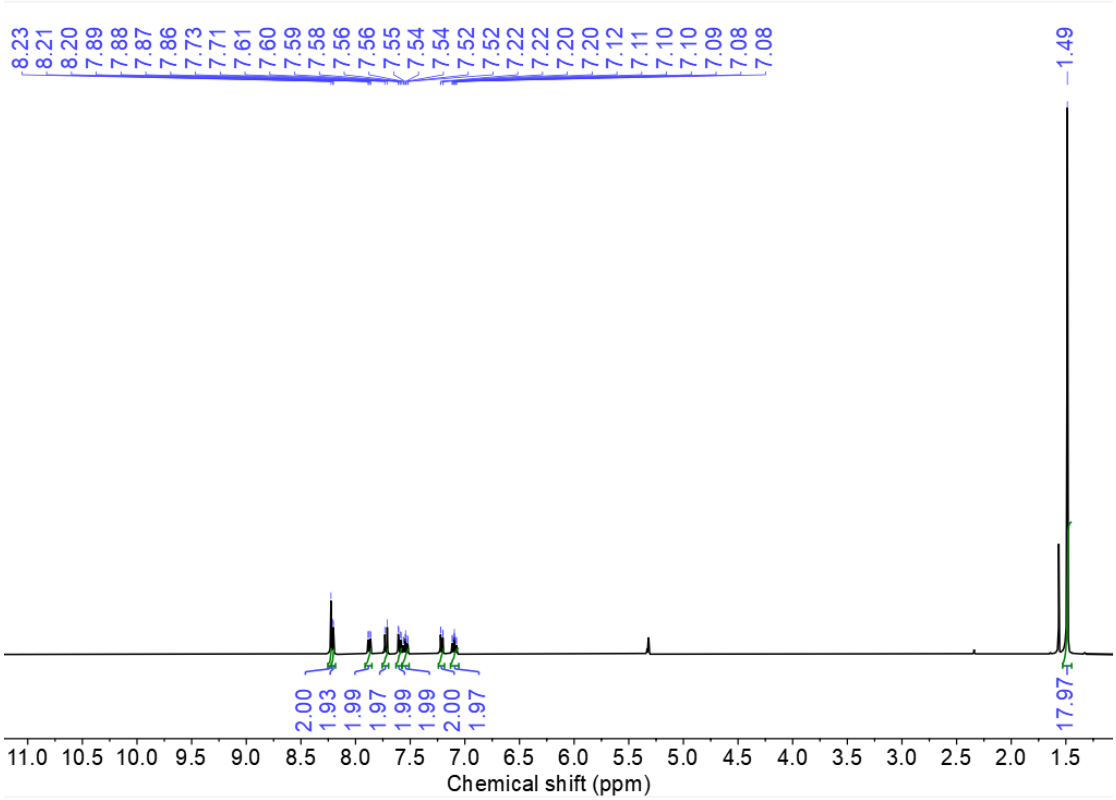

Fig. S33. ^{1}H NMR spectrum of **1** in CD_2Cl_2.

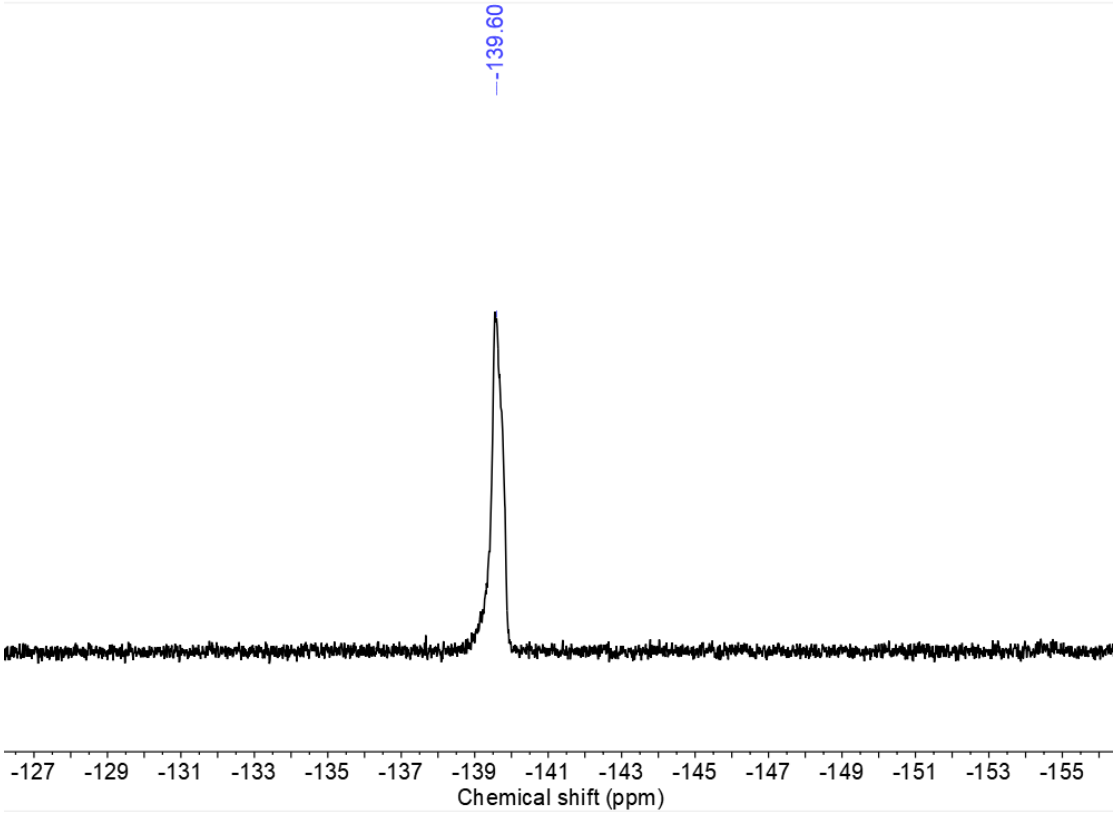

Fig. S34. $^{19}F\{^{1}H\}$ NMR spectrum of **1** in CD_2Cl_2.

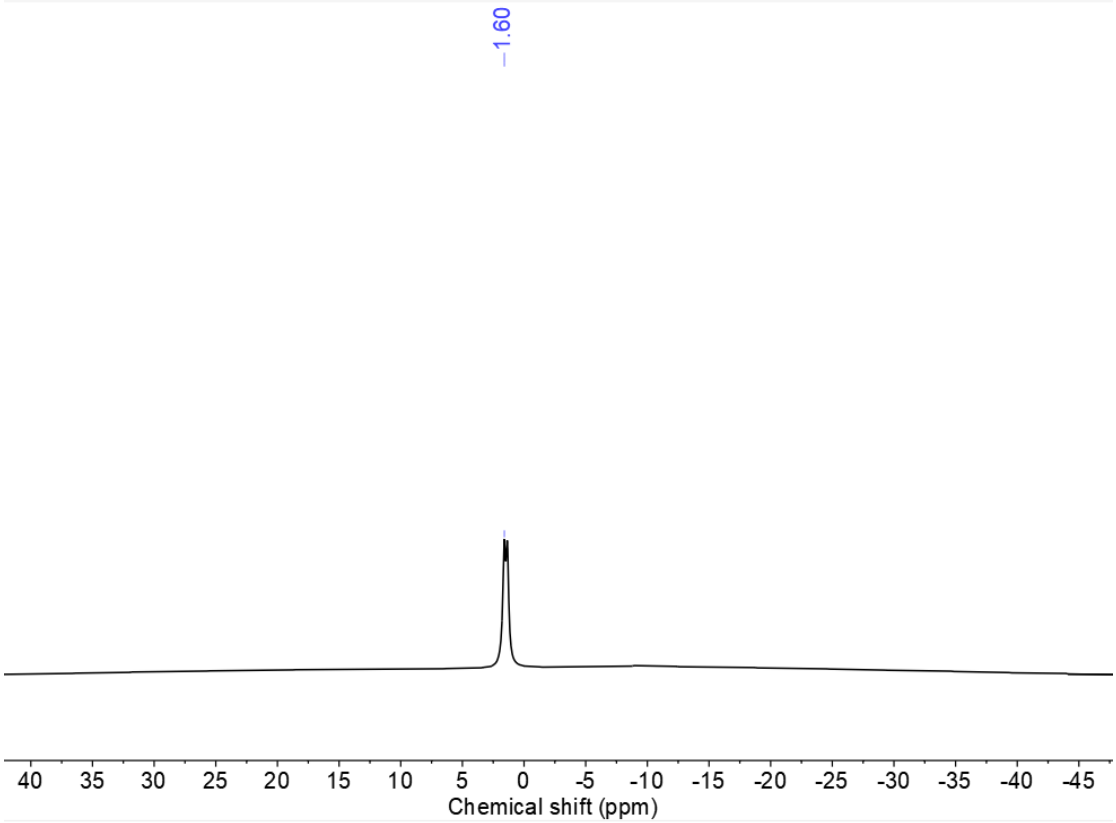

Fig.S35. $^{11}B\{^{1}H\}$ NMR spectrum of **1** in CD_2Cl_2.

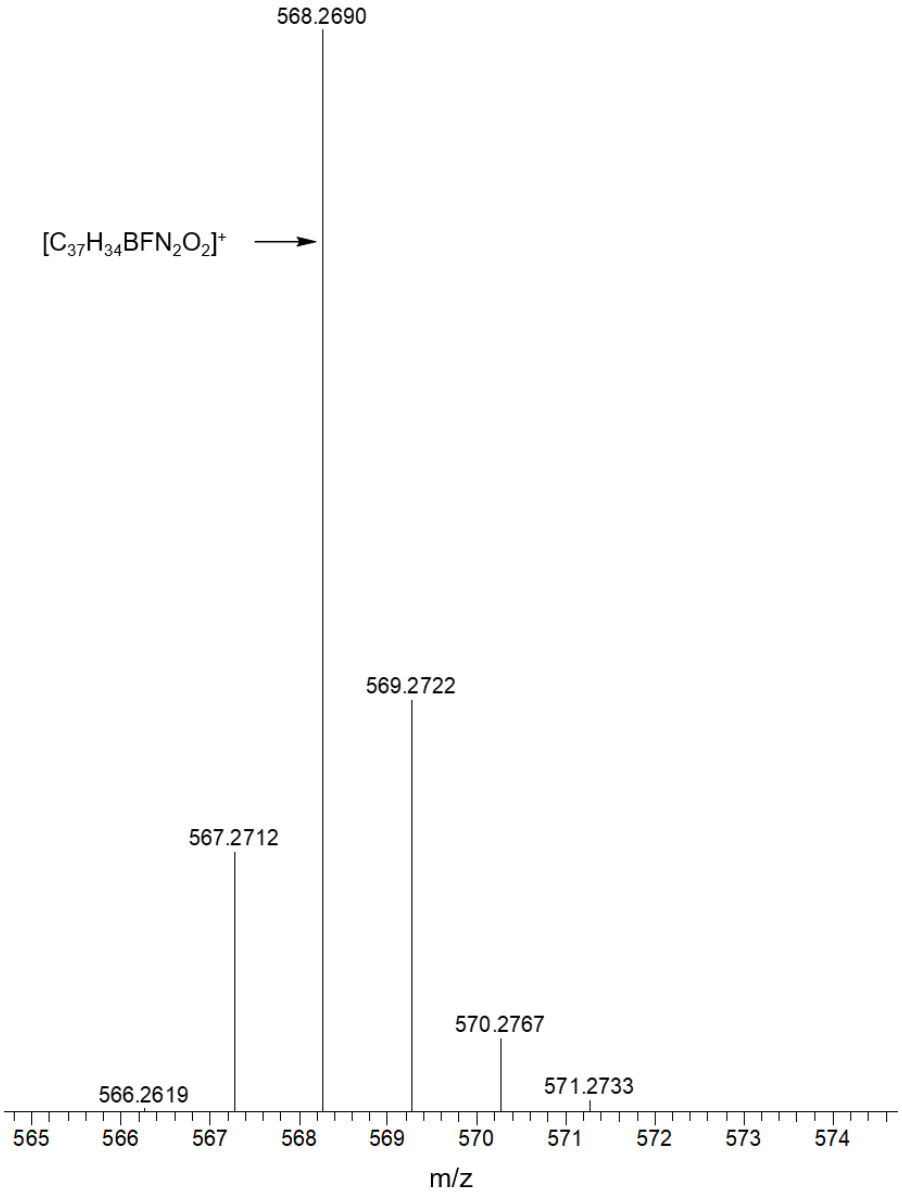

Fig. S36. HR-EI mass spectrum of **1**.

