Electronic Supplementary Material (ESI) for Chemical Science.
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Supporting Information

for

A bis-NHC-CAAC dimer derived dicationic diradical

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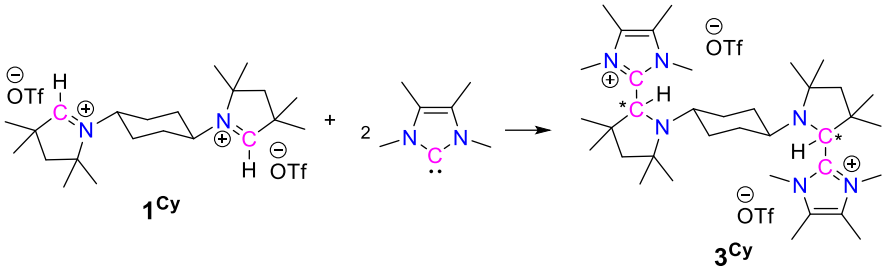
General Considerations

All experiments were carried out either under nitrogen or argon atmosphere using standard Schlenk techniques, PL-HE-2GB Innovative Technology GloveBox, and MBraun Unilab SP GloveBox. Hexane, diethyl ether, THF, and toluene were dried with a PS-MD-5 Innovative Technology solvent purification system. Compounds $\mathbf{1}^{\mathbf{Et}}$,[S1] $\mathbf{1}^{\mathbf{Pr}}$,[S1] and $\mathbf{2}$[S2] were synthesized in accordance with the literature procedures. Compound $\mathbf{1}^{\mathbf{Cy}}$ was synthesized based on a similar procedure as for $\mathbf{1}^{\mathbf{Et}}$ and $\mathbf{1}^{\mathbf{Pr}}$.[S1] All other employed chemicals were purchased commercially (potassium bis(trimethylsilyl)amide - Sigma Aldrich, potassium - Sigma Aldrich, graphite - Sigma Aldrich, diisopropylamine - Avra Chemicals, *n*BuLi - Hychem Laboratories, and AgOTf - Sigma Aldrich) and used as received except for diisopropylamine which was distilled under N_2 over KOH before use. Benzene-d_6 and THF-d_8 were dried and distilled over potassium under argon. CD_3CN was dried and distilled over CaH_2 under argon. NMR spectra were recorded on a BrukerNanoBay 300 MHz NMR spectrometer. ^{1}H and ^{13}C{^{1}H} NMR spectra were referenced to the peaks of residual protons of the deuterated solvent (^{1}H) or the deuterated solvent itself (^{13}C{^{1}H}). ^{19}F{^{1}H} NMR spectra were referenced to external tol-CF_3.

Melting points were determined in closed NMR tubes under argon atmosphere and are uncorrected. Elemental analyses of $\mathbf{6}^{\mathbf{Cy}}$, $\mathbf{7}^{\mathbf{Cy}}$, $\mathbf{3}^{\mathbf{Et}}$, $\mathbf{4}^{\mathbf{Et}}$, $\mathbf{5}^{\mathbf{Et}}$, $\mathbf{8}^{\mathbf{Et}}$ $\mathbf{9}^{\mathbf{Et}}$, $\mathbf{10}^{\mathbf{Et}}$, $\mathbf{8}^{\mathbf{Pr}}$ and $\mathbf{9}^{\mathbf{Pr}}$ were performed on a Perkin Elmer Analyser 240. Elemental analyses of $\mathbf{3}^{\mathbf{Cy}}$, $\mathbf{4}^{\mathbf{Cy}}$, $\mathbf{5}^{\mathbf{Cy}}$ $\mathbf{3}^{\mathbf{Pr}}$, $\mathbf{4}^{\mathbf{Pr}}$ and $\mathbf{5}^{\mathbf{Pr}}$ were performed on an Elementar vario MICRO cube elemental analyzer. HRMS of $\mathbf{3}^{\mathbf{Et}}$, $\mathbf{4}^{\mathbf{Et}}$, $\mathbf{5}^{\mathbf{Et}}$, $\mathbf{8}^{\mathbf{Et}}$, $\mathbf{9}^{\mathbf{Et}}$, and $\mathbf{10}^{\mathbf{Et}}$ were performed on an Exactive Plus Orbitrap-HRMS manufactured by Thermo Scientific. HRMS of $\mathbf{3}^{\mathbf{Cy}}$, $\mathbf{5}^{\mathbf{Cy}}$, $\mathbf{3}^{\mathbf{Pr}}$, $\mathbf{5}^{\mathbf{Pr}}$, and $\mathbf{8}^{\mathbf{Pr}}$ were performed on a Waters Xevo G2-XS QTOF (Waters Corporation) using electrospray ionization (ESI). EPR measurements at 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 simulations were performed using MATLAB 9.8.0.1323502 (R2020a) and the EasySpin 5.2.28 toolbox.[S3] The magnetic susceptibility measurements were performed with Quantum Design MPMS-XL EverCool SQUID magnetometer, between 2 K to 375 K for dc applied fields ranging from -5 to +5 T. Polycrystalline sample (21.5 mg) was introduced in a polypropylene bag and was subjected to the measurement. The temperature dependent data were measured using 1000 Oe and 10000 Oe dc magnetic field. The isothermal magnetization data were acquired at 1.9, 2.5, 5, and 6 K. *M vs H* measurements were performed at 100 K to check for the presence of impurities, where the sample was free from impurities. The magnetic data were corrected for the sample holder and the intrinsic diamagnetic contributions.

