Electronic Supplementary Information

For

Introducing an orthogonally polarized electron-rich alkene: synthesis of a zwitterionic boron-containing *π*-conjugated system

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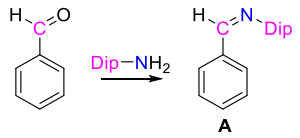
General Considerations

All experiments were carried out under an argon atmosphere using standard Schlenk techniques or in a PL-HE-2GB Innovative Technology GloveBox and MBraun Unilab SP GloveBox. Hexane and pentane were dried by PS-MD-5 Innovative Technology solvent purification system. THF and Benzene were dried and distilled over sodium under argon. Acetonitrile was dried and distilled over CaH_2 under argon. 1,4-Dibromobenzene (Sigma Aldrich), potassium (Sigma Aldrich)), *n*BuLi (Hychem Laboratories), MeOTf (Sigma Aldrich) were commercially purchased and used as are. *N*-Heterocyclic carbene **2** was synthesized following a literature known procedure reported by Kuhn *et al*.[S1] THF-d_8 and C_6D_6 were dried and distilled over potassium under argon. $CDCl_3$ and CD_3CN were dried and distilled over CaH_2 under argon. NMR spectra were recorded on a BrukerNanoBay 300 MHz NMR spectrometer. ^1H and $^{13}C\{^1H\}$ NMR spectra were referenced to the peaks of residual protons of the deuterated solvent (^1H) or the deuterated solvent itself ($^{13}C\{^1H\}$). $^{19}F\{^1H\}$ NMR spectra were referenced to external tol-CF_3.

Elemental analyses of **A**, **1**, **3**, **5**, **6**, **B**, **C**, **D**, and **7** were performed on an Elementar vario MICRO cube elemental analyzer. Melting points were determined in closed NMR tubes under argon atmosphere and are uncorrected. Electrochemical measurements were performed using a METROHM PGStat 204 potentiostat/galvanostat apparatus controlled by the software NOVA 2.1.4 in an argon glove box. A standard three-electrode cell configuration was employed using a glassy carbon disc electrode (d = 3 mm) as working electrode, a platinum wire counter electrode, and a platinum wire serving as pseudo-reference electrode. The redox potentials were referenced to the ferrocene (Fc) / ferrocenium (Fc^+) redox couple. The performed electrochemical methods were cyclic voltammetry (at various scan rates) and differential pulse voltammetry (DPV) (step: 5 mV; modulation amplitude: 25 mV; modulation time: 0.05 s; interval time: 0.5 s). The electrochemical measurements were undertaken at room temperature by dissolving ca. 1.0×10^{-5} mol of analyte in 10 mL THF containing 0.1 M tetrabutylammonium hexafluorophosphate. HRMS of **3** and **8** were measured on LCMS QTOF 6545B (Agilent Technologies) using electrospray ionization (ESI). EPR measurements at the X-band (9.38 GHz) were carried out using a Bruker ELEXSYS E580 CW EPR spectrometer equipped with an Oxford Instruments helium cryostat (ESR900) and a MercuryiTC temperature controller. The spectral analysis was performed using MATLAB 8.6.0.267246 (R2015b) and the Optimization toolbox. The spectral simulations were performed using MATLAB 9.8.0.1323502 (R2020a) and the EasySpin 5.2.28 toolbox.[S2]

Experimental Details and Analytical Data

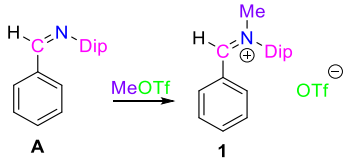
Synthesis of A



A

2,6-Diisopropylaniline (12.928 mL, 103.62 mmol) was added dropwise to a MeOH solution of benzaldehyde (9.614 mL, 94.2 mmol, in 200 mL of MeOH) and then the reaction mixture was stirred for 24 hrs at room temperature. Subsequently all the volatiles were removed under vacuum using a rotary evaporator and the obtained yellow oil was dissolved in 120 mL of DCM. The organic phase was washed with water (3 X 40 mL) and dried over Na_2SO_4. After removing all the volatiles, the resulting yellow dense oil was crystalized by addition of 60 mL of DCM/MeOH (2:1) at −30 °C overnight. The title compound **A** was isolated as yellow crystals. **Yield:** 18.25 g (73 %).[S3] **M.P.:** 63 °C. **^{1}H NMR** (300 MHz, CDCl3, 298): δ = 8.25 (s, 1H, C*H*O), 7.97 (d, $^3J_{(H,H)}$ = 3.18 Hz, 2H, Ph-*H*), 7.57 (m, 3H, Ph-*H*), 7.23-7.16 (m, 3H, Dip-*H*), 3.03 (sept, $^3J_{(H,H)}$ = 6.72 Hz, 2H, Dip-C*H*(CH_3)$_2$), 1.22 (d, $^3J_{(H,H)}$ = 6.84 Hz, 12H, Dip-CH(C*H*$_3$)$_2$) ppm. **^{13}C{^{1}H} NMR** (75.4 MHz, $CDCl_3$,298 K) δ = 162.0 (CH), 149.3 (q), 137.6 (q), 136.1 (q), 131.5 (CH), 128.9 (CH), 128.6 (CH), 124.1 (CH), 123.0 (CH), 28.0 (CH), 23.5 (CH_3) ppm. **Elemental Analysis (%):** calculated for $C_{19}H_{23}N$: C 85.99, H 8.74, N 5.28; found C 85.43, H 8.93, N 5.15.

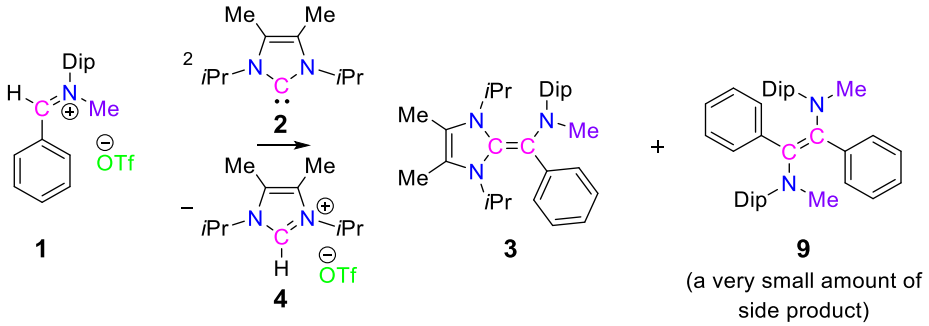
Synthesis of 1



A 1

A precooled (−78 °C) hexane solution of MeOTf (2.225 g, 13.56 mmol, in 15 mL hexane) was added to a precooled (−78 °C) hexane solution of **A** (3.00 g, 11.3 mmol, in 15 mL of hexane). Then the reaction mixture was stirred for 1 hr at −78 °C and after that slowly warmed up to room temperature while stirred overnight. Subsequently, the resulting white precipitate was filtered off, washed with hexane (2 × 10 mL) and dried under vacuum to obtain pure **1**. **Yield:** 4.28 g (88 %). **M.P.:** 140 °C. **^{1}H NMR** (300 MHz, $CDCl_3$, 298 K): δ = 9.97 (s, 1H, C*H*O), 7.70-7.26 (m, 2H, Ph-*H*), 7.45-7.40 (m, 6H, Ph-*H*, Dip-*H*), 4.20 (s, 3H, NC*H*$_3$), 3.03 (sept, $^3J_{(H,H)}$ = 6.51 Hz, 2H, Dip-C*H*(CH_3)$_2$), 1.30 (d, $^3J_{(H,H)}$ = 6.60 Hz, 6H, Dip-CH(C*H*$_3$)$_2$), 0.92 (d, $^3J_{(H,H)}$ = 6.57 Hz, 6H, Dip-CH(C*H*$_3$)$_2$) ppm. **^{13}C{^{1}H} NMR** (75.4 MHz, $CDCl_3$,298 K) δ = 175.0 (CH), 141.7 (q), 138.6 (CH), 136.1 (q), 135.4 (CH), 132.3 (CH), 129.9 (CH), 126.7 (CH), 122.9 (q), 118.6 (CH), 53.6 (CH_3), 28.5 (CH), 24.5 (CH_3), 24.8 (CH_3), 23.7 (CH_3) ppm. **^{19}F{^{1}H} NMR** (282.2 MHz, $CDCl_3$,298 K) δ = –78.32 ppm.

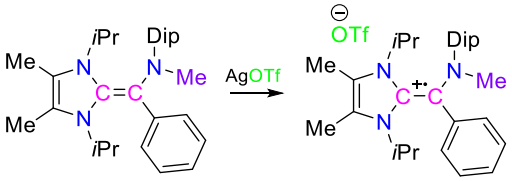
Synthesis of 3



A precooled (−78 °C) THF solution of **2** (2.10 g, 11.60 mmol, in 40 mL THF) was added to a precooled (−78 °C) THF solution of **1** (2.50 g, 5.82 mmol, in 80 mL THF) by cannula. Then the reaction mixture was stirred for 1 hr at −78 °C and after that slowly warmed up to room temperature while stirred overnight. Subsequently, after removing all volatiles the resulting crude mixture was extracted with hot hexane (3 X 100 mL). Then all the combined filtrates were reduced to about 200 mL and kept at room temperature overnight to obtain the title compound **3** as dark red cubic crystals suitable for single crystal X-ray diffraction. **Yield:** 1.418 g (65 %). **M.P.:** 152 °C (decomp.). **^{1}H NMR** (300 MHz, C_6D_6, 298): δ = 7.24 (t, $^3J_{(H,H)}$ = 6.67 Hz, 2H, Ph-*H*), 7.03 (br. s, 3H, Ph-*H*), 6.42 (t, $^3J_{(H,H)}$ = 6.45 Hz, 1H, Dip-*H*), 6.32 (br. s, 2H, Dip-*H*), 4.93 (t, $^3J_{(H,H)}$ = 6.45 Hz, 2H, *i*Pr$_2$Me$_2$NHC-C*H*(CH$_3$)$_2$), 3.60 (br. s, 2H, Dip-C*H*(CH$_3$)$_2$), 3.35 (s, 3H, NC*H*$_3$), 3.35 (s, 3H, NC*H*$_3$), 1.55 (s, 6H, *i*Pr$_2$*Me*$_2$NHC), 1.14 (br. s, 12H, *iPr*$_2$Me$_2$NHC), 0.88 (br. s, 12H, Dip-CH(C*H*$_3$)$_2$) ppm. **^{13}C{^{1}H} NMR** (75.4 MHz, C_6D_6, 298 K): δ = 153.0 (PhC=*C*N), 147.3 (q), 146.7 (q), 145.5 (q), 128.5 (CH), 123.8 (CH), 123.7 (CH), 123.2 (q), 112.1 (CH), 107.7(CH), 70.6 (Ph*C*=CN), 50.5 (CH), 40.2 (CH$_3$), 27.7 (CH), 24.3 (CH$_3$), 20.9 (CH$_3$), 9.5 (CH$_3$) ppm. **UV/Vis (THF):** λ_{max} (ε) = 317 (1140), 403 (1040) nm (Lmol^{-1}cm^{-1}). **Elemental Analysis (%):** calculated for $C_{31}H_{45}N_3$: C 80.99, H 9.87, N 9.14; found C 81.12, H 10.06, N 9.09. **HRMS (ESI+):** (m/z) calculated for $C_{31}H_{46}N_3$ ([M+H]$^+$): 460.3686, Found: 460.3680.

After concentrating the filtrate to about 80 mL and keeping it overnight at room temperature few colourless crystals had formed. Studying these by the NMR and X-ray diffraction revealed the formation of **9** as the side product (it was not possible to calculate the yield of the product as it was so small in amount). The formation of **9** indicates that *N*-heterocyclic carbene **2** act as a base. Previously this kind of dimerization was known using LiN(SiMe$_3$)$_2$ as a base.[S4] **^{1}H NMR** (300 MHz, C_6D_6, 298): δ = 7.47 (m, 4H, Ph-*H*), 7.03 (m, 4H, Ph-*H,*), 6.89 (m, 8H, Ph-*H*), 3.86 (d, $^3J_{(H,H)}$ = 5.76 Hz, 4H, Dip-C*H*(CH$_3$)$_2$), 2.70 (s, 6H, NC*H*$_3$), 3.35 (s, 3H, NC*H*$_3$), 1.55 (s, 6H, *i*Pr$_2$*Me*$_2$NHC), 1.26 (br. d, $^3J_{(H,H)}$ = 42.15 Hz, 24H, Dip-CH(C*H*$_3$)$_2$) ppm. **^{13}C{^{1}H} NMR** (75.4 MHz, C_6D_6, 298 K): δ = 146.9 (Ph*C*−CH(CH$_3$)$_2$), 144.3 (Ph*C*−N), 140.5 (Ph*C*−C), 132.0 (CH), 129.7 (N*C*=*C*N), 126.9 (CH), 126.7 (CH), 125.9 (CH), 123.7 (CH), 46.4 (CH$_3$), 27.8 (CH), 26.6 (CH$_3$), 23.1 (CH$_3$) ppm.

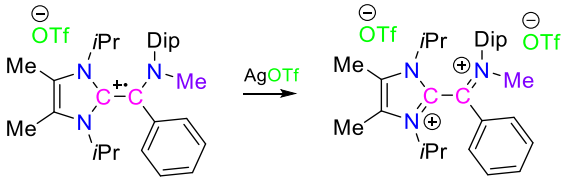
Synthesis of 5



3 **5**

About 30 mL of precooled (−40 °C) CH_3CN was added to a mixture of **3** (0.300 g, 0.65 mmol) and AgOTf (0.205 g, 0.80 mmol) at −40 °C. Then the reaction mixture was stirred for 30 minutes at −40 °C and after that slowly warmed up to room temperature while stirred overnight. Subsequently, the reaction mixture was filtered off over a celite pad and the resulting filtrate was dried under vacuum. After washing with pentane, the dark red powder crystalized by layering Et_2O on top of a saturated CH_3CN solution. After 2 days at −35 °C single crystals (also suitable for single crystal X-Ray diffraction studies) of the title compound **5** were obtained. **Yield:** 0.124 g (77 %). **M.P.:** > 200 °C (decomp.). **^{19}F{^{1}H} NMR** (282.2 MHz, THF-D8, 298 K) δ = −78.2 ppm. **UV/Vis (THF):** λ_{max} (ε) = 326 (2846) nm ($Lmol^{-1}cm^{-1}$). **Elemental Analysis (%):** calculated for $C_{32}H_{45}F_3N_3O_3S$: C 63.13, H 7.45, N 6.90, S 5.27; found C 63.40, H 7.36, N 6.98; S 4.99.

Synthesis of 6

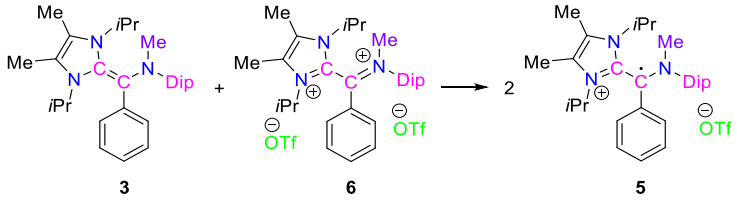


5 **6**

About 30 mL of precooled (−40 °C) CH_3CN was added to a mixture of **3** (0.300 g, 0.65 mmol) and AgOTf (0.410 g, 1.59 mmol) at −40 °C. Then the reaction mixture was stirred for 30 minutes at −40 °C and after that slowly warmed up to room temperature while stirred overnight. Subsequently, the reaction mixture was filtered off over a celite pad and the resulting filtrate was dried under vacuum. The resulting residue was crystalized by the slow evaporation of its acetone (50 mL) solution and resulting in pure compound **6**. Single crystals suitable for single crystal X-Ray diffraction studies were obtained by layering Et_2O on top of a saturated CH_3CN solution after two days at −35 °C. **Yield:** 0.124 g (25 %). **M.P.:** 204 °C. **^{1}H NMR** (300 MHz, CD_3CN, 298): δ = 8.00 (t, $^{3}J_{(H,H)}$ = 7.32 Hz, 1H, Ph-*H*), 7.84 (t, $^{3}J_{(H,H)}$ = 7.81 Hz, 1H, Ph-*H*), 7.67 (d, $^{3}J_{(H,H)}$ = 7.71 Hz, 2H, Ph-*H*), 7.60 (t, $^{3}J_{(H,H)}$ = 7.53 Hz, 2H, Ph-*H* and Dip-*H*), 7.07 (d, $^{3}J_{(H,H)}$ = 8.01 Hz, 2H, Dip-*H*), 4.25 (sept, $^{3}J_{(H,H)}$ = 7.53 Hz, 2H, Dip-C*H*$(CH_3)_2$), 4.08 (s, 3H, NC*H*$_3$), 2.58 (s, 6H, *i*Pr$_2$*Me*$_2$NHC), 3.35 (q, $^{3}J_{(H,H)}$ = 7.53 Hz, 2H, NHC-C*H*$(CH_3)_2$), 1.76 (d, $^{3}J_{(H,H)}$ = 6.87 Hz, 6H, Dip-CH(C*H*$_3)_2$), 1.49 (d, $^{3}J_{(H,H)}$ = 6.66 Hz, 6H, Dip-CH(C*H*$_3)_2$),, 1.39 (d, $^{3}J_{(H,H)}$ = 6.27 Hz, 6H, *i*Pr$_2$*Me*$_2$NHC), 1.00 (d, $^{3}J_{(H,H)}$ = 6.63 Hz, 6H, *i*Pr$_2$*Me*$_2$NHC) ppm. **^{13}C{^{1}H} NMR** (75.4 MHz,

CD_3CN,298 K) δ = 167.4 (q), 143.0 (CH), 140.6 (q), 137.8 (q), 135.4 (CH), 134.7 (q), 134.2 (CH), 132.3 (CH), 129.4 (q), 128.6(CH), 128.0 (q), 123.7 (q), 119.5 (q), 56.5 (CH), 55.2 (CH_3), 30.5 (CH), 24.1 (CH_3), 23.1 (CH_3), 20.66 (CH_3), 20.64 (CH_3), 11.0 (CH_3) ppm. **$^{19}F\{^1H\}$ NMR** (282.2 MHz, CD_3CN,298 K) δ = −79.3 ppm. **UV/Vis (THF):** λ_{max} (ε) = 317 (1118), 408 (389.4) nm ($Lmol^{-1}cm^{-1}$). **Elemental Analysis (%):** calculated for $C_{33}H_{44}F_6N_3O_6S_2$: C 52.37, H 5.86, N 5.55, S 8.47; found C 52.24, H 5.85, N 5.47, S 8.27.

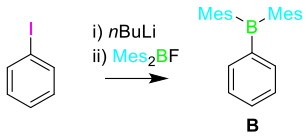
Comproportionation Reaction Between 3 and 6



3 6 5

In a 2 mL volumetric flask 0.606 mL (6.598 X 10^{-4} mM) of a stock solution of **3** with a concentration of 1.087 mM was mixed with 1 mL (6.598 X 10^{-4} mM) of a stock solution of **6** with a concentration of 0.6598 mM at room temperature. After gentle shacking the resulting solution a UV/Vis spectrum was recorded which indicates the formation of **5**.

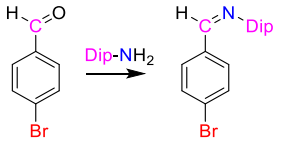
Synthesis of B



B

10 mL of *n*BuLi (16.00 mmol, 1.6 M *n*-hexane) was added dropwise to a solution of iodobenzene (1.366 mL, 12.25 mmol) in 40 mL THF at −78 °C. After completion of the addition, the resulting reaction mixture was stirred for one hour at −78 °C. Then the precooled (at −78 °C) THF solution of Mes_2BF (3.258 g, 12.25 mmol, in 20 mL THF) was added by cannula followed by stirring the reaction mixture for one hour at −78 °C. Afterwards the reaction mixture was allowed to warm up slowly to room temperature while stirred overnight. Subsequently all volatiles were removed and the resulting oily residue was dissolved in 60 mL ethyl acetate. The organic phase was washed with 3×30 mL H_2O and dried over anhydrous Na_2SO_4. After that all volatiles were removed under vacuum and the resulting yellow oily crude product was triturated with pentane to obtain the title compound **B** as fine white powder. **Yield:** 0.88 g (22 %). **^{1}H NMR** (300 MHz, $CDCl_3$, 298): δ = 7.54 (d, $^3J_{(H,H)}$ = 7.17 Hz, 2H, Ph-*H*), 7.47 (d, $^3J_{(H,H)}$ = 6.84 Hz, 1H, Ph-*H*), 7.36 (t, $^3J_{(H,H)}$ = 7.09 Hz, 1H, Ph-*H*), 6.85 (s, 4H, Mes-*H*), 2.33 (s, 6H, Mes-C*H*$_3$), 2.03 (s, 12H, Mes-*CH*$_3$) ppm.[S5]

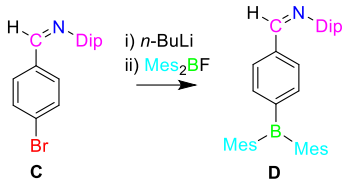
Synthesis of C



C

2,6-Diisopropylaniline (3.705 mL, 29.7 mmol) was added dropwise to a solution of 4-bromobenzaldehyde (5.00 g, 27.0 mmol) in 210 mL MeOH at room temperature and the reaction mixture was stirred overnight. The resulting yellow precipitate of compound **C** was collected by filtration. All the volatiles of the filtrate were removed under vacuum using a rotary evaporator and the resulting oily yellow residue was suspended in a minimal amount of methanol (40 mL). Immediately yellow crystalline solids of **C** were formed and collected. **Total Isolated Yield:** 6.074 g (65 %). **M.P.:** 99 °C. **^{1}H NMR** (300 MHz, CDCl3, 298): δ = 8.16 (s, 1H, C*H*O), 7.79 (d, $^{3}J_{(H,H)}$ = 7.98 Hz, 2H, Ph-*H*), 7.65 (d, $^{3}J_{(H,H)}$ = 7.95 Hz, 2H, Ph-*H*), 7.18-7.12 (m, 3H, Dip-*H*), 2.95 (sept, $^{3}J_{(H,H)}$ = 6.76 Hz, 2H, Dip-C*H*$(CH_3)_2$), 1.18 (d, $^{3}J_{(H,H)}$ = 6.81 Hz, 12H, Dip-CH(C*H*$_3)_2$) ppm. **^{13}C{^{1}H} NMR** (75.4 MHz, $CDCl_3$,298 K) δ = 160.1 (CH), 149.0 (q), 137.5 (q), 134.9 (q), 132.1 (CH), 129.9 (CH), 126.0 (q), 124.3 (CH), 123.1 (CH), 28.0 (CH), 23.5 (CH_3) ppm. **Elemental Analysis (%):** calculated for $C_{19}H_{22}BrN$: C 66.28, H 6.44, N 4.07; found C 65.82, H 6.37, N 3.97.

Synthesis of D

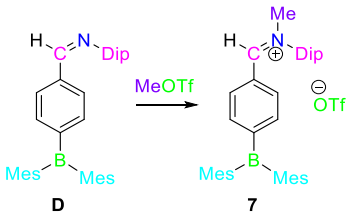


C **D**

13.05 mL *n*-BuLi (20.88 mmol, 1.6 M *n*-hexane) was added dropwise to a solution of **C** (6.00 g, 17.4 mmol) in 60 mL THF at −78 °C. After completion of the addition, the resulting reaction mixture was stirred for one hour at −78 °C. Then the precooled (at −78 °C) THF solution of Mes_2BF (4.666g, 17.4 mmol, in 40 mL THF) was added by cannula followed by stirring the reaction mixture for one hour at −78 °C. Afterwards the reaction mixture was allowed to warm up slowly to room temperature while stirred overnight. Subsequently all volatiles were removed and the resulting oily residue was dissolved in 60 mL DCM. The organic phase was washed with brine (50 mL) and water (2×30 mL) and dried over anhydrous Na_2SO_4. After that all volatiles were removed under vacuum and the resulting yellow oily crude product was triturated with pentane to obtain the title compound **D** as fine yellow powder. **Yield:** 6.800 g (76 %). **M.P.:** 196 °C **^{1}H NMR** (300 MHz, $CDCl_3$, 298): δ = 8.23 (s, 1H, C*H*O), 7.86 (d, $^{3}J_{(H,H)}$ = 7.11 Hz, 2H, Ph-*H*), 7.64 (d, $^{3}J_{(H,H)}$ = 7.50 Hz, 2H, Ph-*H*), 7.18-7.12 (m, 3H, Dip-*H*), 6.86 (s, 4H, Mes-*H*), 2.99 (sept, $^{3}J_{(H,H)}$ = 6.24 Hz, 2H, Dip-C*H*$(CH_3)_2$), 2.33 (s, 6H, Mes-C*H*$_3$), 2.05 (s, 12H, Mes-

CH$_3$), 1.18 (d, $^3J_{(H,H)}$ = 5.88 Hz, 12H, Dip-CH(C*H*$_3$)$_2$) ppm. **^{13}C{^{1}H} NMR** (75.4 MHz, $CDCl_3$, 298 K) δ = 162.2 (CH), 149.2 (q), 140.8 (q), 140.0 (q), 138.5 (q), 137.6 (q), 136.5 (CH), 128.3 (CH), 128.1 (CH), 128.0 (CH), 124.2 (CH), 123.0 (CH), 27.9 (CH), 23.6 (CH_3), 21.2 (CH_3). ppm. **Elemental Analysis (%):** calculated for $C_{37}H_{44}BN$ + 0.33 DCM: C 82.79, H 8.31, N 2.59; found C 82.75, H 8.51, N 2.68.

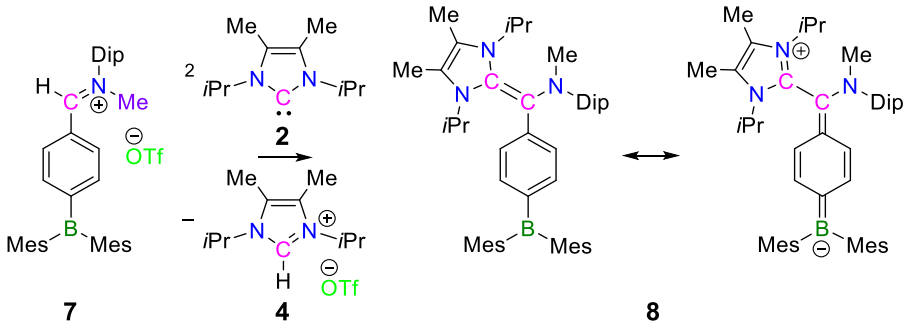
Synthesis of 7



D **7**

A precooled (at −78 °C) DCM solution of MeOTf (1.15 g, 7.00 mmol, in 30 mL DCM) was added to a precooled (at −78 °C) DCM solution of **D** (3.00 g, 5.84 mmol, in 70 mL DCM) by cannula. Then the reaction mixture was stirred for 1 hr at −78 °C and after that slowly warmed up to room temperature while stirred overnight. Subsequently, all volatiles were removed under vacuum and the yellowish crude product was suspended in hexane (50 mL). The resulting white precipitate was filtered off, washed with hexane (2 × 10 mL), and dried under vacuum to obtain pure **7**. Single crystals suitable for single crystal X-Ray diffraction studies were obtained by overlaying a saturated CH_3CN solution of **7** with Et_2O. **Yield:** 6.80 g (76 %). **M.P.:** 120 °C (96 °C decolorised). **^{1}H NMR** (300 MHz, $CDCl_3$, 298): δ = 10.02 (s, 1H, C*H*O), 7.59 (t, $^3J_{(H,H)}$ = 7.77 Hz, 1H, Dip-*H*), 7.47 (d, $^3J_{(H,H)}$ = 7.62 Hz, 2H, Dip-*H*), 7.37 (q, $^3J_{(H,H)}$ = 9.12 Hz, $^3J_{(H,H)}$ = 3.06 Hz, 4H, Ph-*H*), 6.79 (s, 4H, Mes-*H*), 4.20 (s, 3H, N*CH*$_3$), 2.81 (sept, $^3J_{(H,H)}$ = 6.45 Hz, 2H, Dip-C*H*(CH_3)$_2$), 2.28 (s, 6H, Mes-C*H*$_3$), 1.80 (s, 12H, Mes-*CH*$_3$), 1.29 (t, $^3J_{(H,H)}$ = 7.35 Hz, 6H, Dip-CH(C*H*$_3$)$_2$), 0.89 (q, $^3J_{(H,H)}$ = 6.73 Hz, 6H, Dip-CH(C*H*$_3$)$_2$) ppm. **^{13}C{^{1}H} NMR** (75.4 MHz, $CDCl_3$, 298 K) δ = 175.1 (CH), 141.7 (q), 140.8 (q), 140.2 (q), 136.2 (q), 135.7 (CH), 134.4 (CH), 132.2 (CH), 128.6 (CH), 128.1 (q), 126.7 (CH), 53.5 (CH_3), 31.6 (CH_3), 28.5 (CH), 24.8 (CH_3), 23.7 (CH_3), 23.4 (CH_3), 22.6 (CH_3), 21.2 (CH_3), 14.1 (CH_3) ppm. **^{19}F{^{1}H} NMR** (282.2 MHz, $CDCl_3$,298 K): δ = −78.30 ppm. **Elemental Analysis (%):** calculated for $C_{39}H_{47}BF_3NO_3S$: C 69.12, H 6.99, N 2.07, S 4.73; found C 69.15, H 7.24, N 2.04, S 4.55.

Synthesis of 8



A precooled (−78 °C) THF solution of *i*Pr$_2$Me$_2$NHC (1.451 g, 8.05 mmol, in 40 mL THF) was added to a precooled (−78 °C) THF solution of **7** (2.728 g, 4.02 mmol, in 60 mL THF). Then the reaction mixture was stirred for 1 hr at −78 °C and after that slowly warmed up to room temperature while stirred overnight. Subsequently, all volatiles were removed under vacuum and the crude product was extracted with 150 mL benzene by filtering over a celite pad. **Yield:** 1.84 g (65 %). In the extracted product there is a minor amount of imidazolium salt **4** present. Subsequently, we obtained imidazolium salt free compound **8** by extracting it with boiling hot hexane. Single crystals suitable for single crystal X-Ray diffraction studies were obtained from a hot-saturated hexane solution of **8** at room temperature. **M.P.:** > 200 °C. **^{1}H NMR** (300 MHz, C_6D_6, 298): δ = 7.84 (d, $^3J_{(H,H)}$ = 7.17 Hz, 1H, Ph-*H*), 7.32 (d, $^3J_{(H,H)}$ = 7.62 Hz, 1H, Ph-*H*), 7.11 (m, 2H, Ph-*H*), 7.01 (m, 4H, Mes-*H*), 6.89-6.79 (m, 3H, Dip-*H*), 4.90-4.82 (m, 2H, NHC-C*H*(CH$_3$)$_2$), 4.40 (m, 1H, Dip-C*H*(CH$_3$)$_2$), 4.04 (m, 1H, Dip-C*H*(CH$_3$)$_2$), 3.22 (s, 3H, NC*H*$_3$), 2.67 (s, 6H, iPr$_2$*Me*$_2$NHC), 2.63 (s, 3H, *iPr*$_2$Me$_2$NHC), 2.54 (s, 3H, *iPr*$_2$Me$_2$NHC), 2.32 (d, $^3J_{(H,H)}$ = 5.37 Hz, 6H, *iPr*$_2$Me$_2$NHC), 1.50 (s, 3H, Mes-C*H*$_3$), 1.40 (d, $^3J_{(H,H)}$ = 4.80 Hz, 3H, Mes-*CH*$_3$), 1.32 (s, 3H, Mes-*CH*$_3$), 1.18 (d, $^3J_{(H,H)}$ = 5.91 Hz, 3H, Mes-*CH*$_3$),), 1.11-1.04 (m, 6H, Mes-*CH*$_3$), 0.92 (d, $^3J_{(H,H)}$ = 6.33 Hz, 3H, Dip-CH(C*H*$_3$)$_2$), 0.82 (d, $^3J_{(H,H)}$ = 6.54 Hz, 3H, Dip-CH(C*H*$_3$)$_2$), 0.30 (d, $^3J_{(H,H)}$ = 5.67 Hz, 3H, Dip-CH(C*H*$_3$)$_2$), 0.03 (d, $^3J_{(H,H)}$ = 5.82 Hz, 3H, Dip-CH(C*H*$_3$)$_2$) ppm. **^{13}C{^{1}H} NMR** (75.4 MHz, C_6D_6, 298 K) δ = 150.7 (PhC=*C*N), 150.3 (q), 146.3 (q), 145.5 (q), 144.9 (q), 141.4 (CH), 141.14 (q), 141.10 (q), 140.88 (q), 140.84 (q), 139.8 (CH), 134.9 (q), 134.8 (q), 128.2 (CH), 127.9 (CH), 127.8 (CH), 127.54 (CH), 127.47 (CH), 125.3 (CH), 124.5 (q), 124.0 (CH), 123.8 (CH), 123.7 (q), 109.9 (CH), 82.0 (Ph*C*=CN), 51.3 (CH), 50.9 (CH), 42.0 (CH), 31.6 (CH$_3$), 28.1 (CH), 27.4 (CH$_3$), 27.2 (CH), 26.9 (CH), 24.14 (CH$_3$), 24.1 (CH$_3$), 24.0 (CH$_3$), 23.4 (CH$_3$), 23.2 (CH$_3$), 22.7 (CH$_3$), 22.1 (CH$_3$), 21.7 (CH$_3$), 21.2 (CH$_3$), 21.0 (CH$_3$), 19.8 (CH$_3$), 19.1 (CH$_3$), 14.0 (CH$_3$), 9.1 (CH$_3$), 8.8 (CH$_3$), 7.7 (CH$_3$) ppm. **UV/Vis (THF):** λ_{max} (ε) = 505 (3350), nm (Lmol^{-1}cm^{-1}). **HRMS (ESI+):** (m/z) calculated for $C_{49}H_{67}BN_3$ ([M+H]$^+$): 708.5423, Found: 708.5446.

NMR Spectra

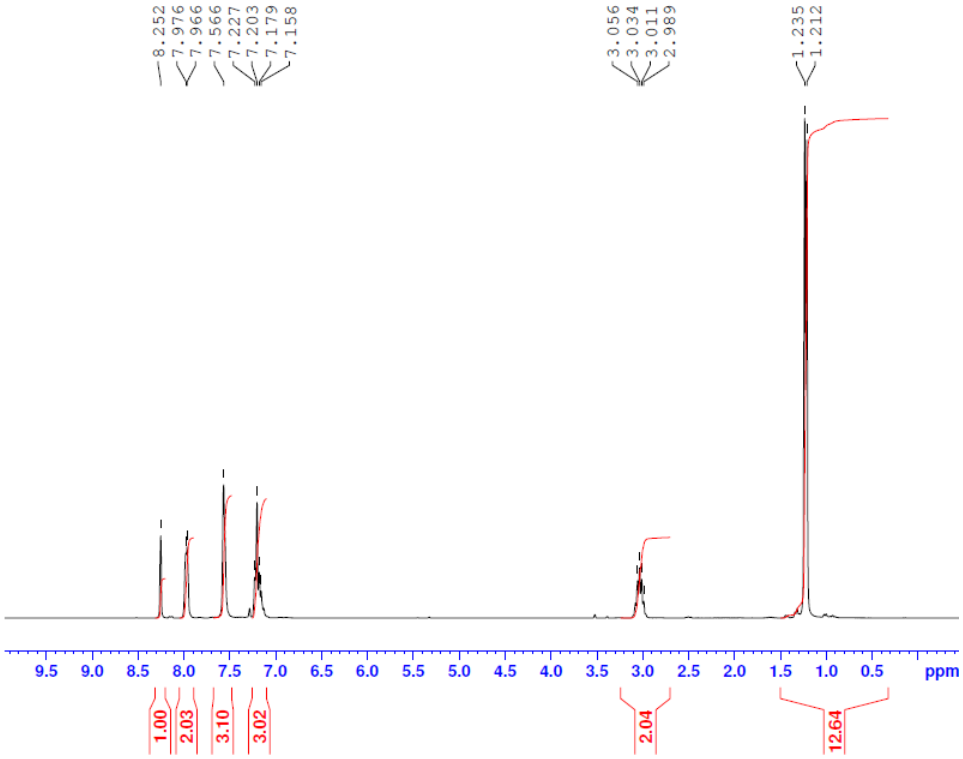


Fig. S1 ^{1}H NMR spectrum of **A** in $CDCl_3$ at room temperature.

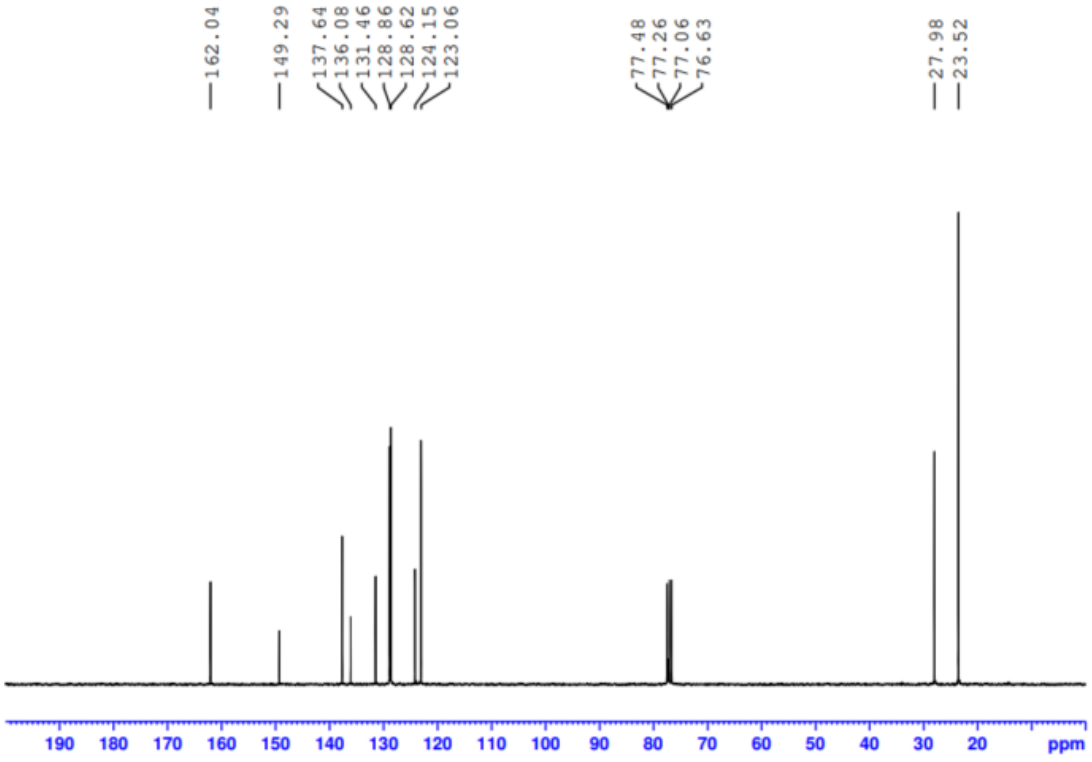


Fig. S2 $^{13}C\{^{1}H\}$ NMR spectrum of **A** in $CDCl_3$ at room temperature.