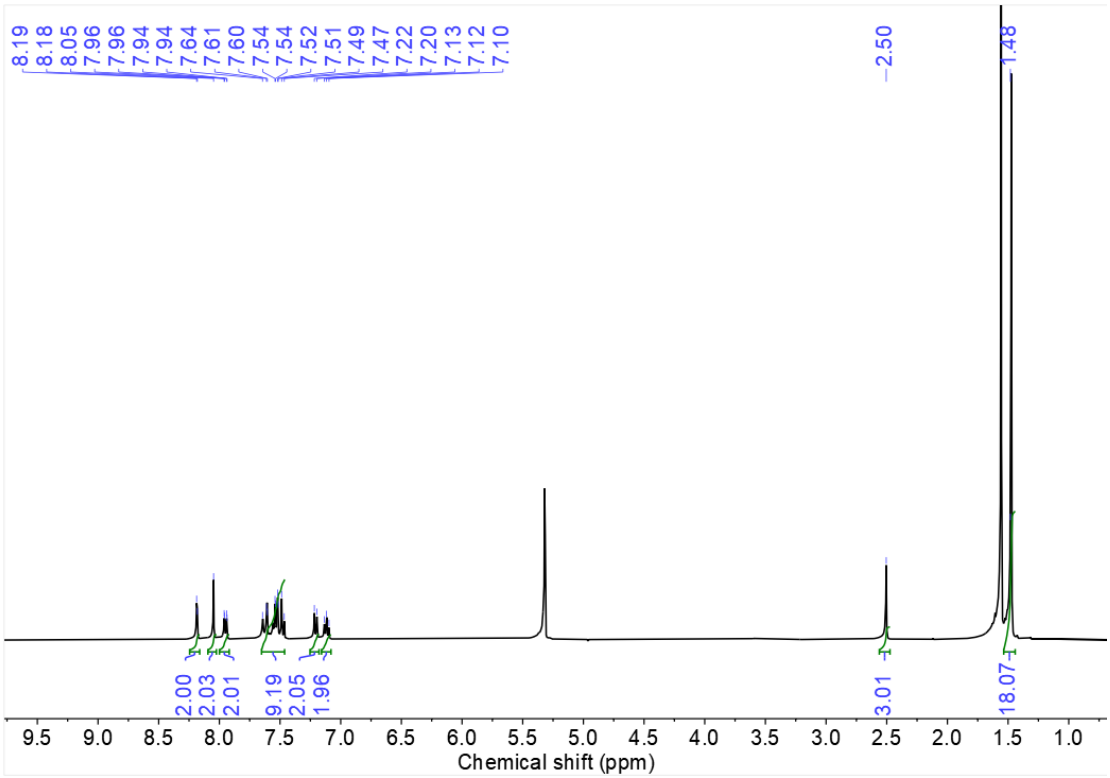

Fig. S37. ^{1}H NMR spectrum of **2** in CD_2Cl_2.

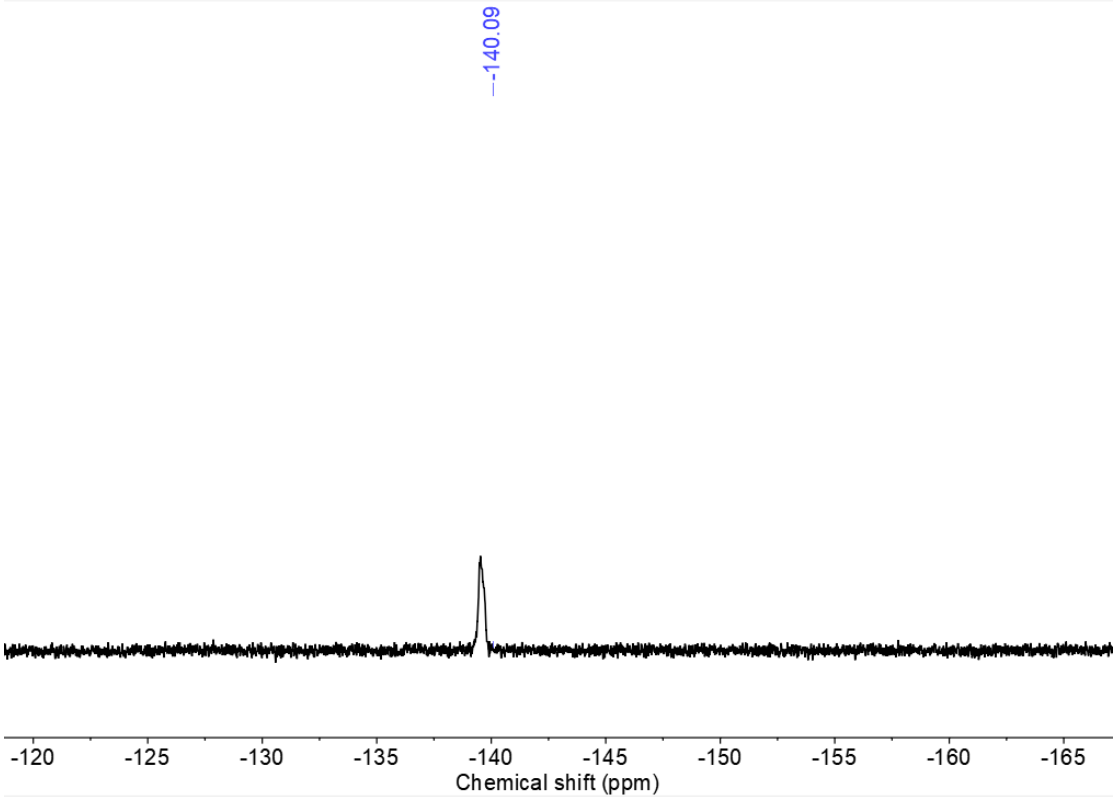

Fig. S38. $^{19}F\{^{1}H\}$ NMR spectrum of **2** in CD_2Cl_2.

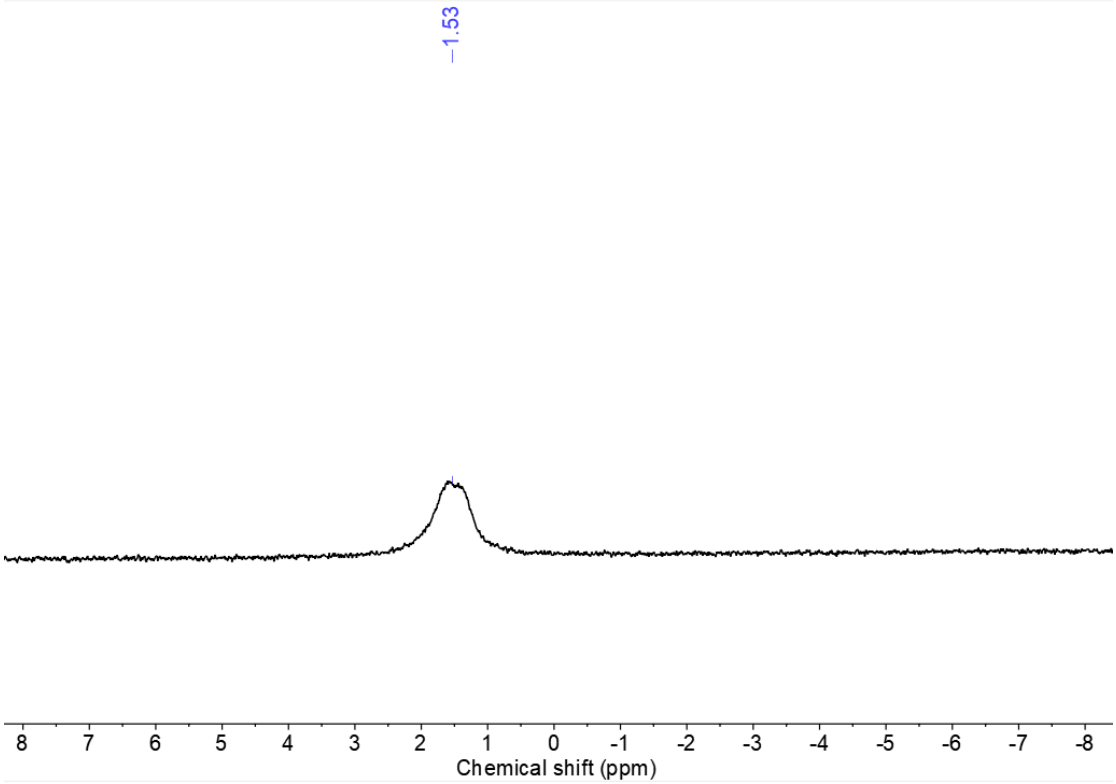

Fig.S39 $^{11}B\{^{1}H\}$ NMR spectrum of **2** in CD_2Cl_2.

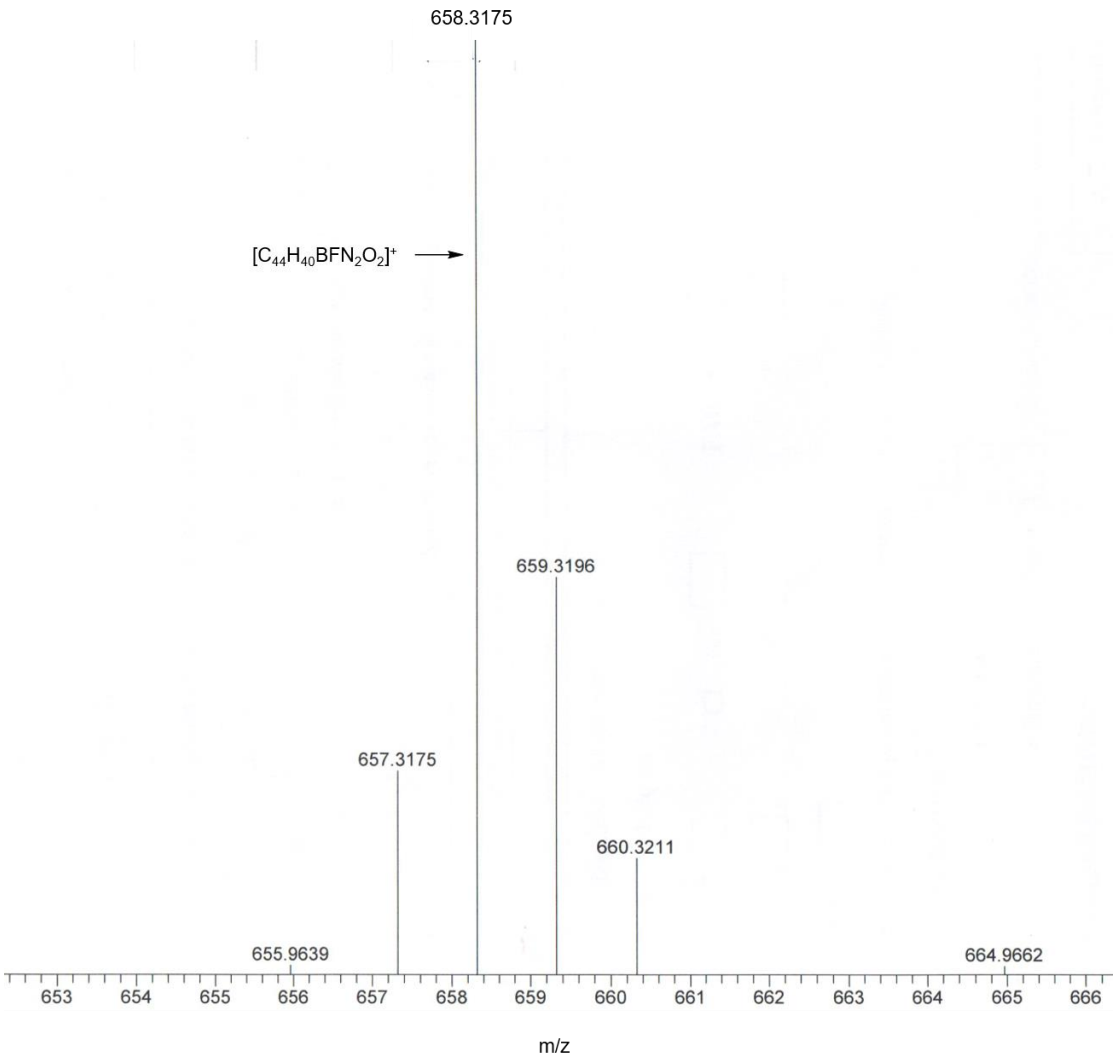

Fig. S40. HR-EI mass spectrum of **2**.