Experimental Details and Analytical Data

Synthesis of 3^{Cy}



$\mathbf{1^{Cy}}$ $\mathbf{3^{Cy}}$

About 80 mL of THF was added to a 100 mL Schlenk flask containing $\mathbf{1^{Cy}}$ (4.617 g, 7.320 mmol) and **2** (2 g, 16.104 mmol) at 0 °C. After stirring for 24 hours at room temperature, the reaction mixture was filtered and the white precipitate was washed with about 50 mL of diethyl ether and dried under vacuum. The ^{1}H NMR spectrum of the residue showed the formation of a mixture of two diastereomers (*dll*- and *meso*-) of $\mathbf{3^{Cy}}$ in an about 59:41 ratio. **Yield:** 5.8 g (90 %). **M.P.:** > 180 °C. $\mathbf{3^{Cy}}$ was crystallized by layering diethyl ether over CH_3CN and THF solution of the crude compound. The obtained crystals were suitable for a single crystal X-ray diffraction study. We used the mixture of diastereomers for the next reaction. **NMR data of the mixture of diastereomers: ^{1}H NMR** (CD_3CN, 25 °C, 300 MHz): δ = 4.51 & 4.52 (s, 2H, C*H*), 3.94 & 3.96 (s, 6H, CH_3-N), 3.68 (s, 6H, CH_3-N), 2.51 (m, 2H, CH_{Cy}), 2.25 (s, 6H, CH_3-C=C), 2.20 (s, 6H, CH_3-C=C), 1.77-1.87 (m, 2H, CH_{2Cy}), 1.77-1.87 (m, 4H, CH_2), 1.66 (m, 2H, CH_{2Cy}), 1.46-1.49 & 1.18 (m, 2H, CH_{2Cy}), 1.38, (s, 6H, CH_3), 1.21 (s, 3H, CH_3), 1.18 (s, 6H, CH_3), 1.12 (s, 3H, CH_3), 0.67 (m, 2H, CH_{2Cy}), 0.67 (s, 6H, CH_3) ppm. **^{13}C{^{1}H} NMR** (CD_3CN, 25 °C, 75 MHz): δ = 145.33 & 145.29 (*C*=N-CH_3), 128.40 (CH_3-*C*=*C*), 128.38 (CH_3-*C*=*C*), 122.125 (q, $^{1}J_{C\text{-}F}$ = 321 Hz, *C*$F_3SO_3^-$), 64.42 & 64.45 (*C*H), 64.11 & 64.13 (*C*$(CH_3)_2$), 55.83 (*C*H_2), 54.33 (*C*H_{Cy}), 43.52 (*C*$(CH_3)_2$), 34.67 & 34.70 (*C*H_3-N), 34.29 (48.95 (*C*H_{2Cy}), 34.02 (*C*H_{2Cy}), 33.16 (*C*H_3-N), 32.74 (C(*C*$H_3)_2$), 30.98 (*C*H_{2Cy}), 30.62 (*C*H_{2Cy}), 29.33 (C(*C*$H_3)_2$), 27.91 (C(*C*$H_3)_2$), 24.23 & 24.07 (C(*C*$H_3)_2$), 9.12 (*C*H_3-C=C), 8.59 (*C*H_3-C=C) ppm. **^{19}F{^{1}H} NMR:** (CD_3CN, 25 °C, 282 MHz): δ = −79.28 ppm. **Elemental analysis:** Calculated (%) for $C_{38}H_{64}F_6N_6O_6S_2$: C, 51.92; H, 7.34; N, 9.56; S, 7.29; Found: C, 51.84; H, 7.30; N, 9.17; S, 7.41. **HRMS-ESI (m/z):** Calculated for $C_{36}H_{64}N_6$ [M-2OTf]: 290.2591, Found: 290.2593.

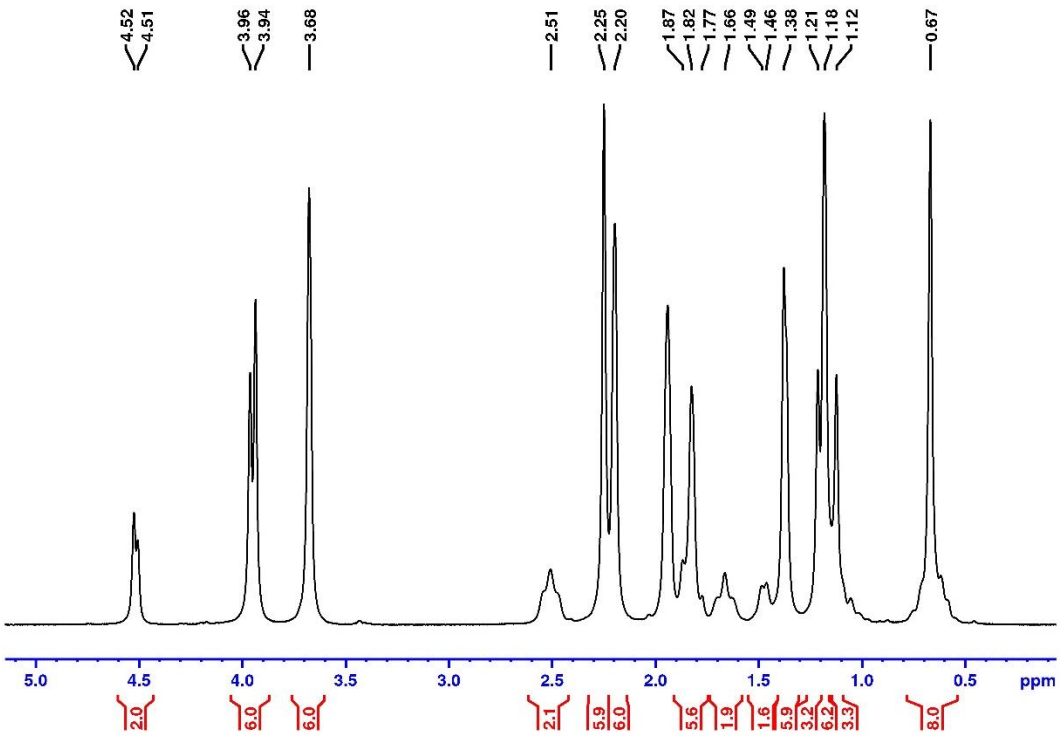


Fig. S1 ^{1}H NMR spectrum of mixture of diastereomers of $\mathbf{3^{Cy}}$ in CD_3CN at RT.

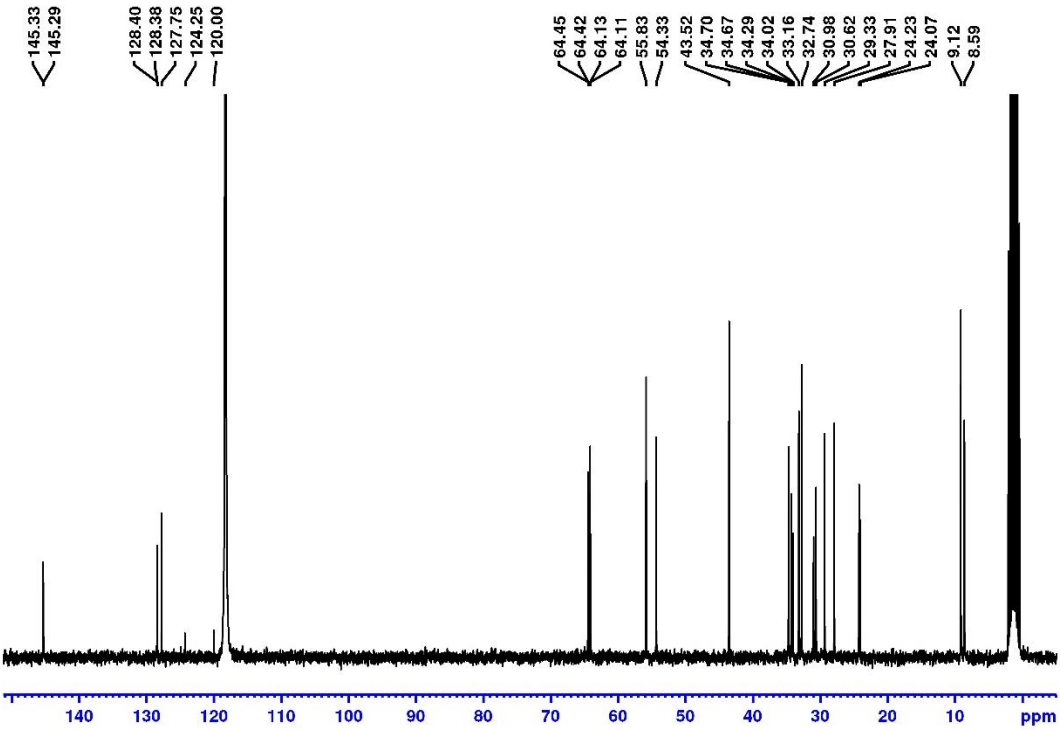


Fig. S2 $^{13}C\{^{1}H\}$ NMR spectrum of mixture of diastereomers of $\mathbf{3^{Cy}}$ in CD_3CN at RT.