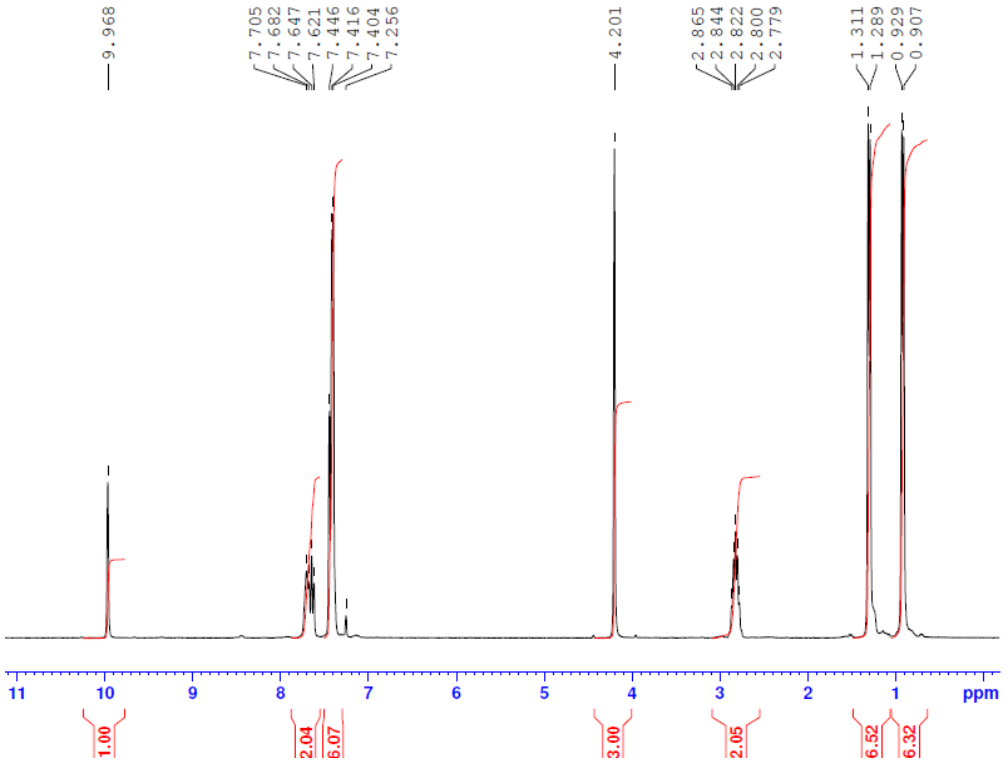


Fig. S3 ^{1}H NMR spectrum of **1** in $CDCl_3$ at room temperature.

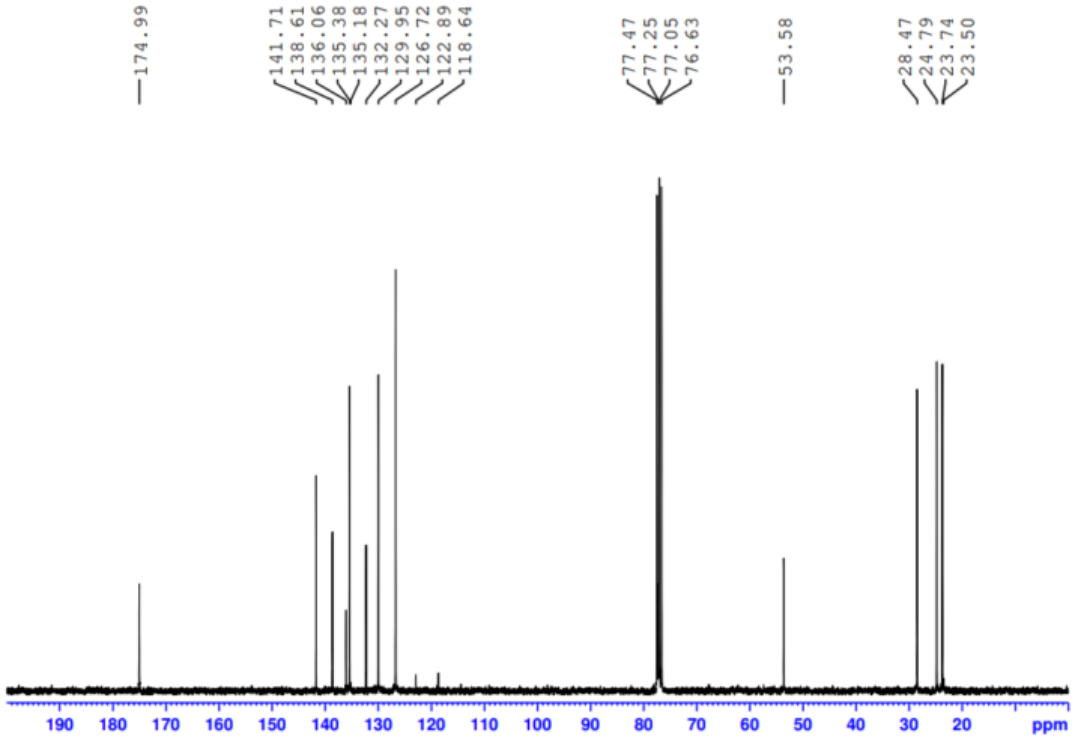


Fig. S4 $^{13}C\{^{1}H\}$ NMR spectrum of **1** in $CDCl_3$ at room temperature.

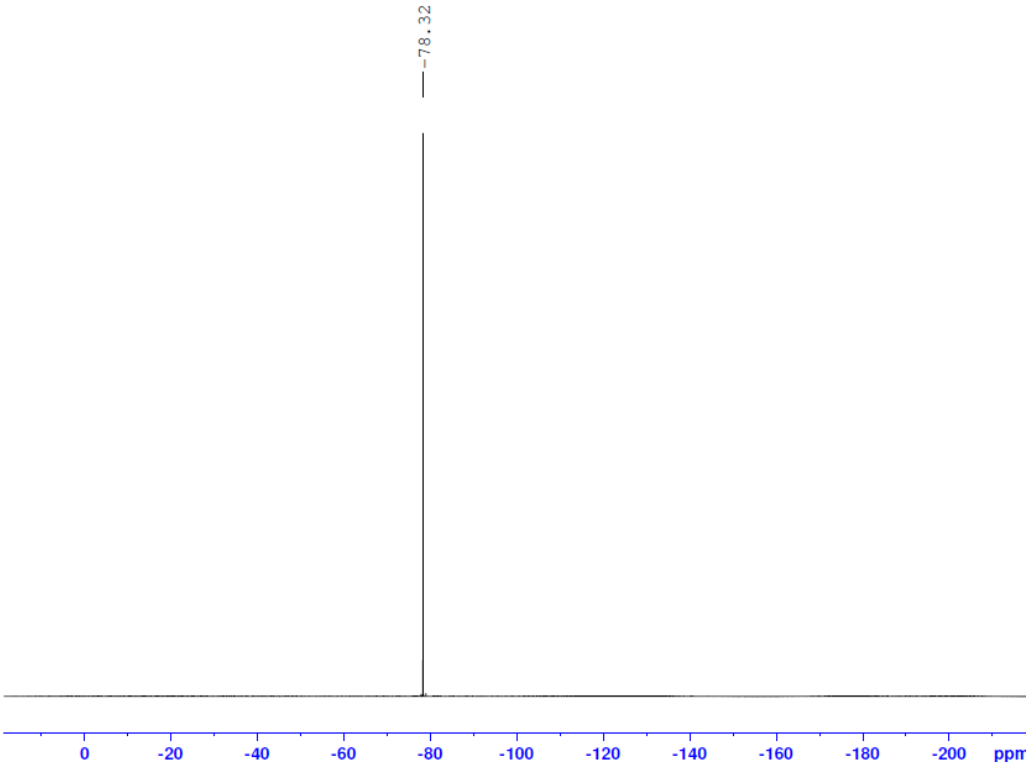


Fig. S5 $^{19}F\{^{1}H\}$ NMR spectrum of **1** in $CDCl_3$ at room temperature.

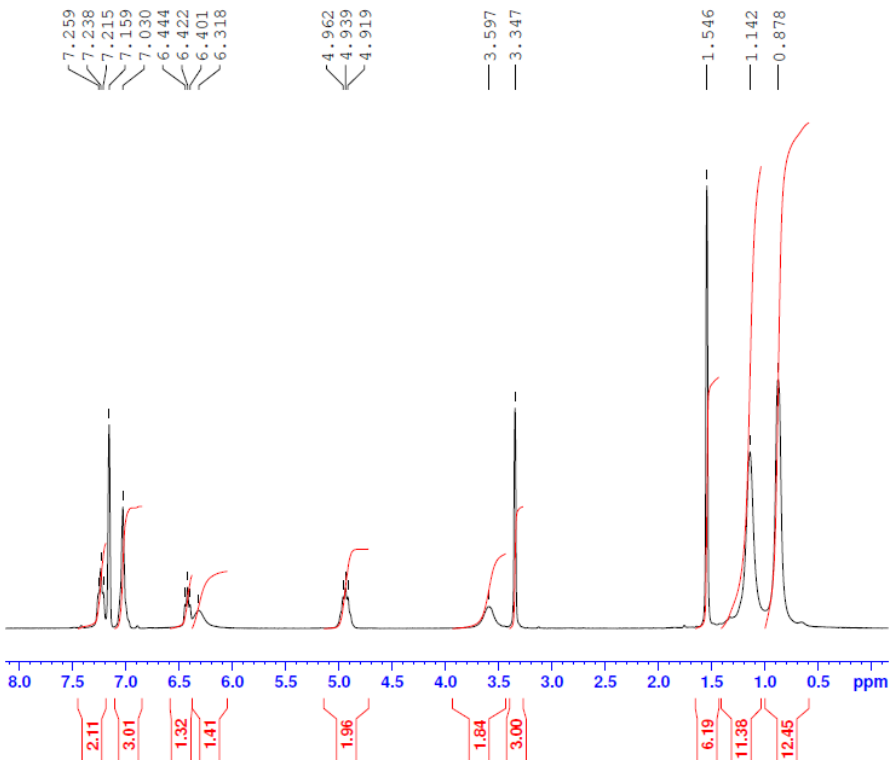


Fig. S6 ^{1}H NMR spectrum of **3** in C_6D_6 at room temperature.

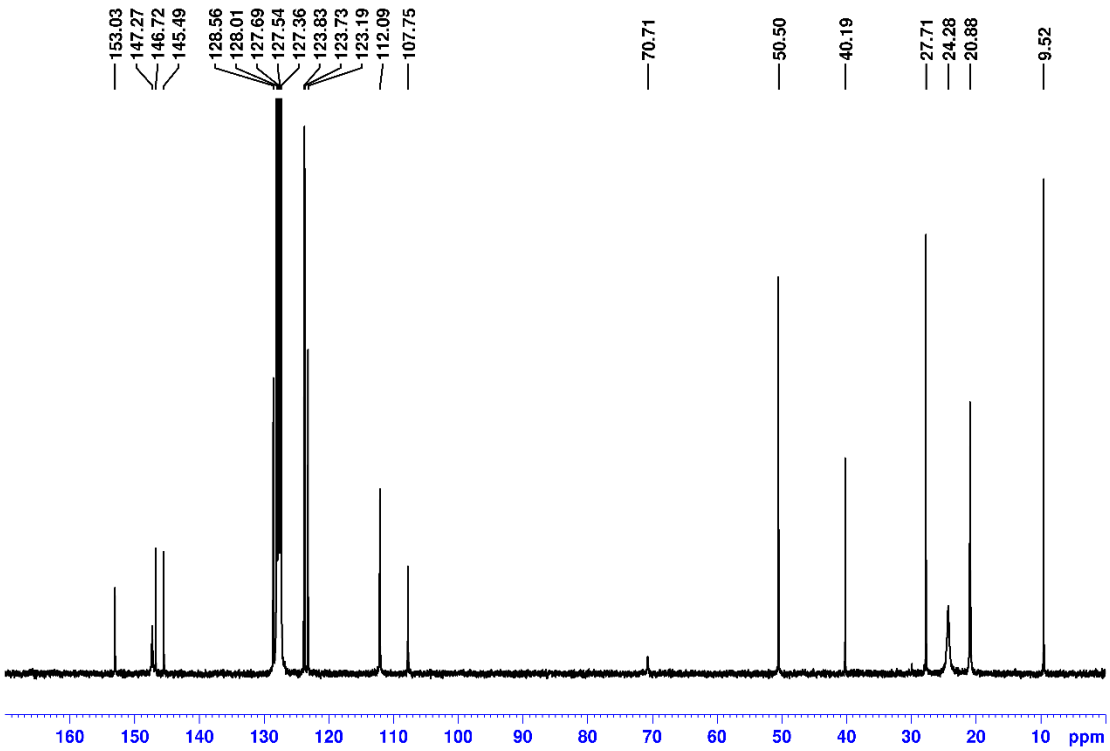


Fig. S7 $^{13}C\{^{1}H\}$ NMR spectrum of **3** in C_6D_6 at room temperature.

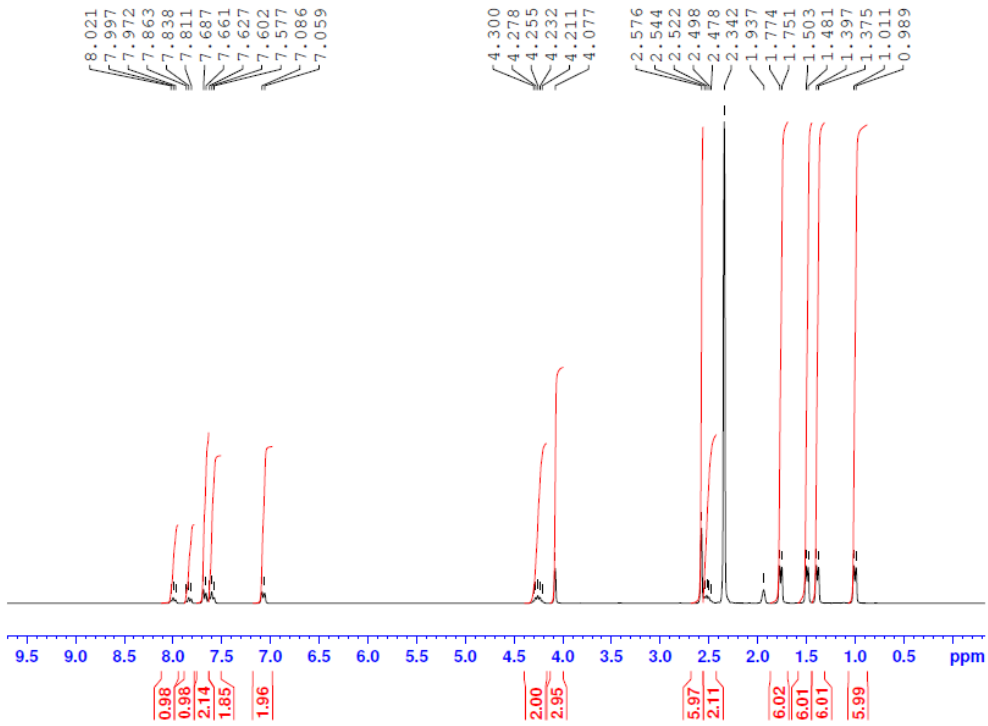


Fig. S8 ^{1}H NMR spectrum of **6** in CD_3CN at room temperature.

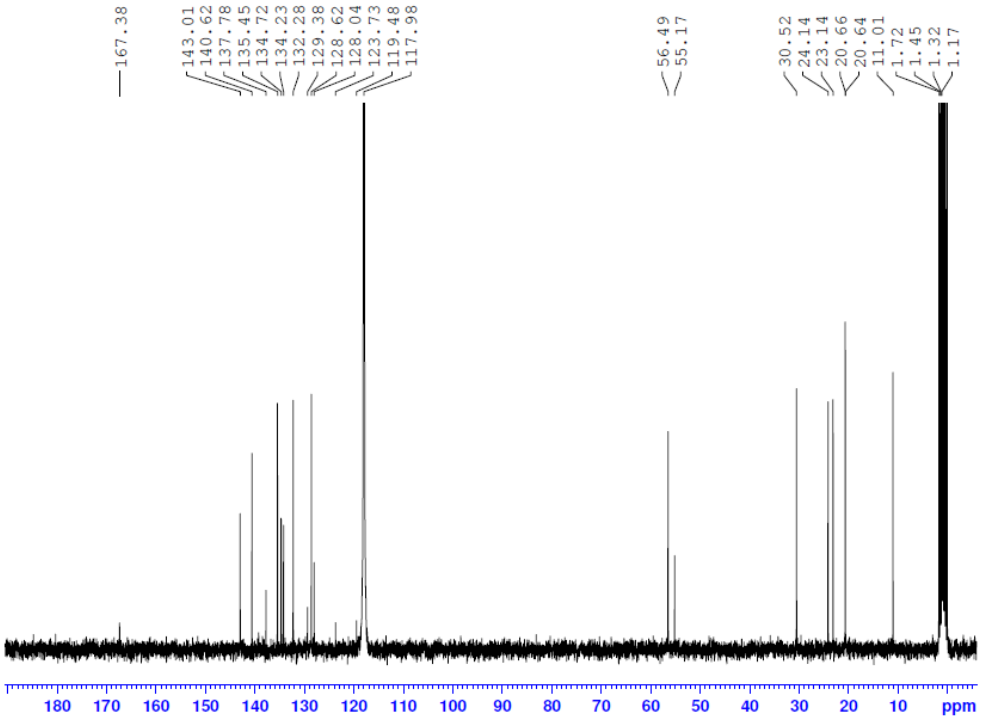


Fig. S9 $^{13}C\{^{1}H\}$ NMR spectrum of **6** in CD_3CN at room temperature.

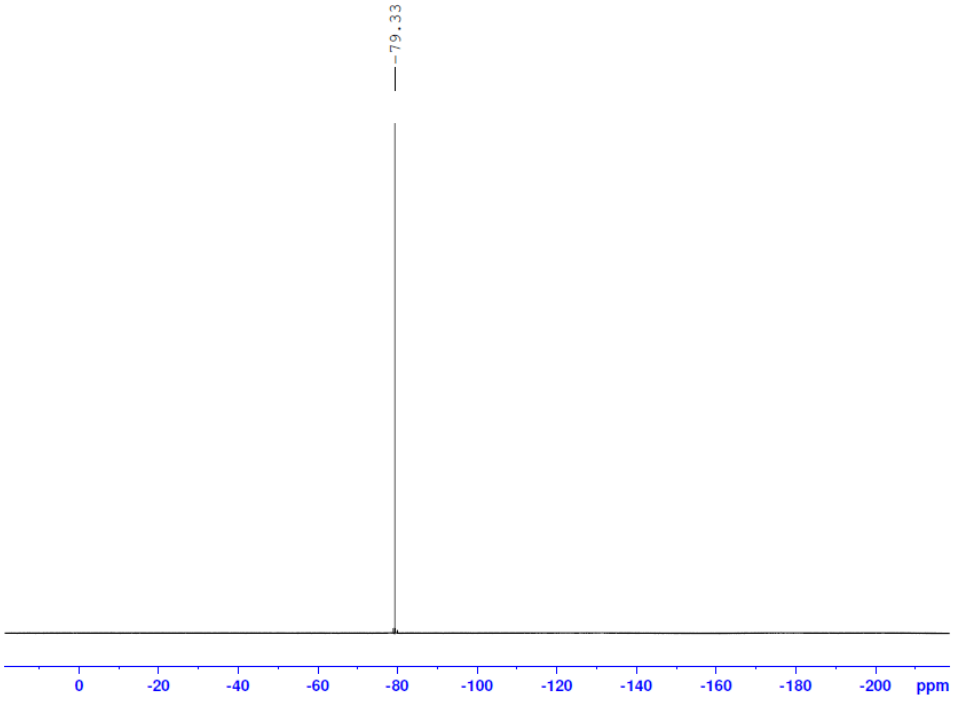


Fig. S10 $^{19}F\{^{1}H\}$ NMR spectrum of **6** in CD_3CN at room temperature.

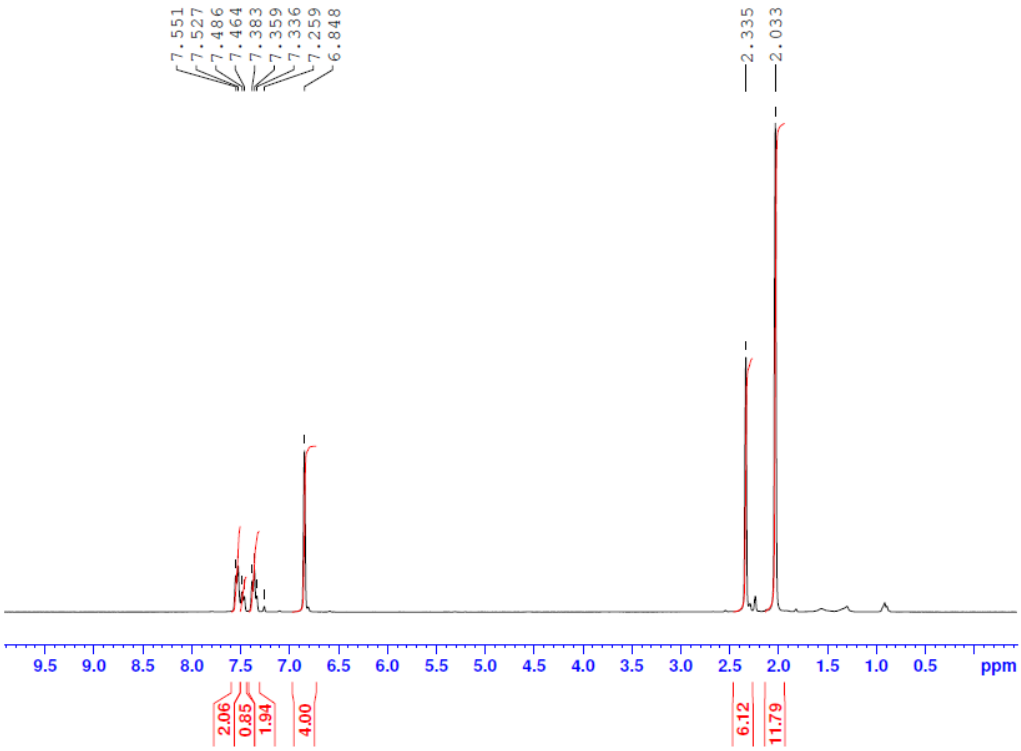


Fig. S11 ^{1}H NMR spectrum of **B** in $CDCl_3$ at room temperature.

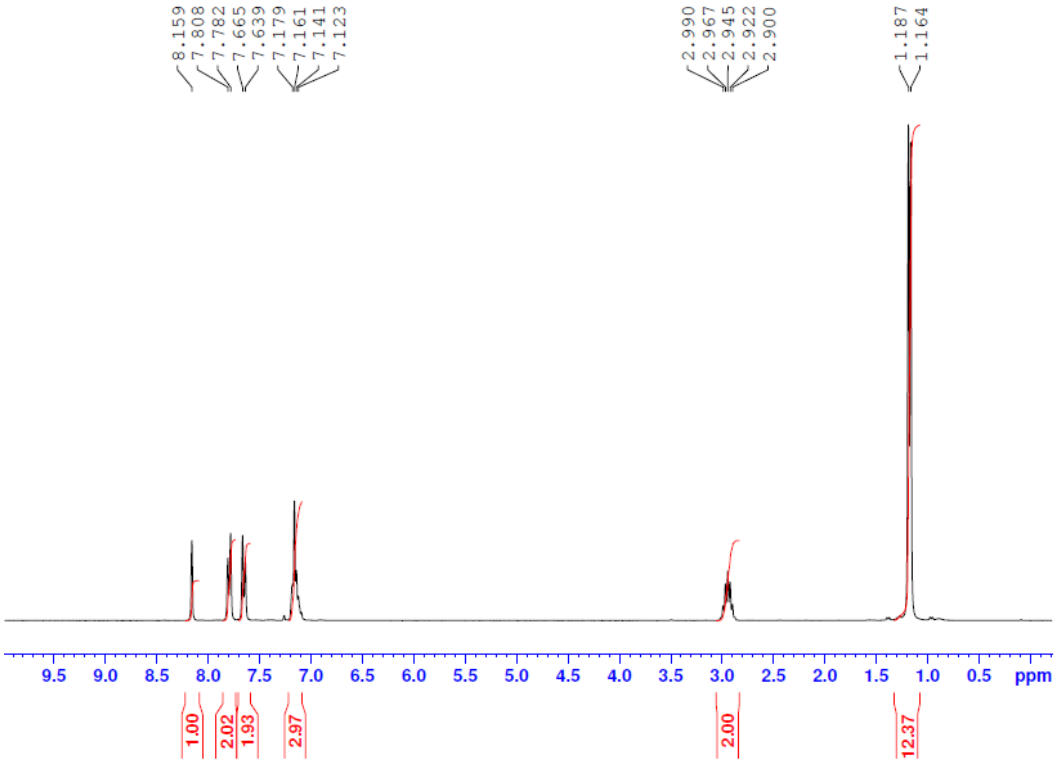


Fig. S12 ^{1}H NMR spectrum of **C** in $CDCl_3$ at room temperature.

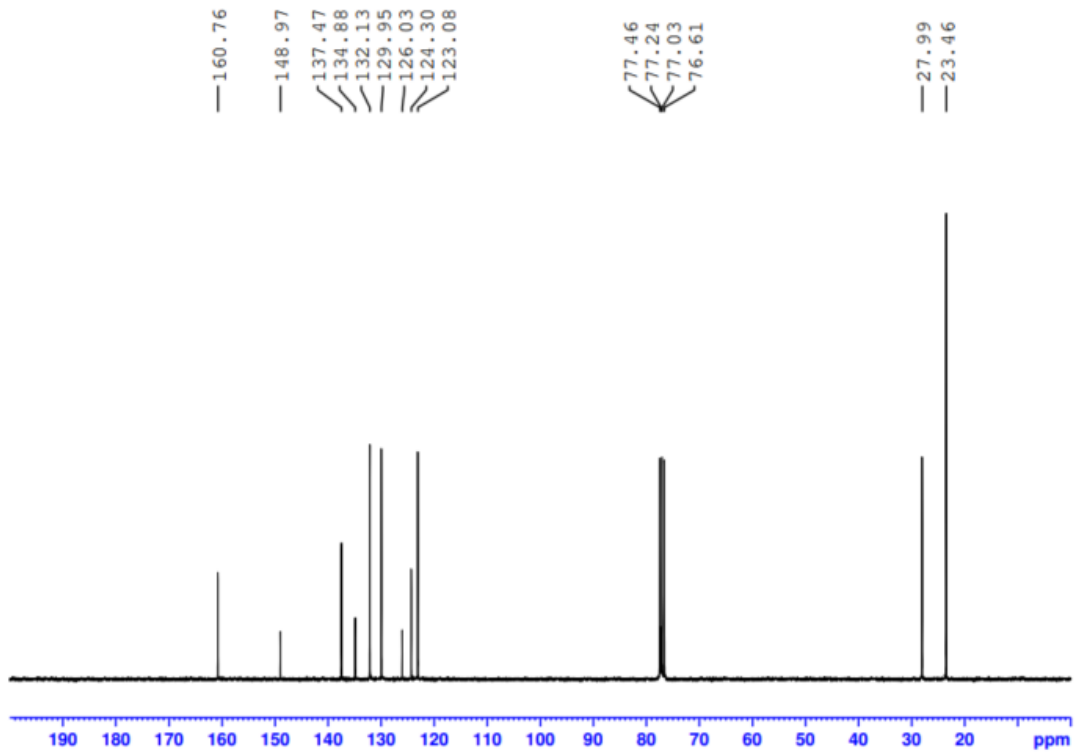


Fig. S13 $^{13}C\{^{1}H\}$ NMR spectrum of **C** in $CDCl_3$ at room temperature.

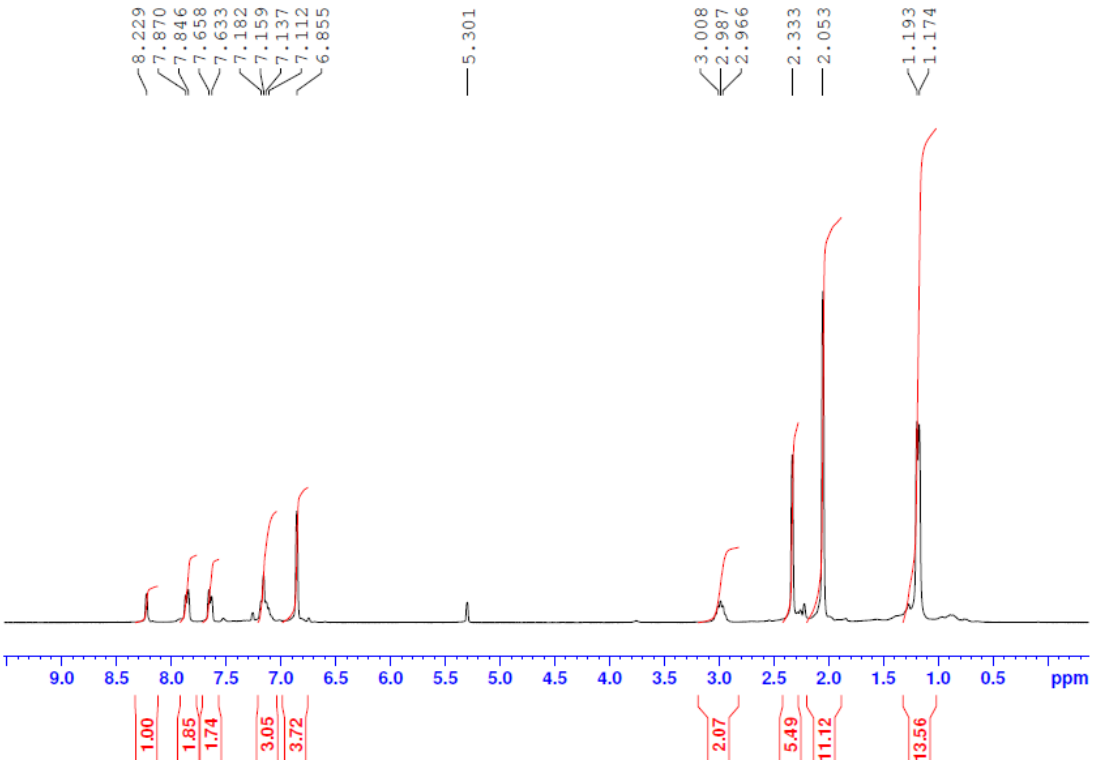


Fig. S14 ^{1}H NMR spectrum of **D** in $CDCl_3$ at room temperature.

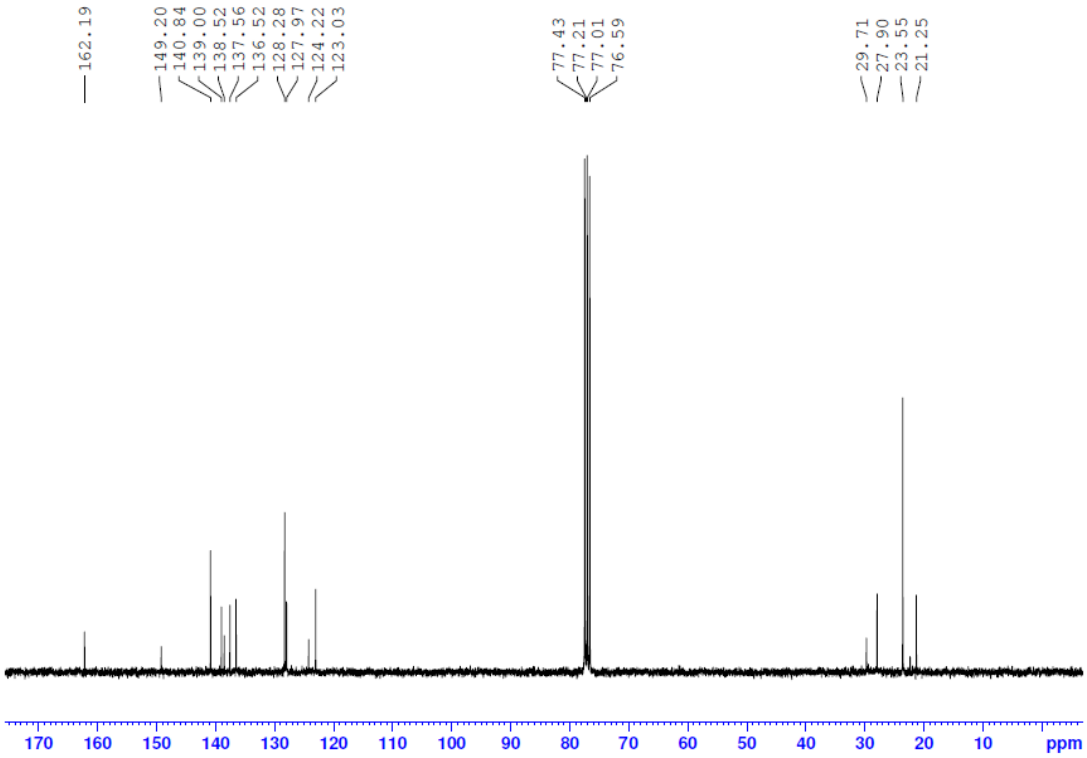


Fig. S15 $^{13}C\{^{1}H\}$ NMR spectrum of **D** in $CDCl_3$ at room temperature.

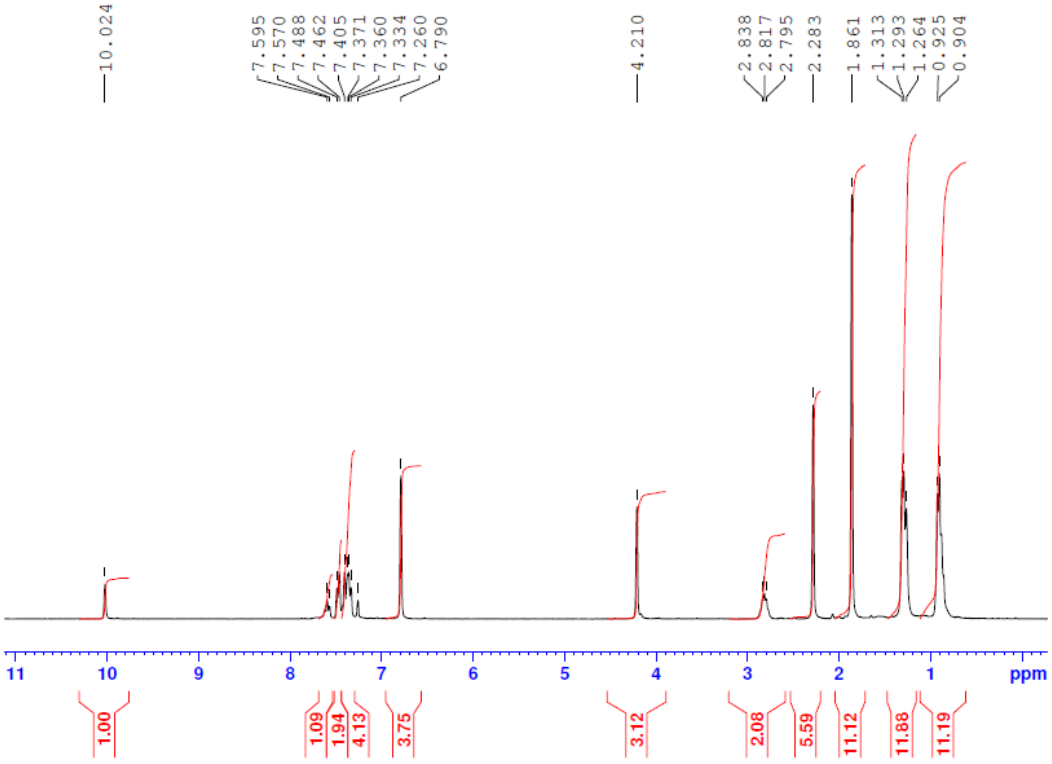


Fig. S16 ^{1}H NMR spectrum of **7** in $CDCl_3$ at room temperature.