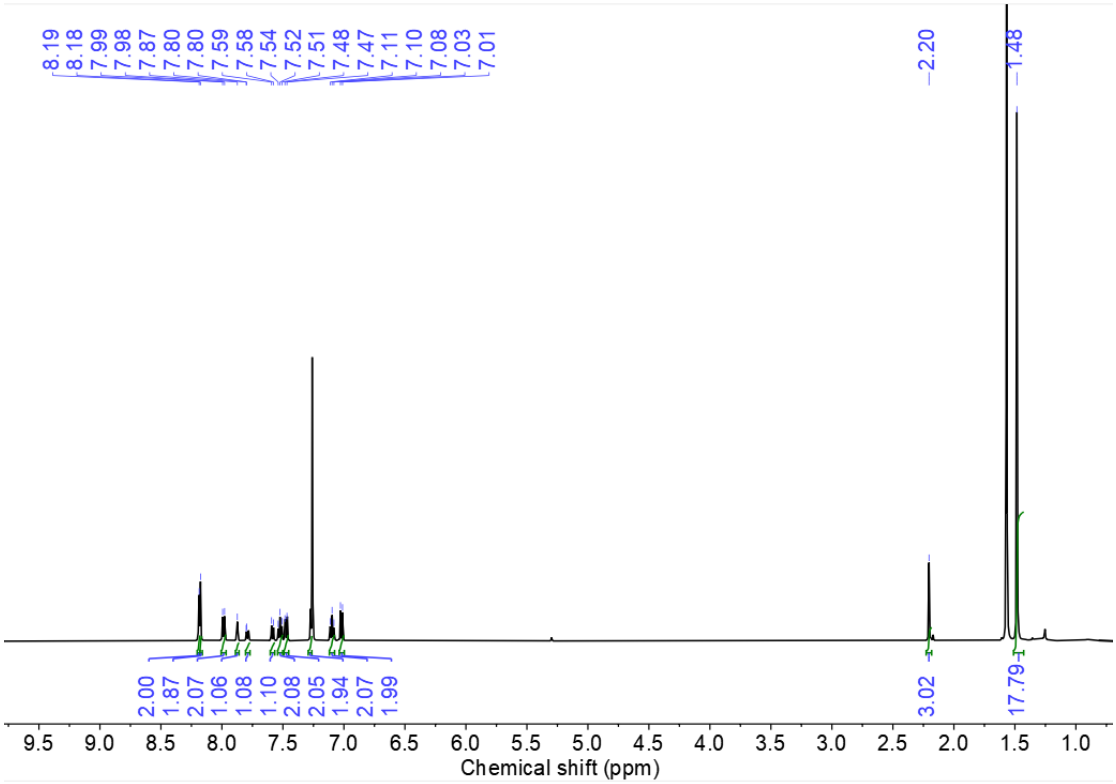

Fig. S41. ^{1}H NMR spectrum of **3** in $CDCl_3$.

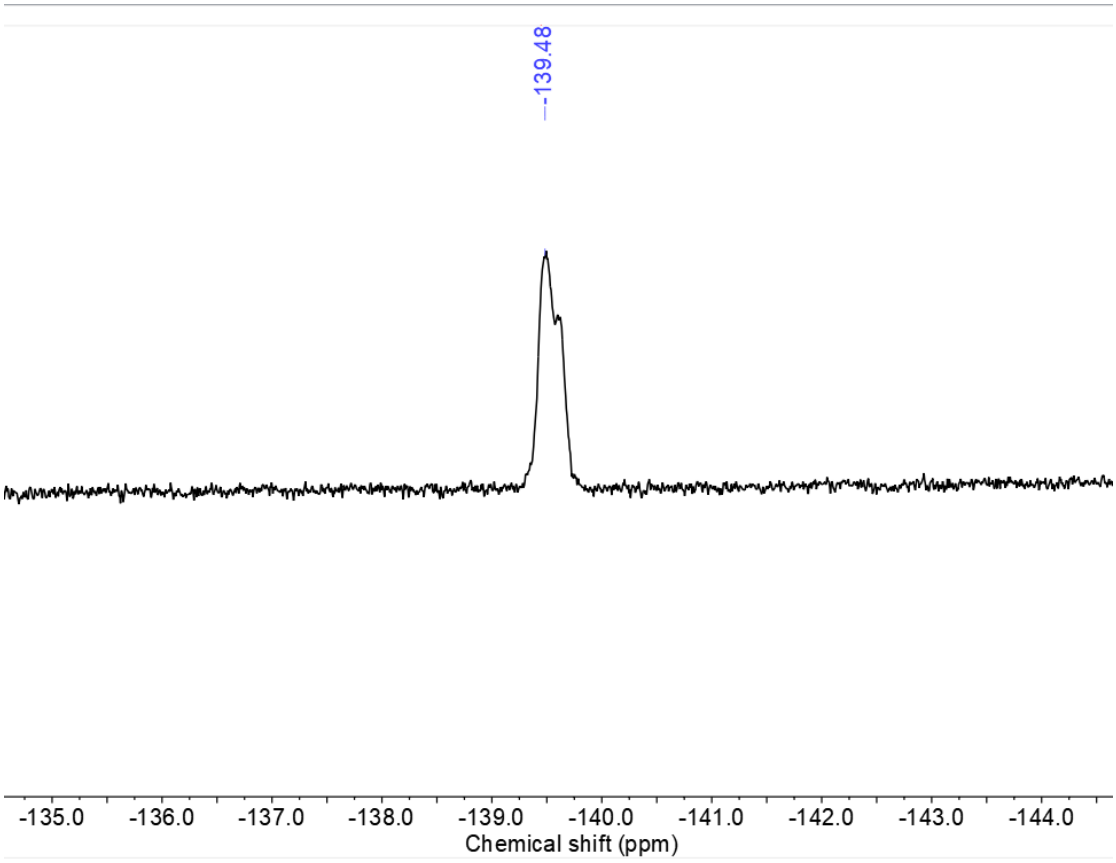

Fig. S42. ^{19}F{^{1}H} NMR spectrum of **3** in $CDCl_3$.

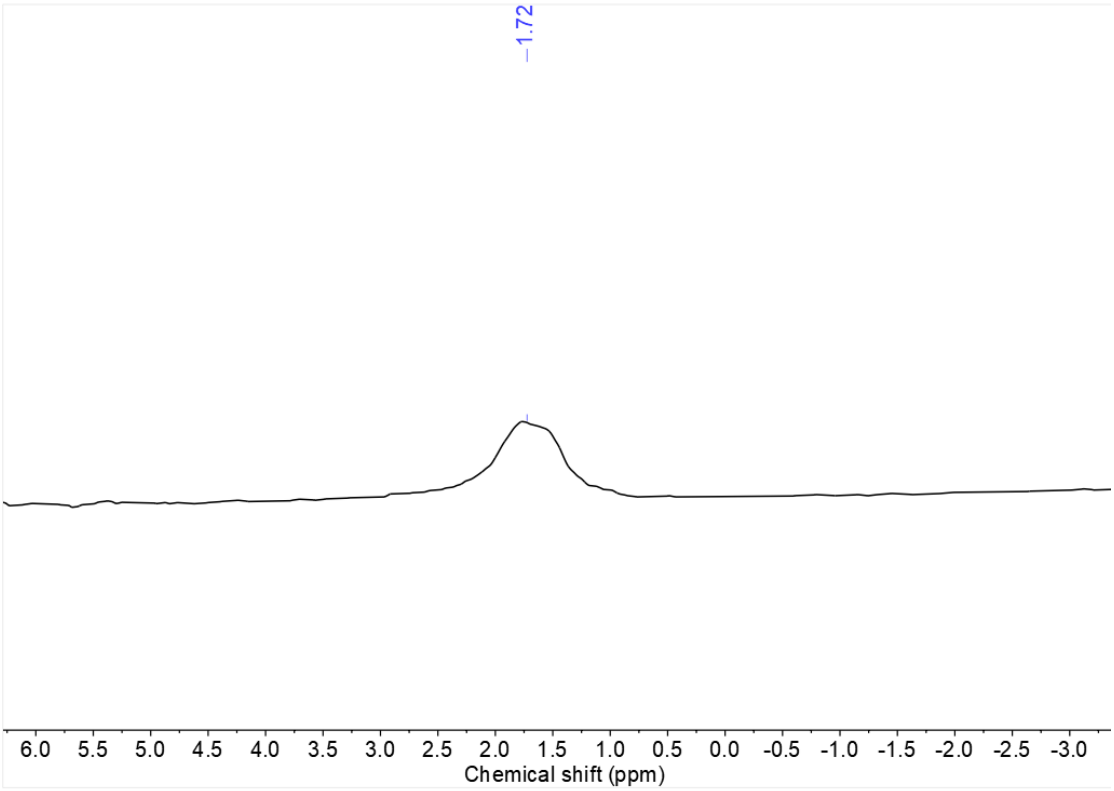

Fig. S43 $^{11}B\{^{1}H\}$ NMR spectrum of **3** in $CDCl_3$.

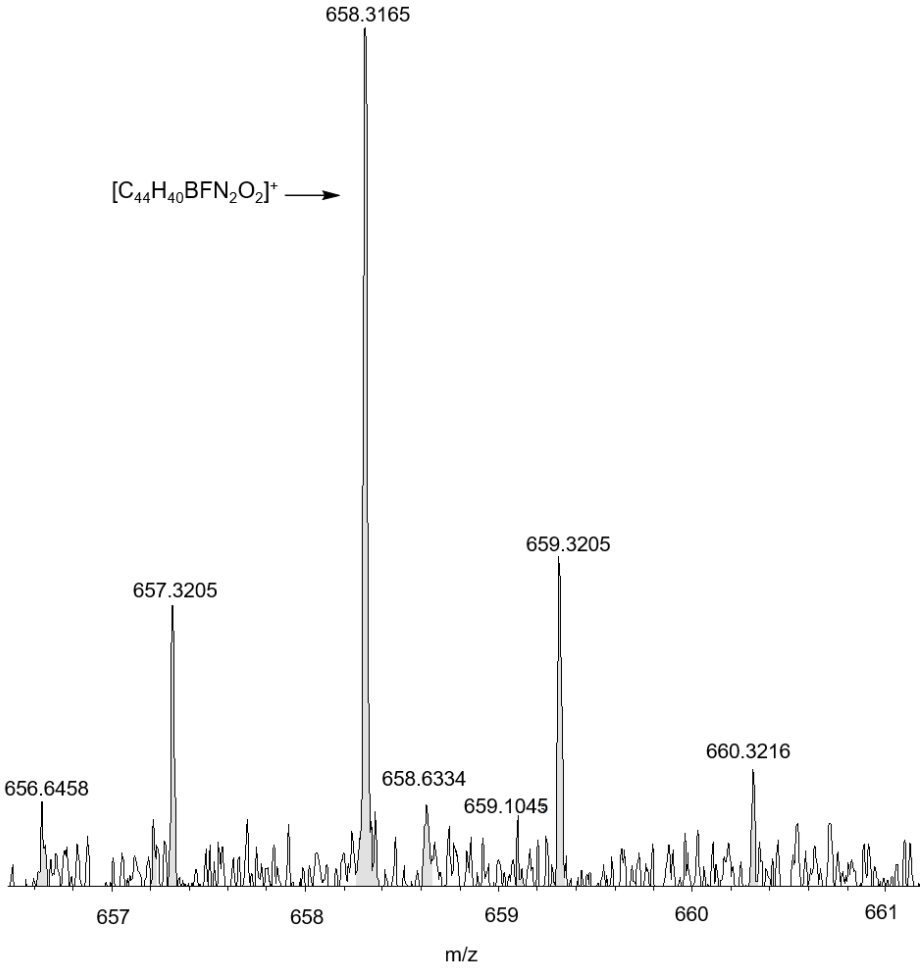

Fig. S44. HR-ESI mass spectrum of **3**.