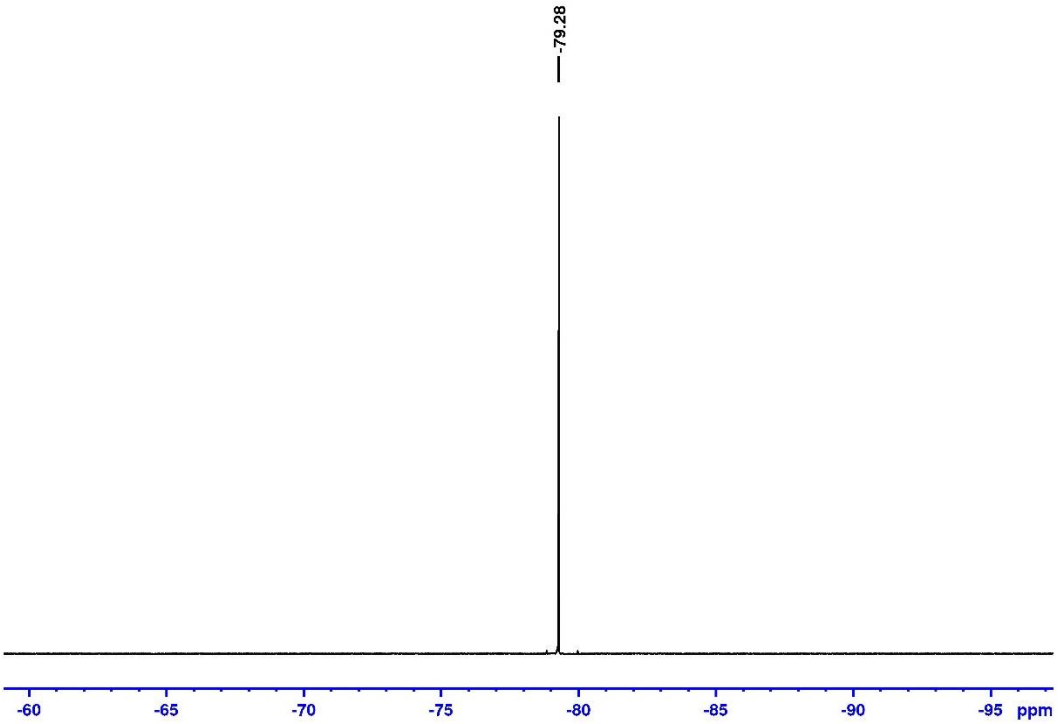
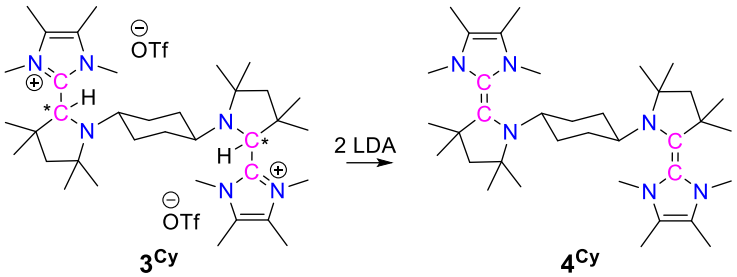


Fig. S3 $^{19}F\{^{1}H\}$ NMR spectrum of mixture of diastereomers of **3^{Cy}** in CD_3CN at RT.

Synthesis of 4^{Cy}



3^{Cy} 4^{Cy}

About 80 mL of toluene was added to a 100 mL Schlenk flask containing **3^{Cy}** (4.0 g, 4.55 mmol) and LDA (1.060 g, 9.895 mmol) at room temperature with stirring. Then the reaction mixture was stirred for 12 hours at room temperature. After that the reaction mixture was heated at 90 °C for three hours and filtered while heated to boiling temperature. The filtrate was evaporated and the white precipitate of **4^{Cy}** was washed with about 10 mL of pentane and dried. The washing pentane solution was kept at −35 °C to increase the amount of **4^{Cy}**. **Yield:** 2.19 g (83 %). **M.P.:** 175 °C. **^{1}H NMR** (C_6D_6, 25 °C, 300 MHz): δ = 3.23 (m, 2H, C*H*$_{Cy}$), 2.98 (s, 6H, C*H*$_3$-N), 2.70 (s, 6H, C*H*$_3$-N), 2.22-2.25 (m, 4H, C*H*$_{2Cy}$), 1.77-1.91 (m, 4H, C*H*$_{2Cy}$), 1.67 (s, 4H, C*H*$_2$), 1.56 (s, 12H, C*H*$_3$-C=C), 1.40 (s, 12H, C*H*$_3$), 1.35 (s, 12H, C*H*$_3$) ppm. **^{13}C{^{1}H} NMR** (C_6D_6, 25 °C, 75 MHz): δ = 144.82 (NC=*C*NN), 121.73 (CH$_3$-*C*=*C*), 120.49 (CH$_3$-*C*=*C*), 109.37 (N*C*=CNN), 62.11 (*C*H$_2$), 60.47 (*C*(CH$_3$)$_2$), 57.55 (*C*H$_{Cy}$), 42.31 (*C*H$_3$-N), 41.01 (*C*(CH$_3$)$_2$), 32.95 (*C*H$_{2Cy}$), 32.26 (*C*H$_3$-N), 28.05 (C(*C*H$_3$)$_2$), 10.10 (*C*H$_3$-C=C), 9.76 (*C*H$_3$-C=C) ppm. Most likely due to high air and moisture sensitivity we were not able to get satisfactory elemental analysis data even after repeating measurements.