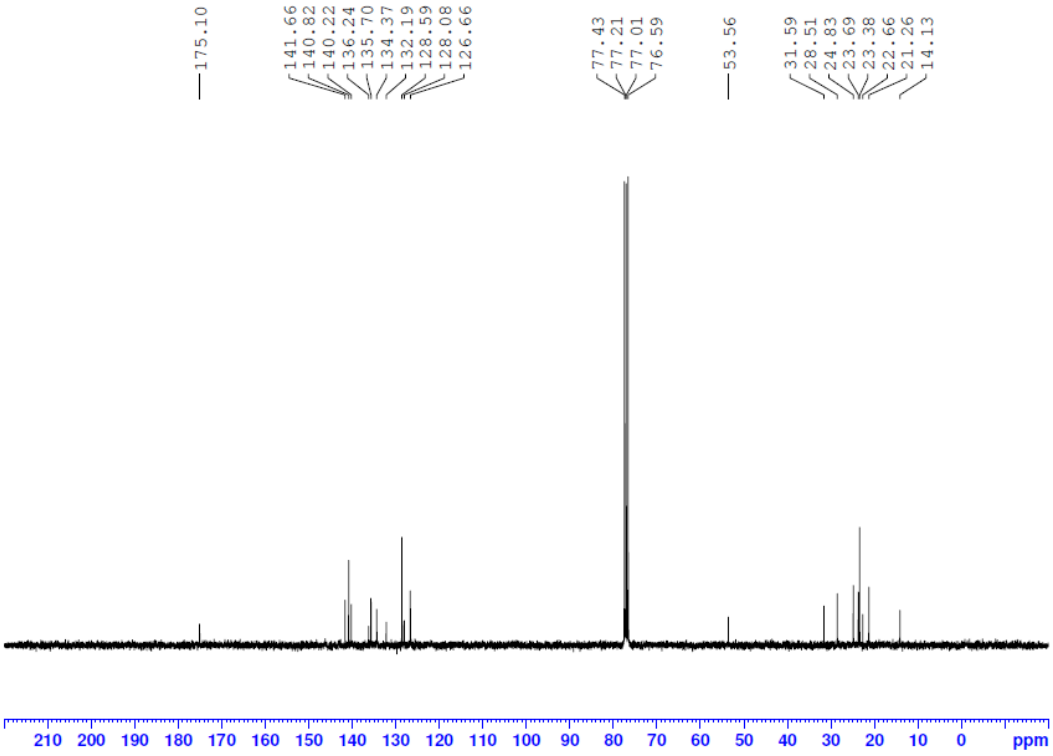


Fig. S17 $^{13}C\{^{1}H\}$ NMR spectrum of **7** in $CDCl_3$ at room temperature.

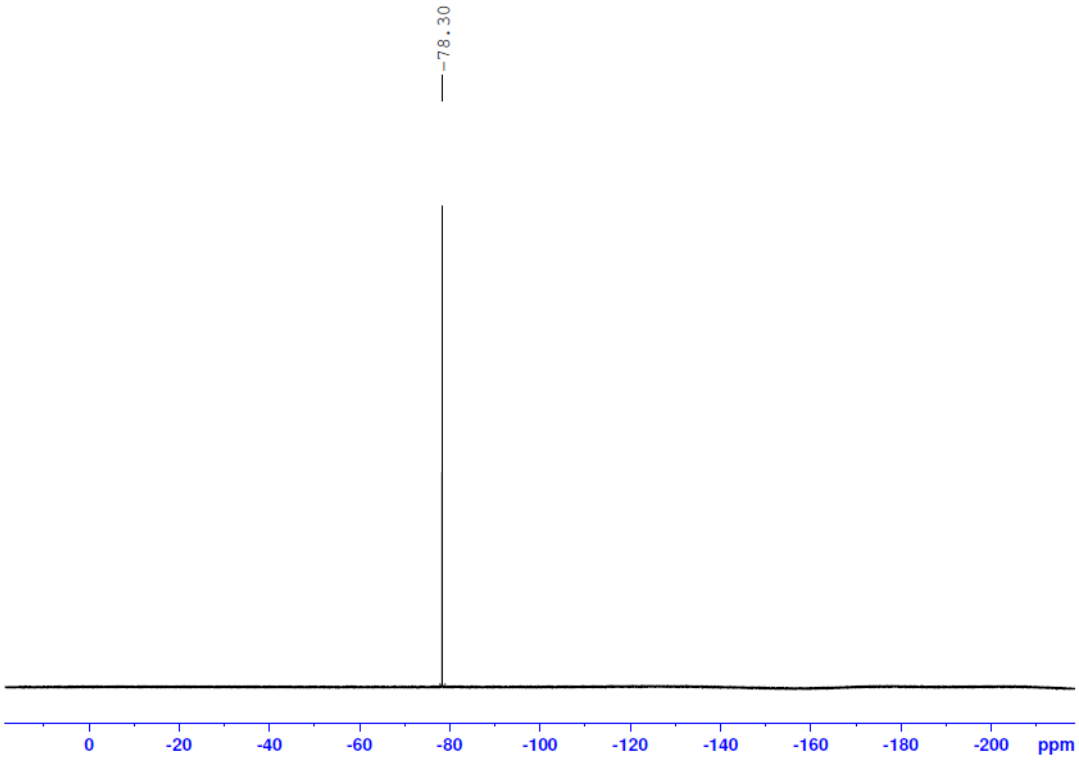


Fig. S18 $^{19}F\{^{1}H\}$ NMR spectrum of **7** in $CDCl_3$ at room temperature.

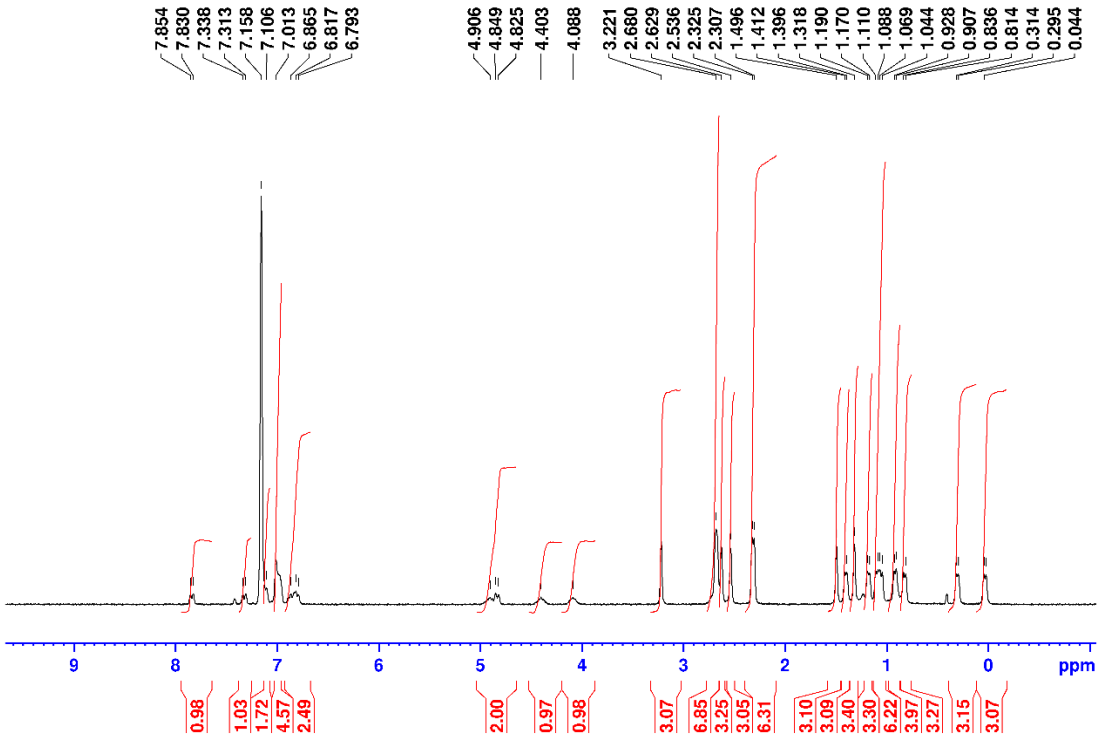


Fig. S19 ^{1}H NMR spectrum of **8** in C_6D_6 at room temperature.

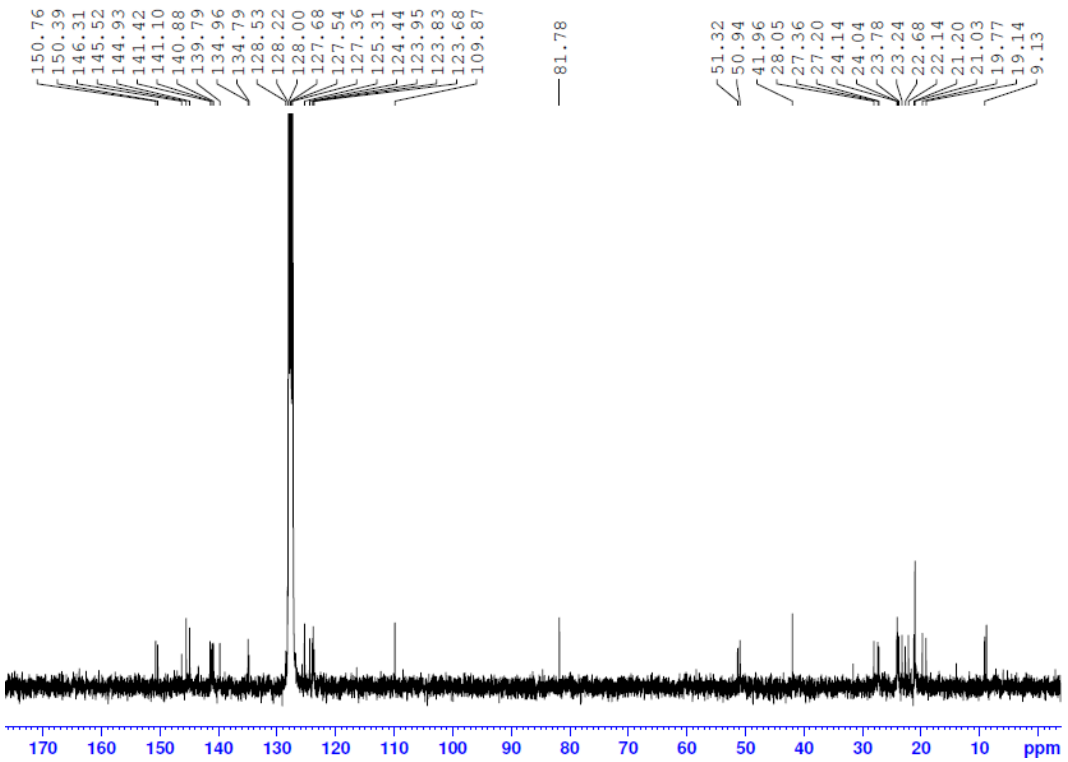


Fig. S20 ^{13}C{^{1}H} NMR spectrum of **8** in C_6D_6 at room temperature.

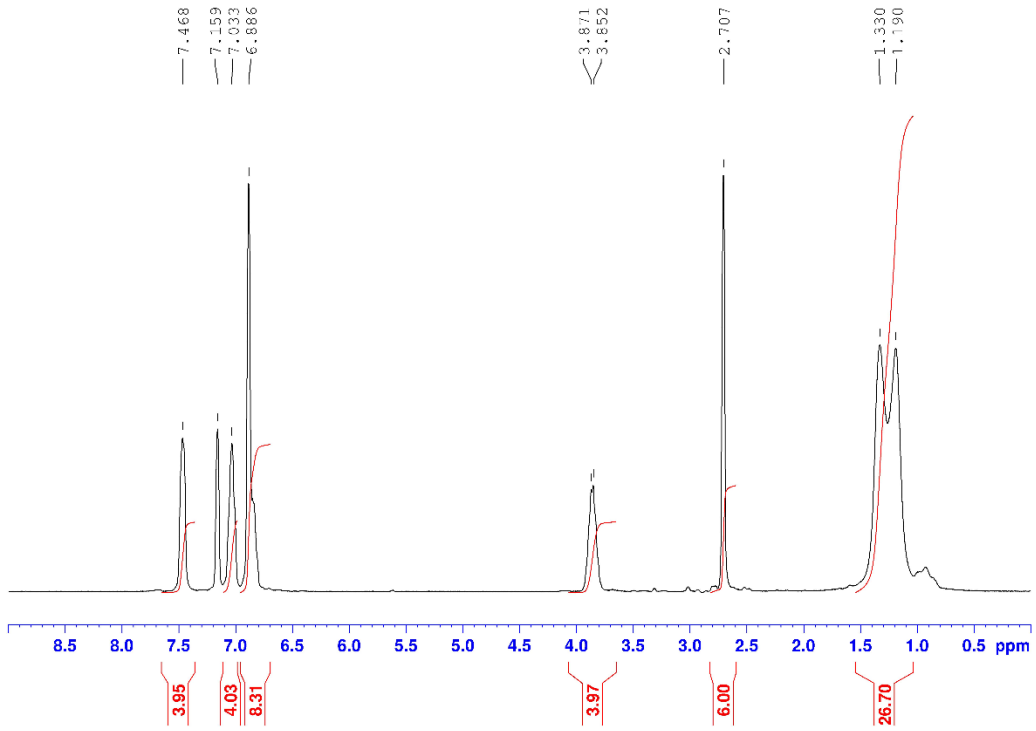


Fig. S21 ^{1}H NMR spectrum of **9** in C_6D_6 at room temperature.

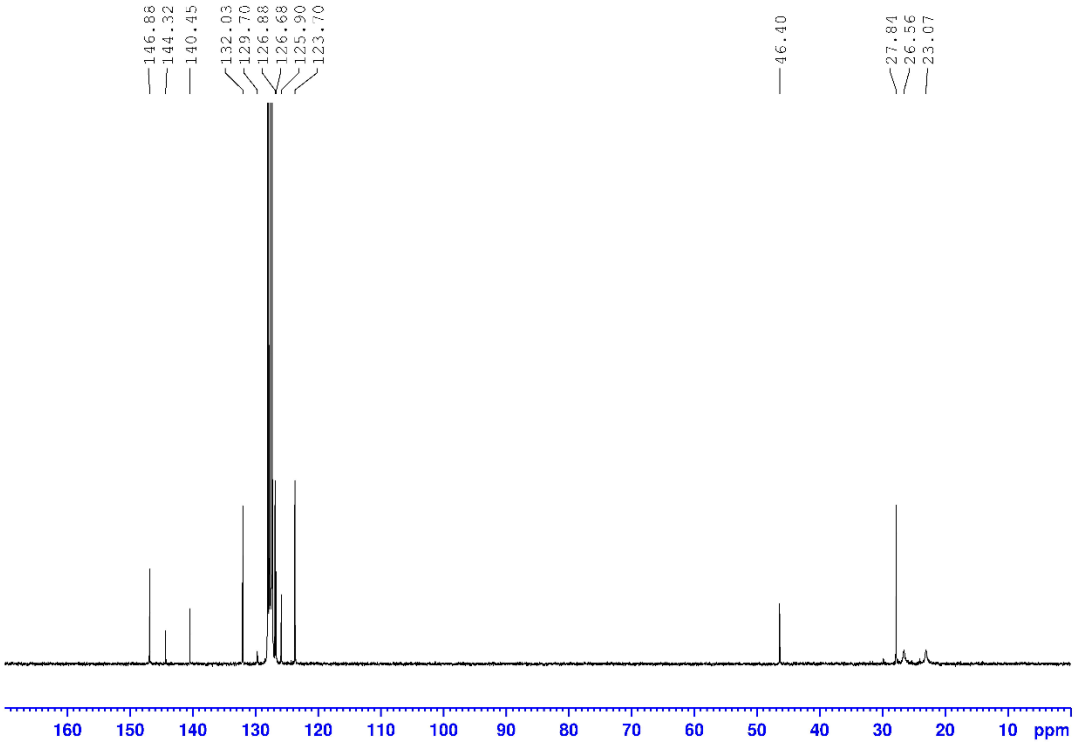


Fig. S22 $^{13}C\{^{1}H\}$ NMR spectrum of **9** in C_6D_6 at room temperature.

UV/Vis Spectra

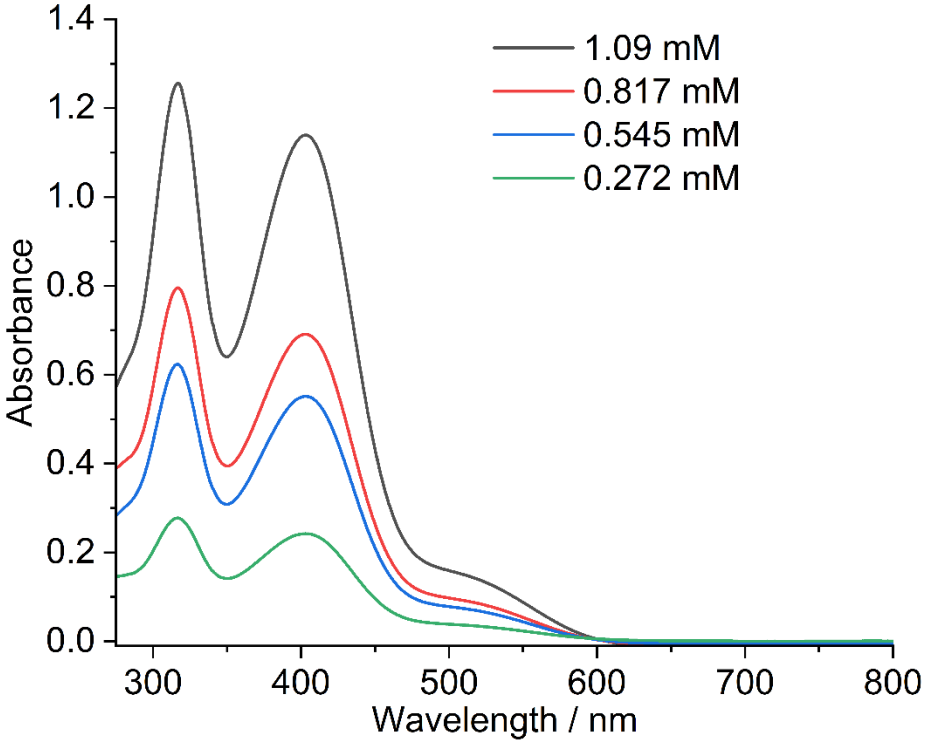


Fig. S23 UV/Vis spectra of **3** in THF at different concentrations at room temperature.

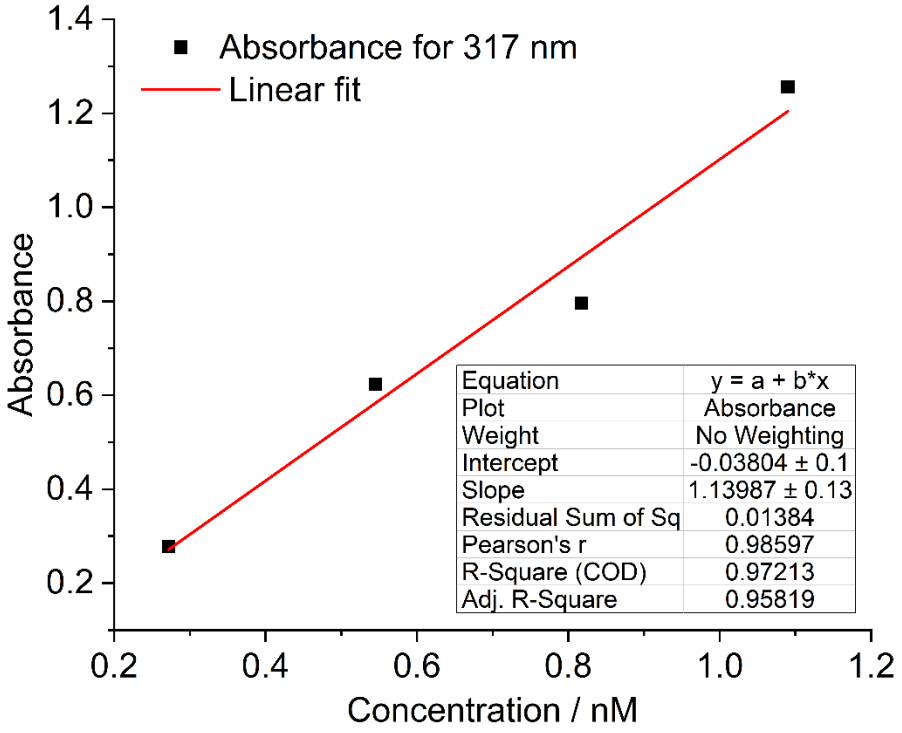


Fig. S24 Linear regression of the absorbance of **3** at 317 nm.

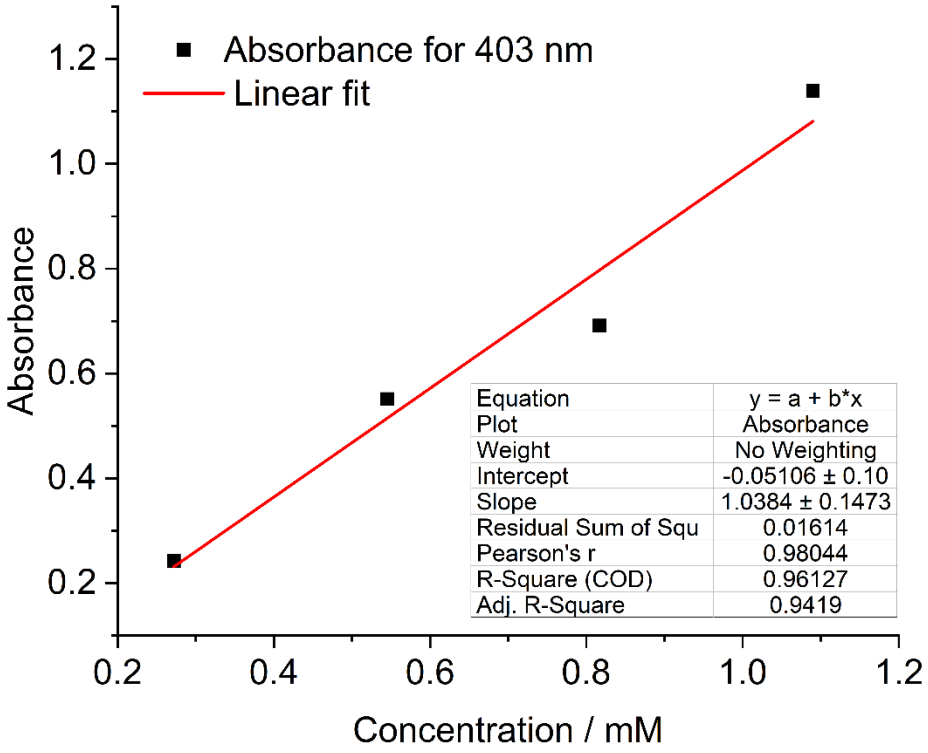


Fig. S25 Linear regression of the absorbance of **3** at 403 nm.

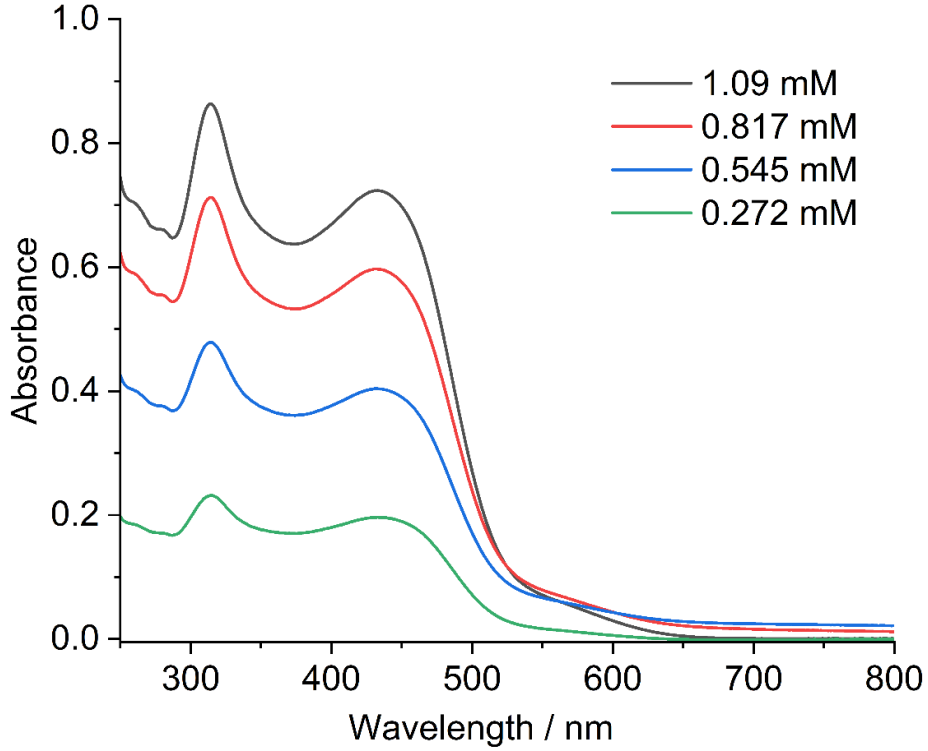


Fig. S26 UV/Vis spectra of **3** in hexane at different concentrations at room temperature.

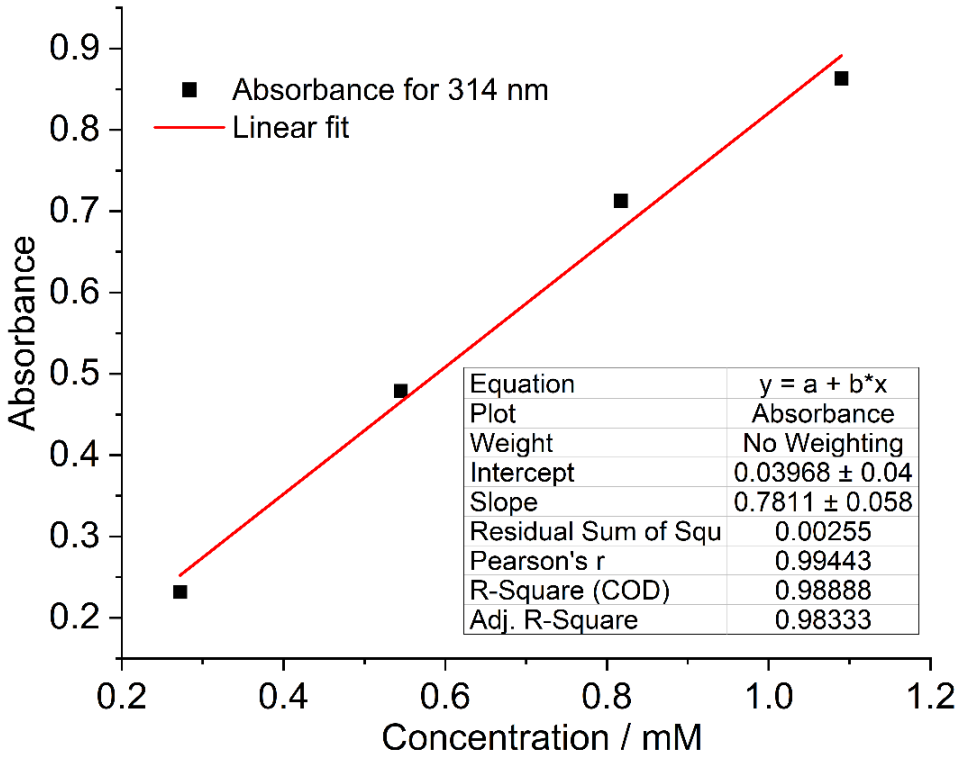


Fig. S27 Linear regression of the absorbance of **3** at 314 nm.

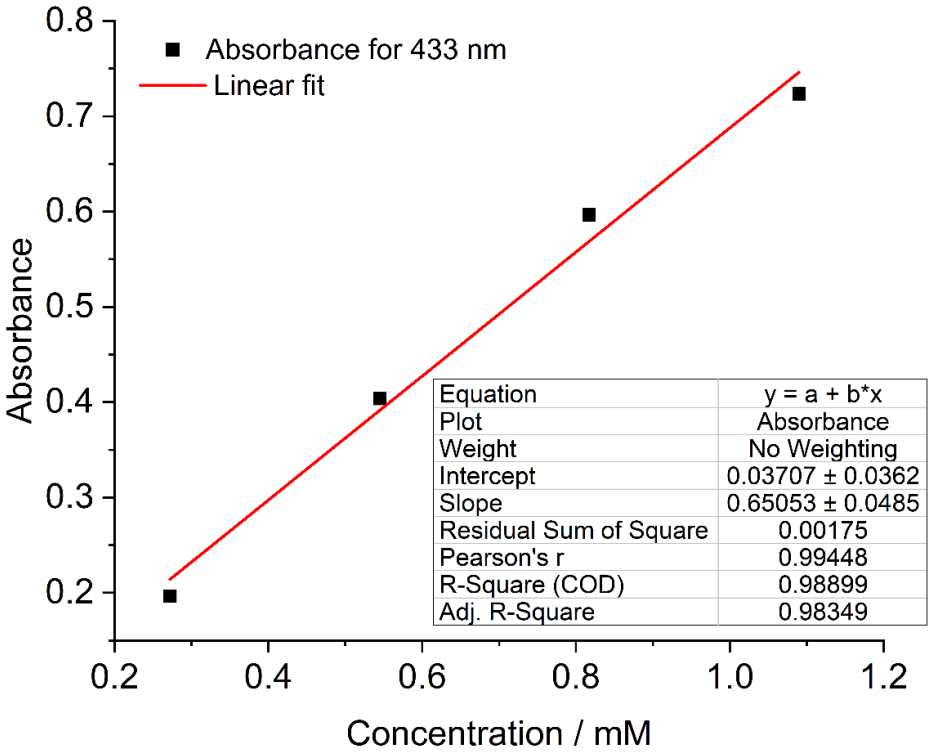


Fig. S28 Linear regression of the absorbance of **3** at 433 nm.

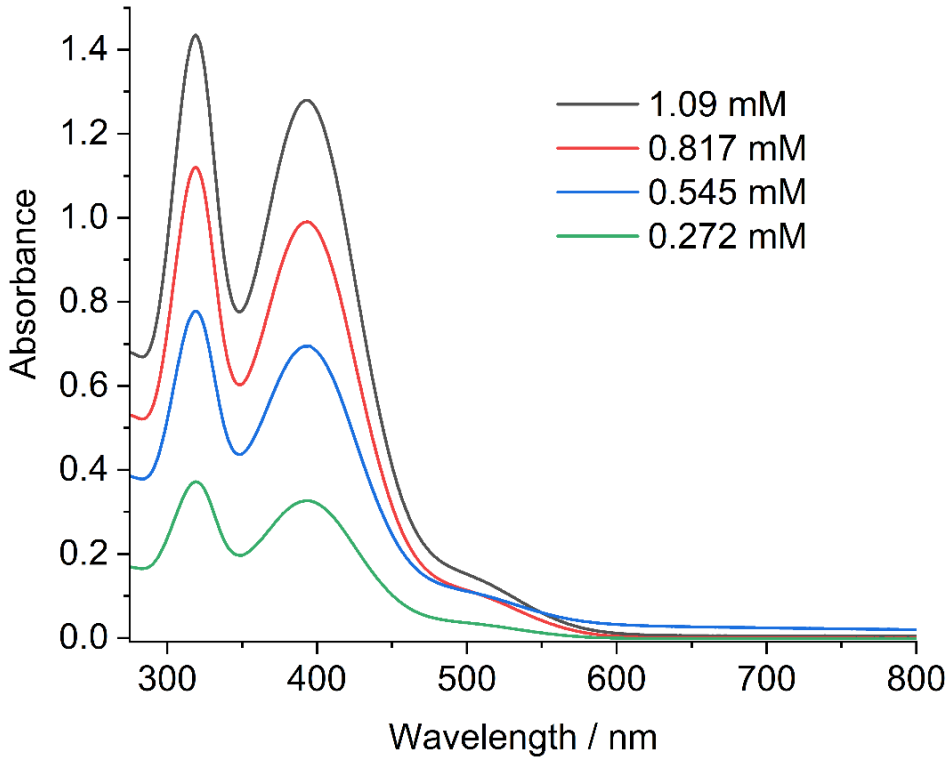


Fig. S29 UV/Vis spectra of **3** in ACN at different concentrations at room temperature.

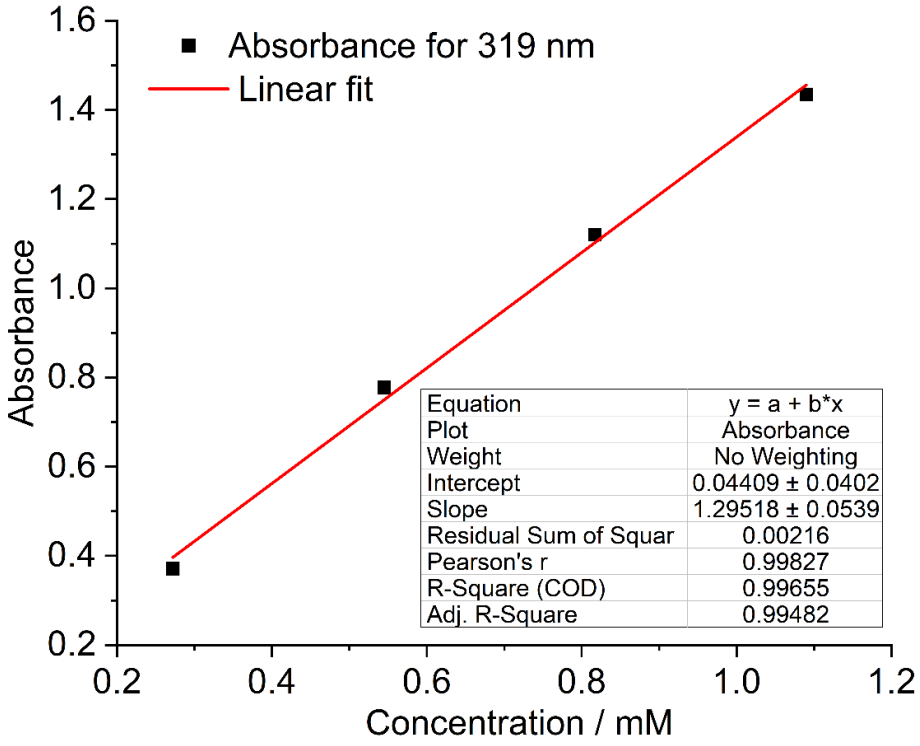


Fig. S30 Linear regression of the absorbance of **3** at 319 nm.

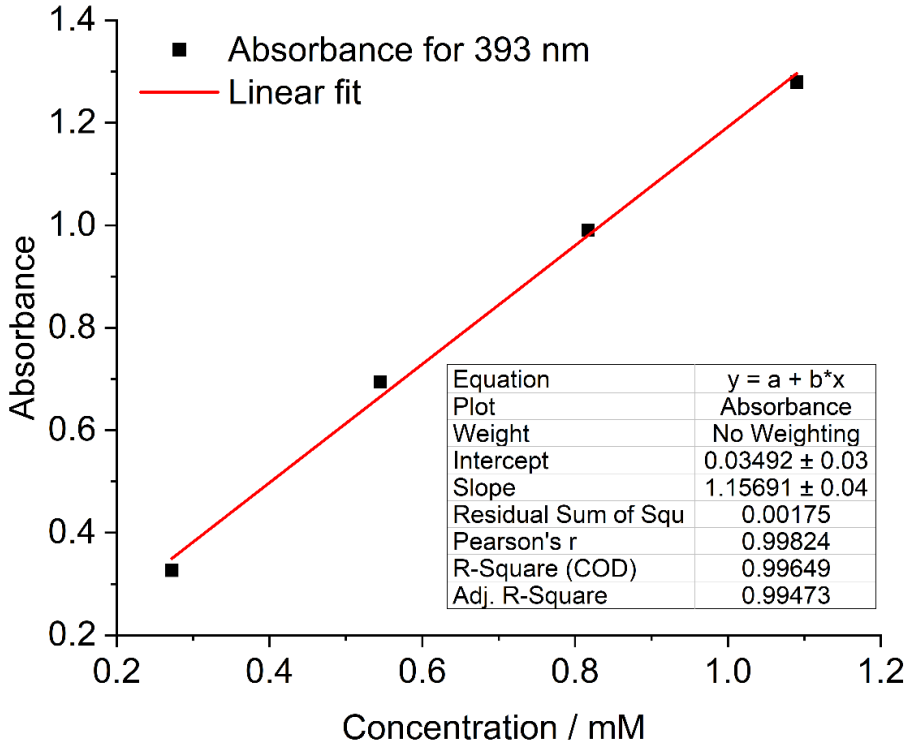


Fig. S31 Linear regression of the absorbance of **3** at 393 nm.

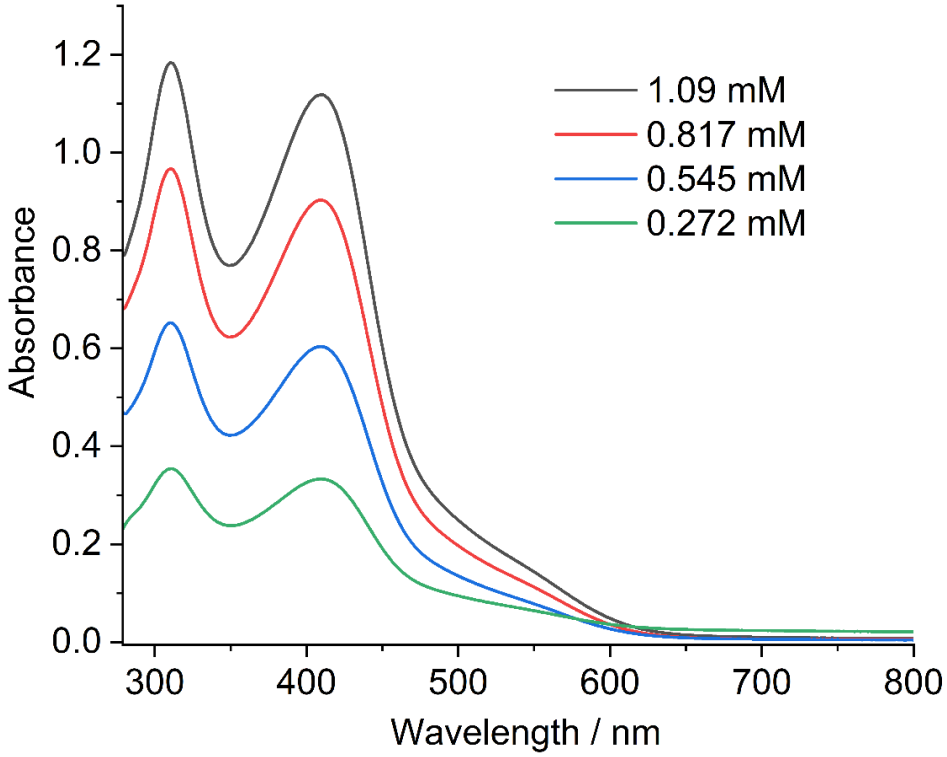


Fig. S32 UV/Vis spectra of **3** in Toluene at different concentrations at room temperature.