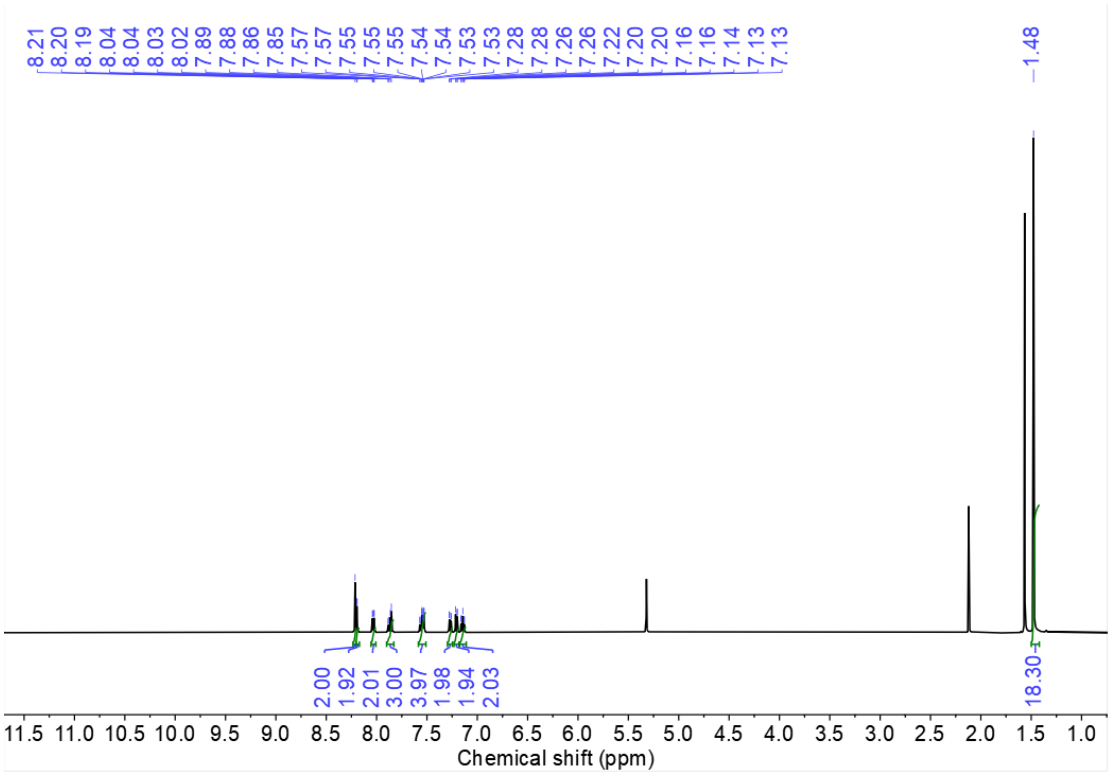

Fig. S45 ^{1}H NMR spectrum of **4** in CD_2Cl_2.

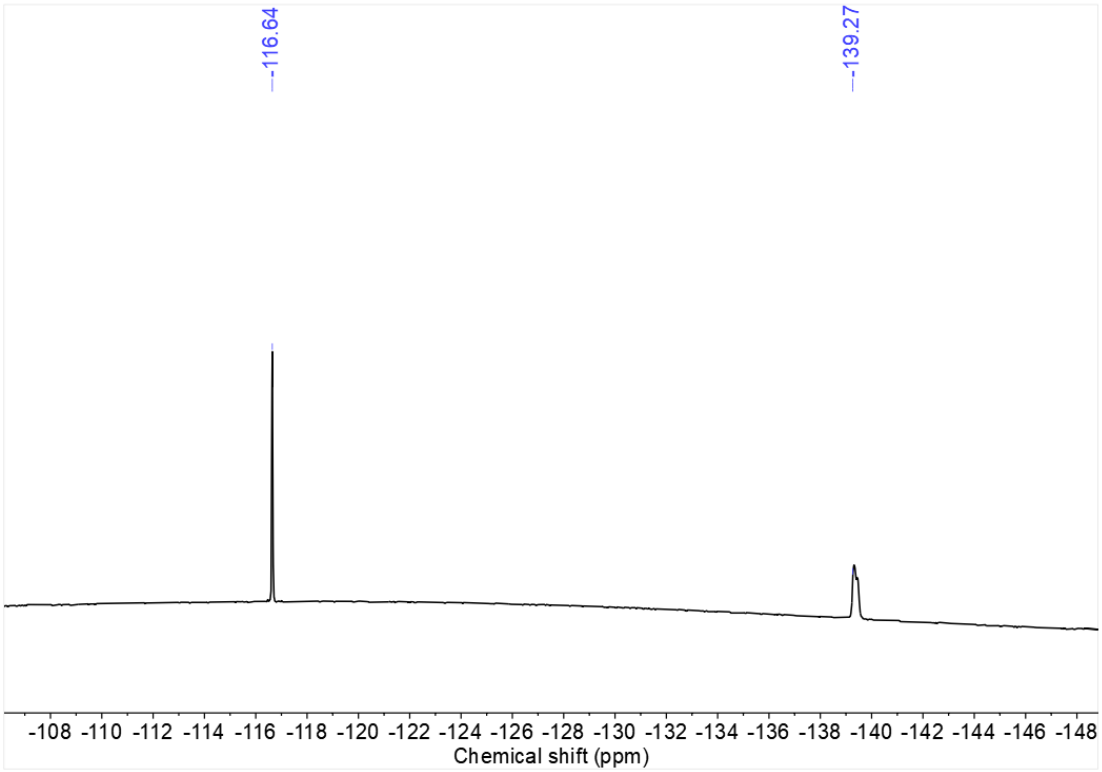

Fig. S46 $^{19}F\{^{1}H\}$ NMR spectrum of **4** in CD_2Cl_2.

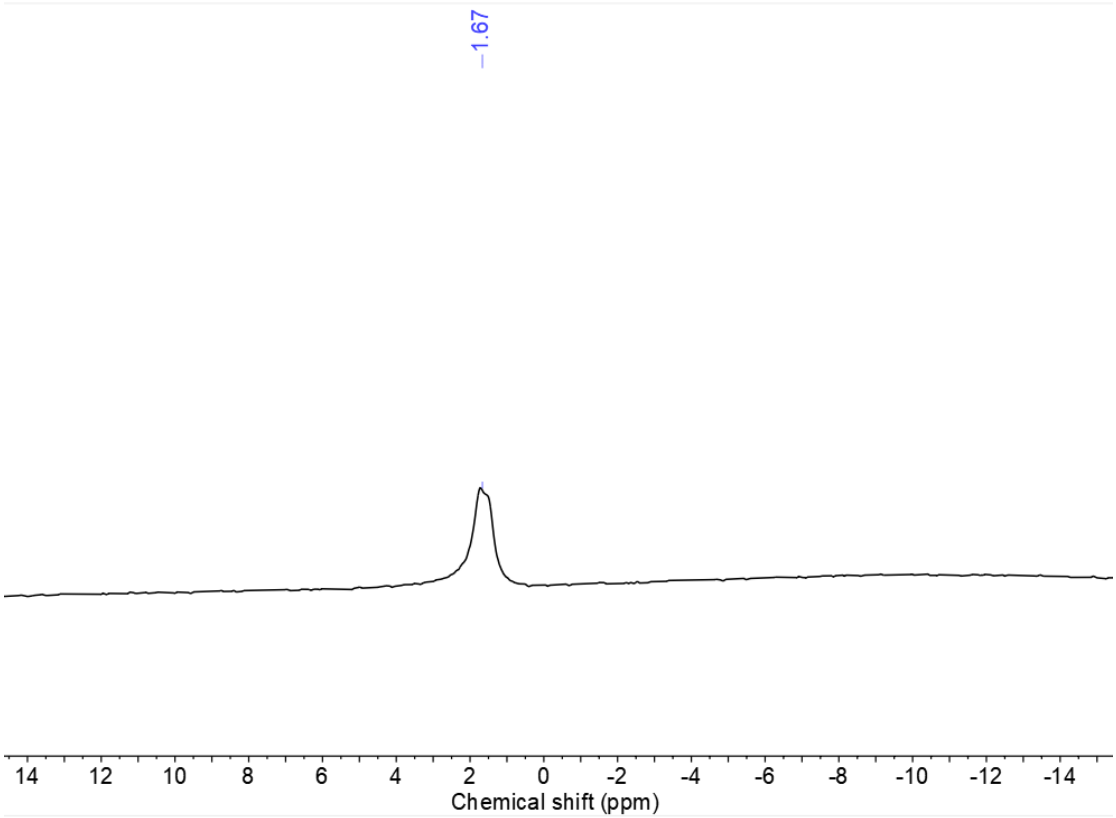

Fig. S47. $^{11}B\{^{1}H\}$ NMR spectrum of **4** in CD_2Cl_2.

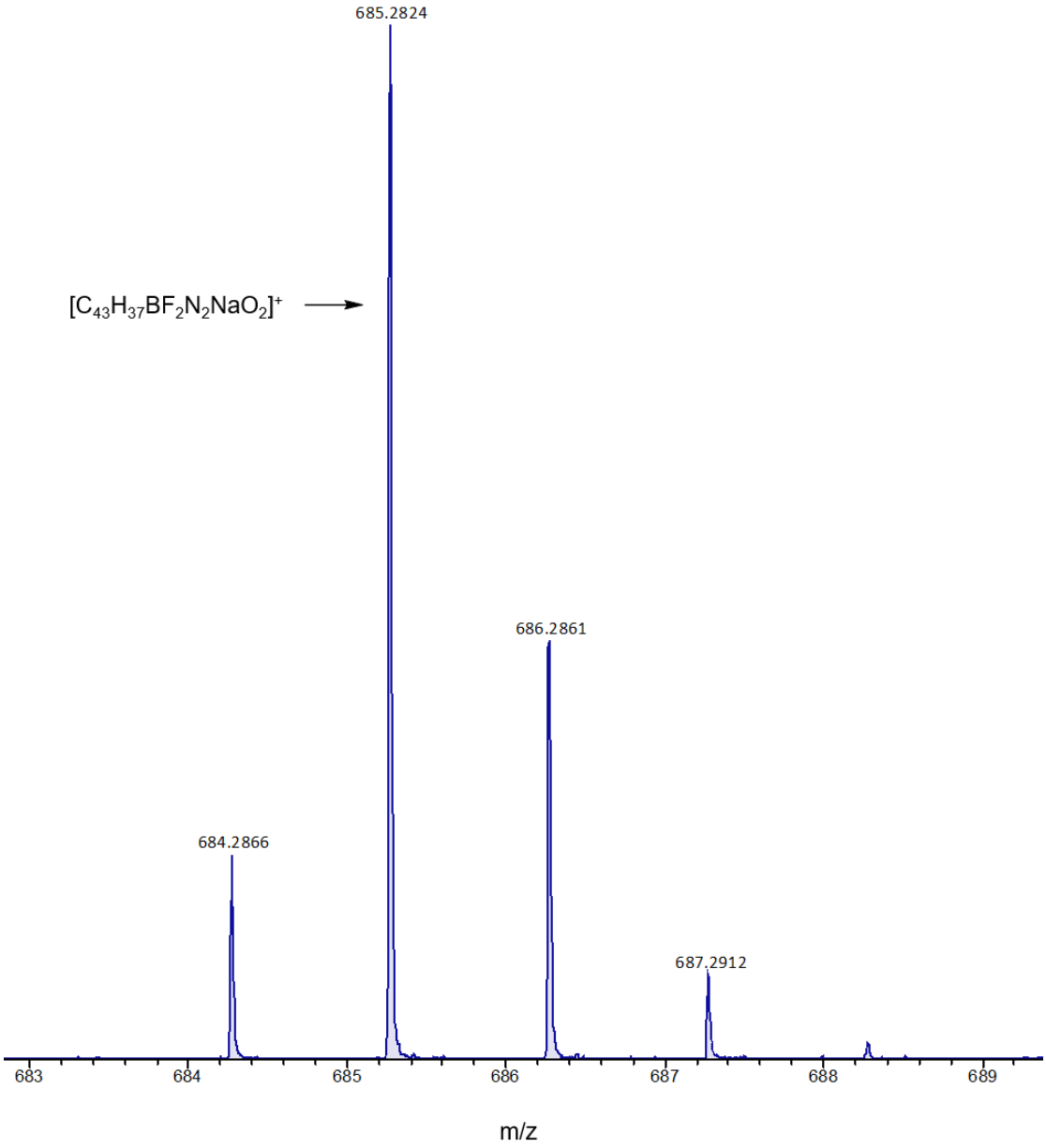

Fig. S48 HR-ESI mass spectrum of **4**.