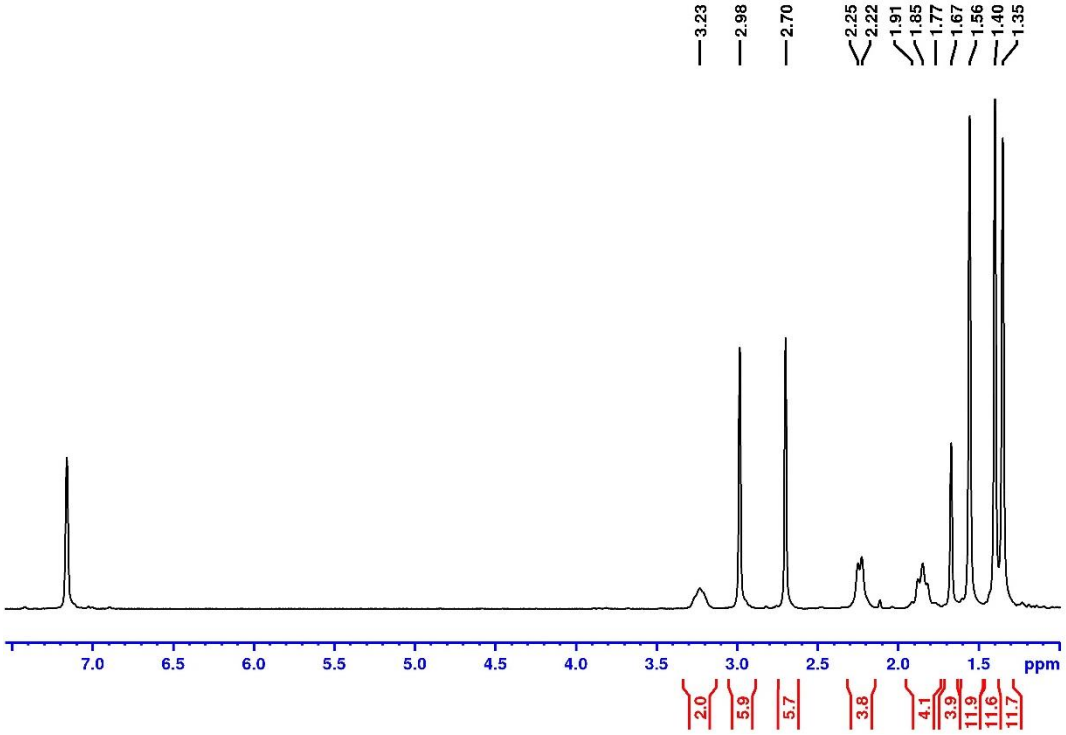


Fig. S4 ^{1}H NMR spectrum of **4^{Cy}** in C_6D_6 at RT.

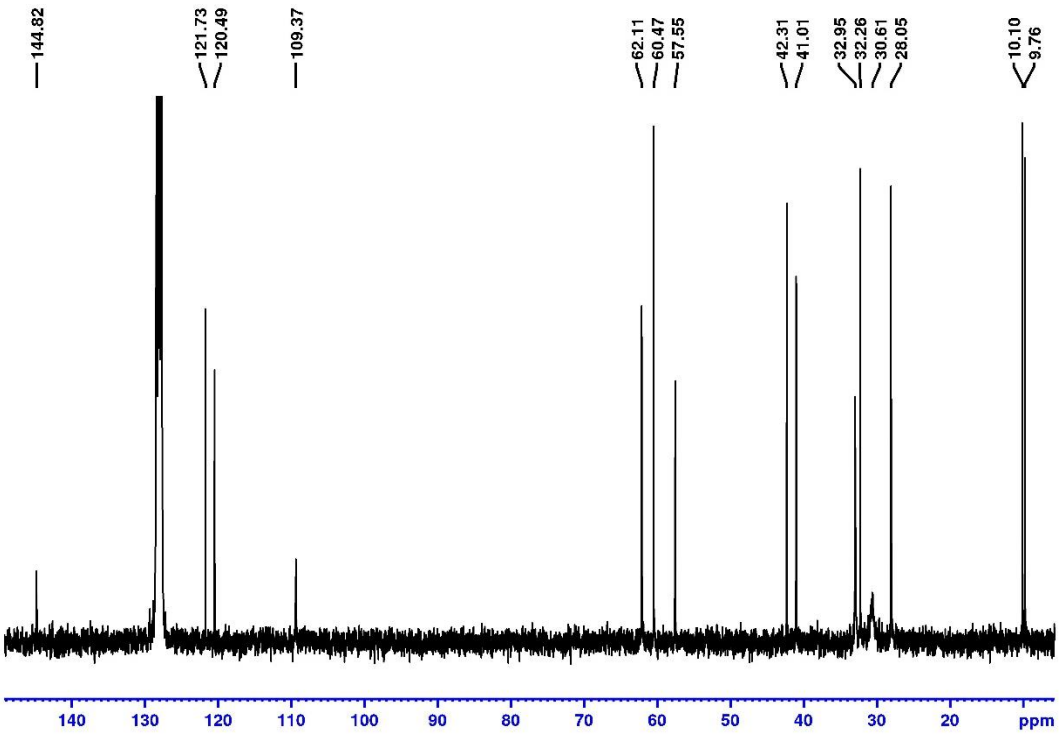


Fig. S5 $^{13}C\{^{1}H\}$ NMR spectrum of **4^{Cy}** in C_6D_6 at RT.

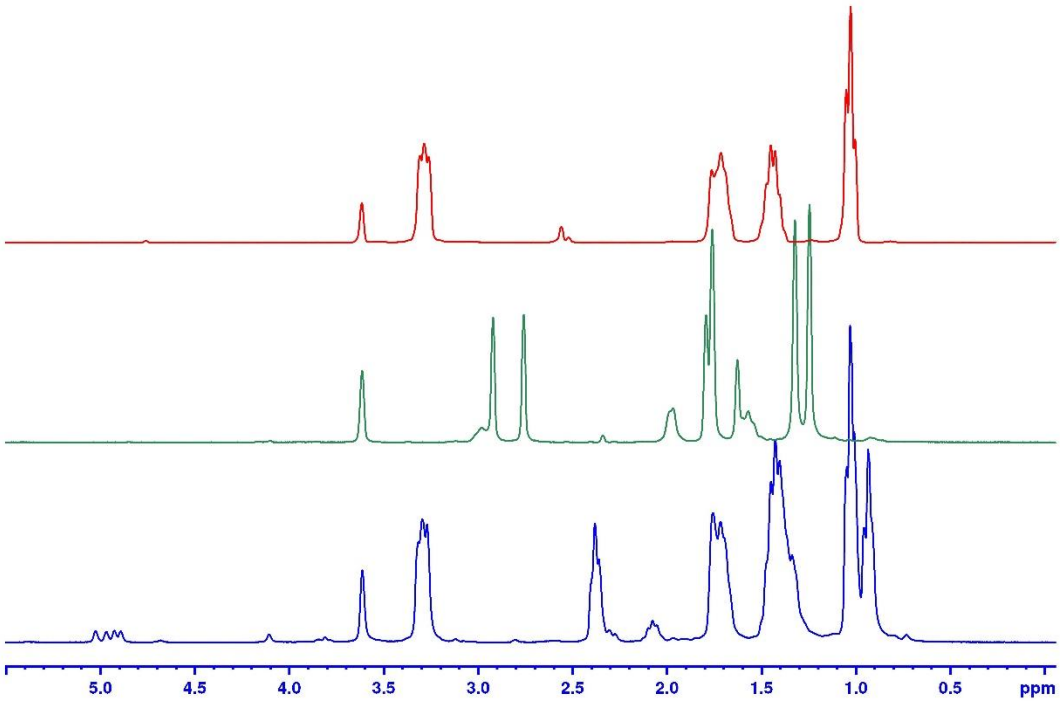


Fig. S6 Overlay of ^{1}H NMR spectra of a mixture of **4^{Cy}** and *n*-Bu_4NPF_6 (Blue), **4^{Cy}** (green) and *n*-Bu_4NPF_6 (red) in THF-d_8 at RT.