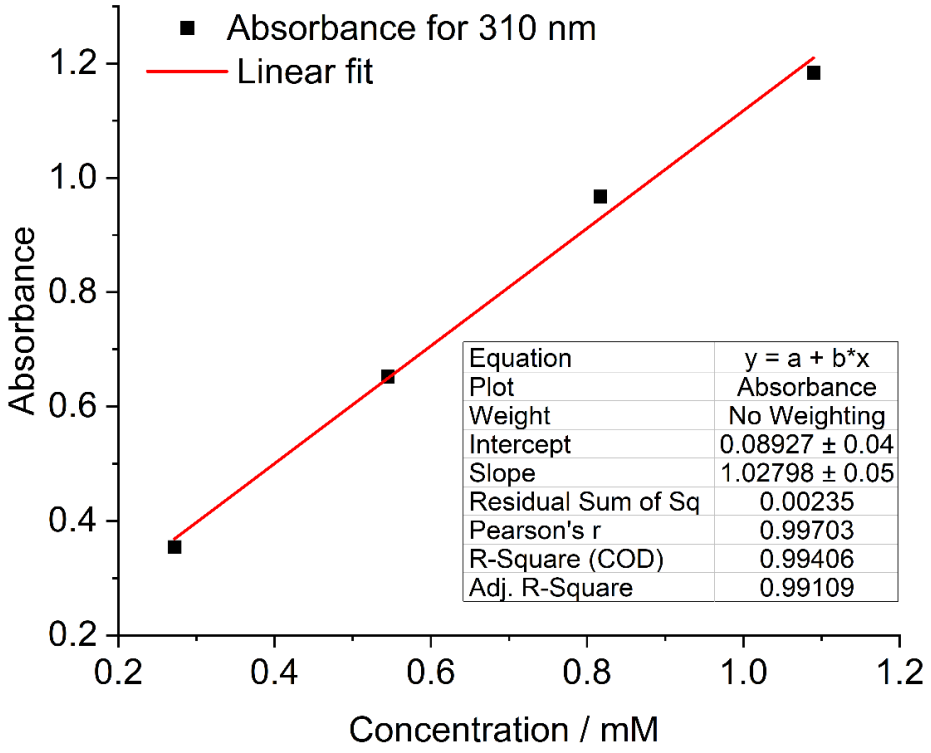


Fig. S33 Linear regression of the absorbance of **3** at 310 nm.

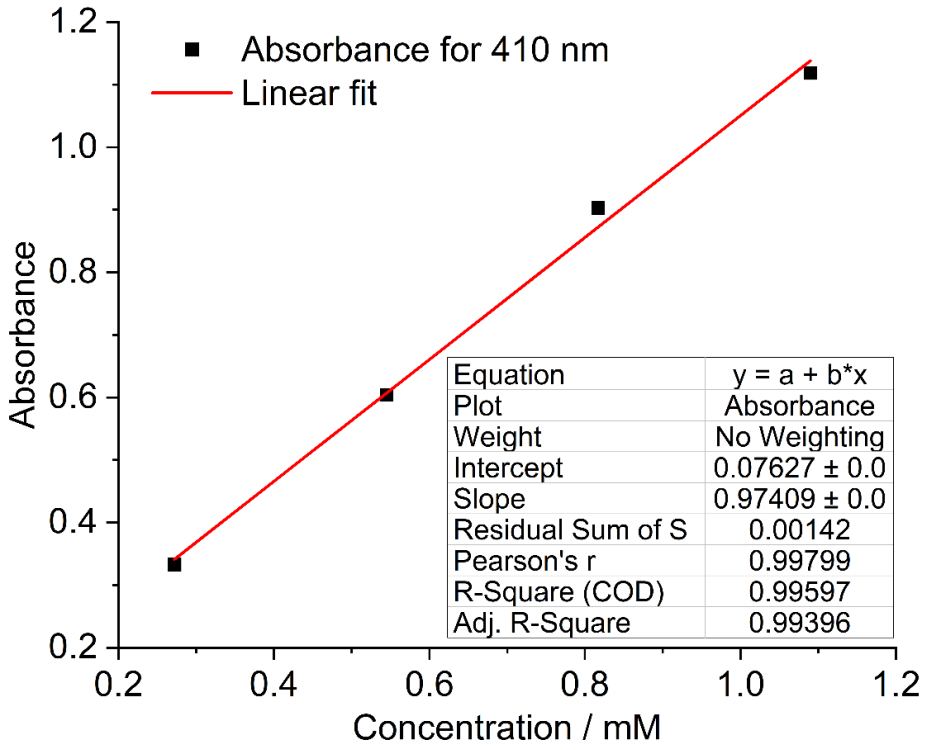


Fig. S34 Linear regression of the absorbance of **3** at 410 nm.

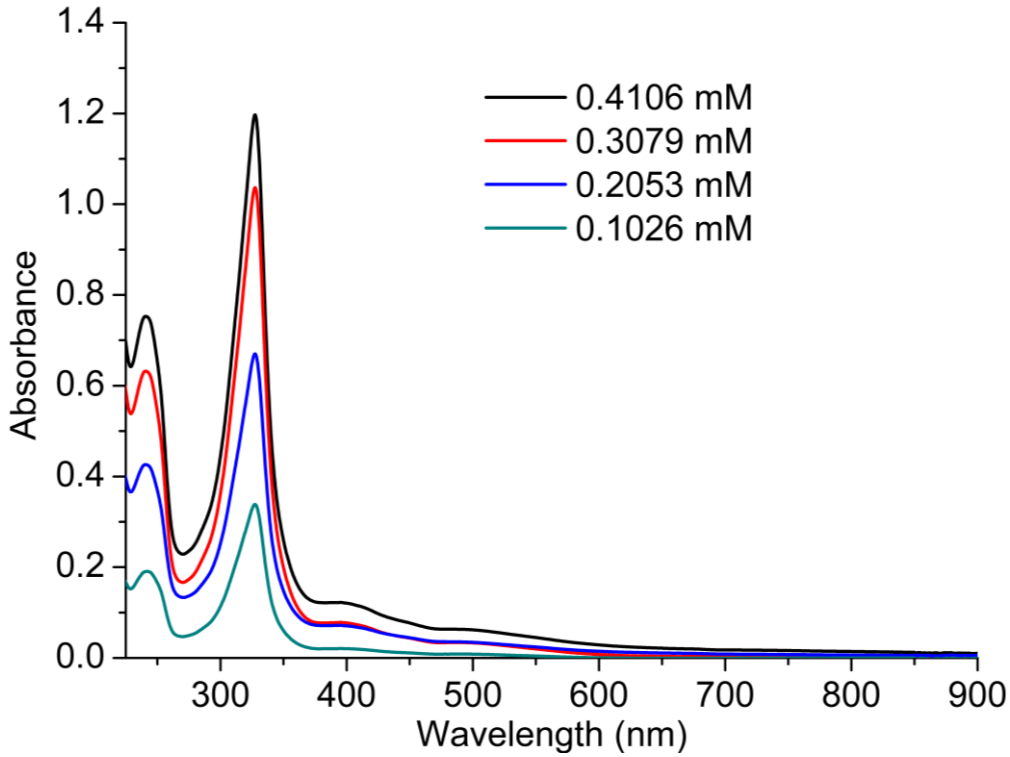


Fig. S35 UV/Vis spectra of **5** in THF at different concentrations at room temperature.

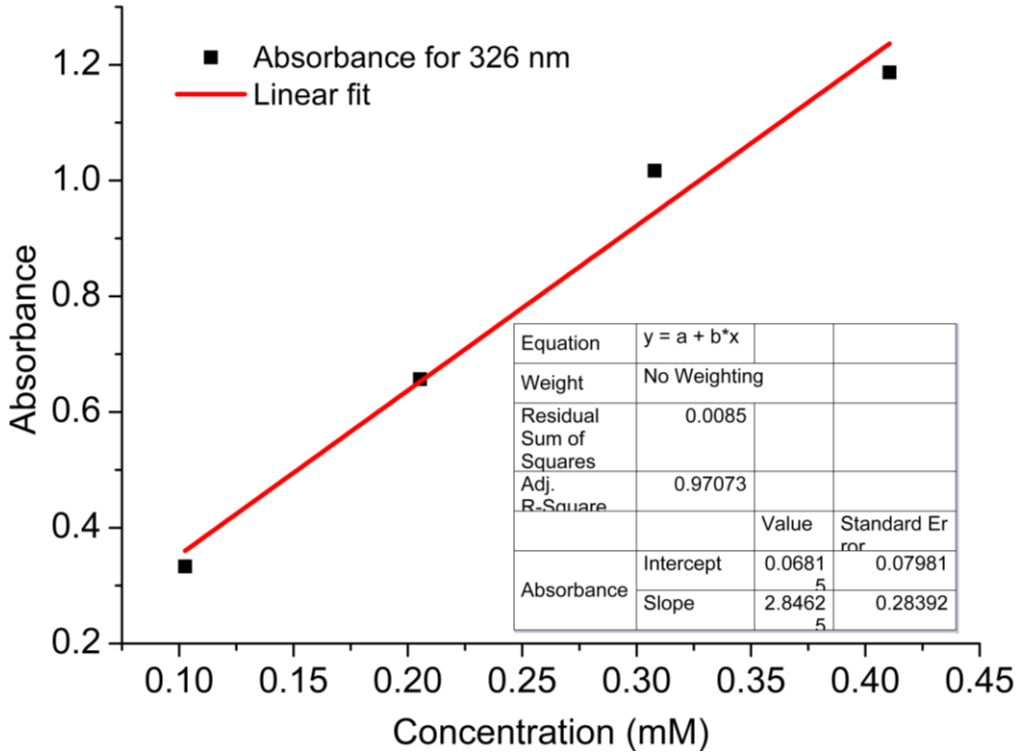


Fig. S36 Linear regression of the absorbance of **5** at 326 nm.

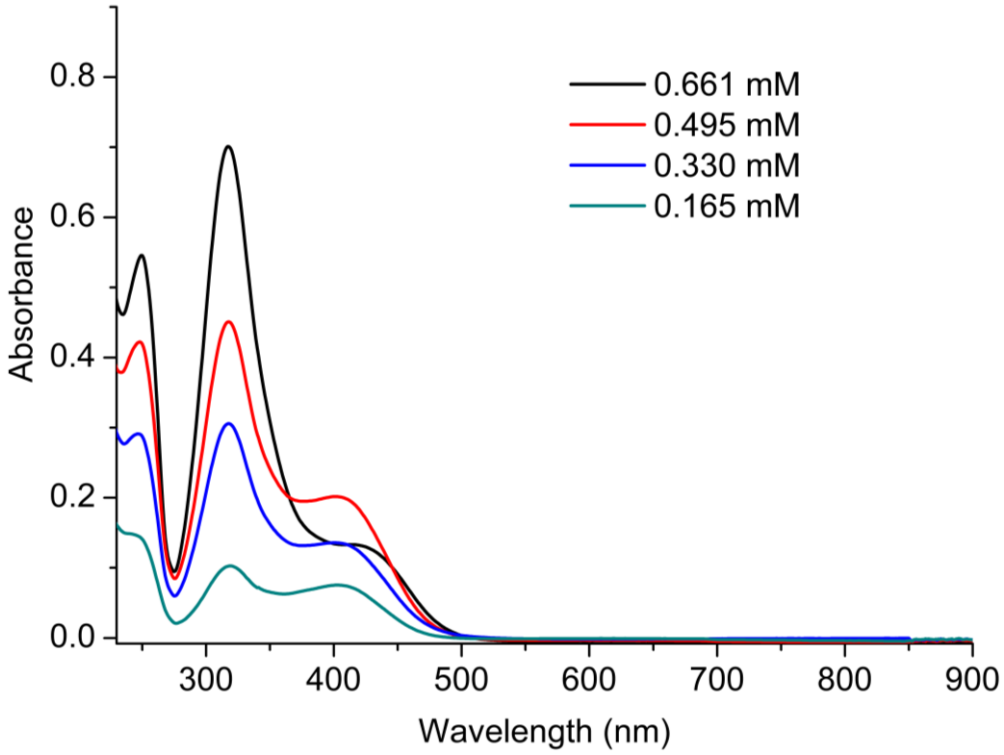


Fig. S37 UV/Vis spectra of **6** in THF at different concentrations at room temperature.

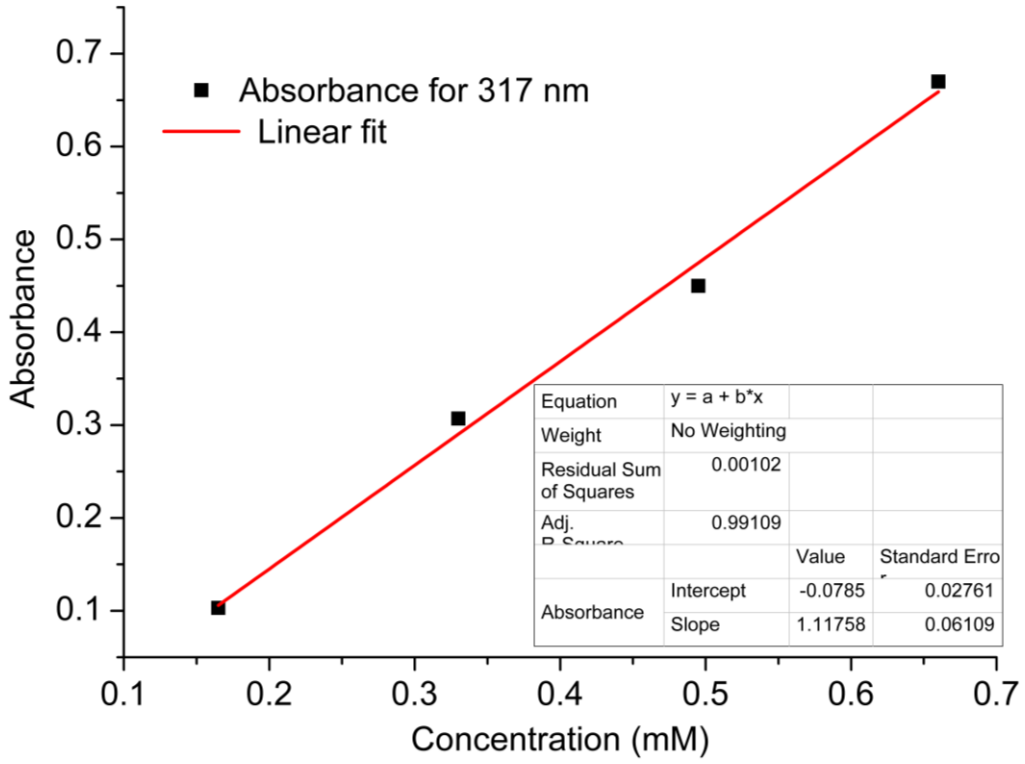


Fig. S38 Linear regression of the absorbance of **6** at 317 nm.

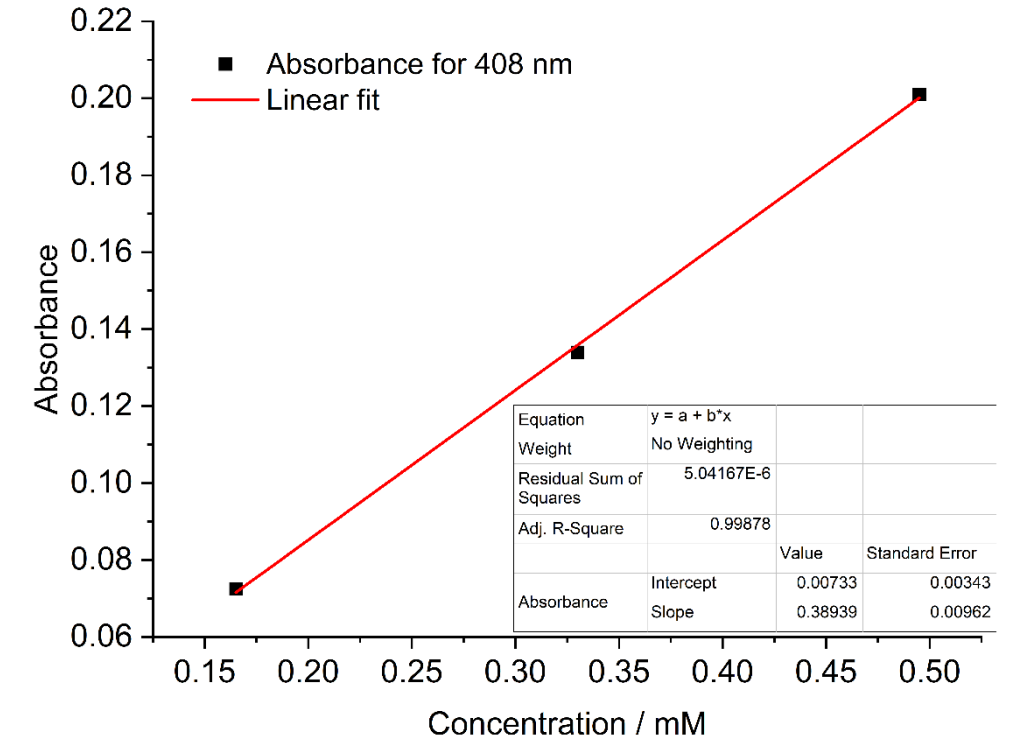


Fig. S39 Linear regression of the absorbance of **6** at 408 nm.

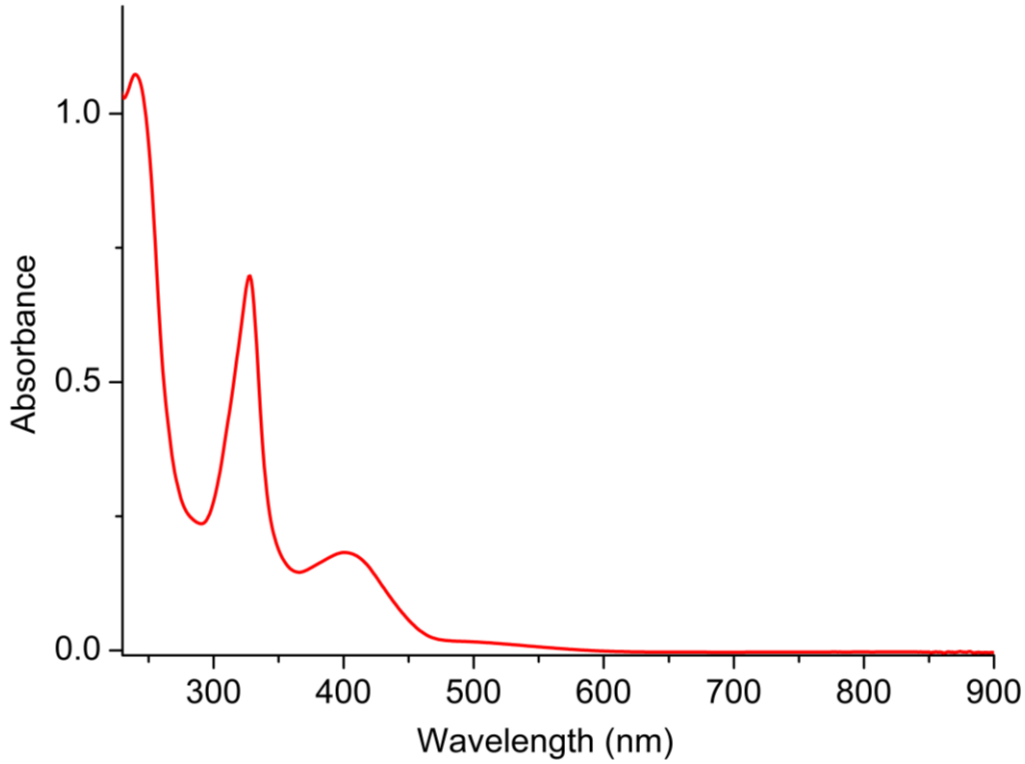


Fig. S40 UV/Vis spectrum of **5** obtained from 1:1 reaction of **3** and **6** in THF at room temperature.

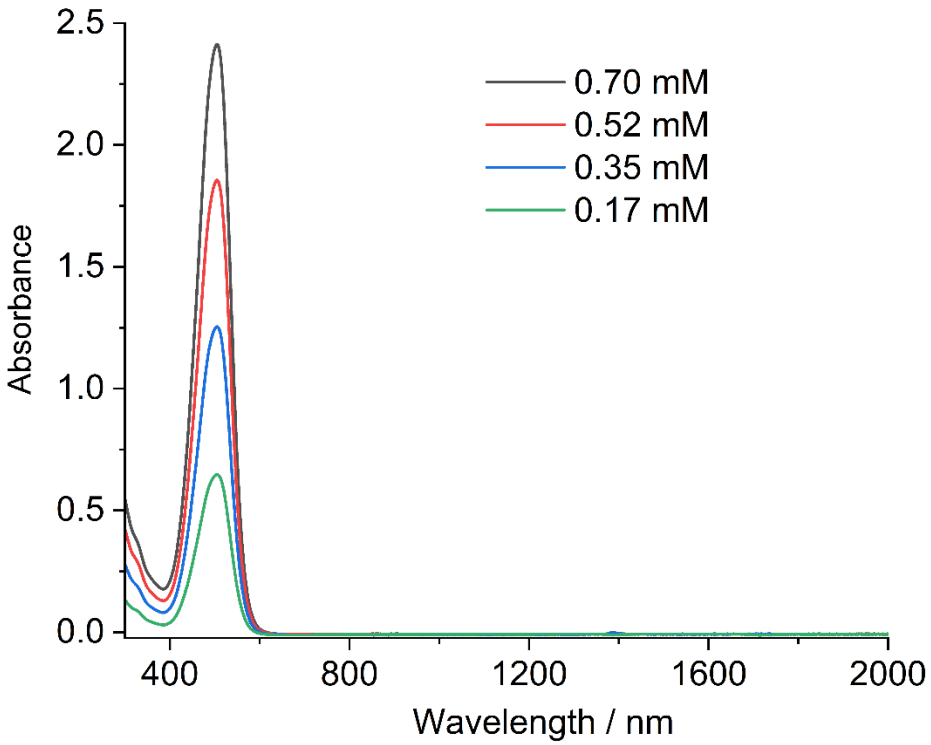


Fig. S41 UV/Vis spectra of **8** in THF at different concentrations at room temperature.

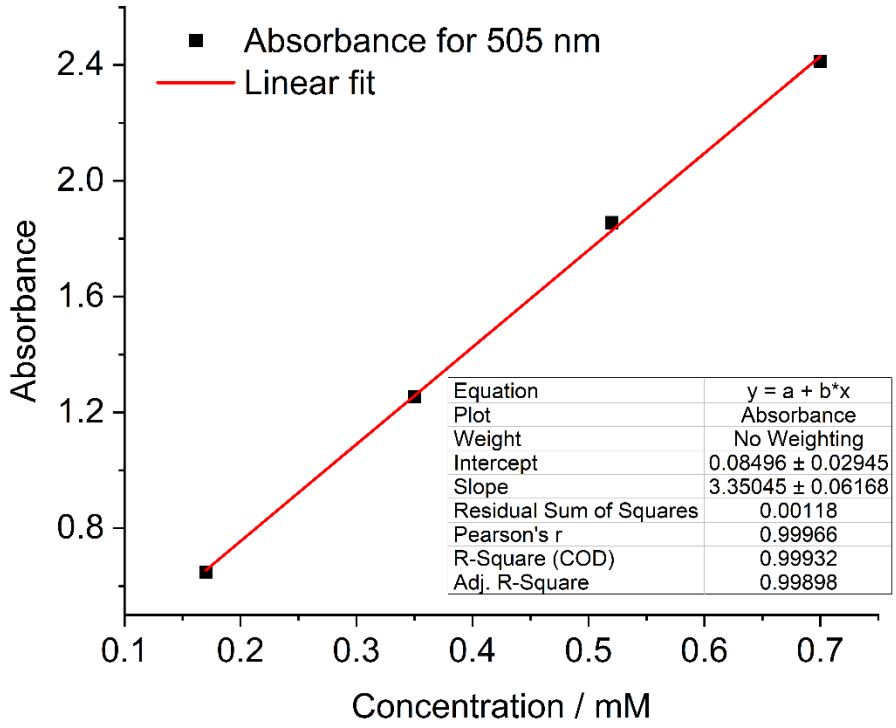


Fig. S42 Linear regression of the absorbance of **8** at 505 nm.

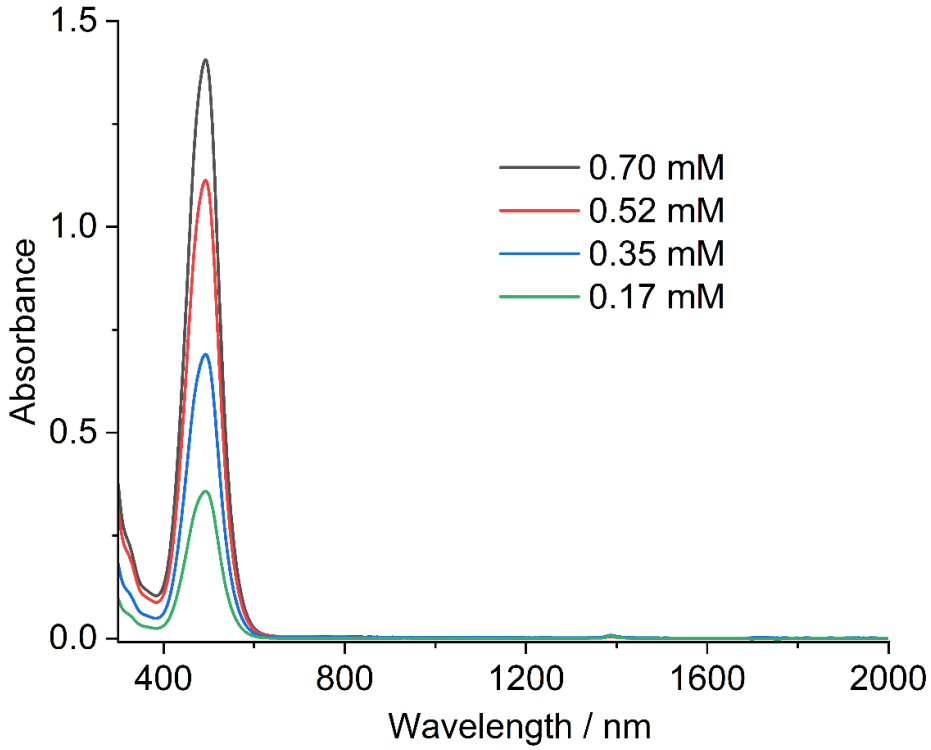


Fig. S43 UV/Vis spectra of **8** in hexane at different concentrations at room temperature.

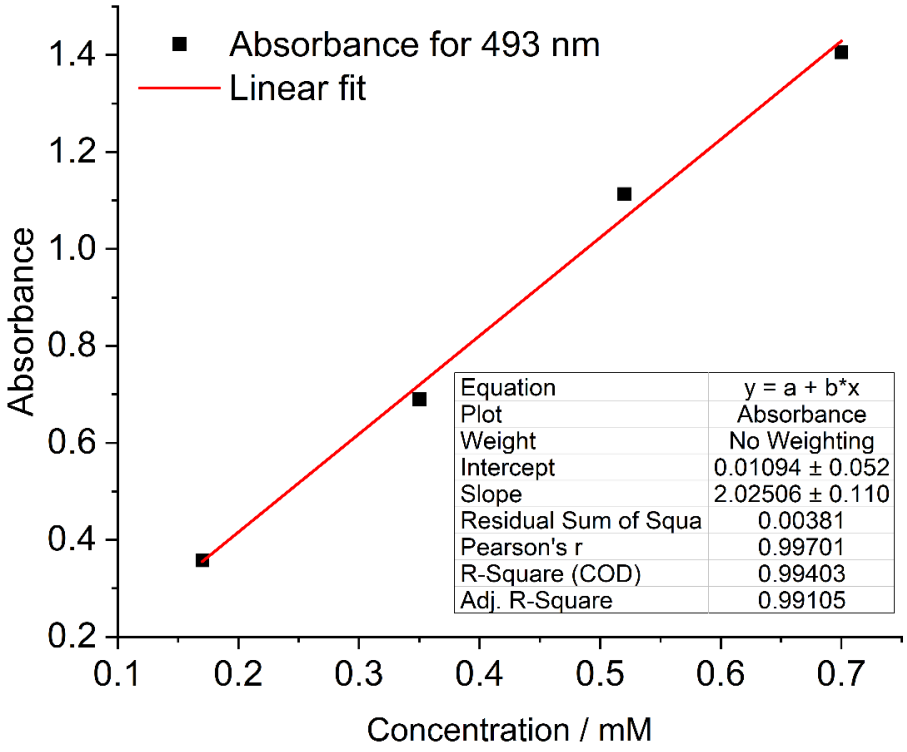


Fig. S44 Linear regression of the absorbance of **8** at 493 nm.

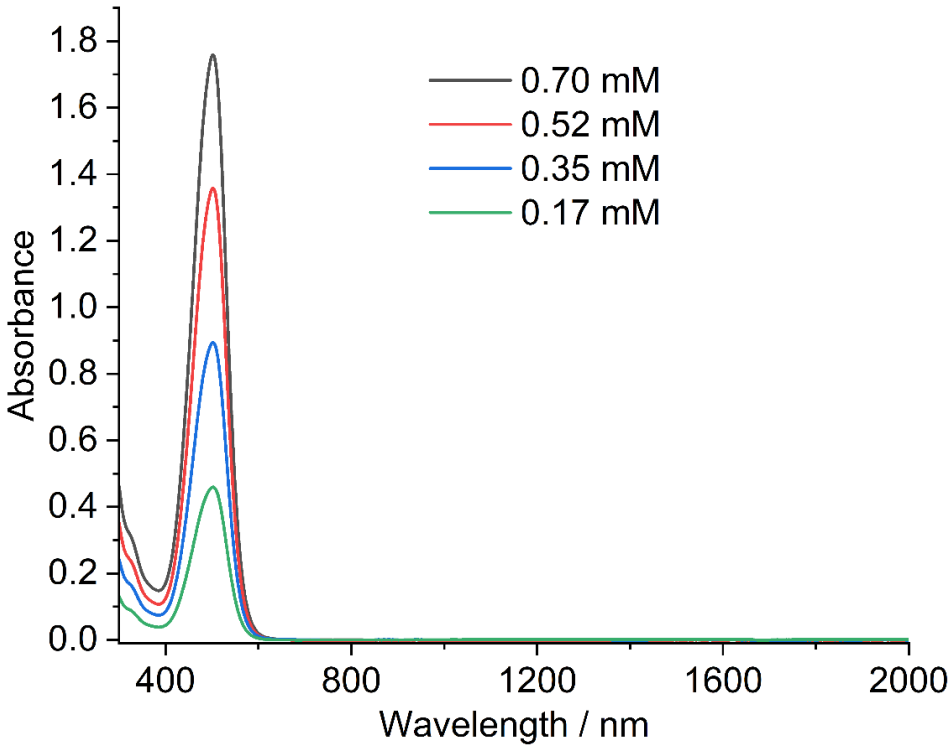


Fig. S45 UV/Vis spectra of **8** in toluene at different concentrations at room temperature.

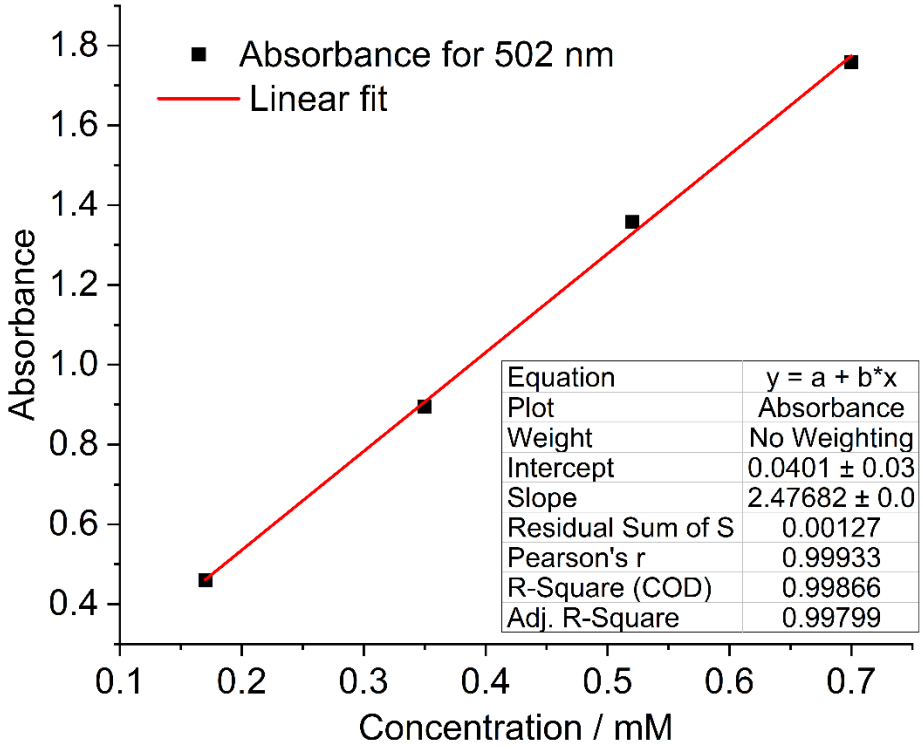


Fig. S46 Linear regression of the absorbance of **8** at 502 nm.

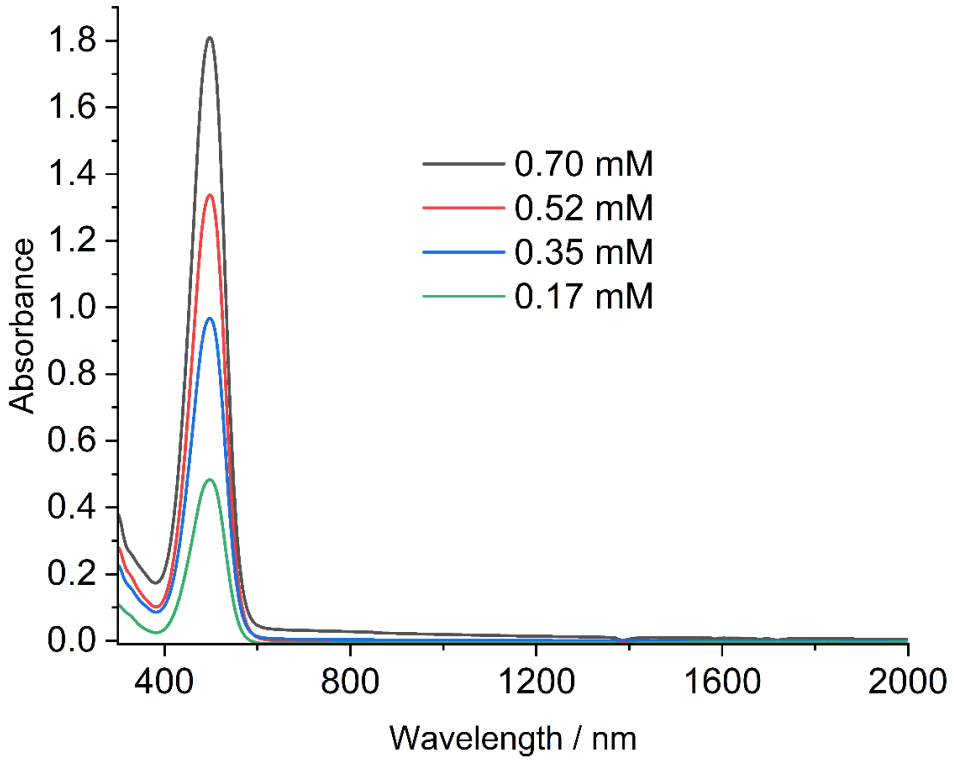


Fig. S47 UV/Vis spectra of **8** in CH_3CN at different concentrations at room temperature.

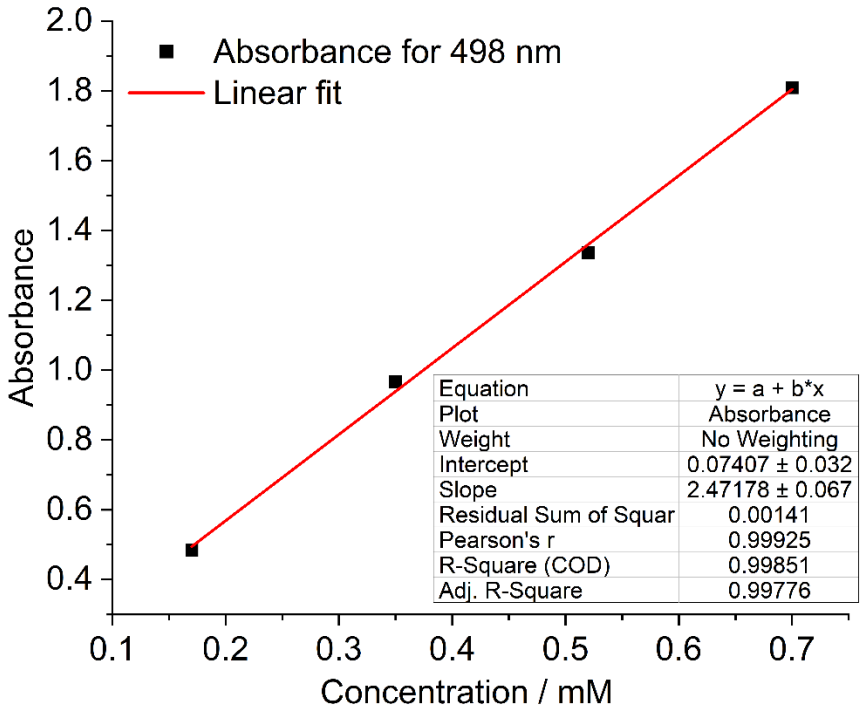


Fig. S48 Linear regression of the absorbance of **8** at 498 nm.