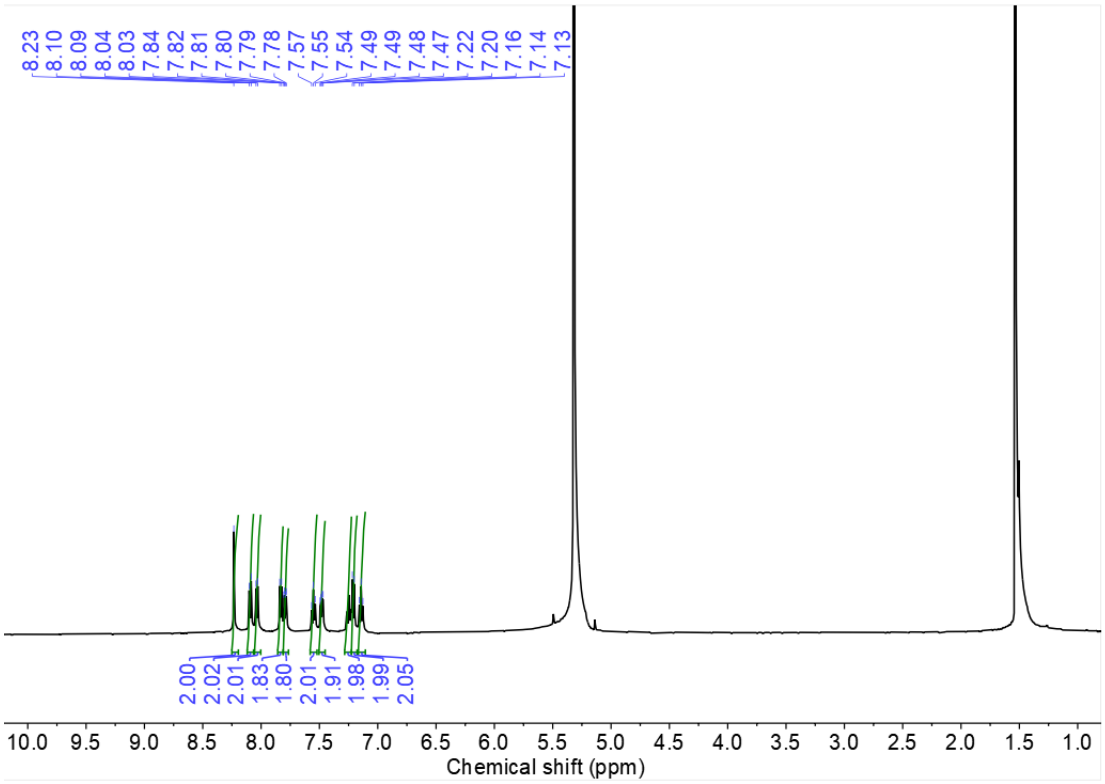

Fig. S49. ^{1}H NMR spectrum of **5** in CD_2Cl_2.

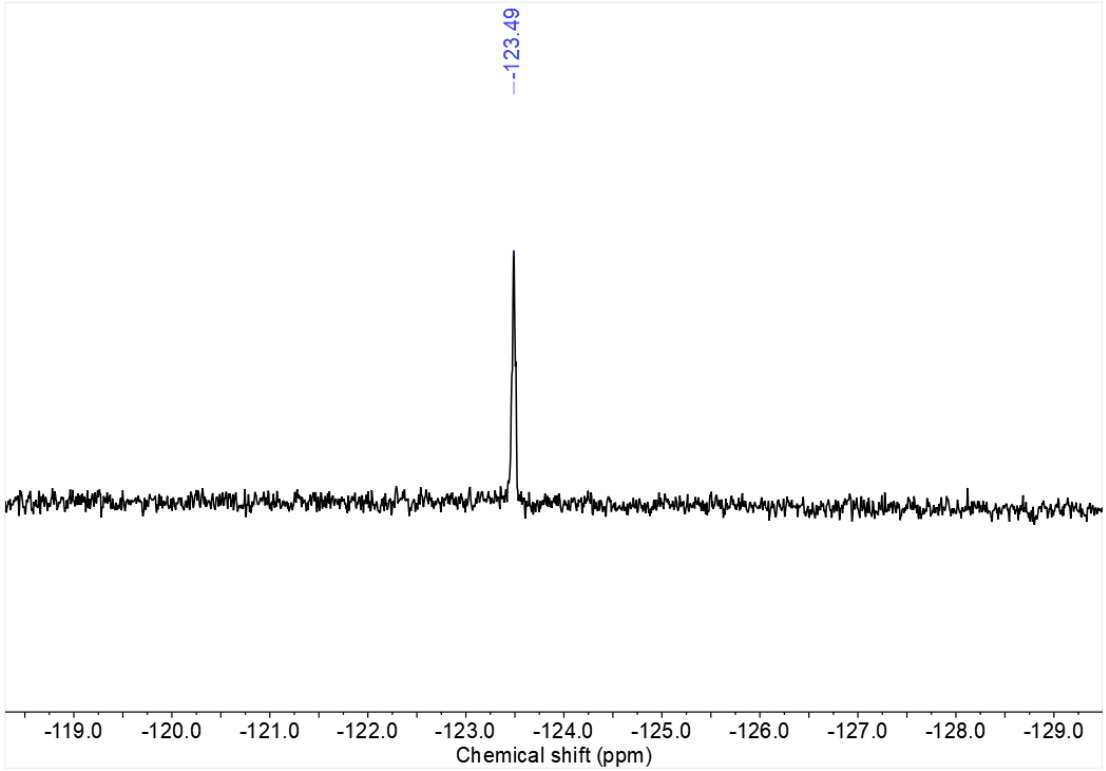

Fig. S50. $^{19}F\{^{1}H\}$ NMR spectrum of **5** in CD_2Cl_2.

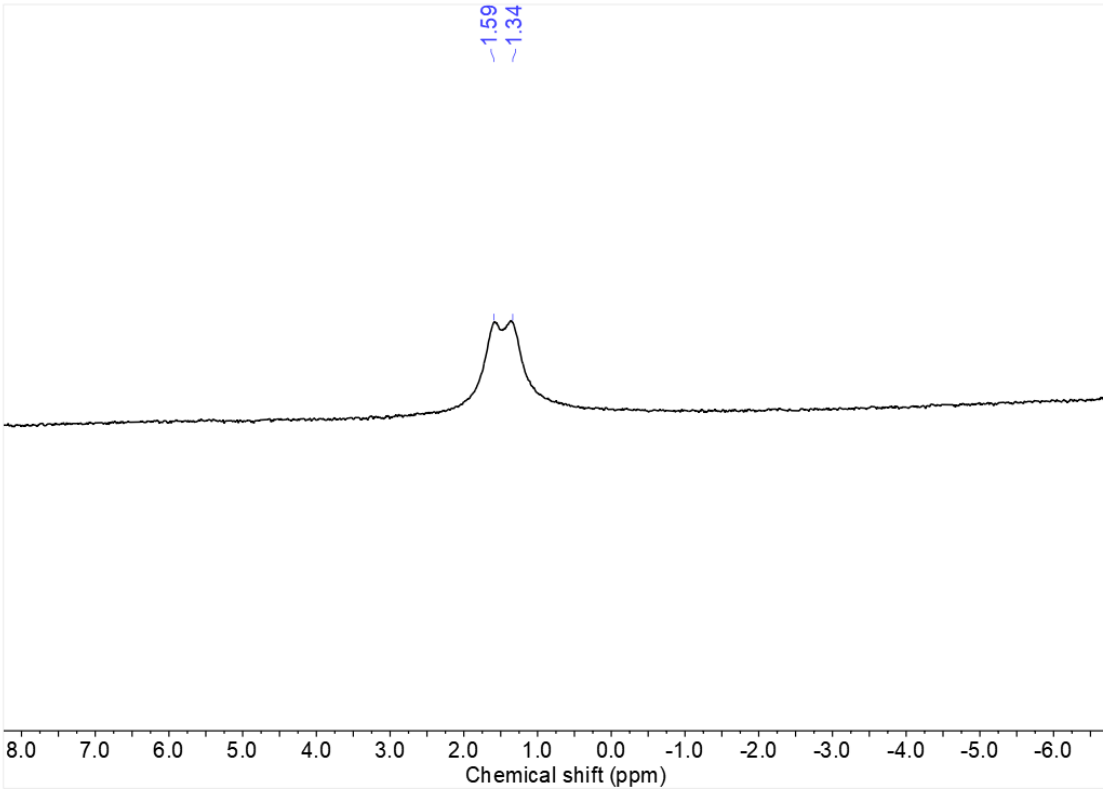

Fig. S51. $^{11}B\{^{1}H\}$ NMR spectrum of **5** in CD_2Cl_2.