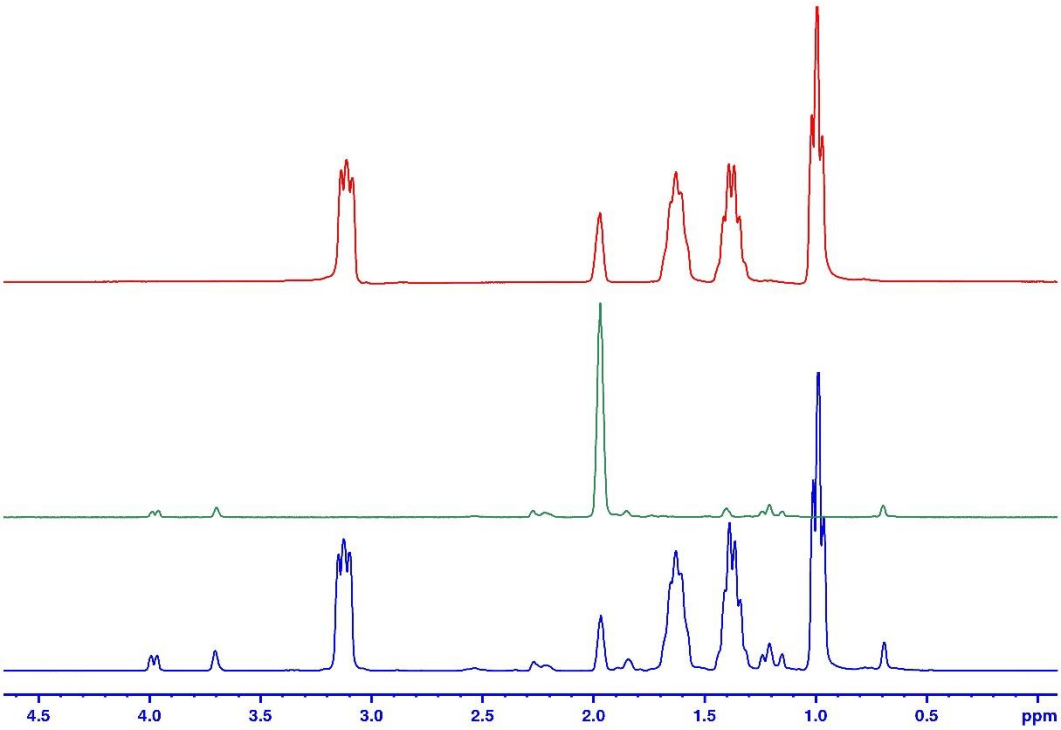
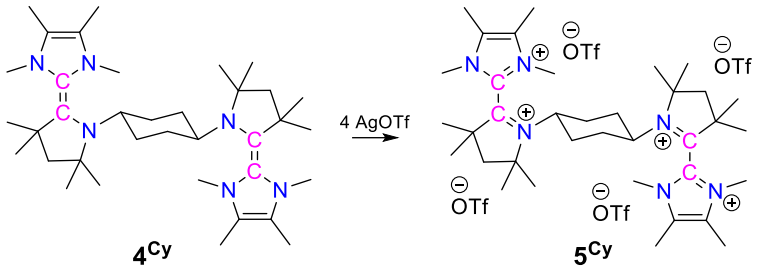


Fig. S7 Overlay of ^{1}H NMR spectra of a mixture of **4^{Cy}** and *n*-Bu_4NPF_6 (Blue), **4^{Cy}** (green) and *n*-Bu_4NPF_6 (red) in CD_3CN at RT.

Synthesis of 5^{Cy}



4^{Cy} 5^{Cy}

20 mL THF solution of **4^{Cy}** (417 mg, 0.72 mmol) was added dropwise to a 10 mL THF solution of AgOTf (824 mg, 3.207 mmol) at room temperature while stirring. Immediately, black colored metallic silver precipitated out. After 1 hour all volatiles were removed under vacuum and the residue was dissolved in acetonitrile (20 mL) and filtered. The filtrate was evaporated and an oily sticky compound was obtained. After that 40 mL of THF was added to this oily compound and then sonicated. A white precipitate of **5^{Cy}** was obtained after sonication. This precipitate was filtered, washed with ether and dried. **Yield:** 750 mg (89 %). **M.P.:** > 180 °C. Acetonitrile solution of **5^{Cy}** was kept for crystallization with DCM diffusion at room temperature for 24 hours. Colorless crystals of **5^{Cy}** were obtained which were also suitable for X-ray structural analysis. **^{1}H NMR** (CD_3CN, 25 °C, 300 MHz): δ = 3.98 (m, 2H, CH_{Cy}), 3.78 (s, 12H, CH_3-N), 2.44 (s, 4H, CH_2), 2.41 (s, 12H, CH_3-C=C), 2.41 (br. 4H, C$H_{2\ Cy}$), 1.84 (s, 12H, CH_3), 1.45 (s, 12H, CH_3), 1.45 (br. 4H, C$H_{2\ Cy}$) ppm. **^{13}C{^{1}H} NMR** (CD_3CN, 25 °C, 75 MHz): δ = 181.09 (*C*=N), 134.78 (CH_3-*C*=*C*), 128.21 (*C*NN), 121.83 (q, $^{1}J_{C\text{-}F}$ = 320.75 Hz, *C*$F_3SO_3^-$), 87.29 (*C*$(CH_3)_2$), 62.92 (*C*H_{Cy}), 57.03 (*C*$(CH_3)_2$), 48.09 (*C*H_2), 37.24 (*C*H_3-N), 31.24 (CH_{2Cy}), 27.89 (C(*C*$H_3)_2$), 27.33 (C(*C*$H_3)_2$), 9.37 (*C*H_3-C=C) ppm. **^{19}F{^{1}H} NMR** (CD_3CN, 25 °C, 282 MHz): δ = −79.27 ppm. **Elemental analysis:** Calculated (%) for $C_{40}H_{62}N_6F_{12}O_{12}S_4$: C, 40.88; H, 5.32; N, 7. 15; S, 10.91; Found: C, 40.72; H, 5.55; N, 6.66; S, 10.11. **HRMS-ESI (m/z):** Calculated for $C_{39}H_{62}N_6F_9O_9S_3$ $[M\text{-}1OTf]^{3+}$: 1025.3592, Found: 1025.3573.