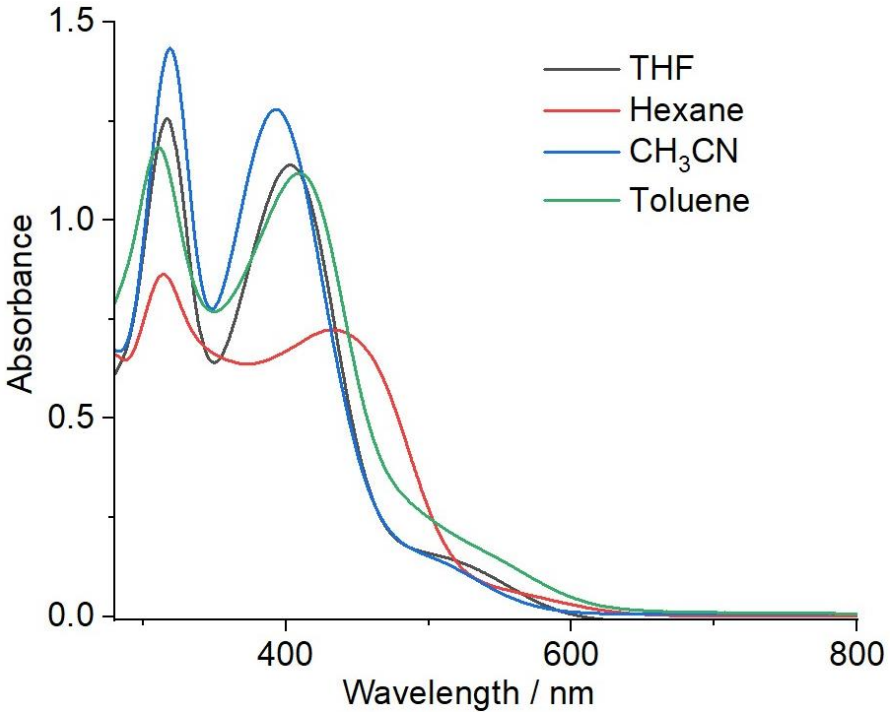


Fig. S49 UV/Vis spectra of **3** in different solvents at room temperature **(**THF - 317 nm (ε = 1140 L mol^{-1} cm^{-1}), - 403 nm (ε =1040 L mol^{-1} cm^{-1}), Hexane - 314 (ε = 781 L mol^{-1} cm^{-1}), - 433 (ε = 651 L mol^{-1} cm^{-1}), CH_3CN - 319 nm (ε = 1295 L mol^{-1} cm^{-1}), - 393 nm (ε = 1157 L mol^{-1} cm^{-1}), and Toluene - 310 nm (ε = 1028 L mol^{-1} cm^{-1}), 410 nm (ε = 974 L mol^{-1} cm^{-1}).

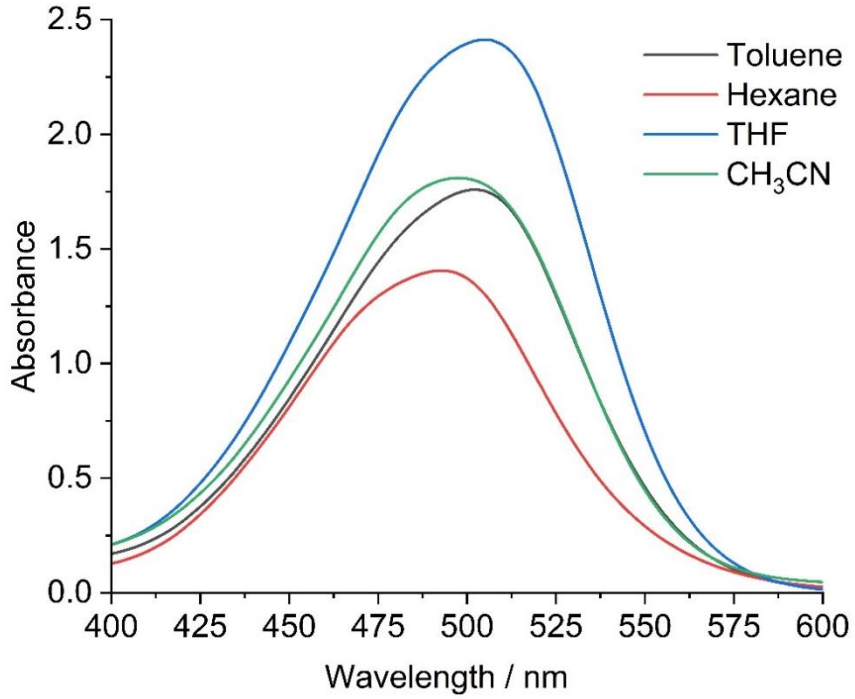


Fig. S50 UV/Vis spectra of **8** in different solvents at room temperature (toluene - 502 nm (ε = 2470 L mol^{-1} cm^{-1}), Hexane - 493 nm (ε = 2020 L mol^{-1} cm^{-1}), THF - 505 nm (ε = 3350 L mol^{-1} cm^{-1})), and CH_3CN - 498 nm (ε = 2470 L mol^{-1} cm^{-1}).

HRMS Spectra of 3 and 8

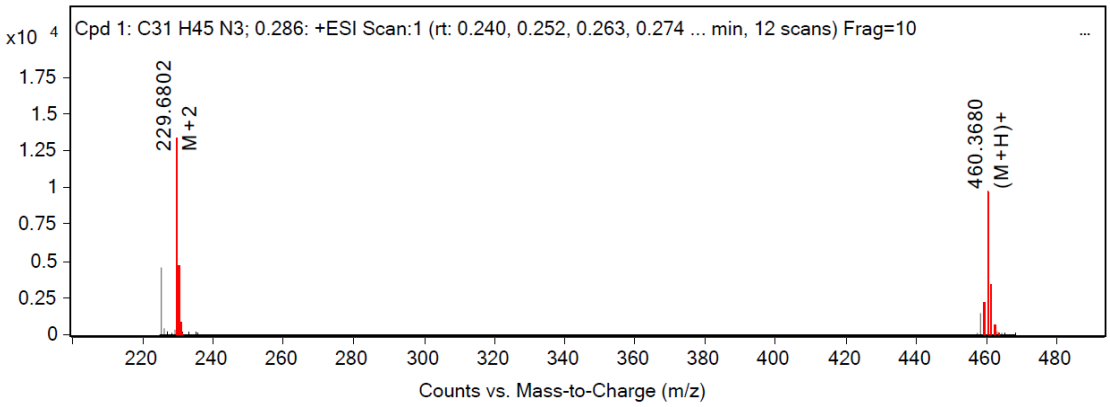


Fig. S51 HRMS Spectrum of **3**.

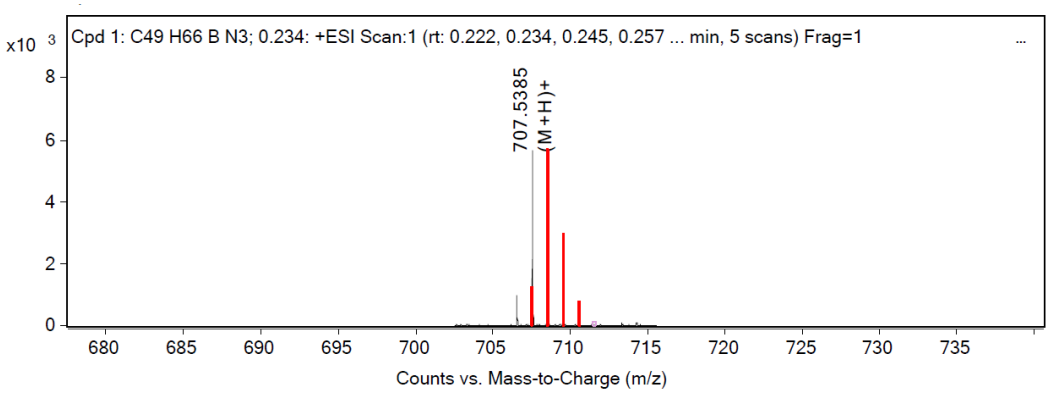


Fig. S52 HRMS Spectrum of **8**.

Cyclic Voltammetry

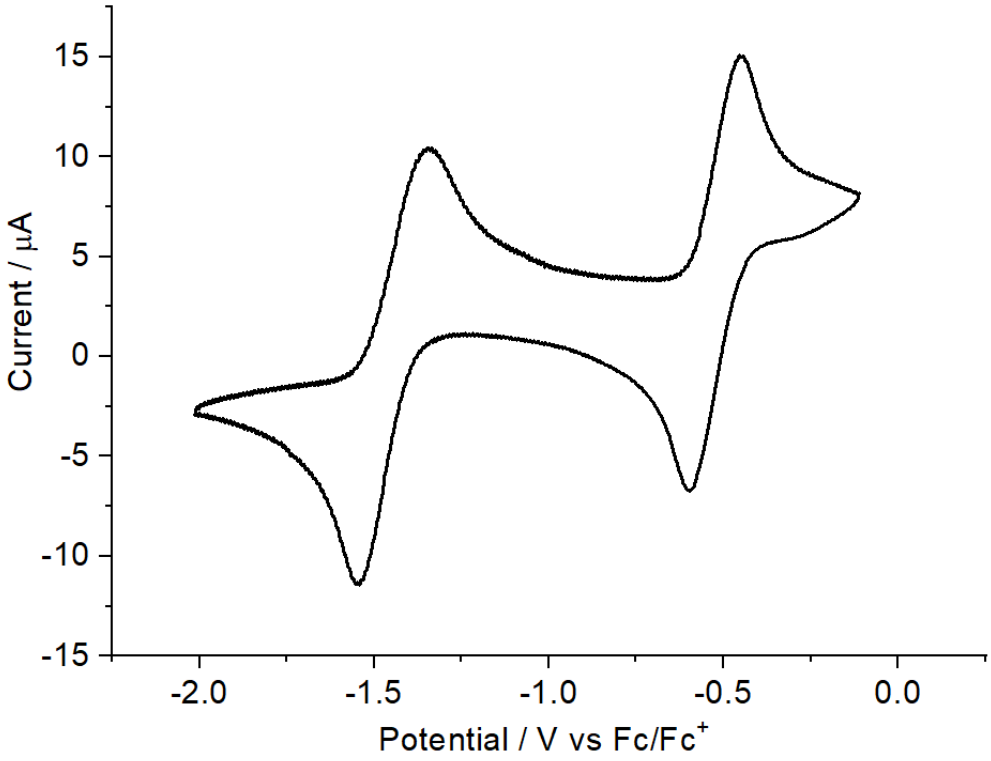


Fig. S53 Cyclic Voltammogram of **3** at 100 mV/s in THF (0.1 M [nBu$_4$N][PF$_6$]) at room temperature.

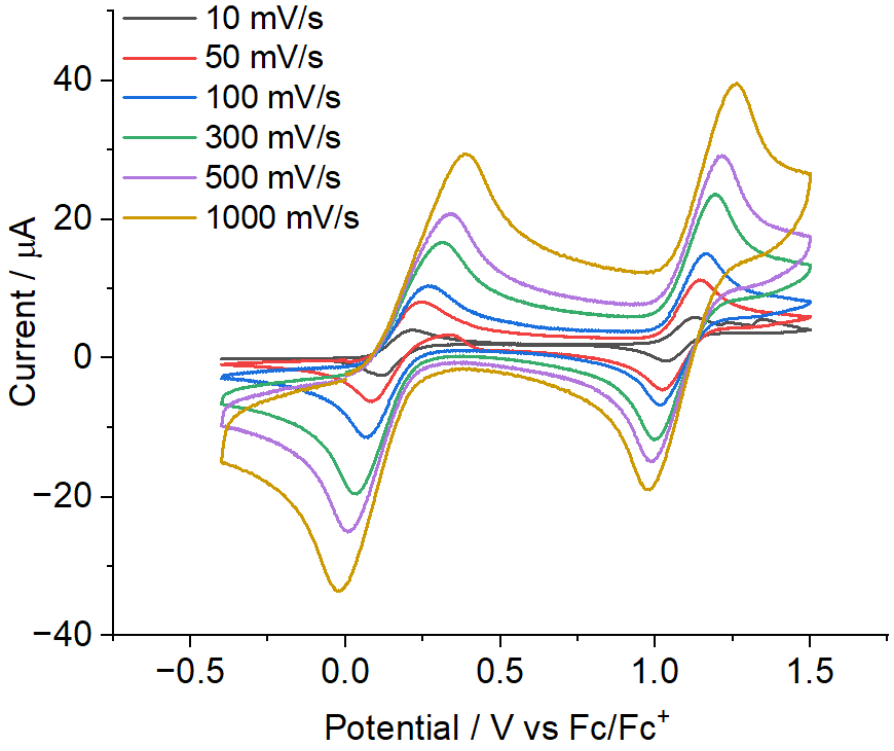


Fig. S54 Cyclic voltammograms of **3** at various scan rates in THF (0.1 M [nBu$_4$N][PF$_6$]) at room temperature.

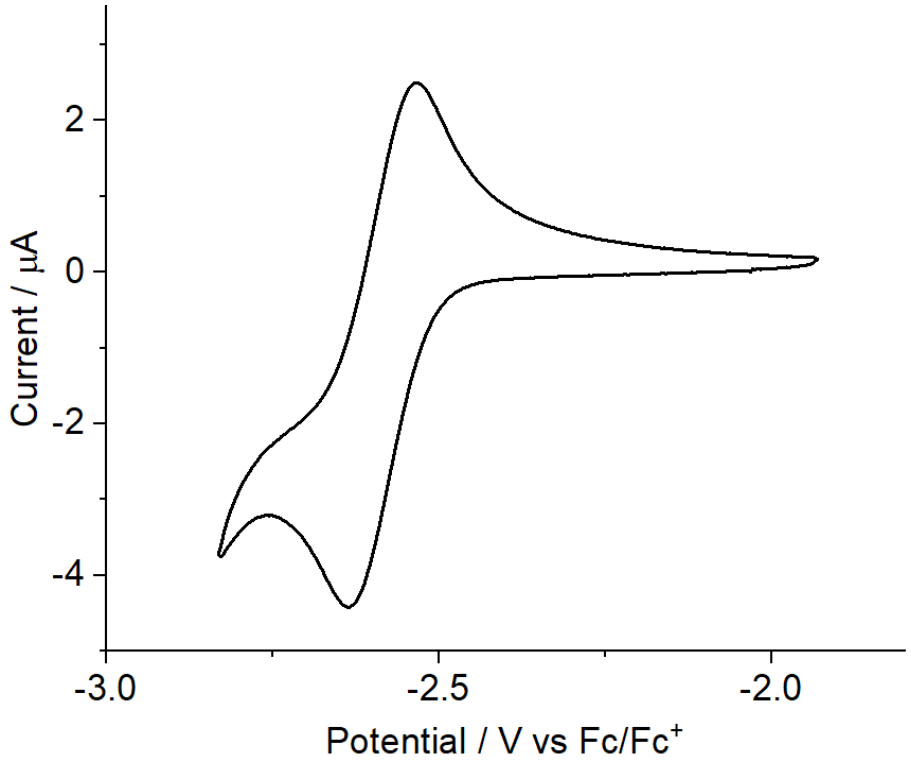


Fig. S55 Cyclic Voltammogram of **B** at 100 mV/s in THF (0.1 M [*n*Bu$_4$N][PF$_6$]) at room temperature.

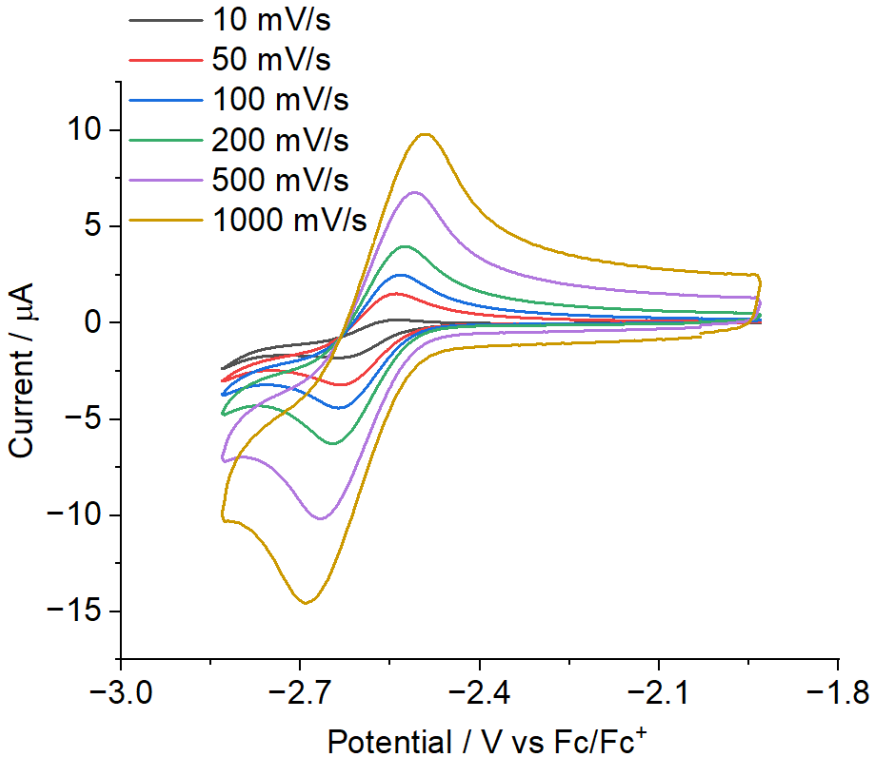


Fig. S56 Cyclic voltammograms of **B** at various scan rates in THF (0.1 M [*n*Bu$_4$N][PF$_6$]) at room temperature.

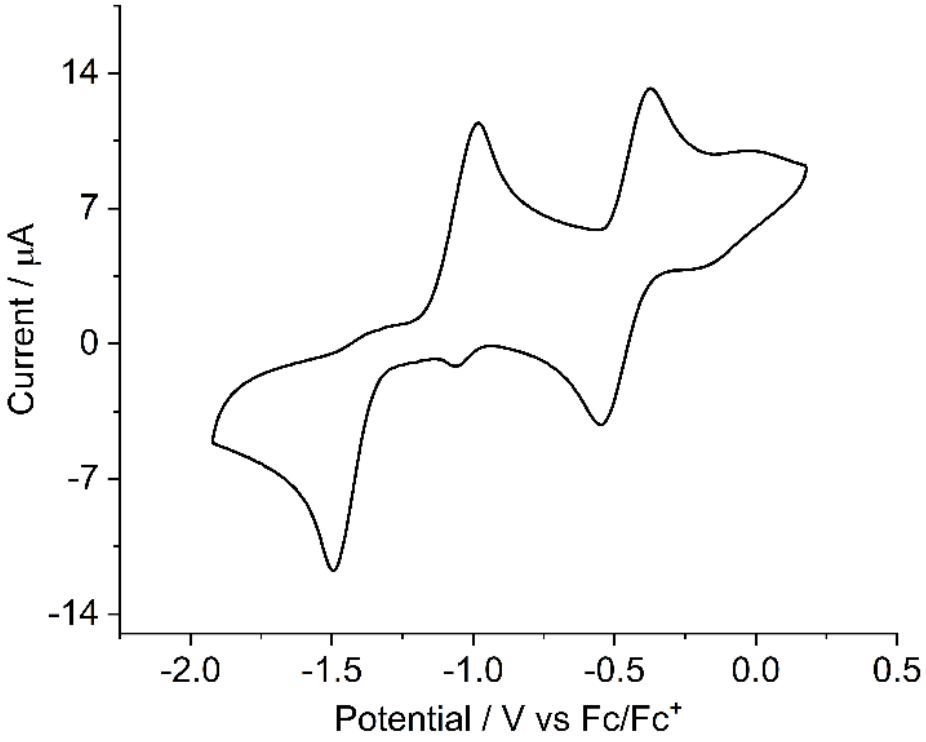


Fig. S57 Cyclic Voltammogram of **8** at 100 mV/s in THF (0.1 M [nBu$_4$N][PF$_6$]) at room temperature.

EPR Spectroscopy

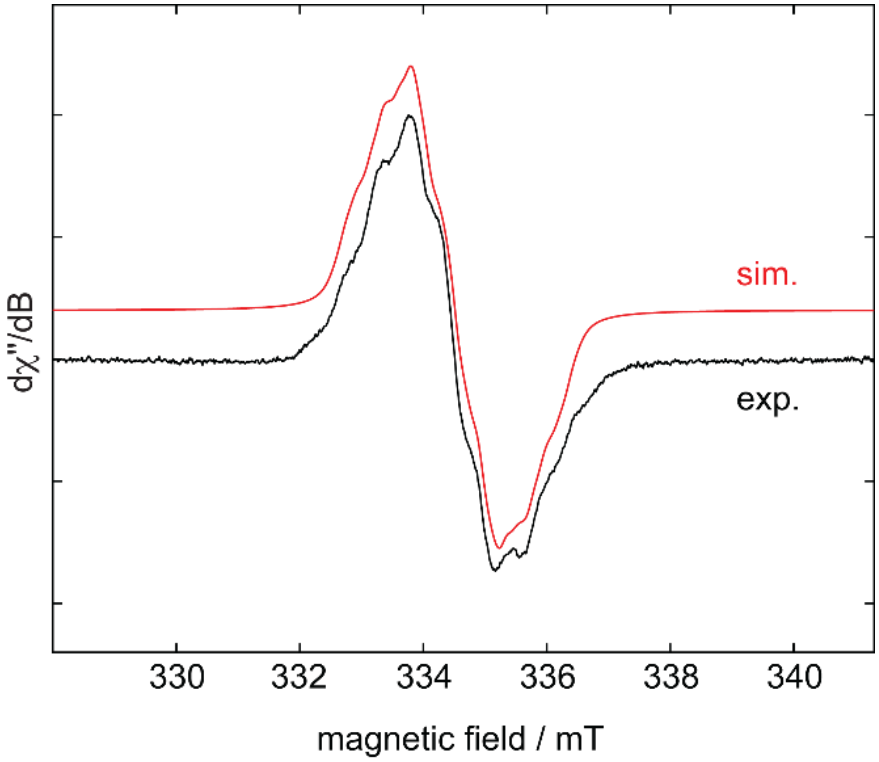


Fig. S58 Experimental (black) and simulated EPR spectra of **5** in acetonitrile. Simulated parameters are: g_{iso} = 2.0023, $a(^{14}N)$ = 15.0 MHz (1N), 12.0 MHz (2N), and $a(^{1}H)$ = 5.0 MHz (3H), 4.0 MHz (2H), and 3.0 MHz (1H).

Molecular Structures of 3, 5, 6, C, D, 7, 8, and 9

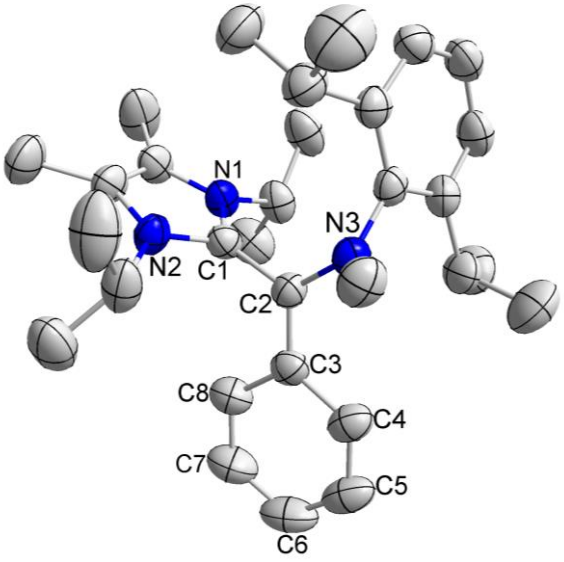


Fig. S59 Molecular structure of **3** with thermal ellipsoids at 50 % probability level. All H atoms are omitted for clarity reasons. Selected bond lengths [Å] and bond angles [°]: N1–C1 1.352(2), N2–C1 1.3598(19), C1–C2 1.450(2), C2–C3 1.414(2), C3–C4 1.418(2), C4–C5 1.383(3), C5–C6 1.378(3), C6–C7 1.379(3), C7–C8 1.367(3), C8–C3 1.423(3), C2–N3 1.438(2); twist angle N2–C1–N1 plane and C3–C2–N3 plane: 86.62°.

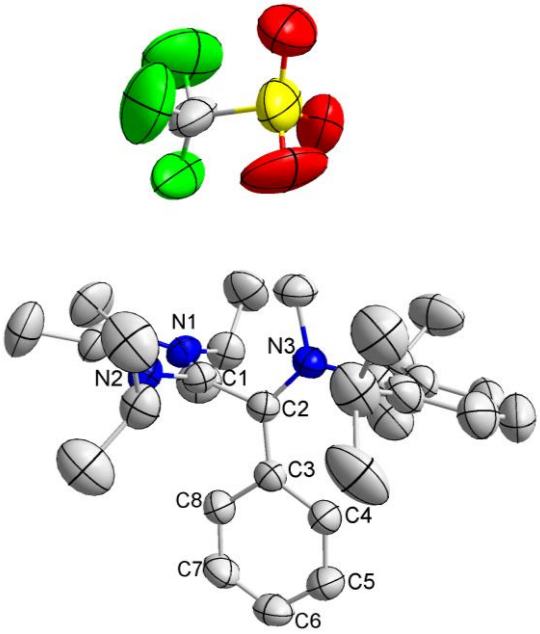


Fig. S60 Molecular structure of **5** with thermal ellipsoids at 50 % probability level. All H atoms are omitted for clarity reasons. Selected bond lengths [Å] and bond angles [°]: N1–C1 1.347(3), N2–C1 1.342(3), C1–C2 1.472(3), C2–C3 1.439(3), C3–C4 1.413(3), C4–C5 1.376(3), C5–C6 1.365(4), C6–C7 1.378(4), C7–C8 1.370(3), C8–C3 1.410(3), C2–N3 1.390(3); twist angle N2–C1–N1 plane and C3–C2–N3 plane: 87.76°.

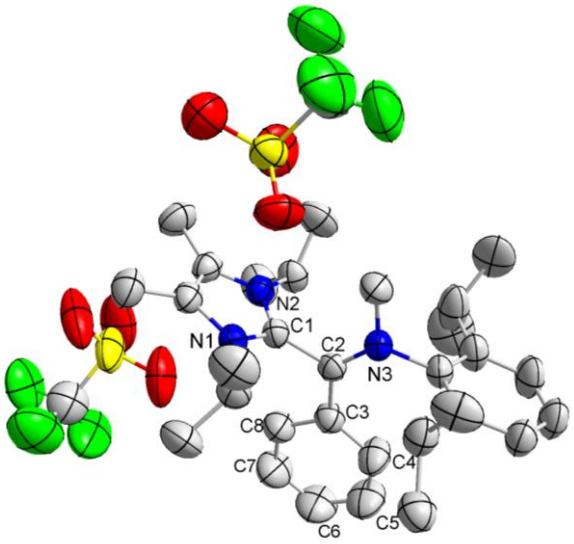


Fig. S61 Molecular structure of **6** with thermal ellipsoids at 50 % probability level. All H atoms are omitted for clarity reasons. Selected bond lengths [Å] and bond angles [°]: N1–C1 1.332(3), N2–C1 1.335(3), C1–C2 1.499(4), C2–C3 1.459(4), C3–C4 1.406(4), C4–C5 1.377(5), C5–C6 1.365(6), C6–C7 1.366(6), C7–C8 1.371(5), C8–C3 1.406(4), C2–N3 1.306(3); twist angle N2–C1–N1 plane and C3–C2–N3 plane: 89.54°.

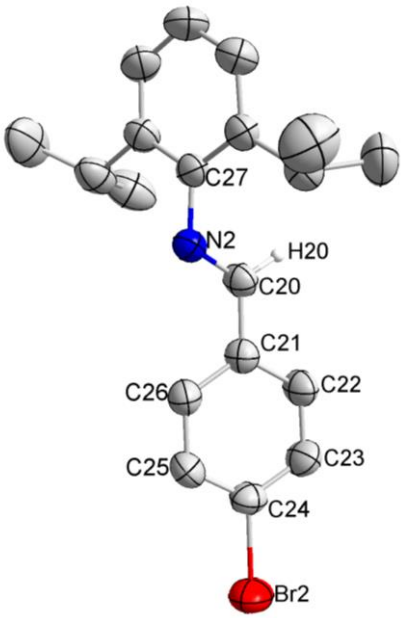


Fig. S62 Molecular structure of **C** with thermal ellipsoids at 50 % probability level. All H atoms are omitted for clarity reasons. Selected bond lengths [Å]: N2–C27 1.413(3), N2–C20 1.262(3), C21–C22 1.387(4), C22–C23 1.371(4), C23–C24 1.348(4), C24–C25 1.389(4), C25–C26 1.363(4), C26–C21 1.371(4), C24–Br2 1.883(3).

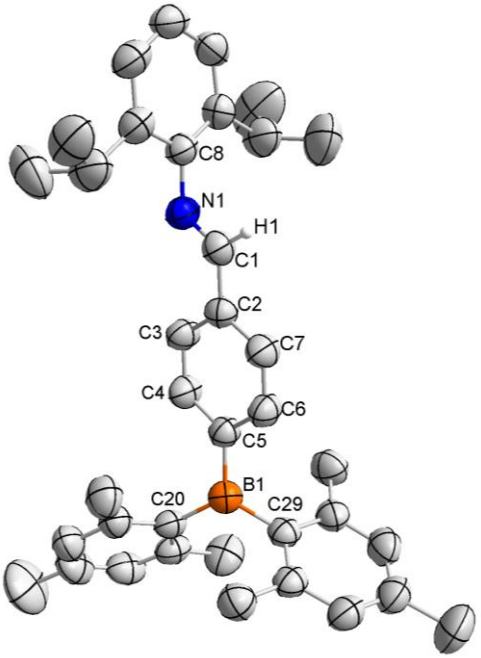


Fig. S63 Molecular structure of **D** with thermal ellipsoids at 50 % probability level. All H atoms are omitted for clarity reasons. Selected bond lengths [Å]: N1–C8 1.432(3), N1–C1 1.241(3), C1–C2 1.472(3), C2–C3 1.389(3), C3–C4 1.377(3), C4–C5 1.399(3), C5–C6 1.398(3), C6–C7 1.377(3), C7–C2 1.375(3), C5–B1 1.566(3), B1–C29 1.579(3), B1–C20 1.572(3).

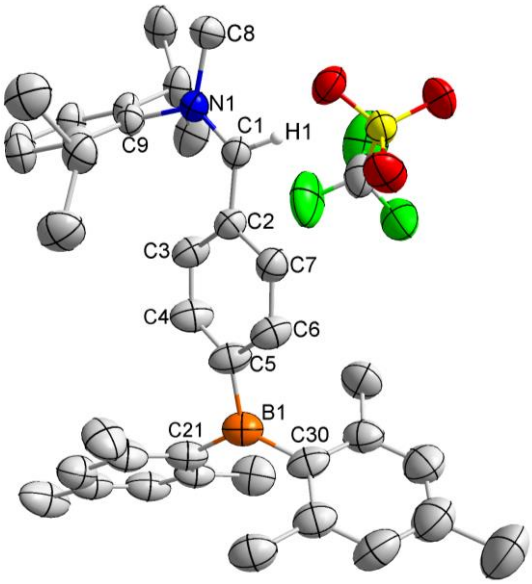


Fig. S64 Molecular structure of **7** with thermal ellipsoids at 50 % probability level. All H atoms are omitted for clarity reasons. Selected bond lengths [Å]: N1–C8 1.474(3), N1–C9 1.465(3),N1–C1 1.285(3), C1–C2 1.444(3), C2–C3 1.390(3), C3–C4 1.378(4), C4–C5 1.400(4), C5–C6 1.389(4), C6–C7 1.373(4), C7–C2 1.389(3), C5–B1 1.586(6), B1–C21 1.553(9), B1–C30 1.567(9).

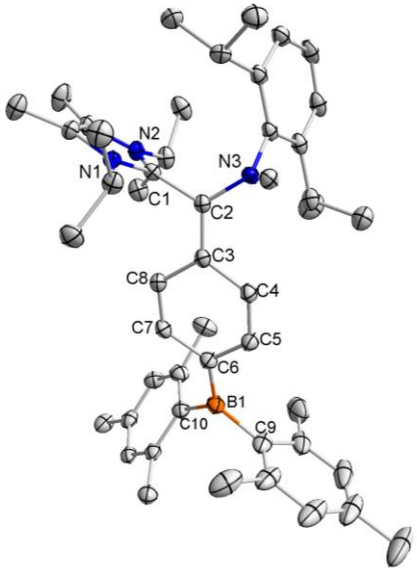


Fig. S65 Molecular structure of **8** with thermal ellipsoids at 50 % probability level. All H atoms are omitted for clarity reasons. Selected bond lengths [Å] and bond angles [°]: N1–C1 1.354(1), N2–C1 1.351(1), C2–N3 1.433(1), C1–C2 1.467(1), C2–C3 1.394(1), C3–C4 1.441(1), C4–C5 1.369(1), C5–C6 1.423(1), C6–C7 1.424(1), C7–C8 1.367(1), C8–C3 1.443(1), C6–B1 1.513(2), B1–C9 1.603(2), B1–C10 1.599(2); twist angle N2–C1–N1 plane and C3–C2–N3 plane: 84.01°.

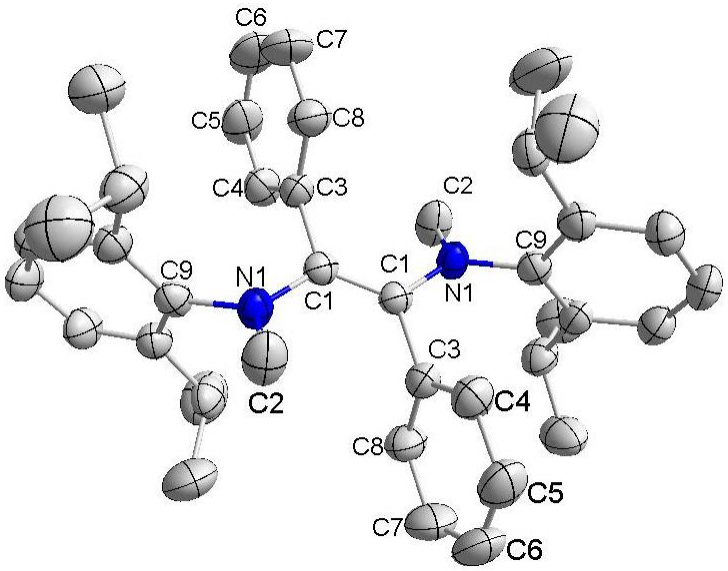


Fig. S66 Molecular structure of **9** with thermal ellipsoids at 50 % probability level. All H atoms are omitted for clarity reasons. Selected bond lengths [Å]: N1–C1 1.4211(16), N1–C9 1.427(8), C2–N1 1.4435(17), C1–C1 1.359(2), C1–C3 1.5004(17), C3–C4 1.3853(19), C4–C5 1.381(2), C5–C6 1.372(3), C6–C7 1.371(3), C7–C8 1.382(2), C8–C3 1.3826(19).

Crystallographic Details

Single-crystal X-ray diffraction data of **3**, **5**, **6**, **D** were collected at 273 K, those of **8**, **C** were collected at 100 K and the diffraction data of **7** were collected at 293K, respectively. Data of the compounds **3**, **5**, **6**, **D** and **9** were collected using a Bruker APEX-II CCD: Kappa single diffractometer with graphite-monochromated molybdenum *Kα* radiation, λ = 0.71073 Å. Data of the compound **C** were collected using a XtaLAB AFC12 (RINC): Kappa single diffractometer with graphite-monochromated molybdenum *Kα* radiation, λ = 0.71073 Å. The data of compound **7** were collected using a STOE IPDS2T. The data of compound **8** were collected using a XtaLAB Synergy Single source at home/near HyPix: Kappa single diffractometer with graphite-monochromated copper *Kα* radiation, λ = 1.54184 Å. Data were integrated using CrysAlisPro 1.171.39.29d (Rigaku Oxford Diffraction, 2017) software or XArea (STOE) software.[S6] Empirical absorption corrections were done using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm. The structures were solved with the SHELXT structure solution program[S7] and refined with the SHELXL refinement package[S8] using Least Squares minimisation in the Olex-2 software.[S9] All non-hydrogen atoms were refined with anisotropic thermal parameters. All the hydrogen atoms were placed in geometrically calculated positions or found in the Fourier difference map and included in the refinement process using a riding model. In the structure of **5** all four *iso*-propyl groups are disordered. All four disorders were modelled with SADI, SIMU and DELU constraints. Occupancies are 52% vs 48%, 68% vs 31%, 84% vs 16%, and 60% vs 40%. The triflate anion is entirely and severely disordered, which was refined with three orientations and SADI, SAME, SIMU and DELU constraints. Occupancies are 42.676%, 39.138%, and 18.136%. The poor parameter to data ratio of this refinement goes back to substantial number of disordered atom positions. In the structure of **6** both of the Dip *iso*-propyl groups are disordered over two orientations each. This was modelled with SADI, SIMU and DELU. Occupancies are 70% vs 30%, and 61% vs 39%. Also both triflate anions are disordered. One appears in three different orientations. This was modelled with SAME, SIMU and DELU constraints. Occupancies are 44%, 44%, and 12%. The second triflate is anchored by its sulfur atom which is not disordered. The other seven atoms are all split. This was modelled with SAME, SIMU and DELU constraints. Occupancies are 82% vs 18%. In the structural data for **D** a badly disordered rather diffuse pentane molecule had to be removed from the refinement by the SQUEEZE/Platon[S10] routine (46 electrons in a void size of 155 Å^3). Further, two *iso*-propyl groups of the DIP are disordered. All C-C distances in the *i*-Pr groups with SADI, and all displacement parameters are constrained with SIMU and DELU. Occupancies are 81% vs 19% and 55% vs 45%. For the refinement of 7 again unresolvable electron density was removed by the SQUEEZE/Platon[S10] routine (311 electrons in a void size of 1752 Å^3). This is accordance with a little less than two acetonitrile molecules per formula and 16 in the unit cell (Z = 8). The solvents are located at sites of symmetry operators and it was not possible to model the disorder in this case due to the very high symmetry of the space group. The entire B(mesityl)$_2$ unit is disordered. This was modelled with SAME, SIMU and DELU constraints and a SADI for the B–C5 distance to the central phenyl moiety. Occupancies are 56% vs 44%. Of the triflate anion only the three fluorine atoms appear in two orientations. This was modelled with SADI for all C-F distances, SIMU and DELU. Occupancies are 53% vs 47%. Half of the molecule of **9** comprises the asymmetric unit. The refined one Dip-substituent substituent is entirely disordered by a small sideways motion. This was modelled with SAME, SIMU and DELU constraints. Occupancies are 71% vs. 29%.