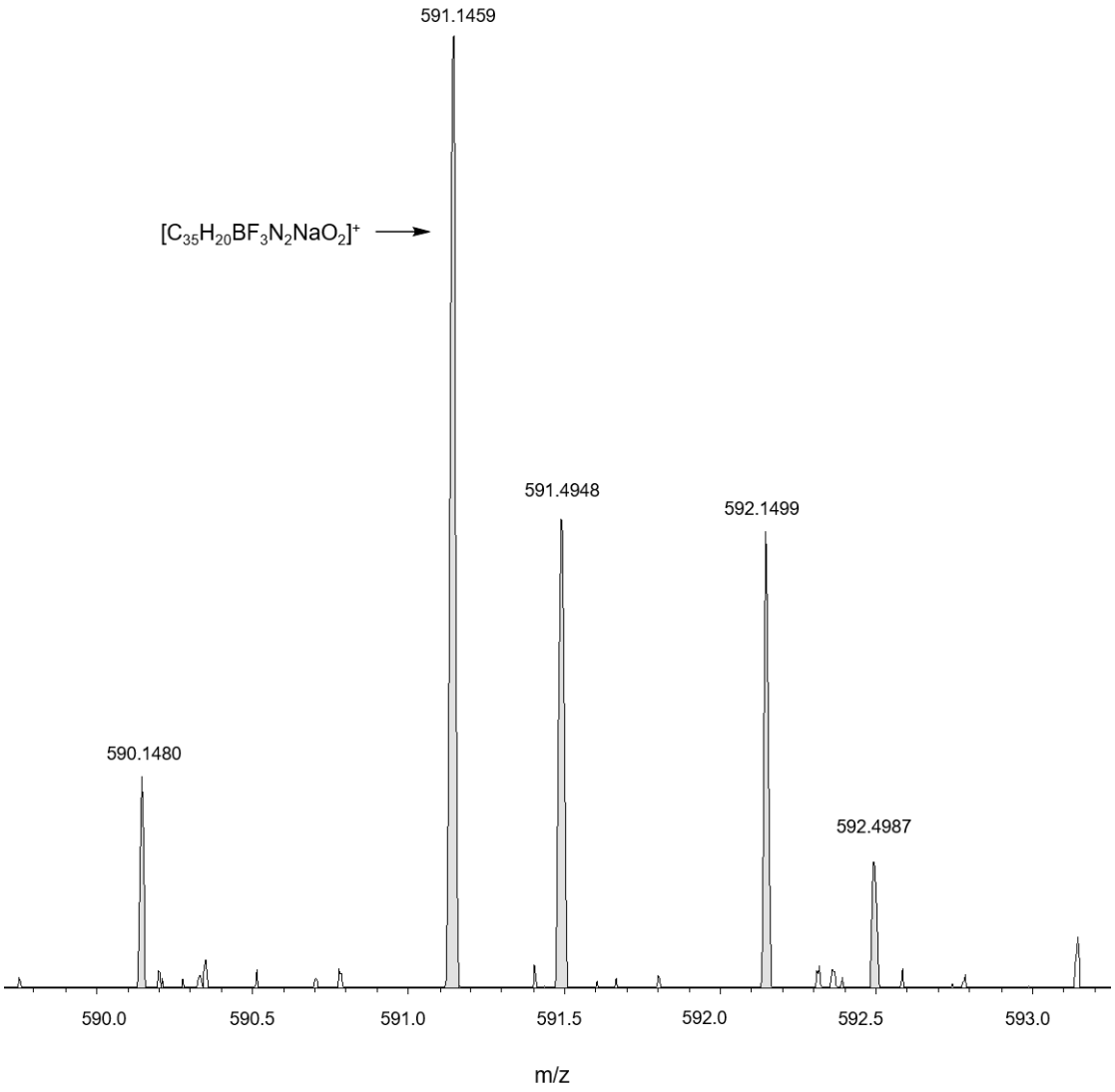

Fig. S52 HR-ESI mass spectrum of **5**.

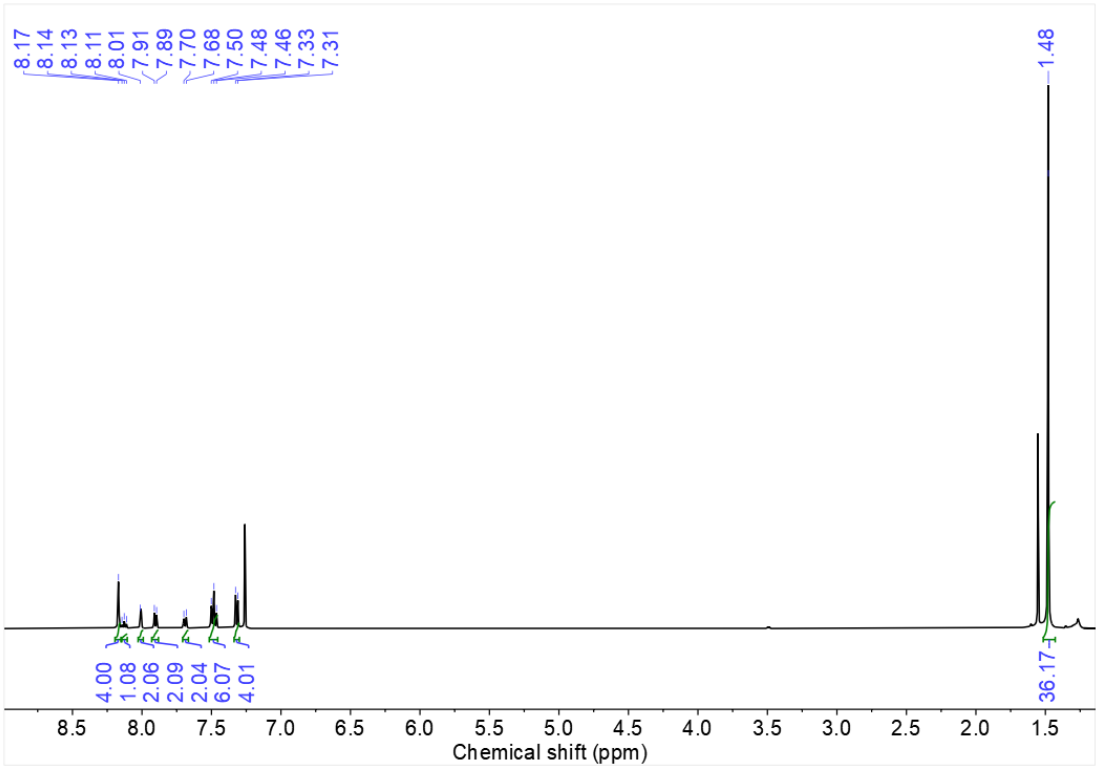

Fig. S53. ^{1}H NMR spectrum of **6** in $CDCl_3$.

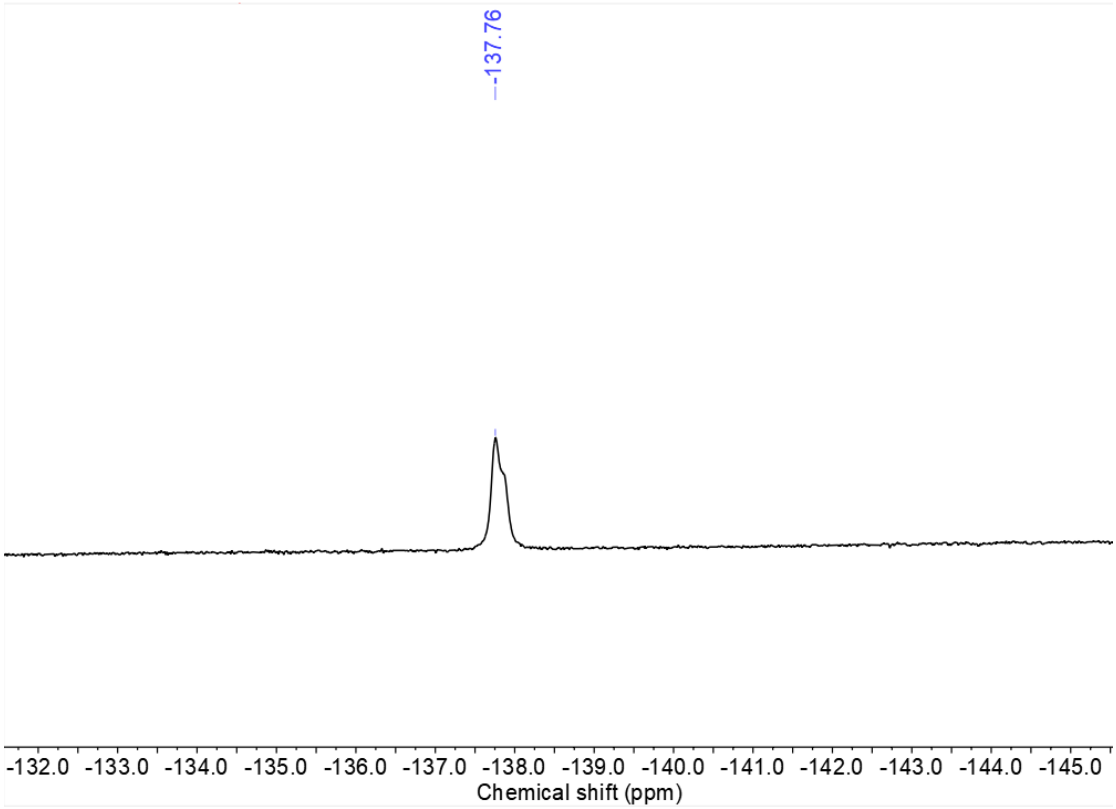

Fig. S54 $^{19}F\{^{1}H\}$ NMR spectrum of **6** in $CDCl_3$.

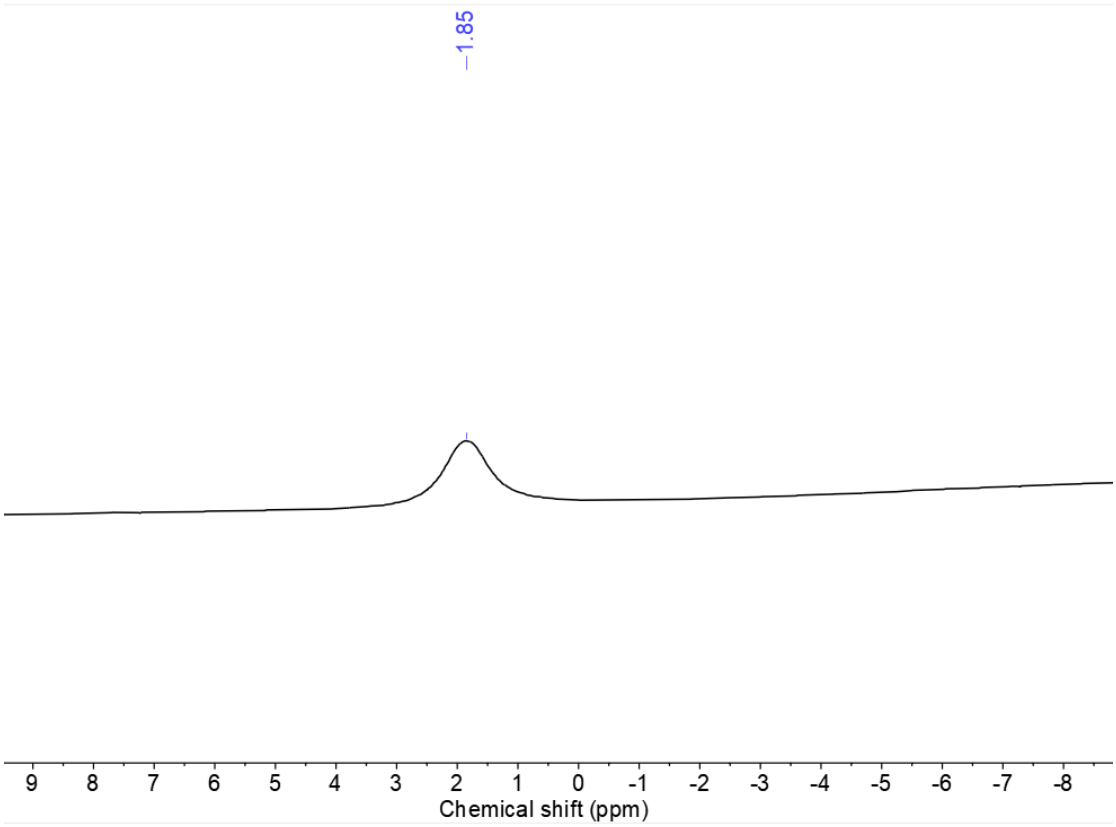

Fig. S55 $^{11}B\{^{1}H\}$ NMR spectrum of **6** in $CDCl_3$.

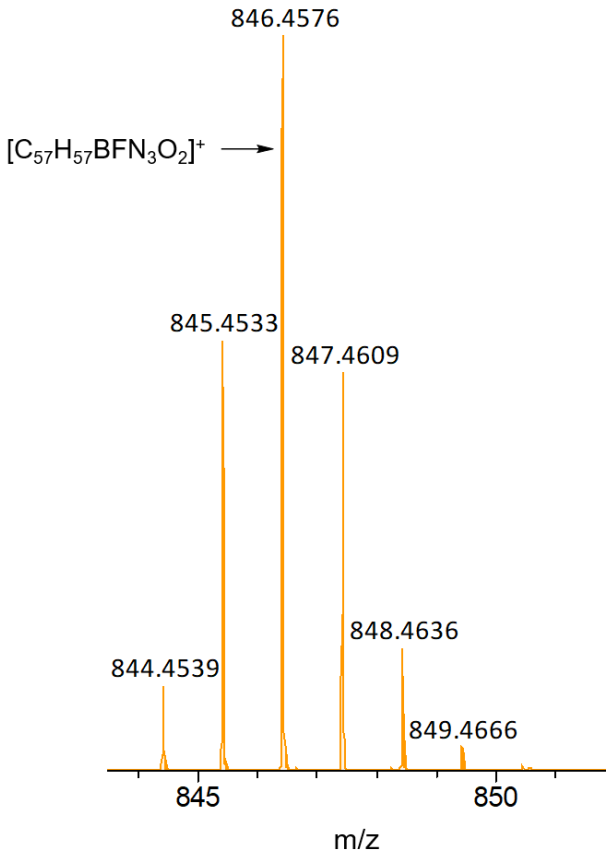

Fig. S56 HR-ESI mass spectrum of **6**.