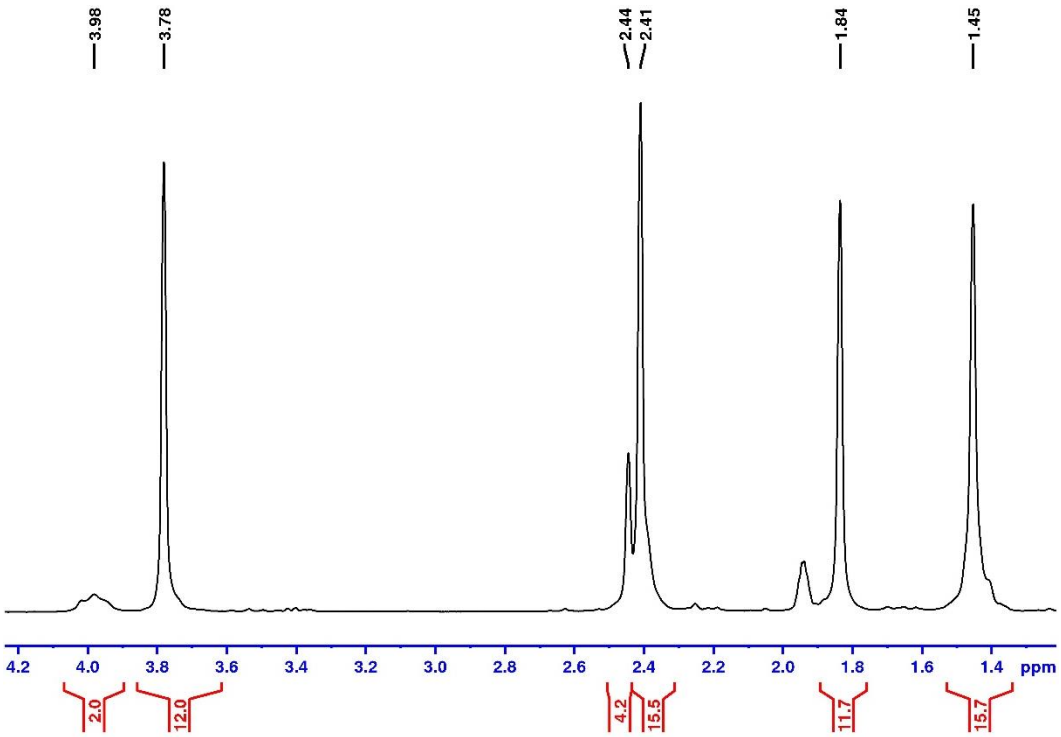


Fig. S8 ^{1}H NMR spectrum of **5**^{Cy} in CD_3CN at RT.

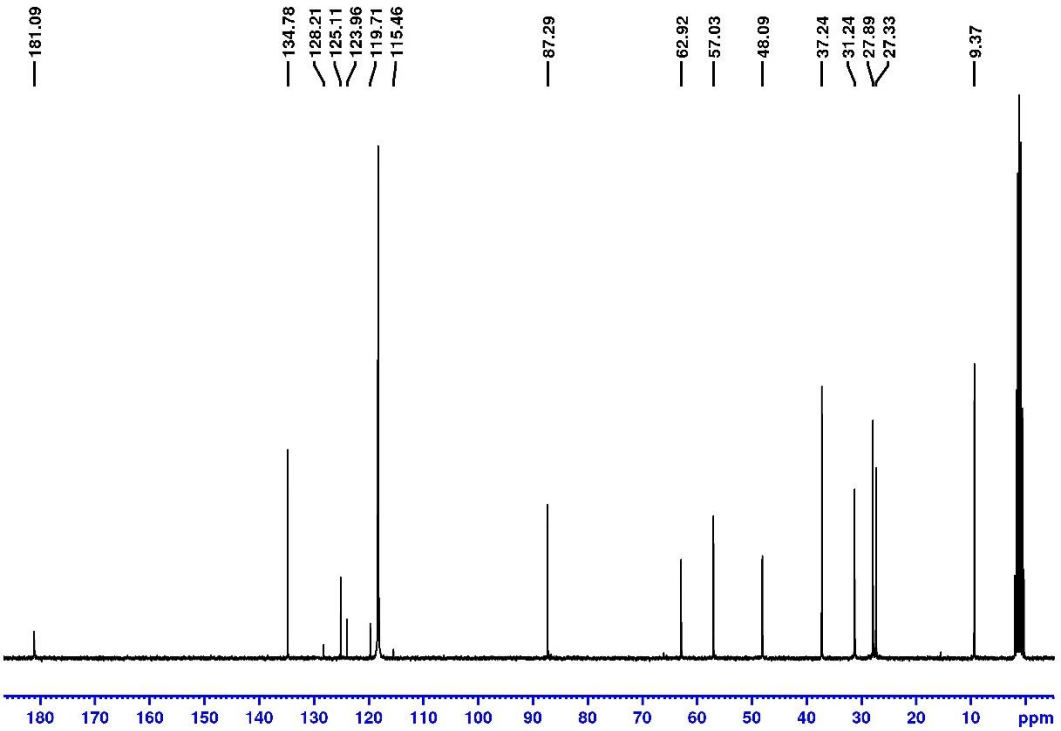


Fig. S9 $^{13}C\{^{1}H\}$ NMR spectrum of **5**^{Cy} in CD_3CN at RT.

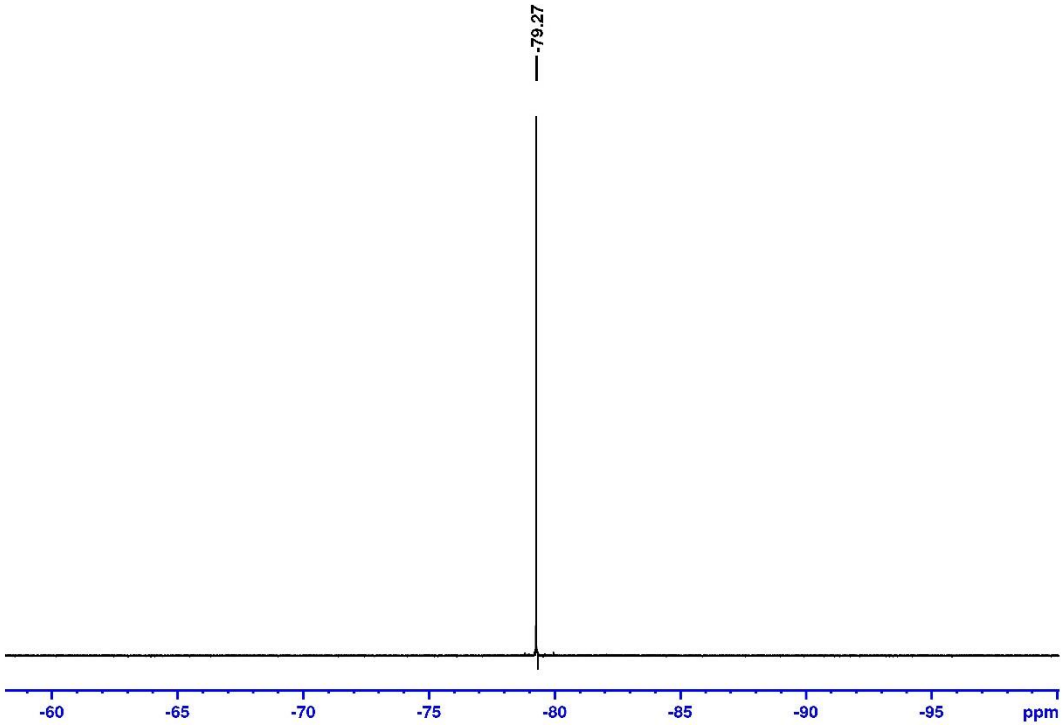
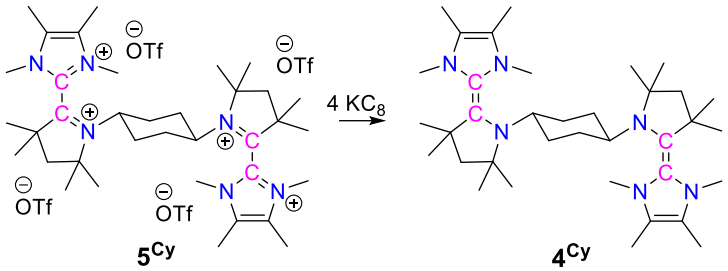


Fig. S10 $^{19}F\{^{1}H\}$ NMR spectrum of $\mathbf{5^{Cy}}$ in CD_3CN at RT.