Table S1. Crystal data and structure refinement for **3** (CCDC 2249364).

Identification code	NC49
Empirical formula	$C_{31}H_{45}N_3$
Formula weight	459.70
Temperature/K	273(2)
Crystal system	triclinic
Space group	P-1
a/Å	9.5583 (19)
b/Å	9.955(2)
c/Å	17.258(4)
α/°	97.09(3)
β/°	99.30(3)
γ/°	116.20(3)
Volume/Å^3	1418.5(7)
Z	2
ρ_{calc}g/cm^3	1.076
μ/mm^{-1}	0.063
F(000)	504.0
Crystal size/mm^3	0.180 x 0.156 x 0.090
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.337 to 27.169
Index ranges	-11 ≤ h ≤ 12, -12 ≤ k ≤ 12, -22 ≤ l ≤ 22
Reflections collected	44022
Independent reflections	6280 [R_{int} = 0.0360, R_{sigma} = 0.0412]
Data/restraints/parameters	6280 / 0 / 319
Goodness-of-fit on F^2	1.027
Final R indexes [I>=2σ (I)]	R_1 = 0.0509, wR_2 = 0.1213
Final R indexes [all data]	R_1 = 0.0892, wR_2 = 0.1395
Largest diff. peak/hole / e Å^{-3}	0.192/-0.151

Table S2. Crystal data and structure refinement for **5** (CCDC 2249365).

Identification code	NC61_1
Empirical formula	$C_{32}H_{45}F_3N_3O_3S$
Formula weight	608.77
Temperature/K	273(2)
Crystal system	Monoclinic
Space group	P 21/n
a/Å	10.953(2)
b/Å	16.805(3)
c/Å	18.971(4)
α/°	90
β/°	106.36(3)
γ/°	90
Volume/Å^3	3350.8(13)
Z	4
ρ_{calc}g/cm^3	1.207
μ/mm^{-1}	0.148
F(000)	1300
Crystal size/mm^3	0.180 × 0.156 × 0.090
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.286 to 25.026
Index ranges	-12 ≤ h ≤ 13, -20 ≤ k ≤ 19, -22 ≤ l ≤ 20
Reflections collected	32861
Independent reflections	5898 [R_{int} = 0.0394, R_{sigma} = 0.0275]
Data/restraints/parameters	5898 / 1245 / 622
Goodness-of-fit on F^2	1.029
Final R indexes [I>=2σ (I)]	R_1 = 0.0652, wR_2 = 0.1637
Final R indexes [all data]	R_1 = 0.0884, wR_2 = 0.1805
Largest diff. peak/hole / e Å^{-3}	0.279/ -0.239

Table S3. Crystal data and structure refinement for **6** (CCDC 2249366).

Identification code	NC60b
Empirical formula	$C_{33}H_{45}F_6N_3O_6S_2$
Formula weight	757.84
Temperature/K	273(2)
Crystal system	Triclinic
Space group	P-1
a/Å	9.4326(19)
b/Å	11.413(2)
c/Å	18.825(4)
α/°	79.77(3)
β/°	82.21(3)
γ/°	76.60(3)
Volume/Å^3	1930.6(7)
Z	2
ρ_{calc}g/cm^3	1.304
μ/mm^{-1}	0.211
F(000)	796
Crystal size/mm^3	0.182 x 0.117 x 0.063
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.011 to 27.149
Index ranges	-12 ≤ h ≤ 12, -14 ≤ k ≤ 14, -24 ≤ l ≤ 24
Reflections collected	59728
Independent reflections	8508 [R_{int} = 0.0791, R_{sigma} = 0.0412]
Data/restraints/parameters	8508 / 1660 / 716
Goodness-of-fit on F^2	1.032
Final R indexes [I>=2σ (I)]	R_1 = 0.0715, wR_2 = 0.1858
Final R indexes [all data]	R_1 = 0.1372, wR_2 = 0.2249
Largest diff. peak/hole / e Å^{-3}	0.599/-0.251

Table S4. Crystal data and structure refinement for **C** (CCDC 2249367).

Identification code	AJ2143
Empirical formula	$C_{51}H_{66}BN_2$
Formula weight	344.28
Temperature/K	100.01(10)
Crystal system	triclinic
Space group	P-1
a/Å	7.2659(7)
b/Å	10.231(2)
c/Å	24.4748(15)
α/°	91.557(13)
β/°	97.622(7)
γ/°	90.170(13)
Volume/Å^3	1802.6(4)
Z	4
ρ_{calc}g/cm^3	1.269
μ/mm^{-1}	2.275
F(000)	712
Crystal size/mm^3	0.762 x 0.760 x 0.572
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.828 to 26.732
Index ranges	-8 ≤ h ≤ 9, -10 ≤ k ≤ 12, -30 ≤ l ≤ 26
Reflections collected	19467
Independent reflections	7171 [R_{int} = 0.0356, R_{sigma} = 0.0496]
Data/restraints/parameters	7171 / 0 / 387
Goodness-of-fit on F^2	1.019
Final R indexes [I>=2σ (I)]	R_1 = 0.0400, wR_2 = 0.0918
Final R indexes [all data]	R_1 = 0.0624, wR_2 = 0.1016
Largest diff. peak/hole / e Å^{-3}	0.583/-0.686

Table S5. Crystal data and structure refinement for **D** (CCDC 2249368).

Identification code	NC31D
Empirical formula	$C_{39.5}H_{50}BN$
Formula weight	556.0
Temperature/K	273(2)
Crystal system	triclinic
Space group	P-1
a/Å	10.200(2)
b/Å	12.537(3)
c/Å	15.057(3)
α/°	93.09(3)
β/°	101.60(3)
γ/°	112.80(3)
Volume/Å^3	1720.0(7)
Z	2
ρ_{calc}g/cm^3	0.992
μ/mm^{-1}	0.056
F(000)	556
Crystal size/mm^3	0.278 x 0.131 x 0.082
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.096 to 27.144
Index ranges	-13 ≤ h ≤ 13, -16 ≤ k ≤ 16, -19 ≤ l ≤ 19
Reflections collected	53371
Independent reflections	7578 [R_{int} = 0.0709, R_{sigma} = 0.0503]
Data/restraints/parameters	7578/ 166 / 405
Goodness-of-fit on F^2	1.021
Final R indexes [I>=2σ (I)]	R_1 = 0.0648, wR_2 = 0.1801
Final R indexes [all data]	R_1 = 0.1329, wR_2 = 0.2187
Largest diff. peak/hole / e Å^{-3}	0.196/ -0.200

Table S6. Crystal data and structure refinement for **7** (CCDC 2249369).

Identification code	NC37
Empirical formula	$C_{39}H_{47}BF_3NO_3S$
Formula weight	677.64
Temperature/K	293(2)
Crystal system	tetragonal
Space group	P 4/n
a/Å	27.406(4)
b/Å	27.406(4)
c/Å	11.871(2)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	8916(3)
Z	8
ρ_{calc}g/cm^3	1.010
μ/mm^{-1}	0.116
F(000)	2880
Crystal size/mm^3	0.241 x 0.216 x 0.201
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	1.870 to 25.020
Index ranges	-32 ≤ h ≤ 32, -32 ≤ k ≤ 32, -14 ≤ l ≤ 14
Reflections collected	65686
Independent reflections	7877 [R_{int} = 0.1391, R_{sigma} = 0.1126]
Data/restraints/parameters	7877 / 1483 / 652
Goodness-of-fit on F^2	0.978
Final R indexes [I>=2σ (I)]	R_1 = 0.0536, wR_2 = 0.1242
Final R indexes [all data]	R_1 = 0.1188, wR_2 = 0.1499
Largest diff. peak/hole / e Å^{-3}	0.266/-0.232

Table S7. Crystal data and structure refinement for **8** (CCDC 2249370).

Identification code	NC39
Empirical formula	$C_{49}H_{66}BN_3$
Formula weight	707.85
Temperature/K	100(2)
Crystal system	Orthorhombic
Space group	Pbca
a/Å	18.03250(10)
b/Å	14.89340(10)
c/Å	32.42450(10)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	8708.09(8)
Z	8
ρ_{calc}g/cm^3	1.080
μ/mm^{-1}	0.460
F(000)	3088
Crystal size/mm^3	0.299 x 0.227 x 0.055
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	3.666 to 80.070
Index ranges	-22 ≤ h ≤ 23, -18 ≤ k ≤ 19, -41 ≤ l ≤ 41
Reflections collected	176472
Independent reflections	9482 [R_{int} = 0.0385, R_{sigma} = 0.0162]
Data/restraints/parameters	9482/0/ 742
Goodness-of-fit on F^2	1.017
Final R indexes [I>=2σ (I)]	R_1 = 0.0412, wR_2 = 0.1072
Final R indexes [all data]	R_1 = 0.0429, wR_2 = 0.1087
Largest diff. peak/hole / e Å^{-3}	0.303/-0.214

Table S8. Crystal data and structure refinement for **9** (CCDC 2287748).

Identification code	NC49carb
Empirical formula	$C_{40}H_{50}N_2$
Formula weight	558.82
Temperature/K	273(2)
Crystal system	monoclinic
Space group	P 21/c
a/Å	10.314 (2)
b/Å	13.131(3)
c/Å	13.121(3)
α/°	90
β/°	105.78(3)
γ/°	90
Volume/Å^3	1709.9(6)
Z	2
ρ_{calc}g/cm^3	1.085
μ/mm^{-1}	0.062
F(000)	608.0
Crystal size/mm^3	0.215 x 0.134 x 0.095
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.338 to 27.126
Index ranges	-13 ≤ h ≤ 11, -16 ≤ k ≤ 16, -16 ≤ l ≤ 16
Reflections collected	27593
Independent reflections	3773 [R_{int} = 0.0535, R_{sigma} = 0.0412]
Data/restraints/parameters	3773 / 828 / 309
Goodness-of-fit on F^2	1.027
Final R indexes [I>=2σ (I)]	R_1 = 0.0448, wR_2 = 0.1075
Final R indexes [all data]	R_1 = 0.0747, wR_2 = 0.1242
Largest diff. peak/hole / e Å^{-3}	0.185/-0.149

Quantum Chemical Calculations

The DFT calculations were performed using the Gaussian 16 (Revision C.01) suite[S11] of electronic structure Programs. The geometries were optimized at the B3LYP/Def2SVP Empirical Dispersion=GD3BJ level of DFT. To verify the stationary point, a frequency analysis was performed on optimized geometries. TD-DFT calculations were performed at the B3LYP/6-311G(2d,p) level. The solvent effect was accounted for with the polarizable continuum model (PCM) including acetonitrile as the solvent.

Table S8. Comparison of **8** with **VIII**.

	Excited state	**λ / nm**	**Energy / eV**	**Major transitions**	**Contribution**	**oscillator strength (*f*)**	**Λ[a]**	**Δ*r*[b] (Å)**	**Dipole moment (D)**
8	1	490.63	2.53	HOMO→LUMO	0.66	0.75	0.60	3.20	12.17
VIII	1	500.94	2.48	HOMO→LUMO	0.70	0.75	0.55	4.34	6.26

[a]Λ (lambda) index is a measure of the degree of overlap of hole and electron of excitations. [b]The Δ*r* index is a quantitative indicator for measuring the charge transfer (CT) length of electron excitation; a larger Δ*r* index implies a longer CT distance. Calculated using Multiwfn 3.8 software.[S12]

Table S9. Singlet–Triplet energy gap for **3** and **8**.

	DFT[a] functional	E_T[b] / Hartree	E_{BS}[b] / Hartree	E_{CS}[b] / Hartree	ΔE_{ST}[d] / kcalmol^{-1}
3	B3LYP-D3	–1371.077019	–	–1371.129387	–32.86
8	B3LYP-D3	-2093.791141	-2093.848498	-2093.848498	–35.99

[a]Def2SVP basis-set. [b]ZPVE corrections are included. BS: Broken symmetry singlet. CS: Closed shell singlet.

Table S10. Dipole moments and HOMO-LUMO energies of **3**, **5**, **6**, **8** and **VIII**.

	Dipole moment (D)	HOMO–LUMO (eV)	HOMO (eV)	LUMO (eV)
3	7.48	2.998	3.352	0.354
5	11.21	3.304	4.408	1.104
6	12.85	2.796	6.463	3.667
8	12.17	3.018	3.823	0.805
VIII	6.26	3.018	4.418	1.400

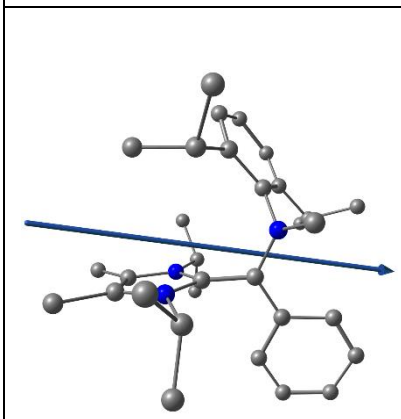
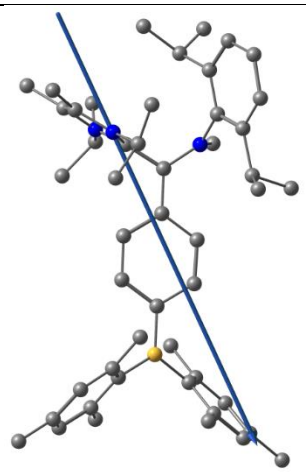
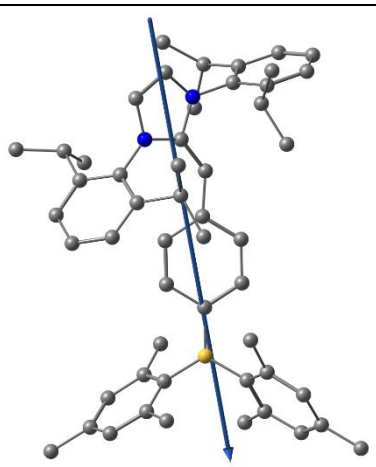
3	**8**	**VIII**
		
7.48 D	12.17 D	6.26 D

Fig. S67 Calculated dipole moments for **3**, **8** and **VIII**.

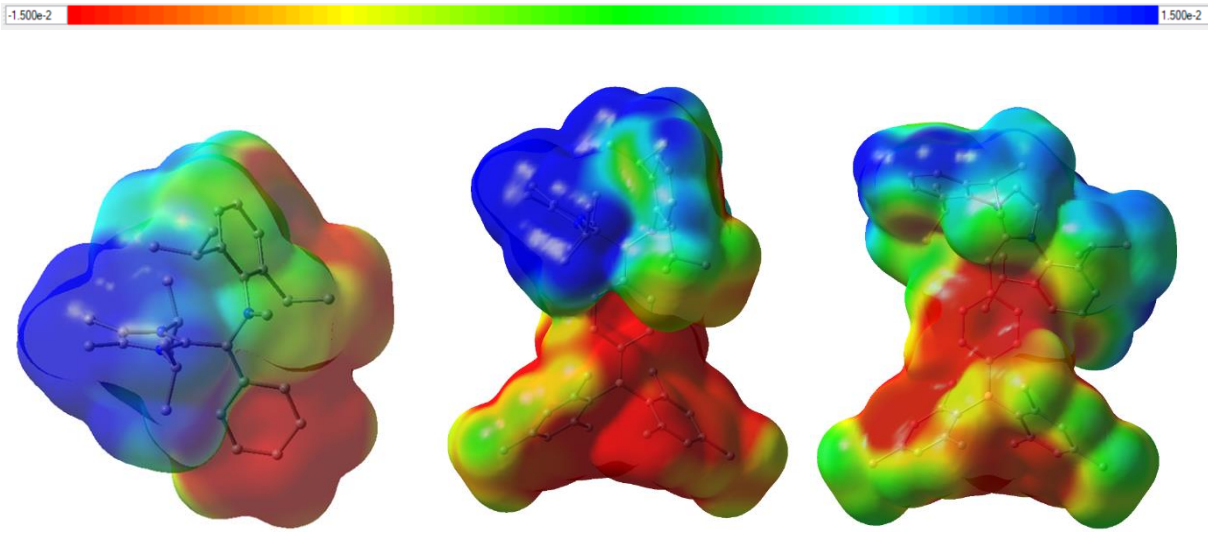


Fig. S68 Molecular electrostatic potential surface of **3**, **8** and **VIII**.

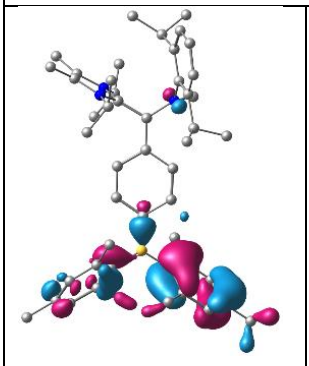
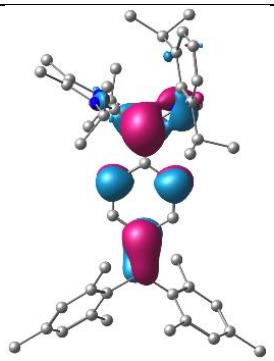
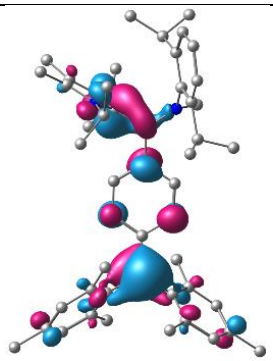
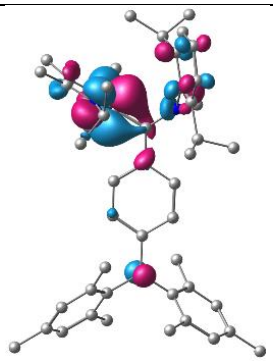
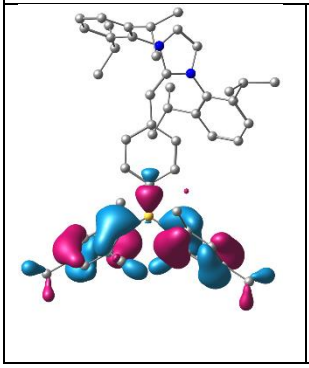
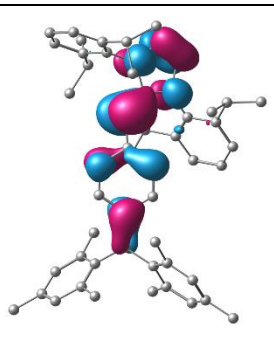
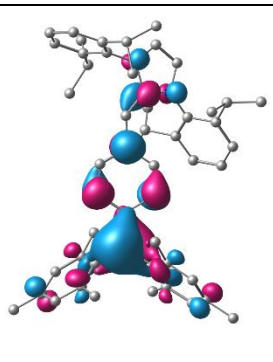
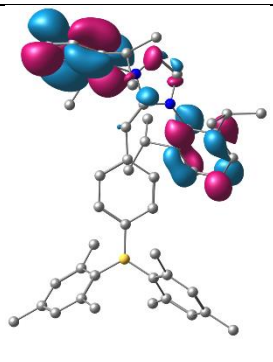
HOMO–1	HOMO	LUMO	LUMO+1
8			
			
VIII			
			

Fig. S69 Frontier Molecular Orbitals of **8** and **VIII**.

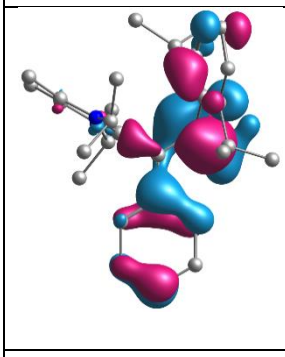
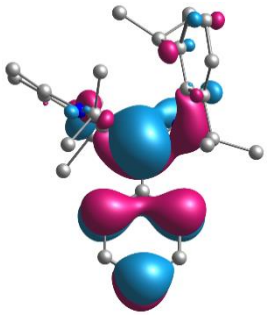
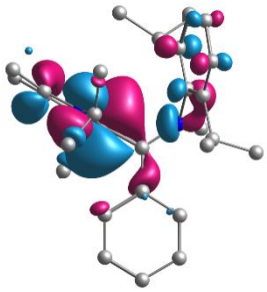
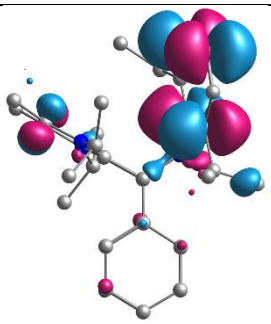
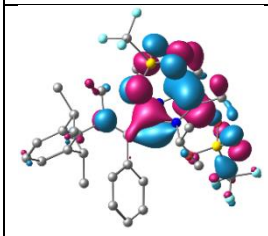
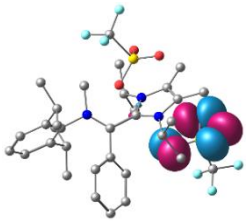
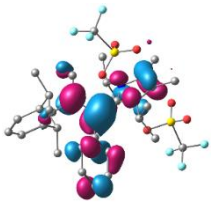
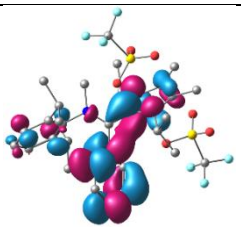
HOMO–1	HOMO	LUMO	LUMO+1
3			
			
6			
			

Fig. S70 Frontier molecular orbitals of **3** and **6**.

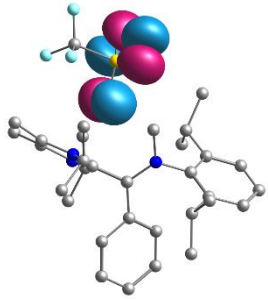
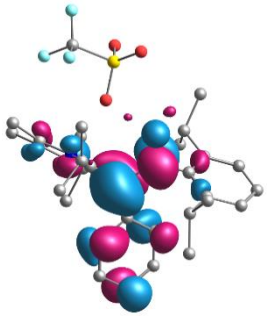
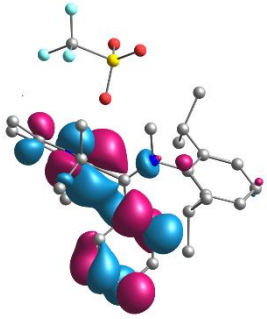
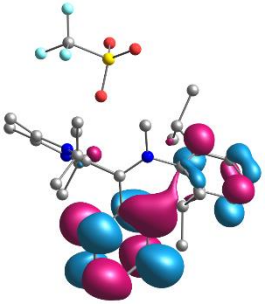
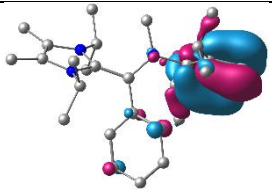
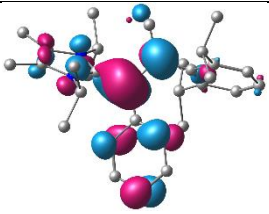
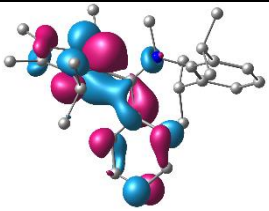
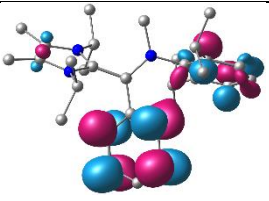
SOMO-α–1	SOMO-α	LUMO-α	LUMO-α+1
5 (including counter anion)			
			
5 (excluding counter anion)			
			

Fig. S71 Frontier molecular orbitals of **5**.

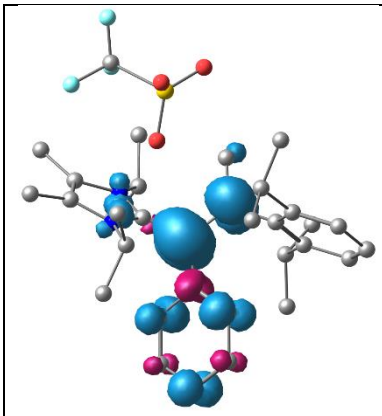
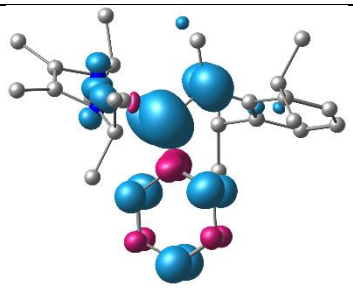
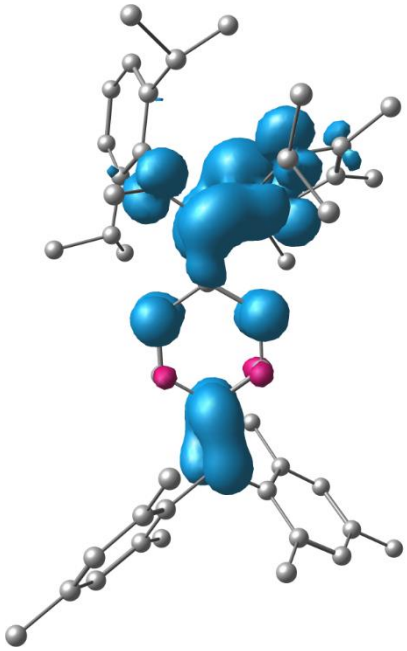
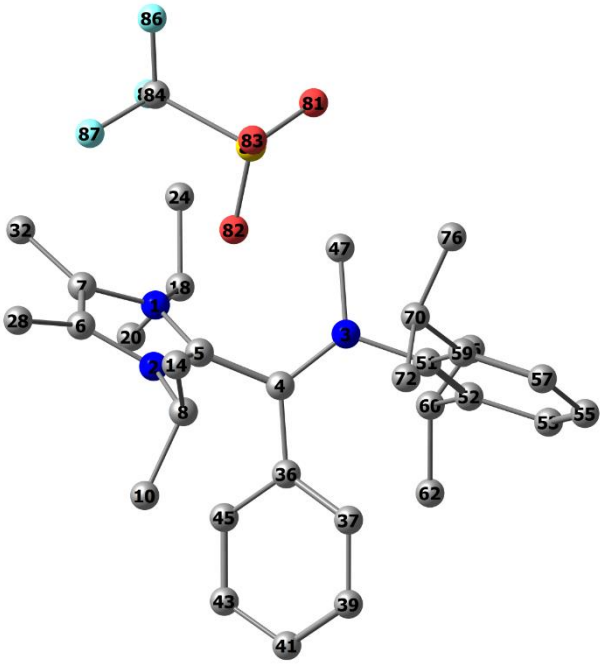
		
5 (including counter ion)	**5** (excluding counter ion)	**8**

Fig. S72 Spin density plot for **5** and **8**.

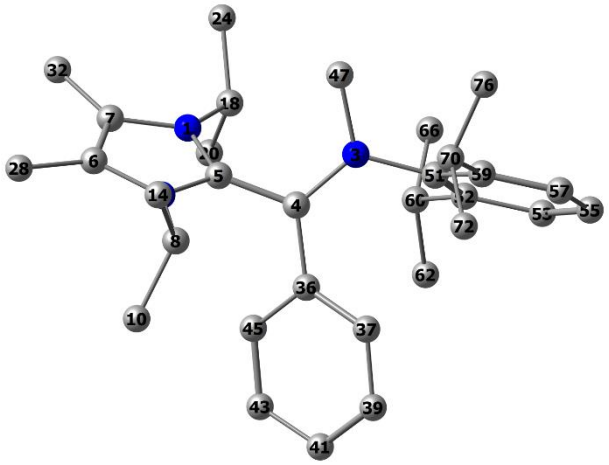
Table S11. Mulliken charges and spin densities for **5** (including countrerion).



		1	2
1	N	-0.179874	0.032062
2	N	-0.149877	0.029278
3	N	-0.259558	0.283233
4	C	-0.010690	0.515349
5	C	0.153647	-0.020242
6	C	-0.058643	0.008720
7	C	-0.071830	0.008100
8	C	-0.002141	0.002689
9	H	0.041452	0.000011
10	C	0.053362	0.000783
11	H	0.003462	0.000580
12	H	0.021001	0.000205
13	H	0.029327	-0.000465
14	C	0.038553	0.001332
15	H	-0.004031	0.000448
16	H	0.065027	-0.000080
17	H	0.014276	-0.000089
18	C	-0.020438	-0.000061
19	H	0.034770	-0.000405
20	C	0.058001	0.001538
21	H	0.016034	0.000054
22	H	0.022033	-0.000151
23	H	0.025642	-0.000080
24	C	0.038530	-0.000084
25	H	0.012784	-0.000002
26	H	0.022920	0.000849
27	H	0.048478	0.000129
28	C	0.117638	-0.000572
29	H	0.009815	0.000524
30	H	0.065895	0.000730
31	H	0.022647	0.000062
32	C	0.117113	-0.000415

33	H	0.018640	0.000713
34	H	0.055525	0.000729
35	H	0.009171	0.000074
36	C	0.067308	-0.106251
37	C	0.003254	0.119491
38	H	-0.006511	-0.005042
39	C	0.024680	-0.062983
40	H	-0.015759	0.002581
41	C	0.012508	0.123649
42	H	-0.015330	-0.005803
43	C	0.037283	-0.059328
44	H	-0.020823	0.002667
45	C	-0.053600	0.114177
46	H	-0.023851	-0.005181
47	C	0.143045	-0.022874
48	H	0.006597	0.026775
49	H	0.048892	0.005174
50	H	0.072822	0.003647
51	C	-0.077057	-0.014291
52	C	0.081872	0.007094
53	C	-0.077748	-0.000806
54	H	-0.027859	0.000598
55	C	0.055073	0.000751
56	H	-0.020850	-0.000048
57	C	-0.065166	-0.000969
58	H	-0.022620	0.001060
59	C	0.060502	0.012585
60	C	-0.044969	-0.000682
61	H	-0.010710	-0.001369
62	C	0.037988	0.000468
63	H	0.000367	0.000027
64	H	0.034116	-0.000186
65	H	0.002619	-0.000089
66	C	0.052039	0.000286
67	H	0.014495	-0.000185
68	H	0.003793	-0.000011
69	H	0.006102	-0.000079
70	C	-0.086278	0.000036
71	H	0.023215	-0.001308
72	C	0.032806	0.000331
73	H	-0.003598	0.000264
74	H	0.002597	0.000027
75	H	0.025180	-0.000007
76	C	0.041867	0.000112
77	H	-0.010894	0.000051
78	H	0.029347	-0.000011
79	H	0.022290	-0.000044
80	S	0.919453	-0.000040
81	O	-0.513209	0.000087
82	O	-0.555471	0.000157
83	O	-0.498174	-0.000039
84	C	0.450145	-0.000029
85	F	-0.186464	-0.000001
86	F	-0.151493	-0.000003
87	F	-0.182481	0.000018

Table S12. Mulliken charges and spin densities for **5** excluding countrerion.



		1	2
1	N	-0.170702	0.046145
2	N	-0.166832	0.047077
3	N	-0.268348	0.224726
4	C	-0.009392	0.505492
5	C	0.075439	-0.019519
6	C	-0.070493	0.013124
7	C	-0.072226	0.014042
8	C	-0.016977	0.002760
9	H	0.053797	-0.002028
10	C	0.042962	0.001123
11	H	0.023391	0.000776
12	H	0.040607	0.000560
13	H	0.040654	-0.000513
14	C	0.038712	0.002561
15	H	0.024738	0.000355
16	H	0.026740	-0.000154
17	H	0.044794	-0.000129
18	C	-0.034282	-0.002177
19	H	0.030549	-0.003977
20	C	0.044627	0.002614
21	H	0.025725	-0.000120
22	H	0.040571	-0.000351
23	H	0.043356	0.000050
24	C	0.033164	0.000615
25	H	0.030040	-0.000132
26	H	0.045393	0.000664
27	H	0.035986	0.000353
28	C	0.111941	-0.001116
29	H	0.029570	0.000430
30	H	0.062522	0.001227
31	H	0.041461	0.000365
32	C	0.114479	-0.001059
33	H	0.045261	0.001096
34	H	0.058016	0.001164
35	H	0.027494	0.000104
36	C	0.076883	-0.117710
37	C	0.000602	0.131300
38	H	-0.015563	-0.005846

39	C	0.029448	-0.070276
40	H	0.001880	0.002799
41	C	0.022070	0.137109
42	H	0.008040	-0.006263
43	C	0.035777	-0.068977
44	H	-0.001635	0.002604
45	C	-0.051087	0.127697
46	H	-0.008755	-0.005727
47	C	0.164685	-0.019399
48	H	0.019687	0.016992
49	H	0.048265	0.003994
50	H	0.039290	0.009408
51	C	-0.038937	-0.020322
52	C	0.072379	0.021059
53	C	-0.065488	-0.009043
54	H	-0.011783	0.000959
55	C	0.060036	0.017753
56	H	-0.000611	-0.000806
57	C	-0.061507	-0.010120
58	H	-0.008717	0.000748
59	C	0.044145	0.024185
60	C	-0.076723	0.001048
61	H	-0.005049	-0.000824
62	C	0.034247	0.000646
63	H	0.009845	0.000092
64	H	0.032878	-0.000212
65	H	0.020120	0.000097
66	C	0.059663	-0.000028
67	H	0.009008	-0.000046
68	H	0.013376	0.000126
69	H	0.021382	0.000265
70	C	-0.079255	-0.000138
71	H	-0.019589	-0.000797
72	C	0.043943	0.000781
73	H	0.022032	0.000127
74	H	0.009068	0.000001
75	H	0.018420	0.000011
76	C	0.048017	0.000326
77	H	0.021601	0.000202
78	H	0.021929	0.000118
79	H	0.013249	-0.000059

Table S13. Summary of TD-DFT calculated first ten low energy transitions of **8**.

Excitation energies and oscillator strengths: HOMO: 193, LUMO: 194

*Excited State 1: Singlet-A 2.5270 eV 490.63 nm f=0.7495 <S**2>=0.000*
193 -> 194 0.65561
193 -> 195 -0.23471

*Excited State 2: Singlet-A 2.6745 eV 463.58 nm f=0.1648 <S**2>=0.000*
193 -> 194 0.24362
193 -> 195 0.65630

*Excited State 3: Singlet-A 3.1594 eV 392.43 nm f=0.0049 <S**2>=0.000*
193 -> 196 0.69620

*Excited State 4: Singlet-A 3.3158 eV 373.92 nm f=0.0221 <S**2>=0.000*
193 -> 197 -0.16400
193 -> 198 0.67265

*Excited State 5: Singlet-A 3.3767 eV 367.17 nm f=0.0376 <S**2>=0.000*
193 -> 197 0.59196
193 -> 198 0.17141
193 -> 199 -0.23681
193 -> 201 0.23820

*Excited State 6: Singlet-A 3.4442 eV 359.98 nm f=0.0051 <S**2>=0.000*
193 -> 197 0.34351
193 -> 199 0.47373
193 -> 201 -0.37070

*Excited State 7: Singlet-A 3.6632 eV 338.46 nm f=0.0074 <S**2>=0.000*
193 -> 199 -0.37461
193 -> 200 0.47755
193 -> 201 -0.35658

*Excited State 8: Singlet-A 3.6789 eV 337.01 nm f=0.0141 <S**2>=0.000*
193 -> 199 0.26331
193 -> 200 0.50983
193 -> 201 0.40542

*Excited State 9: Singlet-A 3.8533 eV 321.76 nm f=0.0027 <S**2>=0.000*
193 -> 202 0.66717
193 -> 203 0.21964

*Excited State 10: Singlet-A 3.9774 eV 311.72 nm f=0.0191 <S**2>=0.000*
192 -> 194 0.67645
193 -> 203 -0.14527

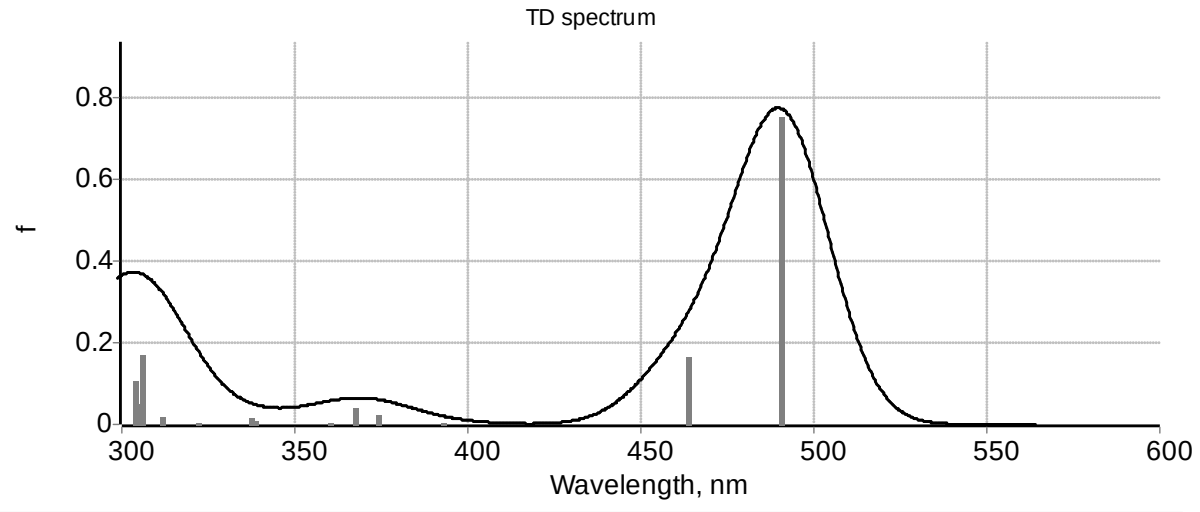


Fig. S73 TD-DFT calculated electronic absorption spectrum of **8**. *f* = oscillator strength

Table S14. Summary of TD-DFT calculated first ten low energy transitions of **3**.