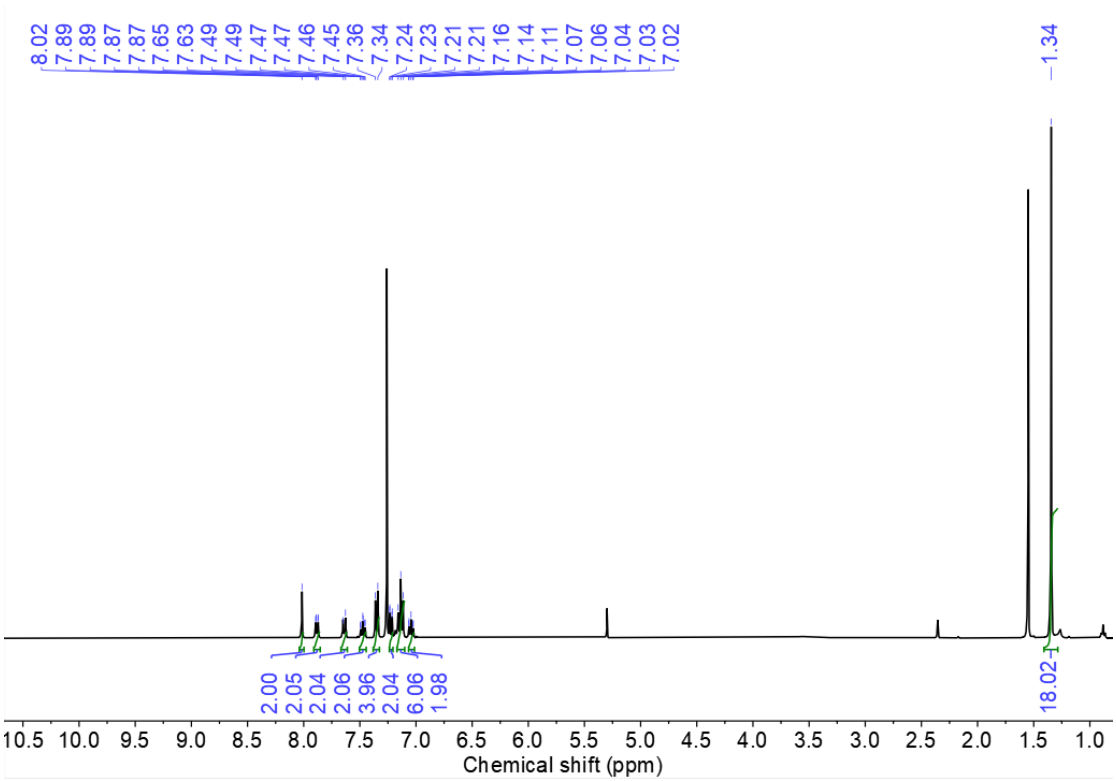

Fig. S57 ^{1}H NMR spectrum of **7** in $CDCl_3$.

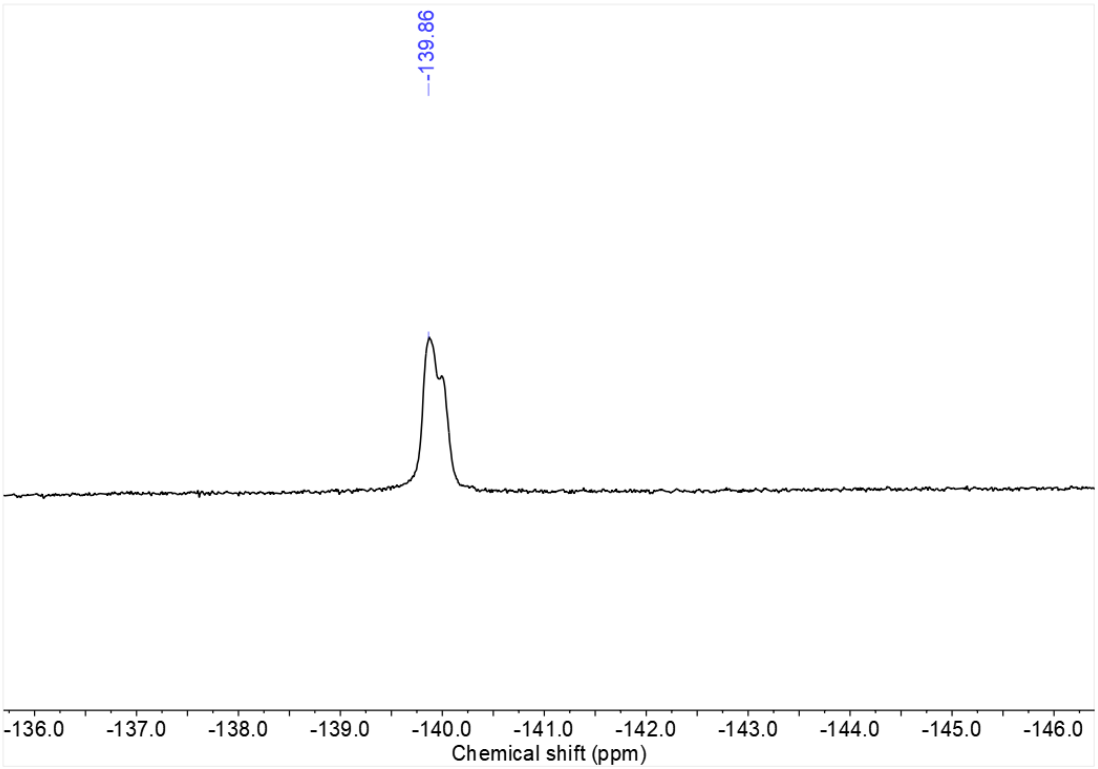

Fig. S58 $^{19}F\{^{1}H\}$ NMR spectrum of **7** in $CDCl_3$.

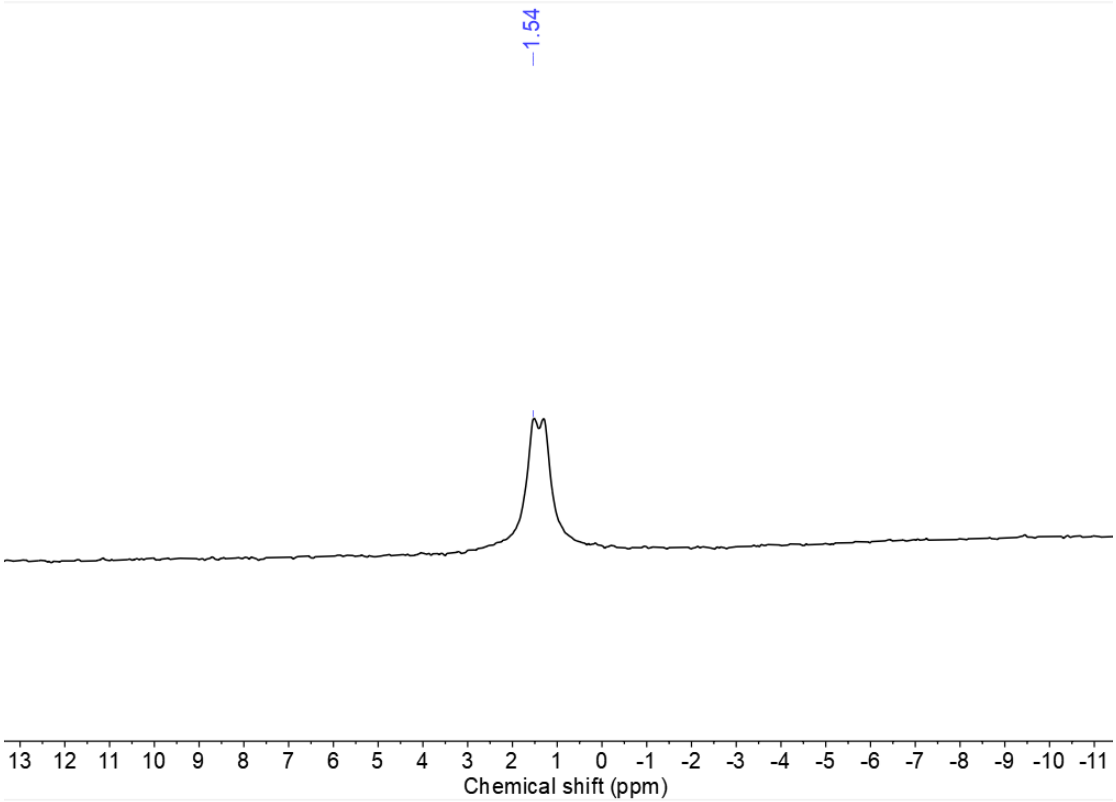

Fig. S59 $^{11}B\{^{1}H\}$ NMR spectrum of **7** in $CDCl_3$.

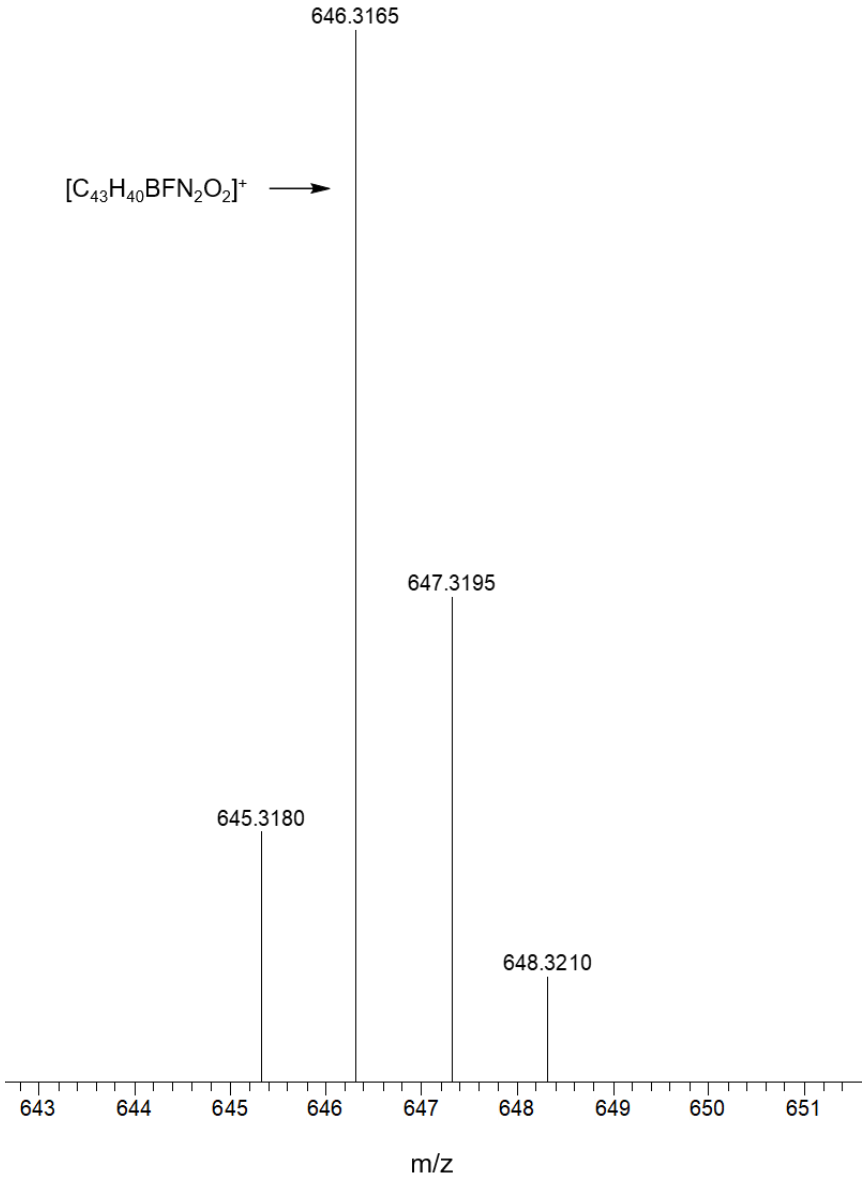

Fig. S60. HR-EI mass spectrum of **7**.