Reduction of 5^{Cy}



THF was added to the mixture of **5^{Cy}** (70 mg, 0.059 mmol) and KC_8 (65 mg, 0.480 mmol) at −30 °C with stirring. After 6 hours stirring at room temperature, solvent and other volatiles were removed under vacuum and the ^1H NMR spectrum of the reaction mixture in C_6D_6 was measured which showed the formation of **4^{Cy}** along with the residual THF solvent.

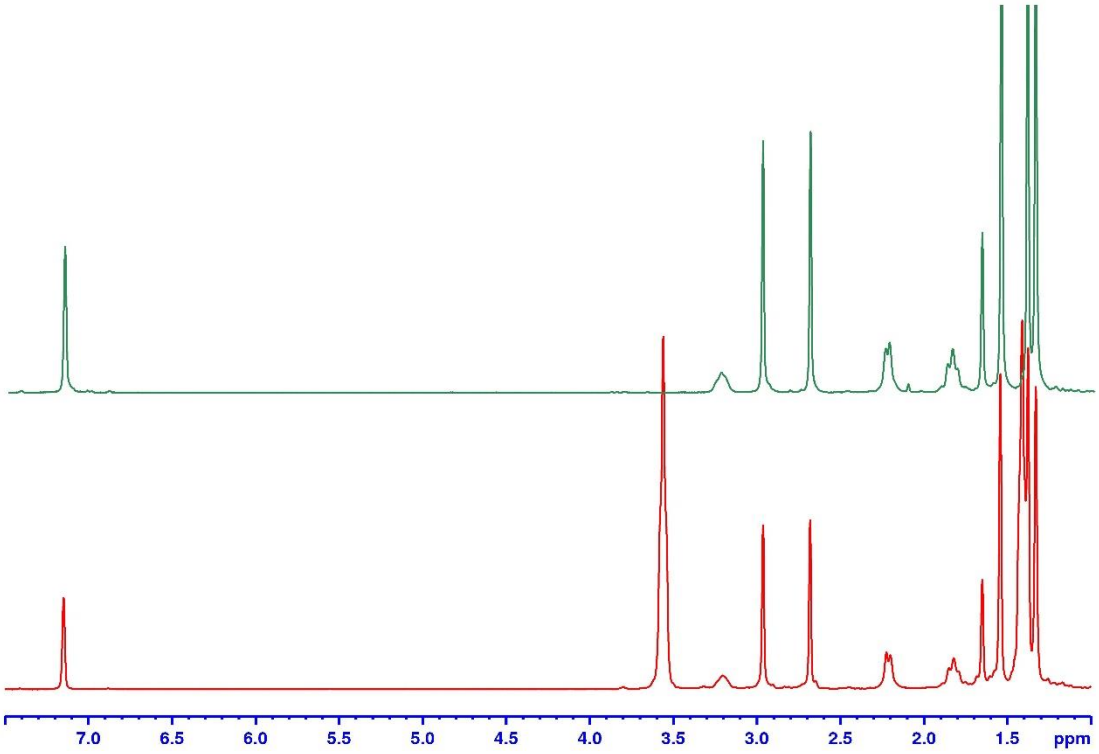
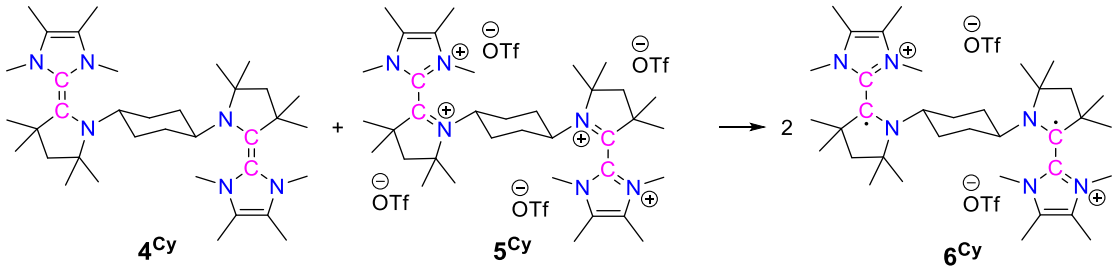


Fig. S11 Overlay of ^1H NMR spectra from the reaction mixture of **5^{Cy}** and excess KC_8 (red) and **4^{Cy}** (green) in C_6D_6 at RT.

Synthesis of 6^{Cy}



5 mL Acetonitrile was added to the mixture of $\mathbf{4^{Cy}}$ (130 mg, 0.225 mmol) and $\mathbf{5^{Cy}}$ (264 mg, 0.225 mmol) at −30 °C and then stirred for 6 hours at room temperature. Then the solvent and other volatiles were removed under reduced pressure and a deep red powder was obtained. **Yield:** 380 mg (96 %). After that about 2 mL of CH_3CN was added to the residue and kept for crystallization at −35 °C. After 24 hours, dark red colored crystals were collected. **M.P.:** Upto 120 °C there was no color change observed. At 130 °C the color changed from red to light yellow without melting (the UV/Vis spectrum of the light yellow colored sample reveals that decomposition of $\mathbf{6^{Cy}}$ has occurred and the ^{1}H NMR spectrum shows the formation of an unidentified mixture of compounds). The resulting light yellow sample does not melt even at 170 °C. **UV/Vis (CH_3CN):** λ_{max} (nm)= 455, 375, 299. **Elemental analysis:** Calculated (%) for $C_{38}H_{62}F_6N_6O_6S_2$: C, 52.04; H, 7.13; N, 9.58; S, 7.31; Found: C, 49.62; H, 7.00; N, 9.18; S, 6.8.

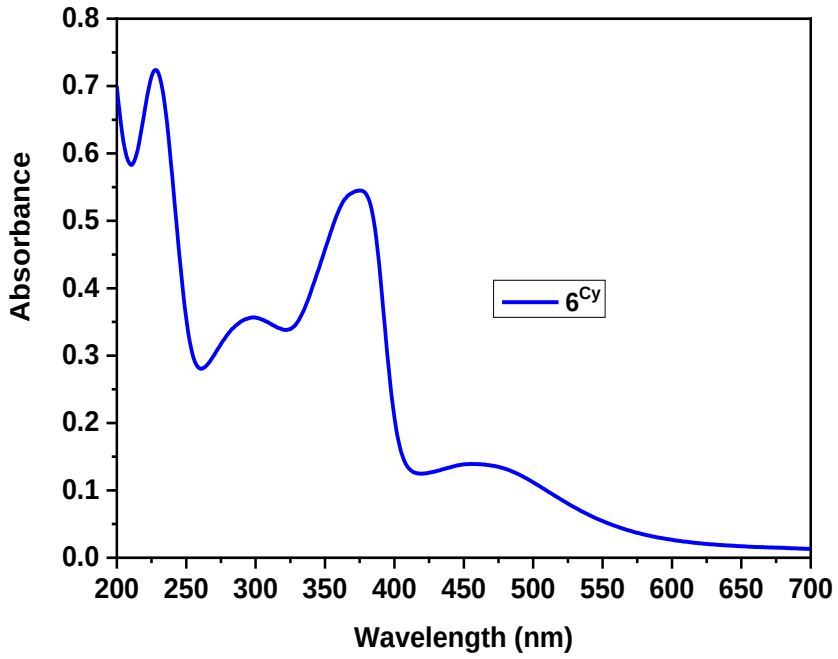


Fig. S12 UV/Vis spectrum of $\mathbf{6^{Cy}}$ in acetonitrile at room temperature.