Excitation energies and oscillator strengths: HOMO: 126, LUMO: 127

*Excited State 1: Singlet-A 2.3447 eV 528.79 nm f=0.0210 <S**2>=0.000*
126 ->127 0.69333
126 ->129 0.11312

*Excited State 2: Singlet-A 2.8495 eV 435.11 nm f=0.0238 <S**2>=0.000*
126 ->128 0.70196

*Excited State 3: Singlet-A 2.9912 eV 414.50 nm f=0.1618 <S**2>=0.000*
126 ->127 -0.11758
126 ->129 0.69331

*Excited State 4: Singlet-A 3.1634 eV 391.94 nm f=0.0290 <S**2>=0.000*
126 ->130 0.70221

*Excited State 5: Singlet-A 3.5407 eV 350.17 nm f=0.0040 <S**2>=0.000*
126 ->131 0.70491

*Excited State 6: Singlet-A 4.0509 eV 306.07 nm f=0.0180 <S**2>=0.000*
126 ->132 0.25608
126 ->133 0.64871

*Excited State 7: Singlet-A 4.1852 eV 296.24 nm f=0.2994 <S**2>=0.000*
126 ->132 0.61779
126 ->133 -0.25250
126 ->134 -0.15458

*Excited State 8: Singlet-A 4.3635 eV 284.14 nm f=0.0516 <S**2>=0.000*
125 ->127 0.69214

*Excited State 9: Singlet-A 4.5566 eV 272.10 nm f=0.0455 <S**2>=0.000*

125 ->128 -0.14360
126 ->134 0.65577
126 ->135 -0.14507

*Excited State 10: Singlet-A 4.6308 eV 267.74 nm f=0.0163 <S**2>=0.000*
125 ->128 0.62968
126 ->135 -0.26165

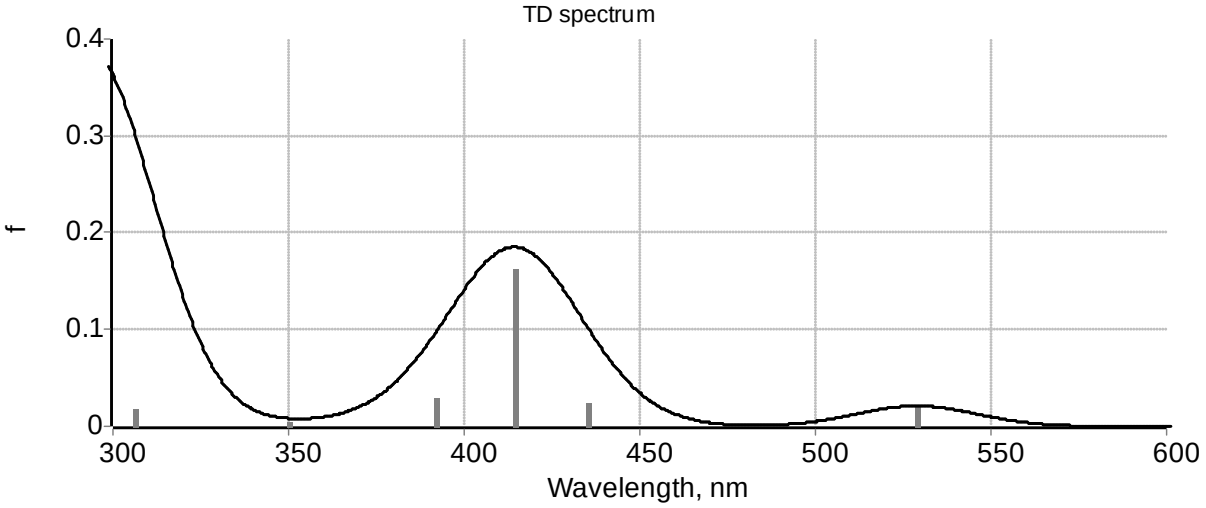


Fig. S74 TD-DFT calculated electronic absorption spectrum of **3**. *f* = oscillator strength

Table S15. Summary of TD-DFT calculated first ten low energy transitions of **5**.

Excitation energies and oscillator strengths: HOMO: 163, LUMO: 164

Excited State 1: 2.053-A 2.3282 eV 532.54 nm f=0.0692 <S**2>=0.804
163A ->164A 0.98212

Excited State 2: 2.063-A 2.7190 eV 455.99 nm f=0.0041 <S**2>=0.814
163A ->165A 0.95194
163A ->167A 0.22441

Excited State 3: 2.047-A 2.9982 eV 413.53 nm f=0.0035 <S**2>=0.797
163A ->166A 0.94583
163A ->167A -0.17149
163A ->168A 0.14435
162B ->163B -0.16450

Excited State 4: 2.059-A 3.1432 eV 394.45 nm f=0.0008 <S**2>=0.810
163A ->165A -0.25618
163A ->167A 0.91407
163A ->168A 0.20111
162B ->163B -0.15829

Excited State 5: 2.209-A 3.2732 eV 378.78 nm f=0.0058 <S**2>=0.970
163A ->166A -0.28519
163A ->167A -0.24853

163A ->168A 0.66161
159B ->163B -0.11883
162B ->163B -0.55068

Excited State 6: 2.363-A 3.5768 eV 346.63 nm f=0.1077 <S**2>=1.146
161A ->167A -0.10583
162A ->164A 0.20305
163A ->168A 0.54458
159B ->163B -0.10469
162B ->163B 0.68324
162B ->164B -0.17976

Excited State 7: 3.361-A 3.6296 eV 341.59 nm f=0.0124 <S**2>=2.574
157A ->166A 0.17646
160A ->164A -0.12943
160A ->165A -0.15032
160A ->166A -0.24889
160A ->167A 0.15697
161A ->165A -0.30989
161A ->166A 0.21409
161A ->167A 0.29265
162A ->166A -0.21752
163A ->168A 0.16508
157B ->166B 0.19491
159B ->166B -0.14452
160B ->164B 0.14616
160B ->165B 0.15465
160B ->166B 0.19234
160B ->167B -0.14068
161B ->165B 0.33541
161B ->166B -0.18903
161B ->167B -0.26396
162B ->163B 0.23170
162B ->166B 0.19567

Excited State 8: 2.671-A 3.8024 eV 326.07 nm f=0.0978 <S**2>=1.533
157A ->164A -0.14149
162A ->164A -0.29482
163A ->164A -0.11422
163A ->168A 0.33638
157B ->164B -0.11560
157B ->167B -0.10576
158B ->163B 0.26284
159B ->163B 0.27562
160B ->163B 0.49839
161B ->163B -0.31266
162B ->164B 0.28526

Excited State 9: 2.285-A 3.9040 eV 317.58 nm f=0.0035 <S**2>=1.055
162A ->169A -0.16696
163A ->169A 0.93625
162B ->168B -0.13723
162B ->169B -0.13151

Excited State 10: 2.302-A 3.9993 eV 310.01 nm f=0.0212 <S**2>=1.075
158A ->165A 0.14307

163A ->168A	0.10239
157B ->163B	0.17885
157B ->167B	-0.10019
159B ->163B	0.52843
160B ->163B	-0.29734
161B ->163B	0.65596

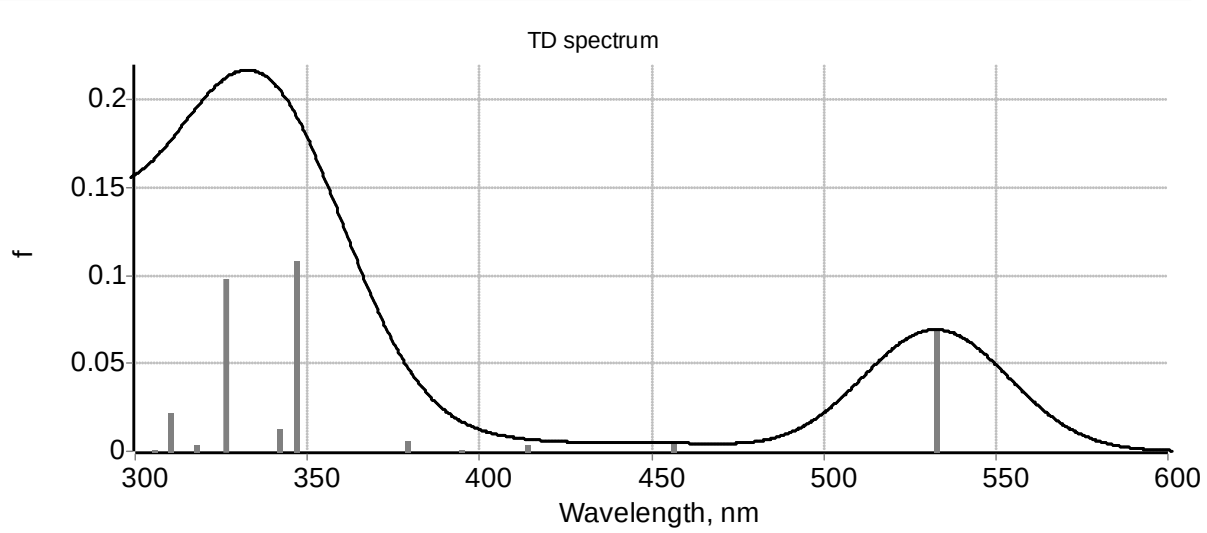


Fig. S75 TD-DFT calculated electronic absorption spectrum of **5**. *f* = oscillator strength

Table S16. Summary of TD-DFT calculated first ten low energy transitions of **6**.

Excitation energies and oscillator strengths: HOMO: 199, LUMO: 200

*Excited State 1: Singlet-A 2.8956 eV 428.18 nm f=0.1225 <S**2>=0.000*
196 ->200 -0.32826
199 ->200 0.61764

*Excited State 2: Singlet-A 2.9561 eV 419.42 nm f=0.0022 <S**2>=0.000*
198 ->200 0.70569

*Excited State 3: Singlet-A 3.0347 eV 408.56 nm f=0.0028 <S**2>=0.000*
197 ->200 0.70209

*Excited State 4: Singlet-A 3.1371 eV 395.21 nm f=0.1817 <S**2>=0.000*
196 ->200 0.61827
199 ->200 0.31902

*Excited State 5: Singlet-A 3.2555 eV 380.85 nm f=0.0083 <S**2>=0.000*
195 ->200 0.70033

*Excited State 6: Singlet-A 3.4797 eV 356.30 nm f=0.0411 <S**2>=0.000*
193 ->200 -0.10202
194 ->200 0.69468

*Excited State 7: Singlet-A 3.8290 eV 323.80 nm f=0.1131 <S**2>=0.000*
193 ->200 0.68757

*Excited State 8: Singlet-A 3.9278 eV 315.65 nm f=0.0009 <S**2>=0.000*
191 ->200 0.19711
192 ->200 0.66844

*Excited State 9: Singlet-A 4.0657 eV 304.95 nm f=0.0077 <S**2>=0.000*
188 ->200 0.18295
190 ->200 -0.22335
191 ->200 0.61363
192 ->200 -0.18654

*Excited State 10: Singlet-A 4.1828 eV 296.41 nm f=0.0078 <S**2>=0.000*
188 ->200 -0.23803
189 ->200 -0.12789
190 ->200 0.58917
191 ->200 0.25934

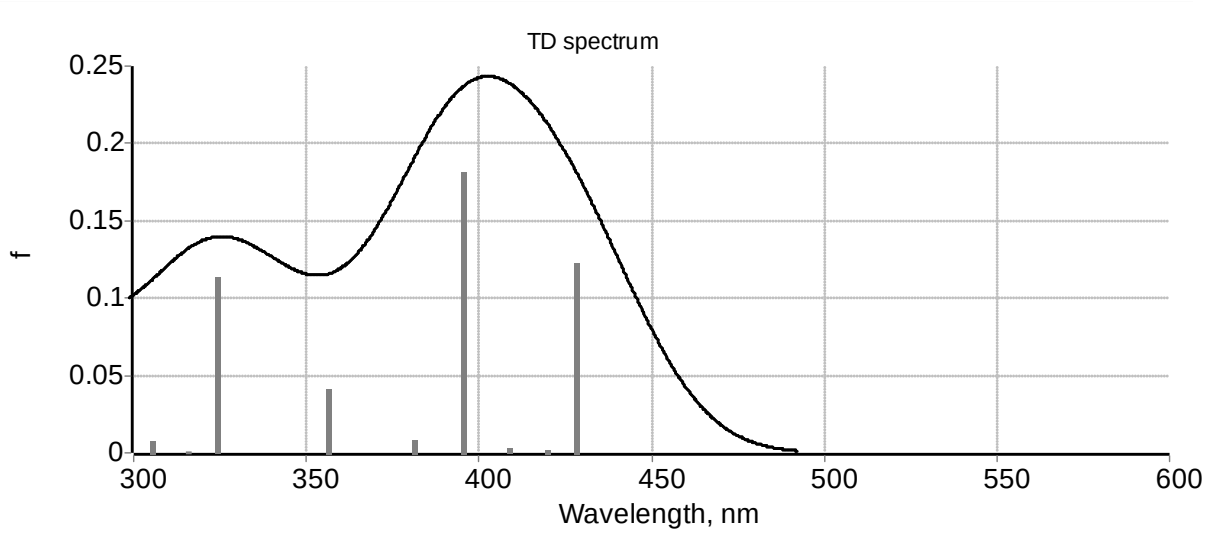
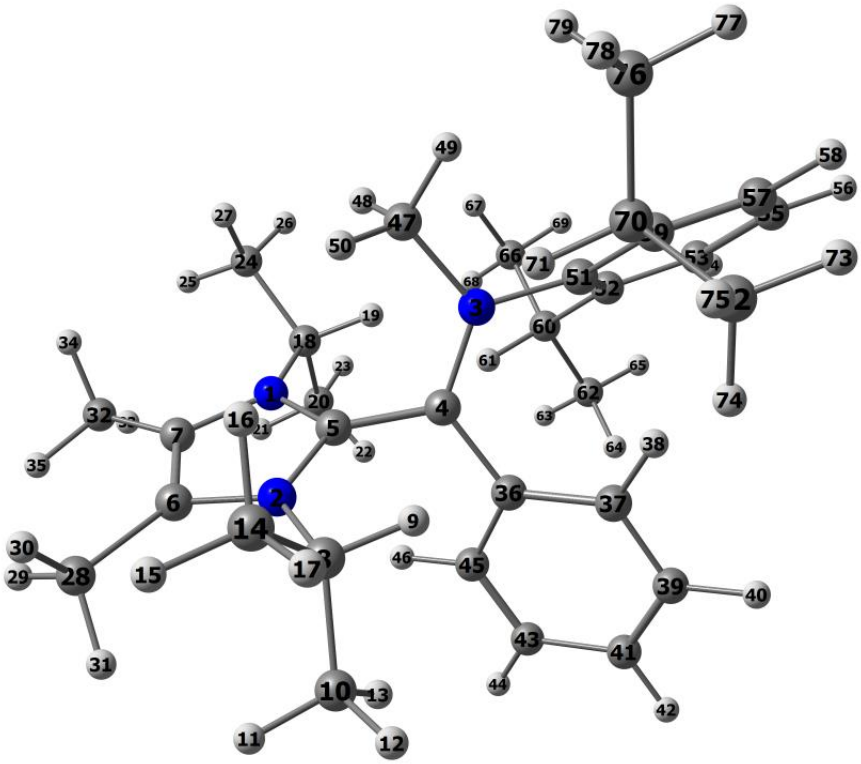


Fig. S76 TD-DFT calculated electronic absorption spectrum of **6**. *f* = oscillator strength

Table S17. Isotropic Fermi Contact Couplings of **5**.



Atom	a.u.	MegaHertz	Gauss	10(-4) cm-1
1 N(14)	0.02918	9.42909	3.36453	3.14521
2 N(14)	0.02825	9.12787	3.25705	3.04473
3 N(14)	0.03564	11.51479	4.10876	3.84092
4 C(13)	0.03389	38.09967	13.59491	12.70868
5 C(13)	-0.02466	-27.71866	-9.89071	-9.24595
6 C(13)	-0.00094	-1.05667	-0.37705	-0.35247
7 C(13)	-0.00051	-0.57825	-0.20633	-0.19288
8 C(13)	0.00320	3.59184	1.28166	1.19811
9 H(1)	-0.00037	-1.64813	-0.58810	-0.54976
10 C(13)	0.00002	0.02284	0.00815	0.00762
11 H(1)	0.00046	2.07494	0.74039	0.69213
12 H(1)	0.00029	1.30064	0.46410	0.43385
13 H(1)	0.00001	0.05211	0.01859	0.01738
14 C(13)	0.00183	2.05866	0.73458	0.68670
15 H(1)	0.00010	0.45659	0.16292	0.15230
16 H(1)	-0.00005	-0.20794	-0.07420	-0.06936
17 H(1)	-0.00009	-0.38496	-0.13736	-0.12841
18 C(13)	0.00043	0.48207	0.17202	0.16080
19 H(1)	0.00021	0.95321	0.34013	0.31796
20 C(13)	0.00122	1.36820	0.48821	0.45638
21 H(1)	-0.00005	-0.22064	-0.07873	-0.07360
22 H(1)	-0.00003	-0.14138	-0.05045	-0.04716
23 H(1)	-0.00001	-0.03262	-0.01164	-0.01088
24 C(13)	0.00193	2.17123	0.77475	0.72424
25 H(1)	-0.00006	-0.25054	-0.08940	-0.08357
26 H(1)	0.00015	0.65886	0.23510	0.21977
27 H(1)	0.00004	0.16458	0.05873	0.05490
28 C(13)	-0.00030	-0.34000	-0.12132	-0.11341
29 H(1)	0.00024	1.08758	0.38808	0.36278
30 H(1)	0.00061	2.74817	0.98061	0.91669

31	H(1)	0.00016	0.72888	0.26008	0.24313
32	C(13)	0.00013	0.14571	0.05199	0.04860
33	H(1)	0.00057	2.56269	0.91443	0.85482
34	H(1)	0.00046	2.06512	0.73689	0.68885
35	H(1)	0.00003	0.13774	0.04915	0.04595
36	C(13)	-0.02230	-25.07196	-8.94630	-8.36311
37	C(13)	0.01692	19.02181	6.78745	6.34499
38	H(1)	-0.00193	-8.62879	-3.07897	-2.87825
39	C(13)	-0.00821	-9.22489	-3.29167	-3.07709
40	H(1)	0.00089	3.96849	1.41605	1.32374
41	C(13)	0.01012	11.37327	4.05827	3.79372
42	H(1)	-0.00201	-8.99472	-3.20954	-3.00032
43	C(13)	-0.00759	-8.52828	-3.04310	-2.84473
44	H(1)	0.00077	3.42680	1.22277	1.14306
45	C(13)	0.01633	18.35862	6.55081	6.12378
46	H(1)	-0.00169	-7.55870	-2.69713	-2.52131
47	C(13)	-0.00786	-8.84109	-3.15472	-2.94907
48	H(1)	0.00728	32.54852	11.61412	10.85702
49	H(1)	0.00165	7.38319	2.63451	2.46277
50	H(1)	0.00291	13.02851	4.64890	4.34584
51	C(13)	-0.00909	-10.21702	-3.64569	-3.40803
52	C(13)	0.01310	14.72305	5.25355	4.91108
53	C(13)	0.00060	0.67693	0.24154	0.22580
54	H(1)	0.00040	1.80301	0.64336	0.60142
55	C(13)	0.00122	1.37501	0.49064	0.45865
56	H(1)	-0.00025	-1.13453	-0.40483	-0.37844
57	C(13)	-0.00040	-0.44447	-0.15860	-0.14826
58	H(1)	0.00023	1.03184	0.36819	0.34419
59	C(13)	0.00808	9.08816	3.24288	3.03148
60	C(13)	-0.00069	-0.77525	-0.27663	-0.25860
61	H(1)	-0.00004	-0.16258	-0.05801	-0.05423
62	C(13)	0.00109	1.22532	0.43723	0.40872
63	H(1)	-0.00001	-0.02886	-0.01030	-0.00963
64	H(1)	0.00006	0.27337	0.09755	0.09119
65	H(1)	0.00005	0.24524	0.08751	0.08180
66	C(13)	0.00007	0.08160	0.02912	0.02722
67	H(1)	0.00002	0.09395	0.03352	0.03134
68	H(1)	0.00007	0.30787	0.10986	0.10269
69	H(1)	0.00016	0.70775	0.25254	0.23608
70	C(13)	-0.00044	-0.49007	-0.17487	-0.16347
71	H(1)	0.00002	0.07185	0.02564	0.02397
72	C(13)	0.00071	0.80342	0.28668	0.26799
73	H(1)	0.00001	0.03492	0.01246	0.01165
74	H(1)	-0.00001	-0.05840	-0.02084	-0.01948
75	H(1)	-0.00000	-0.01271	-0.00454	-0.00424
76	C(13)	0.00016	0.18104	0.06460	0.06039
77	H(1)	0.00010	0.44050	0.15718	0.14694
78	H(1)	0.00008	0.34414	0.12280	0.11479
79	H(1)	0.00002	0.07473	0.02666	0.02493

Cartesian Coordinates

3-Singlet

N	-0.919721000	0.418902000	1.569917000
N	-2.044891000	1.017246000	-0.199274000
N	0.716967000	-0.375547000	-1.331908000
C	0.452997000	0.764148000	-0.506100000
C	1.271950000	1.937835000	-0.484326000
C	0.921576000	3.088119000	0.291415000
H	0.004123000	3.073045000	0.887130000
C	1.712321000	4.232371000	0.315347000
H	1.400499000	5.078957000	0.935197000
C	2.888762000	4.318835000	-0.441667000
H	3.504498000	5.220295000	-0.424124000
C	3.241118000	3.216731000	-1.230341000
H	4.147834000	3.256138000	-1.842228000
C	2.463689000	2.061816000	-1.260496000
H	2.774997000	1.227420000	-1.887690000
C	-0.780895000	0.738469000	0.249342000
C	-2.966300000	0.865921000	0.831814000
C	-2.255763000	0.495289000	1.949427000
C	-4.442759000	1.013742000	0.680132000
H	-4.925855000	0.979026000	1.665203000
H	-4.868971000	0.198968000	0.073064000
H	-4.722950000	1.965203000	0.205591000
C	-2.774724000	0.157427000	3.307037000
H	-3.807089000	0.515207000	3.414515000
H	-2.176688000	0.622217000	4.102653000
H	-2.779106000	-0.929633000	3.486606000
C	0.245586000	0.023011000	2.388019000
H	1.048306000	0.003182000	1.638599000
C	0.605232000	1.085261000	3.425074000
H	0.731561000	2.066484000	2.947077000
H	1.562996000	0.815921000	3.895649000
H	-0.145431000	1.168481000	4.226481000
C	0.093202000	-1.383698000	2.960281000
H	-0.618525000	-1.428669000	3.797716000
H	1.069909000	-1.720738000	3.336359000
H	-0.217805000	-2.091688000	2.179481000
C	-2.261004000	1.644302000	-1.519543000
H	-1.283444000	1.521913000	-2.003656000
C	-2.513154000	3.145816000	-1.370912000
H	-3.460639000	3.360661000	-0.852753000
H	-2.564344000	3.608433000	-2.368226000
H	-1.688679000	3.618907000	-0.819528000
C	-3.314817000	0.934600000	-2.367093000
H	-3.148607000	-0.150637000	-2.389996000
H	-3.246793000	1.306499000	-3.400484000
H	-4.339395000	1.123816000	-2.017754000
C	0.844126000	-1.647043000	-0.693689000
C	2.032108000	-1.962149000	0.024961000
C	2.152052000	-3.215611000	0.631931000
H	3.067245000	-3.462541000	1.172659000
C	1.136024000	-4.169789000	0.542481000
H	1.256478000	-5.149356000	1.011661000
C	-0.033227000	-3.854605000	-0.140055000
H	-0.839963000	-4.590051000	-0.193779000
C	-0.206505000	-2.598124000	-0.742140000
C	3.184641000	-0.973461000	0.077621000
H	2.753171000	0.031487000	0.034872000
C	4.015225000	-1.045673000	1.362976000
H	4.597874000	-1.978169000	1.439565000
H	3.379995000	-0.972858000	2.260510000
H	4.732379000	-0.210479000	1.390697000
C	4.078038000	-1.139616000	-1.161944000
H	4.567233000	-2.127973000	-1.162558000
H	4.861178000	-0.365015000	-1.186563000
H	3.487932000	-1.055824000	-2.086191000
C	-1.542612000	-2.279512000	-1.394483000
H	-1.520130000	-1.217019000	-1.654203000
C	-1.758365000	-3.076212000	-2.689317000
H	-0.940827000	-2.902261000	-3.404549000
H	-2.706434000	-2.792916000	-3.176610000
H	-1.798070000	-4.158508000	-2.484801000
C	-2.715759000	-2.474711000	-0.422289000
H	-2.855748000	-3.534389000	-0.156887000
H	-3.658154000	-2.123694000	-0.875069000
H	-2.556060000	-1.912567000	0.509526000
C	0.564697000	-0.311008000	-2.773667000
H	-0.481703000	-0.362653000	-3.141329000
H	1.117504000	-1.137588000	-3.248546000
H	0.994450000	0.633878000	-3.143207000

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.697947 (Hartree/Particle)

Thermal correction to Energy= 0.734755

Thermal correction to Enthalpy= 0.735699

Thermal correction to Gibbs Free Energy= 0.632692

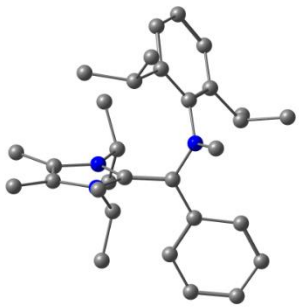
Sum of electronic and zero-point Energies= -1371.129387

Sum of electronic and thermal Energies= -1371.092578

Sum of electronic and thermal Enthalpies= -1371.091634

Sum of electronic and thermal Free Energies= -1371.194641

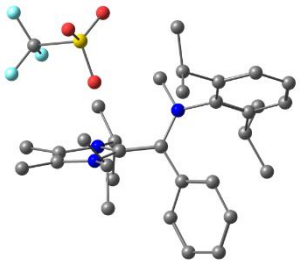
Charge = 0 Multiplicity = 1



3-Triplet

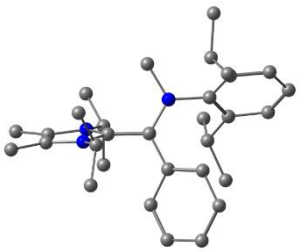
N	-1.184058000	0.124653000	1.574167000
N	-2.048643000	-1.035693000	-0.164171000
N	0.978632000	0.083831000	-1.290748000
H	3.514490000	1.852665000	-1.857989000
C	1.063654000	-2.877728000	-1.132881000
H	0.315072000	-2.232196000	-1.608545000

C	-0.187792000	0.586153000	-0.695660000	C	1.746585000	-3.705988000	-2.232150000
C	-0.668745000	1.913250000	-0.979473000	H	2.279242000	-3.063192000	-2.950501000
C	-1.925110000	2.344553000	-0.455137000	H	1.004394000	-4.300417000	-2.789505000
H	-2.523299000	1.648893000	0.130349000	H	2.483641000	-4.406646000	-1.807378000
C	-2.393788000	3.635082000	-0.667293000	C	0.322649000	-3.778294000	-0.133396000
H	-3.360409000	3.927728000	-0.248480000	H	1.021982000	-4.417961000	0.427368000
C	-1.644781000	4.561400000	-1.407234000	H	-0.379697000	-4.445937000	-0.656756000
H	-2.019248000	5.573986000	-1.572486000	H	-0.243401000	-3.168071000	0.585168000
C	-0.403775000	4.166982000	-1.924114000	C	1.239426000	0.159649000	-2.717013000
H	0.199745000	4.878195000	-2.494671000	H	1.473218000	-0.842009000	-3.117304000
C	0.078389000	2.879165000	-1.716704000	H	2.086817000	0.819271000	-2.973540000
H	1.056414000	2.617838000	-2.115458000	H	0.344771000	0.534090000	-3.231679000
C	-0.881598000	-0.312830000	0.253185000	- Thermochemistry -			
C	-2.927722000	-1.136015000	0.922540000	----------			
C	-2.380611000	-0.475787000	1.987940000	Temperature 298.150 Kelvin. Pressure 1.00000 Atm.			
C	-4.212787000	-1.894919000	0.877390000				
H	-4.755565000	-1.778155000	1.824314000	Zero-point correction= 0.696025			
H	-4.049412000	-2.973839000	0.718357000	(Hartree/Particle)			
H	-4.880376000	-1.546685000	0.072934000	Thermal correction to Energy= 0.733230			
C	-2.937787000	-0.330243000	3.364488000	Thermal correction to Enthalpy= 0.734174			
H	-3.867075000	-0.906072000	3.463827000	Thermal correction to Gibbs Free Energy= 0.628324			
H	-3.167369000	0.721283000	3.605190000	Sum of electronic and zero-point Energies= -			
H	-2.242424000	-0.694433000	4.138147000	1371.077019			
C	-0.069515000	0.558672000	2.415066000	Sum of electronic and thermal Energies= -			
H	0.637363000	0.990046000	1.693882000	1371.039814			
C	-0.441225000	1.685043000	3.380532000	Sum of electronic and thermal Enthalpies= -			
H	-1.014423000	2.464663000	2.856780000	1371.038870			
H	0.476735000	2.143043000	3.780879000	Sum of electronic and thermal Free Energies= -			
H	-1.029689000	1.333499000	4.239378000	1371.144720			
C	0.642468000	-0.616978000	3.092045000				
H	-0.000069000	-1.097998000	3.846832000	Charge = 0 Multiplicity = 3			
H	1.562671000	-0.278101000	3.592923000				
H	0.922219000	-1.366896000	2.338213000				
C	-2.342490000	-1.295773000	-1.571675000				
H	-1.381431000	-1.129618000	-2.078828000				
C	-3.348289000	-0.308952000	-2.181719000				
H	-4.334904000	-0.393753000	-1.700628000				
H	-3.481551000	-0.521563000	-3.254776000				
H	-3.004959000	0.727690000	-2.076928000				
C	-2.749968000	-2.747831000	-1.853412000				
H	-2.095525000	-3.450603000	-1.323419000				
H	-2.673325000	-2.949172000	-2.933395000				
H	-3.788401000	-2.952182000	-1.558193000				
C	1.961501000	-0.563742000	-0.465654000				
C	2.866265000	0.238691000	0.277997000				
C	3.854292000	-0.392965000	1.043887000				
H	4.558078000	0.212865000	1.616755000				
C	3.963097000	-1.781324000	1.078949000				
H	4.744773000	-2.256324000	1.676869000				
C	3.063929000	-2.559301000	0.355849000				
H	3.139565000	-3.647995000	0.400602000				
C	2.049190000	-1.972722000	-0.413422000				
C	2.819542000	1.760315000	0.223035000				
H	1.796662000	2.051921000	-0.039188000				
C	3.146813000	2.434627000	1.561972000				
H	4.208165000	2.323644000	1.835192000				
H	2.544352000	2.021784000	2.384567000				
H	2.939125000	3.514244000	1.498506000				
C	3.748739000	2.295568000	-0.879576000				
H	4.800530000	2.056268000	-0.652364000				
H	3.657669000	3.390115000	-0.969934000				
5							
N	-1.025776000	1.877585000	0.931300000	H	5.750779000	0.423323000	1.889800000
N	-0.971786000	1.523829000	-1.225835000	C	3.731726000	-0.476487000	3.630427000
N	1.151798000	-0.511766000	0.702740000	H	2.874402000	-1.110123000	3.905725000
C	1.020969000	0.685702000	0.014976000	H	3.774216000	0.371760000	4.332999000
C	-0.284243000	1.337201000	-0.070036000	H	4.645913000	-1.074997000	3.772813000
C	-2.175241000	2.153843000	-0.947620000	C	0.826177000	-2.681570000	-1.148439000
C	-2.216462000	2.373460000	0.408912000	H	0.129496000	-1.878895000	-0.879255000

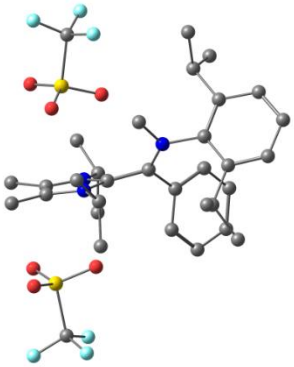
C	-0.524785000	0.981857000	-2.537141000	C	1.052487000	-2.590526000	-2.665290000
H	0.312149000	0.329430000	-2.266860000	H	1.707432000	-3.398018000	-3.031468000
C	0.004594000	2.101268000	-3.433647000	H	1.516019000	-1.632485000	-2.951246000
H	-0.797048000	2.796481000	-3.727437000	H	0.089690000	-2.675016000	-3.192345000
H	0.416124000	1.660703000	-4.353952000	C	0.132399000	-3.999801000	-0.773600000
H	0.803135000	2.671442000	-2.941709000	H	0.727976000	-4.875520000	-1.081500000
C	-1.568762000	0.107217000	-3.233920000	H	-0.851917000	-4.053331000	-1.263135000
H	-2.333422000	0.698403000	-3.755218000	H	-0.050137000	-4.065422000	0.308358000
H	-2.045397000	-0.576758000	-2.522380000	S	-2.845337000	-1.962868000	-0.001457000
H	-1.046693000	-0.490087000	-3.996133000	O	-2.436814000	-2.753491000	1.172318000
C	-0.518103000	2.047797000	2.309345000	O	-1.903768000	-0.856685000	-0.353068000
H	0.410268000	1.465616000	2.321782000	O	-3.380047000	-2.687059000	-1.163739000
C	-0.139752000	3.506062000	2.575794000	C	-4.292614000	-0.961202000	0.635936000
H	-1.013875000	4.172399000	2.543917000	F	-3.933335000	-0.280275000	1.749689000
H	0.596845000	3.863265000	1.841674000	F	-5.339833000	-1.719813000	0.943238000
H	0.309480000	3.589532000	3.576894000	F	-4.689071000	-0.045153000	-0.266560000
C	-1.462788000	1.468779000	3.363965000				
H	-2.300245000	2.144356000	3.582946000	- Thermochemistry -			
H	-0.904603000	1.320405000	4.300394000	----------			
H	-1.875450000	0.501761000	3.049872000	Temperature 298.150 Kelvin. Pressure 1.00000 Atm.			
C	-3.246523000	2.421926000	-1.947898000				
H	-3.953182000	3.160619000	-1.548009000	Zero-point correction= 0.729869			
H	-3.810336000	1.502241000	-2.163883000	(Hartree/Particle)			
H	-2.845897000	2.815149000	-2.891245000	Thermal correction to Energy= 0.775339			
C	-3.336162000	2.935997000	1.216831000	Thermal correction to Enthalpy= 0.776284			
H	-3.003121000	3.698827000	1.934400000	Thermal correction to Gibbs Free Energy= 0.651490			
H	-3.855683000	2.139934000	1.770042000	Sum of electronic and zero-point Energies= -			
H	-4.070078000	3.404929000	0.549384000	2332.041658			
C	2.108631000	1.324130000	-0.733830000	Sum of electronic and thermal Energies= -			
C	3.100235000	0.647203000	-1.485110000	2331.996187			
H	3.092238000	-0.436422000	-1.552416000	Sum of electronic and thermal Enthalpies= -			
C	4.088494000	1.352041000	-2.170188000	2331.995243			
H	4.833440000	0.794881000	-2.743364000	Sum of electronic and thermal Free Energies= -			
C	4.131527000	2.749402000	-2.140425000	2332.120037			
H	4.912494000	3.292613000	-2.676661000				
C	3.153552000	3.439923000	-1.416444000	Charge = 0 Multiplicity = 2			
H	3.166734000	4.531929000	-1.377556000				
C	2.163070000	2.741354000	-0.732039000				
H	1.415659000	3.300059000	-0.165629000				
C	0.193471000	-0.996019000	1.688714000				
H	0.531273000	-0.747591000	2.711603000				
H	0.103560000	-2.084632000	1.611866000				
H	-0.801923000	-0.599973000	1.491373000				
C	2.277991000	-1.376746000	0.509642000				
C	3.473085000	-1.145065000	1.215266000				
C	4.539400000	-2.029637000	1.004818000				
H	5.482200000	-1.872176000	1.533522000				
C	4.411715000	-3.109498000	0.131878000				
H	5.253335000	-3.790259000	-0.017933000				
C	3.212218000	-3.326045000	-0.548093000				
H	3.121733000	-4.176178000	-1.228023000				
C	2.120896000	-2.465323000	-0.377103000				
C	3.615079000	0.021496000	2.181203000				
H	2.695085000	0.619476000	2.109568000				
C	4.783642000	0.944938000	1.807969000				
H	4.818758000	1.813212000	2.485564000				
H	4.683941000	1.316474000	0.778227000				

5, excluding the counter ion

N	2.312872000	1.023941000	-0.687750000	C	-1.731199000	3.685034000	-0.357507000
N	2.484000000	-1.076696000	-0.086686000	H	-1.463578000	3.432993000	-1.396499000
N	-0.740809000	0.050426000	-0.929909000	H	-1.028741000	4.452446000	0.005971000
C	0.185888000	-0.132950000	0.082185000	H	-2.735329000	4.136179000	-0.380203000
C	1.603402000	-0.050430000	-0.244948000	C	-2.545647000	-2.076824000	-1.790223000
C	3.765985000	-0.641934000	-0.410407000	H	-1.445788000	-2.073530000	-1.770035000
C	3.658458000	0.677218000	-0.792035000	C	-2.994456000	-3.308330000	-0.985217000
C	2.050054000	-2.457293000	0.257717000	H	-4.090678000	-3.406063000	-0.972339000
H	0.958453000	-2.370753000	0.319342000	H	-2.650959000	-3.259944000	0.059253000
C	2.552293000	-2.898816000	1.630602000	H	-2.586118000	-4.227752000	-1.433408000
H	3.636255000	-3.079521000	1.645271000	C	-2.995951000	-2.196957000	-3.255098000