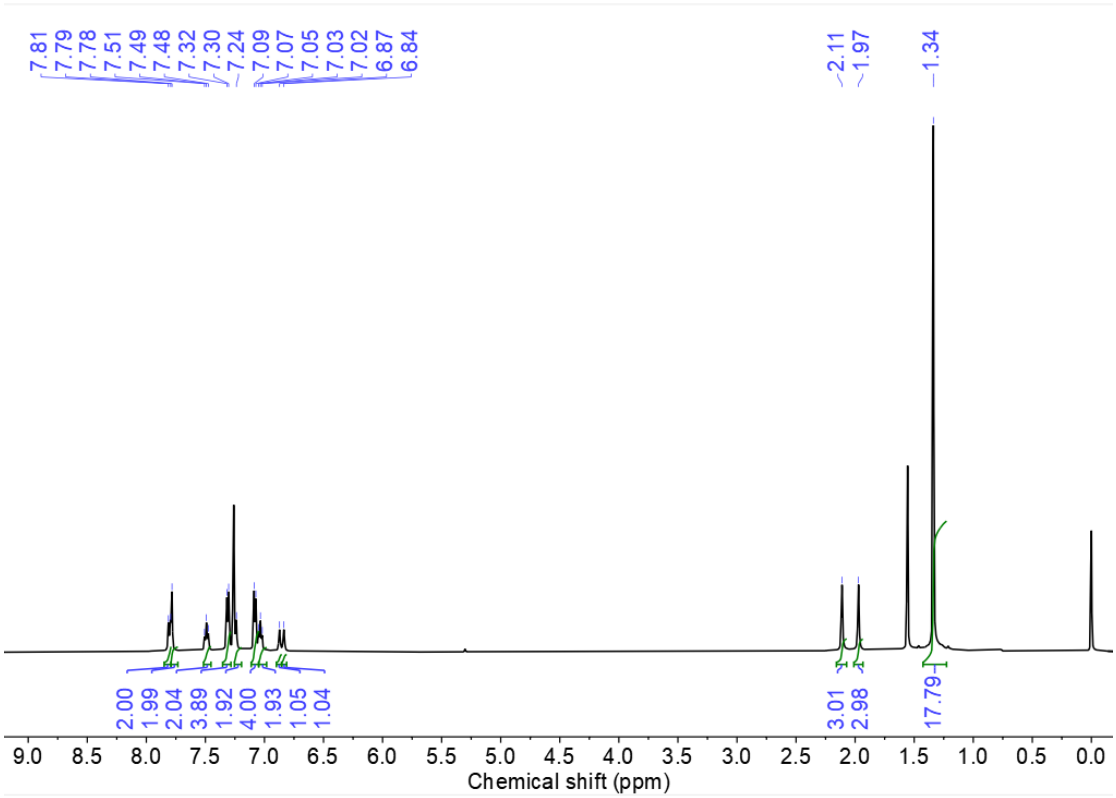

Fig. S61. ^{1}H NMR spectrum of **8** in $CDCl_3$.

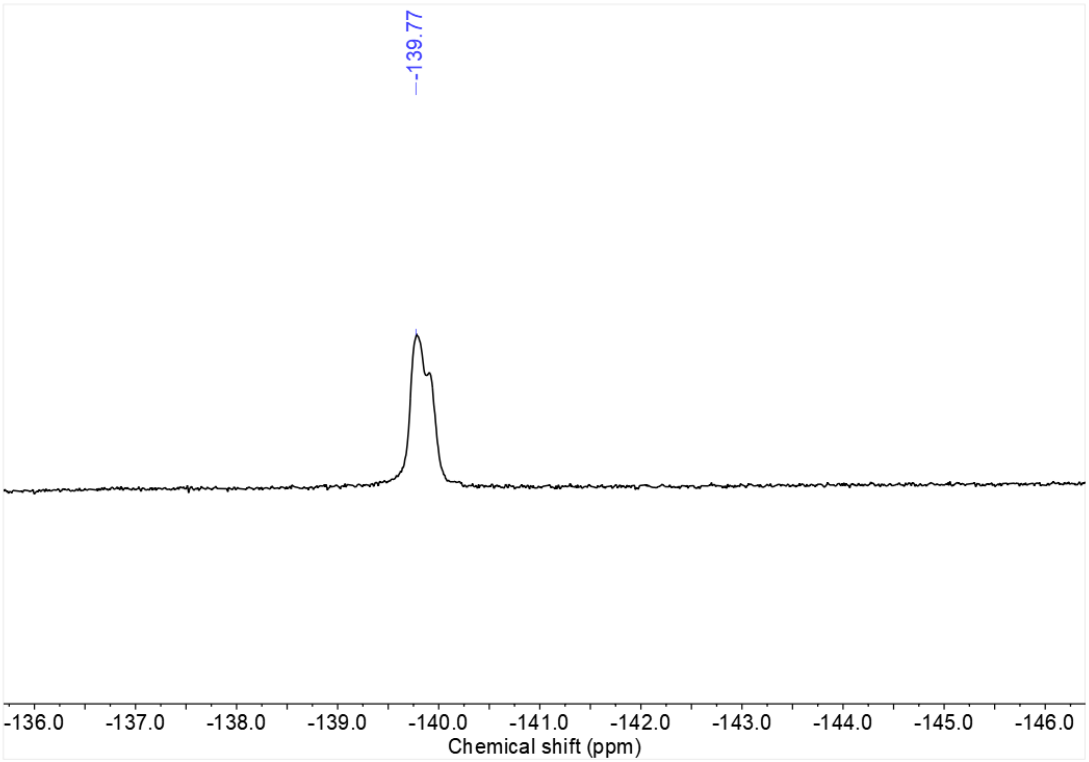

Fig. S62 $^{19}F\{^{1}H\}$ NMR spectrum of **8** in $CDCl_3$.

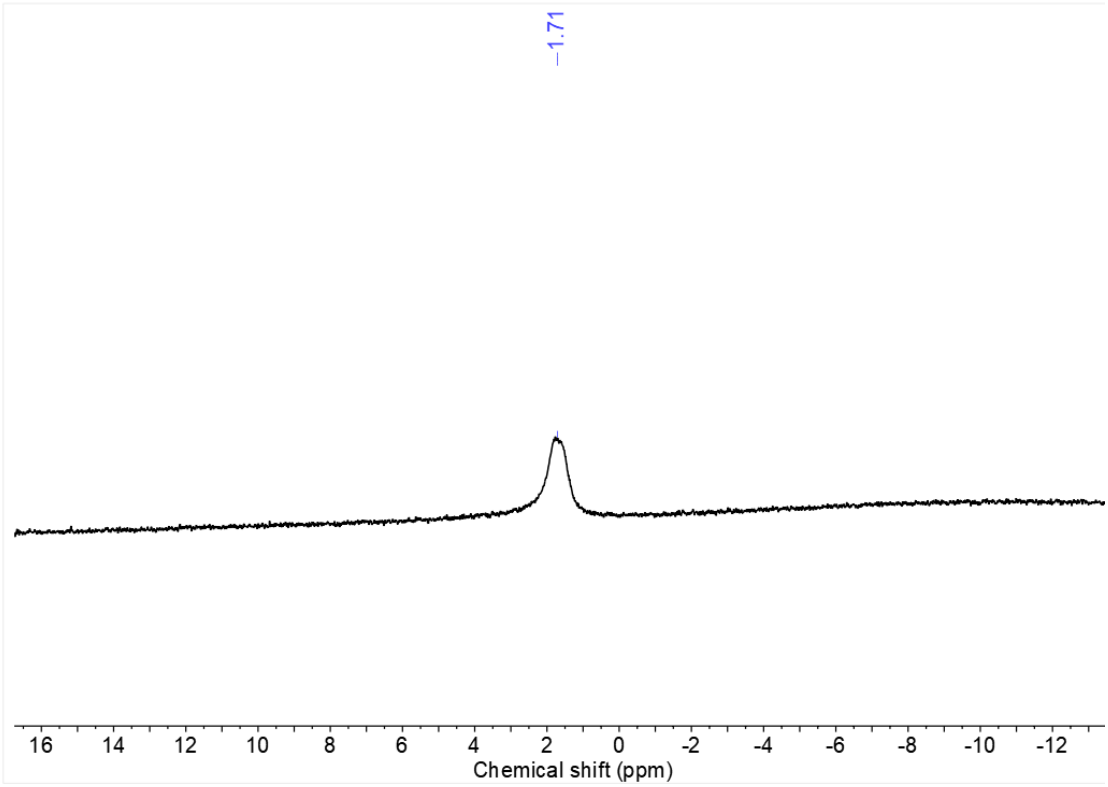

Fig. S63. $^{11}B\{^{1}H\}$ NMR spectrum of **8** in $CDCl_3$.

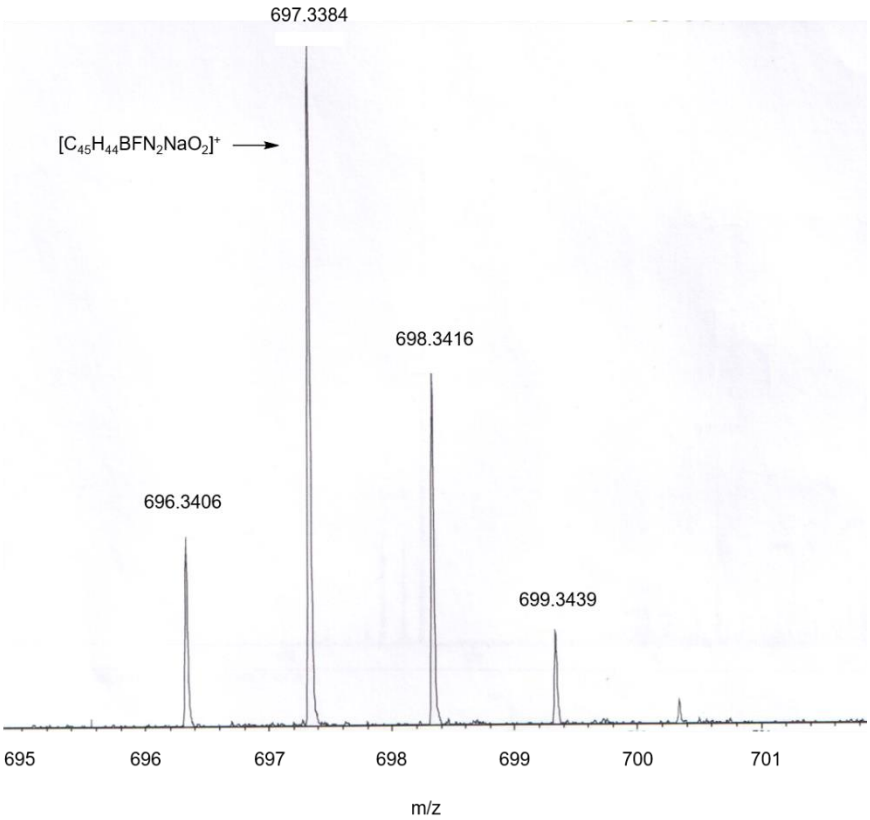

Fig. S64. HR-ESI mass spectrum of **8**.

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