H	2.058266000	-3.843265000	1.901979000	H	-4.093070000	-2.257304000	-3.326588000
H	2.301569000	-2.155634000	2.399248000	H	-2.581954000	-3.106872000	-3.716926000
C	2.372089000	-3.440000000	-0.867311000	H	-2.678237000	-1.332710000	-3.858889000
H	3.445219000	-3.660866000	-0.943539000				
H	2.020436000	-3.061164000	-1.838976000	- Thermochemistry -			
H	1.855586000	-4.390197000	-0.667170000	----------			
C	1.725606000	2.383264000	-0.798721000	Temperature 298.150 Kelvin. Pressure 1.00000 Atm.			
H	0.647749000	2.202025000	-0.799502000				
C	2.048359000	3.216917000	0.440719000	Zero-point correction= 0.700079			
H	3.126727000	3.406995000	0.542435000	(Hartree/Particle)			
H	1.691780000	2.719408000	1.353813000	Thermal correction to Energy= 0.737309			
H	1.540782000	4.189512000	0.365816000	Thermal correction to Enthalpy= 0.738253			
C	2.073015000	3.082543000	-2.112361000	Thermal correction to Gibbs Free Energy= 0.631791			
H	3.084301000	3.508186000	-2.114024000	Sum of electronic and zero-point Energies= -			
H	1.368278000	3.913644000	-2.260976000	1370.963423			
H	1.978263000	2.401674000	-2.970885000	Sum of electronic and thermal Energies= -			
C	4.992016000	-1.491750000	-0.373588000	1370.926194			
H	5.885966000	-0.857717000	-0.422550000	Sum of electronic and thermal Enthalpies= -			
H	5.036785000	-2.188825000	-1.224643000	1370.925250			
H	5.055256000	-2.082335000	0.549185000	Sum of electronic and thermal Free Energies= -			
C	4.740510000	1.594775000	-1.253001000	1371.031711			
H	4.729192000	2.554166000	-0.717203000				
H	4.665424000	1.808764000	-2.330047000	Charge = 1 Multiplicity = 2			
H	5.718480000	1.130197000	-1.077321000				
C	-0.164407000	-0.411575000	1.472117000				
C	-1.342225000	-1.087997000	1.868450000				
H	-2.040905000	-1.451521000	1.121013000				
C	-1.621751000	-1.306656000	3.215342000				
H	-2.537708000	-1.834541000	3.489785000				
C	-0.744253000	-0.865071000	4.211418000				
H	-0.972917000	-1.036038000	5.265126000				
C	0.430122000	-0.200899000	3.840512000				
H	1.123366000	0.155926000	4.605470000				
C	0.714014000	0.023365000	2.496469000				
H	1.625882000	0.562608000	2.231726000				
C	-0.302831000	0.129759000	-2.318986000				
H	0.065050000	1.134636000	-2.582587000				
H	-1.148781000	-0.087383000	-2.977773000				
H	0.495502000	-0.600408000	-2.521068000				
C	-2.149743000	0.223261000	-0.684597000				
C	-2.624079000	1.360001000	0.006539000				
C	-4.008123000	1.495178000	0.176647000				
H	-4.397926000	2.370185000	0.699484000				
C	-4.896079000	0.541645000	-0.314391000				
H	-5.971512000	0.673125000	-0.177692000				
C	-4.407347000	-0.588125000	-0.967085000				
H	-5.107147000	-1.345807000	-1.325143000				
C	-3.033298000	-0.779914000	-1.151393000				
C	-1.702156000	2.442698000	0.546487000				
H	-0.681889000	2.046689000	0.533988000				
C	-1.997555000	2.791459000	2.011431000				
H	-1.244793000	3.499671000	2.392006000				
H	-1.970278000	1.891365000	2.643392000				
H	-2.982977000	3.266475000	2.133516000				
6							
N	-0.797197000	0.833984000	1.244328000	C	4.608878000	-1.061099000	-2.303639000
N	-0.808086000	1.151187000	-0.932667000	H	5.456646000	-1.757456000	-2.402471000
N	1.638735000	-0.970255000	0.546906000	H	4.905879000	-0.105089000	-2.760665000
C	0.524268000	-0.818770000	-0.152475000	H	3.775092000	-1.464152000	-2.897983000
C	0.123920000	-1.836818000	-1.145280000	C	0.617955000	-3.436740000	1.783439000
C	1.028089000	-2.403508000	-2.065616000	H	0.017984000	-2.565065000	1.496347000
H	2.051417000	-2.046618000	-2.115491000	C	-0.192568000	-4.667947000	1.358028000
C	0.601264000	-3.391905000	-2.943503000	H	-0.292448000	-4.718114000	0.264260000
H	1.304719000	-3.811757000	-3.665327000	H	-1.203652000	-4.620925000	1.790779000
C	-0.725532000	-3.844110000	-2.904830000	H	0.271465000	-5.604276000	1.704891000
H	-1.054039000	-4.627379000	-3.591980000	C	0.795648000	-3.377226000	3.309647000
C	-1.627682000	-3.279439000	-2.003208000	H	1.364303000	-4.246584000	3.675524000
H	-2.669117000	-3.606205000	-1.979547000	H	-0.184155000	-3.373178000	3.812327000
C	-1.215142000	-2.267282000	-1.134221000	H	1.342131000	-2.472700000	3.619465000
H	-1.942689000	-1.795943000	-0.470645000	S	-4.314456000	0.573840000	0.128660000

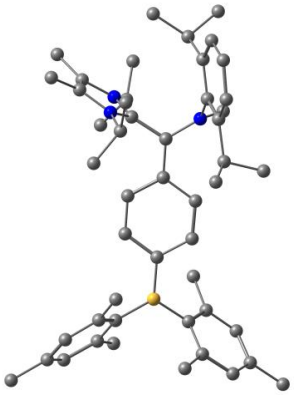
C	-0.365666000	0.321397000	0.057152000	O	-4.333356000	1.564189000	-0.965675000
C	-1.482129000	1.992147000	1.009995000	O	-4.471900000	1.117838000	1.493465000
C	-1.463263000	2.208231000	-0.367599000	O	-3.246954000	-0.463788000	0.005122000
C	-0.723234000	0.115573000	2.546887000	C	-5.854514000	-0.437680000	-0.149260000
H	-0.000278000	-0.683771000	2.373275000	F	-6.945016000	0.327308000	-0.115690000
C	-2.052812000	-0.557246000	2.886611000	F	-5.969634000	-1.381769000	0.791236000
H	-2.885653000	0.156326000	2.936134000	F	-5.798450000	-1.043962000	-1.341909000
H	-1.944764000	-1.064594000	3.857797000	S	1.953558000	3.037527000	-0.145124000
H	-2.331900000	-1.288472000	2.117598000	O	2.135460000	1.715669000	-0.813444000
C	-0.173563000	1.007271000	3.664215000	O	1.328432000	2.944508000	1.200786000
H	0.602007000	1.691051000	3.293968000	O	1.443156000	4.111409000	-1.009924000
H	0.259530000	0.364942000	4.445660000	C	3.715925000	3.511782000	0.245580000
H	-0.964543000	1.604130000	4.134053000	F	4.468413000	3.498704000	-0.857416000
C	-0.661271000	0.901892000	-2.400604000	F	3.784013000	4.718998000	0.797652000
H	0.055596000	0.079890000	-2.458449000	F	4.241610000	2.622726000	1.110472000
C	-2.002348000	0.437525000	-2.969471000				
H	-2.759096000	1.231465000	-2.925734000	- Thermochemistry -			
H	-2.414869000	-0.403883000	-2.402105000	----------			
H	-1.854983000	0.138979000	-4.018313000	Temperature 298.150 Kelvin. Pressure 1.00000 Atm.			
C	-0.048246000	2.066014000	-3.177817000				
H	-0.770888000	2.866526000	-3.374731000	Zero-point correction= 0.762315			
H	0.276197000	1.670190000	-4.152371000	(Hartree/Particle)			
H	0.821578000	2.485826000	-2.664008000	Thermal correction to Energy= 0.816019			
C	-2.072813000	2.879340000	2.042563000	Thermal correction to Enthalpy= 0.816963			
H	-1.289075000	3.534201000	2.456008000	Thermal correction to Gibbs Free Energy= 0.673575			
H	-2.553779000	2.312013000	2.844166000	Sum of electronic and zero-point Energies= -			
H	-2.855779000	3.493275000	1.584363000	3292.941412			
C	-1.947724000	3.413900000	-1.084642000	Sum of electronic and thermal Energies= -			
H	-1.088863000	4.071935000	-1.295084000	3292.887707			
H	-2.661535000	3.947505000	-0.447768000	Sum of electronic and thermal Enthalpies= -			
H	-2.471178000	3.157593000	-2.010254000	3292.886763			
C	2.165157000	-0.010043000	1.525775000	Sum of electronic and thermal Free Energies= -			
H	1.631465000	0.940530000	1.498975000	3293.030151			
H	3.210538000	0.190355000	1.282934000				
H	2.121119000	-0.475146000	2.519876000	Charge = 0 Multiplicity = 1			
C	2.446992000	-2.179207000	0.467508000				
C	3.709778000	-2.096837000	-0.157474000				
C	4.498383000	-3.253979000	-0.155831000				
H	5.478578000	-3.228761000	-0.635435000				
C	4.051916000	-4.433274000	0.437450000				
H	4.684684000	-5.323580000	0.425697000				
C	2.798820000	-4.480208000	1.044259000				
H	2.459136000	-5.408368000	1.506538000				
C	1.964876000	-3.354852000	1.077485000				
C	4.223390000	-0.828640000	-0.833601000				
H	3.427207000	-0.071436000	-0.833052000				
C	5.424205000	-0.239053000	-0.072150000				
H	6.301253000	-0.903028000	-0.137894000				
H	5.205417000	-0.086767000	0.994997000				
H	5.696685000	0.738322000	-0.496872000				



8-Broken Symmetry Singlet

B	3.873234000	-0.000351000	0.120377000	- Thermochemistry -			
N	-2.706247000	-1.548580000	0.420915000	----------			
N	-3.149970000	1.702017000	-0.492127000	Temperature 298.150 Kelvin. Pressure 1.00000 Atm.			
N	-3.138533000	1.504030000	1.677634000				
C	-1.960223000	-0.329032000	0.396239000	Zero-point correction= 1.038773			
C	-0.550076000	-0.262919000	0.344421000	(Hartree/Particle)			
C	0.150138000	0.993592000	0.382813000	Thermal correction to Energy= 1.097059			
H	-0.422656000	1.921942000	0.465010000	Thermal correction to Enthalpy= 1.098003			
C	1.524977000	1.063561000	0.305145000	Thermal correction to Gibbs Free Energy= 0.944093			
H	2.004084000	2.046999000	0.321294000	Sum of electronic and zero-point Energies= -			
C	2.352561000	-0.090796000	0.221849000	2093.848498			
C	1.658470000	-1.332387000	0.224848000	Sum of electronic and thermal Energies= -			
H	2.245268000	-2.253794000	0.163741000	2093.790212			
C	0.282396000	-1.430227000	0.277243000	Sum of electronic and thermal Enthalpies= -			
H	-0.188716000	-2.412097000	0.252913000	2093.789268			
C	-2.722055000	0.906409000	0.524431000	Sum of electronic and thermal Free Energies= -			
C	-3.831896000	2.673979000	1.385082000	2093.943178			
C	-3.835984000	2.801040000	0.015030000				
C	-2.851544000	1.380081000	-1.906384000	Charge = 0 Multiplicity = 1			

H	-2.385263000	0.390701000	-1.824771000
C	-1.811014000	2.331565000	-2.494536000
H	-2.192400000	3.357286000	-2.614143000
H	-1.518871000	1.968124000	-3.491258000
H	-0.908226000	2.354769000	-1.868453000
C	-4.119093000	1.239971000	-2.743754000
H	-4.851282000	0.593654000	-2.240401000
H	-3.860044000	0.759025000	-3.697773000
H	-4.585395000	2.208365000	-2.975834000
C	-2.694410000	1.015610000	3.001928000
H	-2.239427000	0.046512000	2.759962000
C	-1.592282000	1.909012000	3.572580000
H	-0.756468000	1.989219000	2.863995000
H	-1.207255000	1.462173000	4.501539000
H	-1.956437000	2.919541000	3.813367000
C	-3.849534000	0.777628000	3.972303000
H	-4.273370000	1.711880000	4.365707000
H	-3.475879000	0.200033000	4.830896000
H	-4.655763000	0.197712000	3.502990000
C	-4.490038000	3.548809000	2.398073000
H	-3.815623000	3.810351000	3.225474000
H	-5.381074000	3.066513000	2.830829000
H	-4.816871000	4.485011000	1.927489000
C	-4.493358000	3.851072000	-0.816162000
H	-5.414177000	3.478535000	-1.292554000
H	-3.832682000	4.219866000	-1.612324000
H	-4.768352000	4.708280000	-0.188018000
C	-2.681002000	-2.404741000	1.593274000
H	-3.299578000	-2.052418000	2.444765000
H	-1.645625000	-2.499711000	1.956749000
H	-3.035504000	-3.412800000	1.326708000
C	-3.708371000	-1.752838000	-0.577286000
C	-3.320058000	-2.122414000	-1.894870000
C	-4.308658000	-2.345371000	-2.858478000
H	-4.016065000	-2.640572000	-3.867389000
C	-5.665139000	-2.221005000	-2.551647000
H	-6.422194000	-2.415866000	-3.315164000
C	-6.042327000	-1.835402000	-1.270040000
H	-7.102619000	-1.715683000	-1.033993000
C	-5.082256000	-1.575605000	-0.279340000
C	-1.853765000	-2.333618000	-2.235100000
H	-1.270395000	-1.658049000	-1.601054000
C	-5.547665000	-1.073641000	1.078784000
H	-4.648956000	-0.794442000	1.637664000
C	-6.277233000	-2.163584000	1.877428000
H	-7.201047000	-2.476992000	1.364762000
H	-6.557924000	-1.799290000	2.879733000
H	-5.646394000	-3.056082000	2.002001000
C	-6.408177000	0.193027000	0.957230000
H	-5.890617000	0.970731000	0.376777000
H	-6.634570000	0.605964000	1.954335000
H	-7.370328000	-0.012038000	0.462300000
C	4.558053000	1.368643000	-0.302341000
C	4.217786000	2.009172000	-1.520049000
C	4.854849000	3.203786000	-1.891052000
H	4.590201000	3.670366000	-2.845521000
C	5.817320000	3.811526000	-1.083667000
C	6.148582000	3.178245000	0.120908000
H	6.902800000	3.632223000	0.771952000
C	5.551009000	1.976282000	0.512313000
C	3.189788000	1.444189000	-2.477977000
H	2.177363000	1.811480000	-2.241828000
H	3.130938000	0.349061000	-2.435607000
H	3.418855000	1.741484000	-3.513156000
C	5.984465000	1.349977000	1.817821000
H	6.669702000	2.013052000	2.366379000
H	6.494689000	0.388884000	1.652817000
H	5.125970000	1.138063000	2.473523000
C	6.485769000	5.102483000	-1.484659000
H	6.159471000	5.434202000	-2.481690000
H	7.583415000	4.997163000	-1.505506000



H	6.256796000	5.911224000	-0.769665000
C	-1.429972000	-3.767533000	-1.878953000
H	-1.963412000	-4.500612000	-2.506467000
H	-1.656999000	-3.996183000	-0.827508000
H	-0.347424000	-3.903708000	-2.030564000
C	-1.493983000	-2.001410000	-3.686872000
H	-1.832595000	-0.991039000	-3.968133000
H	-1.931598000	-2.713650000	-4.404999000
H	-0.401351000	-2.037616000	-3.817488000
C	4.771476000	-1.271848000	0.428531000
C	4.684939000	-1.940314000	1.675507000
C	5.510048000	-3.043577000	1.942989000
H	5.439788000	-3.532429000	2.920014000
C	6.418272000	-3.534199000	1.003372000
C	6.498226000	-2.874220000	-0.229131000
H	7.204368000	-3.236897000	-0.983155000
C	5.708097000	-1.758284000	-0.522266000
C	3.736194000	-1.498019000	2.769626000
H	4.116255000	-1.798253000	3.758356000
H	2.738958000	-1.949825000	2.643180000
H	3.577254000	-0.411582000	2.774435000
C	5.874818000	-1.094272000	-1.869921000
H	6.548117000	-1.676173000	-2.516577000
H	6.287566000	-0.078842000	-1.770009000
H	4.913074000	-0.989849000	-2.395183000
C	7.283539000	-4.734869000	1.292691000
H	8.346691000	-4.522773000	1.091625000
H	7.193836000	-5.054686000	2.341620000
H	7.003108000	-5.592170000	0.656616000

8-Closed shell Singlet

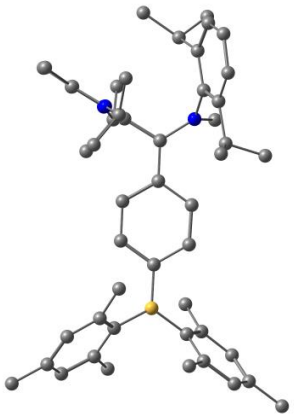
B	3.873233000	-0.000347000	0.120328000
N	-2.706213000	-1.548651000	0.420751000
N	-3.150124000	1.701977000	-0.491935000
N	-3.138497000	1.503903000	1.677818000
C	-1.960223000	-0.329068000	0.396247000
C	-0.550071000	-0.262941000	0.344411000
C	0.150136000	0.993570000	0.382824000
H	-0.422658000	1.921918000	0.465053000
C	1.524976000	1.063547000	0.305127000
H	2.004082000	2.046986000	0.321296000
C	2.352558000	-0.090804000	0.221780000
C	1.658475000	-1.332398000	0.224748000
H	2.245281000	-2.253799000	0.163613000
C	0.282403000	-1.430243000	0.277160000
H	-0.188711000	-2.412111000	0.252812000
C	-2.722076000	0.906347000	0.524548000
C	-3.831942000	2.673821000	1.385371000
C	-3.836154000	2.800940000	0.015324000
C	-2.851709000	1.380212000	-1.906231000
H	-2.385424000	0.390823000	-1.824759000
C	-1.811195000	2.331805000	-2.494235000
H	-2.192529000	3.357596000	-2.613408000
H	-1.519251000	1.968693000	-3.491134000
H	-0.908307000	2.354735000	-1.868285000
C	-4.119254000	1.240226000	-2.743636000
H	-4.851535000	0.594006000	-2.240291000
H	-3.860231000	0.759210000	-3.697625000
H	-4.585432000	2.208668000	-2.975767000
C	-2.694293000	1.015427000	3.002069000
H	-2.239227000	0.046388000	2.760013000
C	-1.592227000	1.908872000	3.572775000
H	-0.756423000	1.989181000	2.864194000
H	-1.207166000	1.462001000	4.501704000
H	-1.956440000	2.919364000	3.813628000
C	-3.849380000	0.777249000	3.972440000
H	-4.273387000	1.711425000	4.365839000
H	-3.475642000	0.199714000	4.831035000
H	-4.655506000	0.197200000	3.503116000
C	-4.490097000	3.548561000	2.398438000

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 1.038773 (Hartree/Particle)
Thermal correction to Energy= 1.097059
Thermal correction to Enthalpy= 1.098004
Thermal correction to Gibbs Free Energy= 0.944090
Sum of electronic and zero-point Energies= -2093.848498
Sum of electronic and thermal Energies= -2093.790212
Sum of electronic and thermal Enthalpies= -2093.789268
Sum of electronic and thermal Free Energies= -2093.943182

Charge = 0 Multiplicity = 1



H	-3.815777000	3.809795000	3.226006000
H	-5.381297000	3.066335000	2.830941000
H	-4.816668000	4.484933000	1.928009000
C	-4.493741000	3.850915000	-0.815771000
H	-5.414487000	3.478221000	-1.292181000
H	-3.833160000	4.219926000	-1.611914000
H	-4.768914000	4.708005000	-0.187545000
C	-2.681055000	-2.404848000	1.593091000
H	-3.299406000	-2.052354000	2.444669000
H	-1.645656000	-2.500144000	1.956429000
H	-3.035899000	-3.412788000	1.326537000
C	-3.708353000	-1.752782000	-0.577464000
C	-3.320033000	-2.122219000	-1.895089000
C	-4.308622000	-2.345033000	-2.858739000
H	-4.016024000	-2.640121000	-3.867681000
C	-5.665105000	-2.220649000	-2.551915000
H	-6.422154000	-2.415388000	-3.315469000
C	-6.042299000	-1.835187000	-1.270270000
H	-7.102590000	-1.715460000	-1.034224000
C	-5.082236000	-1.575551000	-0.279518000
C	-1.853738000	-2.333401000	-2.235320000
H	-1.270374000	-1.657847000	-1.601251000
C	-5.547661000	-1.073787000	1.078672000
H	-4.648960000	-0.794646000	1.637593000
C	-6.277205000	-2.163870000	1.877155000
H	-7.200998000	-2.477227000	1.364423000
H	-6.557923000	-1.799725000	2.879506000
H	-5.646345000	-3.056366000	2.001613000
C	-6.408213000	0.192872000	0.957322000
H	-5.890692000	0.970678000	0.376971000
H	-6.634587000	0.605649000	1.954496000
H	-7.370376000	-0.012143000	0.462394000
C	4.558063000	1.368637000	-0.302378000
C	4.217847000	2.009135000	-1.520132000
C	4.854958000	3.203709000	-1.891144000
H	4.590362000	3.670283000	-2.845628000
C	5.817429000	3.811454000	-1.083737000
C	6.148607000	3.178223000	0.120873000
H	6.902791000	3.632201000	0.771956000
C	5.550980000	1.976277000	0.512291000
C	3.189844000	1.444131000	-2.478039000
H	2.177330000	1.810928000	-2.241517000
H	3.131425000	0.348960000	-2.436061000
H	3.418565000	1.741889000	-3.513158000
C	5.984346000	1.350014000	1.817853000
H	6.669597000	2.013074000	2.366409000
H	6.494520000	0.388881000	1.652923000
H	5.125807000	1.138184000	2.473528000
C	6.486025000	5.102305000	-1.484832000
H	6.159040000	5.434472000	-2.481486000
H	7.583619000	4.996572000	-1.506636000
H	6.257974000	5.910886000	-0.769370000
C	-1.429937000	-3.767326000	-1.879214000
H	-1.963371000	-4.500387000	-2.506754000
H	-1.656966000	-3.996005000	-0.827777000
H	-0.347388000	-3.903489000	-2.030827000
C	-1.493952000	-2.001153000	-3.687080000
H	-1.832545000	-0.990767000	-3.968309000
H	-1.931577000	-2.713364000	-4.405230000
H	-0.401320000	-2.037371000	-3.817695000
C	4.771479000	-1.271831000	0.428525000
C	4.684914000	-1.940265000	1.675503000
C	5.510031000	-3.043523000	1.943034000
H	5.439729000	-3.532365000	2.920061000
C	6.418302000	-3.534136000	1.003472000
C	6.498301000	-2.874164000	-0.229042000
H	7.204481000	-3.236842000	-0.983033000
C	5.708170000	-1.758251000	-0.522222000
C	3.736123000	-1.497976000	2.769587000
H	4.116168000	-1.798165000	3.758336000
H	2.738912000	-1.949835000	2.643125000

H	3.577132000	-0.411547000	2.774358000
C	5.874903000	-1.094258000	-1.869884000
H	6.548467000	-1.675992000	-2.516413000
H	6.287325000	-0.078697000	-1.769968000
H	4.913199000	-0.990160000	-2.395292000
C	7.283708000	-4.734690000	1.292857000
H	8.347061000	-4.521869000	1.093585000
H	7.192629000	-5.055586000	2.341335000
H	7.004661000	-5.591475000	0.655490000

8-Triplet

B	3.830595000	-0.062582000	0.208921000
N	-2.771991000	-1.548725000	0.411409000
N	-2.603231000	1.935773000	-0.460026000
N	-3.492679000	1.375018000	1.549308000
C	-2.023240000	-0.364928000	0.448966000
C	-0.590806000	-0.351126000	0.500104000
C	0.105259000	0.888558000	0.685523000
H	-0.470589000	1.795538000	0.864403000
C	1.479927000	0.967792000	0.595272000
H	1.964415000	1.939145000	0.725918000
C	2.296042000	-0.168926000	0.341453000
C	1.605574000	-1.404733000	0.191868000
H	2.190504000	-2.309013000	0.002782000
C	0.229329000	-1.499964000	0.252940000
H	-0.231295000	-2.473542000	0.098923000
C	-2.801314000	0.862660000	0.422084000
C	-3.790041000	2.726738000	1.275652000
C	-3.277992000	3.051277000	0.050607000
C	-2.321528000	1.645639000	-1.872324000
H	-1.846927000	0.655855000	-1.840048000
C	-1.297524000	2.598191000	-2.488057000
H	-1.705142000	3.602515000	-2.669506000
H	-0.965019000	2.197925000	-3.458239000
H	-0.416041000	2.686396000	-1.836260000
C	-3.612645000	1.512852000	-2.686336000
H	-4.292554000	0.795615000	-2.204439000
H	-3.393197000	1.145206000	-3.700186000
H	-4.132166000	2.478006000	-2.786204000
C	-3.179987000	0.860723000	2.901335000
H	-2.891090000	-0.184946000	2.728443000
C	-1.979338000	1.572152000	3.535015000
H	-1.093441000	1.505466000	2.891603000
H	-1.731808000	1.106735000	4.502020000
H	-2.195907000	2.635601000	3.719755000
C	-4.381614000	0.840375000	3.849072000
H	-4.651347000	1.842804000	4.206870000
H	-4.128088000	0.237408000	4.734467000
H	-5.263979000	0.394925000	3.374886000
C	-4.586738000	3.585729000	2.199129000
H	-4.080142000	3.764600000	3.161461000
H	-5.564019000	3.128697000	2.424024000
H	-4.772718000	4.566105000	1.741926000
C	-3.348686000	4.361039000	-0.661144000
H	-3.799228000	4.274726000	-1.661818000
H	-2.346308000	4.800119000	-0.791149000
H	-3.953011000	5.074563000	-0.086853000
C	-2.487890000	-2.694453000	1.259558000
H	-3.415146000	-3.038329000	1.748088000
H	-1.772055000	-2.400338000	2.038248000
H	-2.067508000	-3.552427000	0.708683000
C	-3.769536000	-1.713993000	-0.619152000
C	-3.354706000	-2.025980000	-1.942585000
C	-4.333031000	-2.238296000	-2.921758000
H	-4.024448000	-2.479965000	-3.940059000
C	-5.690400000	-2.159038000	-2.620708000
H	-6.437864000	-2.334851000	-3.398089000
C	-6.086468000	-1.849777000	-1.323567000
H	-7.150716000	-1.776248000	-1.090222000
C	-5.145302000	-1.615806000	-0.311335000

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 1.036463 (Hartree/Particle)

Thermal correction to Energy= 1.095126

Thermal correction to Enthalpy= 1.096070

Thermal correction to Gibbs Free Energy= 0.939277

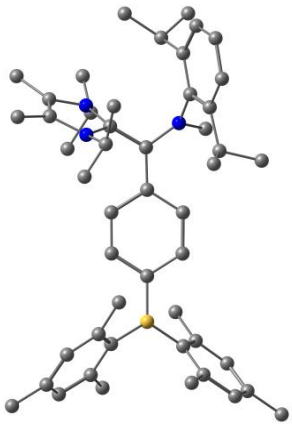
Sum of electronic and zero-point Energies= -2093.791141

Sum of electronic and thermal Energies= -2093.732478

Sum of electronic and thermal Enthalpies= -2093.731534

Sum of electronic and thermal Free Energies= -2093.888328

Charge = 0 Multiplicity = 3

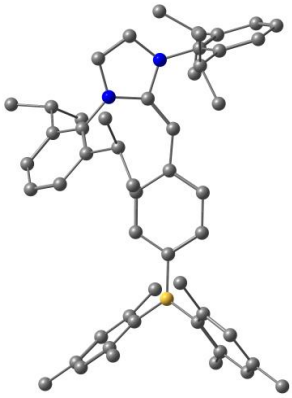


C	-1.889545000	-2.195351000	-2.320387000	
H	-1.289098000	-1.651133000	-1.587013000	
C	-5.644260000	-1.235288000	1.070996000	
H	-4.762275000	-0.990602000	1.674077000	
C	-6.379297000	-2.398983000	1.753717000	
H	-7.296253000	-2.669970000	1.205774000	
H	-6.672144000	-2.125762000	2.780622000	
H	-5.748472000	-3.299846000	1.807032000	
C	-6.528926000	0.019091000	1.006475000	
H	-5.983024000	0.859255000	0.554454000	
H	-6.854116000	0.322451000	2.014097000	
H	-7.439221000	-0.161661000	0.413789000	
C	4.481938000	1.330355000	-0.161336000	
C	4.067718000	2.051177000	-1.310867000	
C	4.675819000	3.273205000	-1.633503000	
H	4.354930000	3.802379000	-2.536459000	
C	5.682097000	3.831165000	-0.842273000	
C	6.089326000	3.116883000	0.291531000	
H	6.879639000	3.530530000	0.926194000	
C	5.522009000	1.885275000	0.632783000	
C	2.995514000	1.535310000	-2.247074000	
H	1.986348000	1.798963000	-1.891180000	
H	3.009202000	0.440262000	-2.337573000	
H	3.117090000	1.965278000	-3.252935000	
C	6.041086000	1.170749000	1.859709000	
H	6.728280000	1.813585000	2.429376000	
H	6.578577000	0.248674000	1.590416000	
H	5.225700000	0.868745000	2.534454000	
C	6.311932000	5.157474000	-1.184946000	
H	5.985629000	5.517469000	-2.172055000	
H	7.412271000	5.089954000	-1.193931000	
H	6.045497000	5.929559000	-0.442541000	
C	-1.475682000	-3.675051000	-2.248152000	
H	-2.019595000	-4.269572000	-3.000291000	
H	-1.694571000	-4.112196000	-1.263353000	
H	-0.396018000	-3.786034000	-2.437382000	
C	-1.531195000	-1.616807000	-3.695879000	
H	-1.867698000	-0.575500000	-3.801523000	
H	-1.972697000	-2.197064000	-4.521512000	
H	-0.438851000	-1.635272000	-3.833391000	
C	4.730931000	-1.342824000	0.431225000	
C	4.640225000	-2.103327000	1.625317000	
C	5.470361000	-3.217306000	1.816273000	
H	5.398098000	-3.777120000	2.754116000	
C	6.389822000	-3.629865000	0.849314000	
C	6.476010000	-2.878002000	-0.328976000	
H	7.191432000	-3.178360000	-1.101295000	
C	5.680787000	-1.748229000	-0.545256000	
C	3.686165000	-1.738420000	2.742135000	
H	4.024018000	-2.164722000	3.698848000	
H	2.670483000	-2.118280000	2.546400000	
H	3.585520000	-0.651003000	2.867584000	
C	5.859579000	-0.981590000	-1.835949000	
H	6.515623000	-1.526766000	-2.530530000	
H	6.300533000	0.010904000	-1.656463000	
H	4.900192000	-0.807162000	-2.346292000	
C	7.258991000	-4.844680000	1.054172000	
H	8.318700000	-4.620606000	0.849113000	
H	7.185070000	-5.226171000	2.083461000	
H	6.967862000	-5.663055000	0.373071000	
VIII				
C	-0.094911000	0.869935000	-0.379394000	- Thermochemistry -
C	-1.480885000	0.825031000	-0.330504000	----------
C	-2.212761000	-0.363846000	-0.549980000	Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
C	-1.447524000	-1.513405000	-0.864971000	
C	-0.064592000	-1.478229000	-0.928390000	Zero-point correction= 1.019591
C	0.670756000	-0.292420000	-0.646151000	(Hartree/Particle)
C	2.112965000	-0.381885000	-0.683570000	Thermal correction to Energy= 1.076759
B	-3.756334000	-0.395231000	-0.470012000	Thermal correction to Enthalpy= 1.077703

C	3.135187000	0.285032000	-0.037694000
N	3.167321000	1.287332000	0.929852000
C	4.488879000	1.499720000	1.351847000
C	5.287437000	0.662901000	0.658795000
N	4.481045000	-0.062454000	-0.219283000
C	2.067645000	1.977103000	1.527777000
C	4.913690000	-1.252462000	-0.883519000
C	1.219376000	1.285011000	2.412844000
C	0.146426000	1.992683000	2.969613000
C	-0.064263000	3.334155000	2.660395000
C	0.794074000	4.000632000	1.784610000
C	1.876957000	3.336288000	1.196350000
C	5.378064000	-1.193539000	-2.214613000
C	5.796117000	-2.395657000	-2.804503000
C	5.748304000	-3.603917000	-2.110855000
C	5.279458000	-3.636664000	-0.799580000
C	4.854987000	-2.464784000	-0.160759000
C	5.407713000	0.070306000	-3.069916000
C	4.337449000	-2.524677000	1.270083000
C	3.048048000	-3.353774000	1.367861000
C	5.414427000	-3.035774000	2.237924000
C	4.003753000	0.458764000	-3.561517000
C	6.129125000	1.276008000	-2.448976000
C	2.764252000	4.018660000	0.160294000
C	1.465531000	-0.177358000	2.752126000
C	2.465483000	-0.302895000	3.913182000
C	0.177135000	-0.957746000	3.026696000
C	2.340992000	3.620793000	-1.265556000
C	2.813982000	5.542881000	0.303848000
C	-4.511272000	-1.768255000	-0.257021000
C	-5.537353000	-2.182066000	-1.148838000
C	-6.198788000	-3.396771000	-0.944161000
C	-5.903352000	-4.226989000	0.144249000
C	-4.910256000	-3.806118000	1.030666000
C	-4.206419000	-2.607398000	0.843571000
C	-3.149617000	-2.252201000	1.867240000
C	-5.941036000	-1.336800000	-2.335478000
C	-6.633464000	-5.531550000	0.338605000
C	-4.568966000	0.955437000	-0.597787000
C	-4.413640000	1.796383000	-1.727300000
C	-5.158952000	2.980476000	-1.829142000
C	-6.047899000	3.383452000	-0.830944000
C	-6.194428000	2.550987000	0.285961000
C	-5.488418000	1.350735000	0.410362000
C	-5.726028000	0.499810000	1.637184000
C	-3.477579000	1.459276000	-2.868673000
C	-6.827160000	4.669544000	-0.939729000
H	0.400306000	1.822893000	-0.229330000
H	-2.025904000	1.747012000	-0.111998000
H	-1.967373000	-2.454422000	-1.065037000
H	0.489334000	-2.388428000	-1.175501000
H	2.488081000	-1.227700000	-1.261774000
H	4.714406000	2.236028000	2.115871000
H	6.360909000	0.511739000	0.688905000
H	-0.541986000	1.483546000	3.644460000
H	-0.911274000	3.866598000	3.099450000
H	0.606127000	5.047832000	1.546770000
H	6.162236000	-2.376328000	-3.833997000
H	6.078426000	-4.525030000	-2.597127000
H	5.242537000	-4.586371000	-0.261442000
H	5.990023000	-0.212257000	-3.962889000
H	4.087244000	-1.504369000	1.585032000
H	2.665598000	-3.345513000	2.400772000
H	2.264904000	-2.943591000	0.714384000
H	3.220309000	-4.404202000	1.083229000
H	5.042695000	-3.006644000	3.274586000
H	6.323596000	-2.416895000	2.184125000
H	5.702042000	-4.075865000	2.015295000
H	4.067446000	1.304002000	-4.265769000
H	3.516738000	-0.381789000	-4.078860000
H	3.351852000	0.754882000	-2.727929000

Thermal correction to Gibbs Free Energy= 0.923095
Sum of electronic and zero-point Energies= -2151.614594
Sum of electronic and thermal Energies= -2151.557427
Sum of electronic and thermal Enthalpies= -2151.556483
Sum of electronic and thermal Free Energies= -2151.711091

Charge = 0 Multiplicity = 1



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H	5.521736000	1.768801000	-1.678197000
H	3.791070000	3.648875000	0.304635000
H	1.923764000	-0.643158000	1.871366000
H	3.420170000	0.191712000	3.677758000
H	2.063050000	0.156063000	4.830888000
H	2.678243000	-1.362754000	4.127640000
H	0.400931000	-2.032437000	3.110405000
H	-0.543528000	-0.825581000	2.207813000
H	-0.305382000	-0.652288000	3.969180000
H	3.011305000	4.081410000	-2.008882000
H	2.369493000	2.532730000	-1.414835000
H	1.314055000	3.960674000	-1.474653000
H	3.567521000	5.960482000	-0.381681000
H	3.077558000	5.848249000	1.328411000
H	1.850261000	6.010995000	0.047540000
H	-6.976597000	-3.702089000	-1.651222000
H	-4.674165000	-4.428315000	1.899669000
H	-2.155807000	-2.612041000	1.557393000
H	-3.049909000	-1.169027000	2.016233000
H	-3.380140000	-2.711542000	2.840524000
H	-5.075523000	-1.057064000	-2.955143000
H	-6.651285000	-1.876147000	-2.979042000
H	-6.414373000	-0.395916000	-2.016220000
H	-7.725075000	-5.395550000	0.269170000
H	-6.352285000	-6.264054000	-0.437616000
H	-6.407414000	-5.980120000	1.317345000
H	-5.040416000	3.605335000	-2.719966000
H	-6.888076000	2.842884000	1.080933000
H	-6.367219000	1.023040000	2.361590000
H	-6.209980000	-0.453854000	1.377212000
H	-4.785217000	0.243496000	2.148142000
H	-3.351754000	0.377805000	-3.009802000
H	-3.846617000	1.887982000	-3.812948000
H	-2.468063000	1.864131000	-2.691240000
H	-6.682028000	5.149099000	-1.919054000
H	-7.907394000	4.497398000	-0.801893000
H	-6.517064000	5.390429000	-0.163896000

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