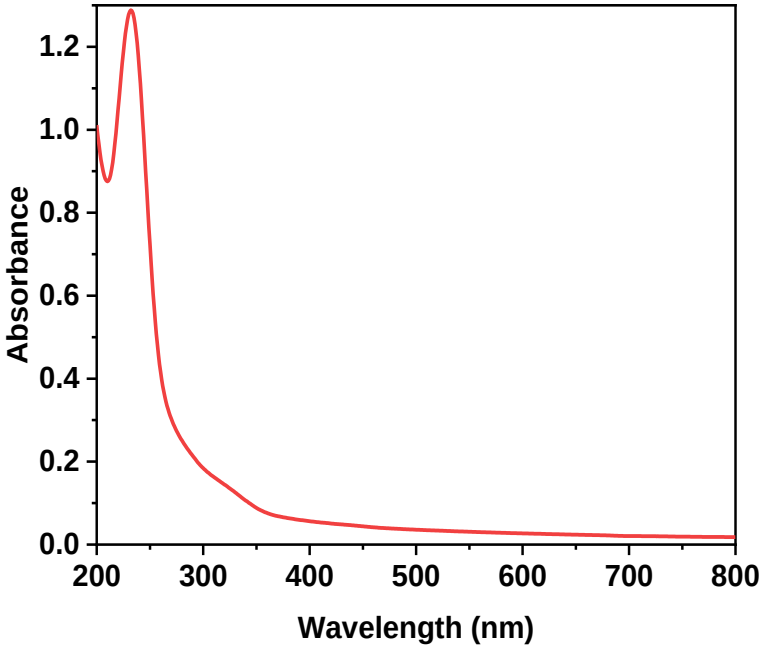


Fig. S13 UV/Vis spectrum of the light-yellow solid, which was obtained after heating solid **6**^{Cy} at 130 °C for 10 minutes in a closed sealed NMR tube in acetonitrile measured at room temperature.

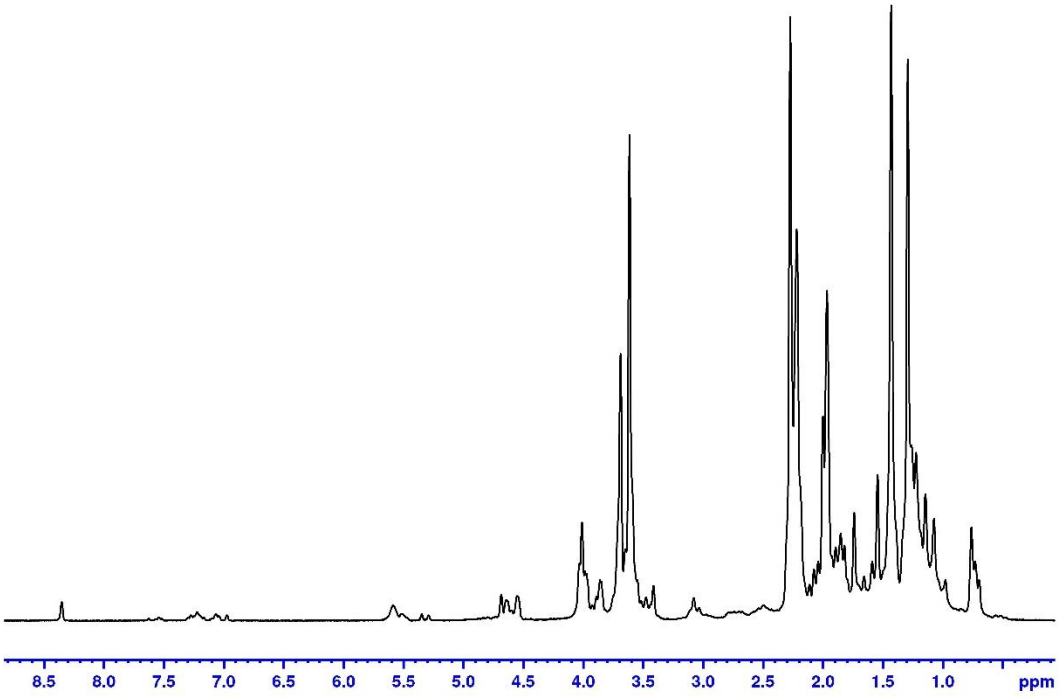
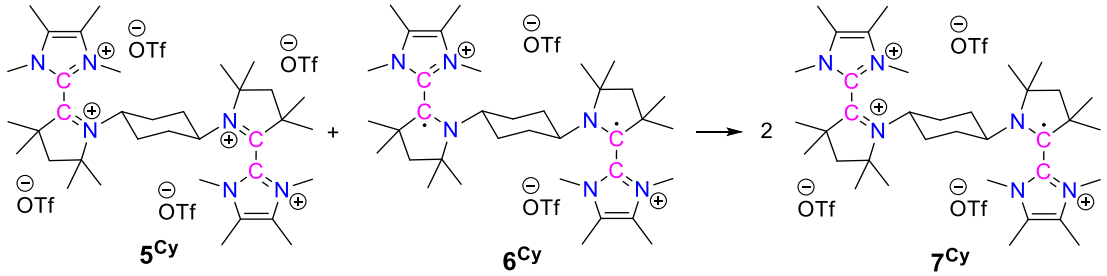


Fig. S14 ^{1}H NMR spectrum of the light-yellow solid, which was obtained after heating solid **6**^{Cy} at 130 °C for 10 minutes in closed sealed NMR tube measured in CD_3CN at RT.

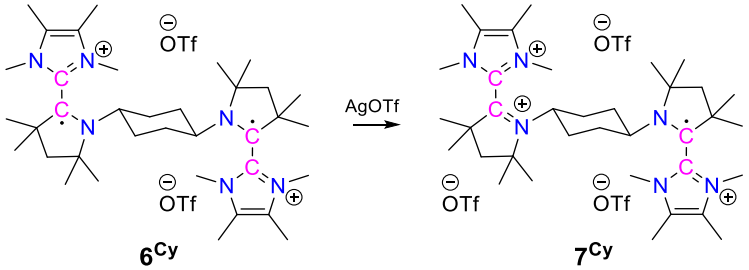
Synthesis of 7^{Cy}

Method I



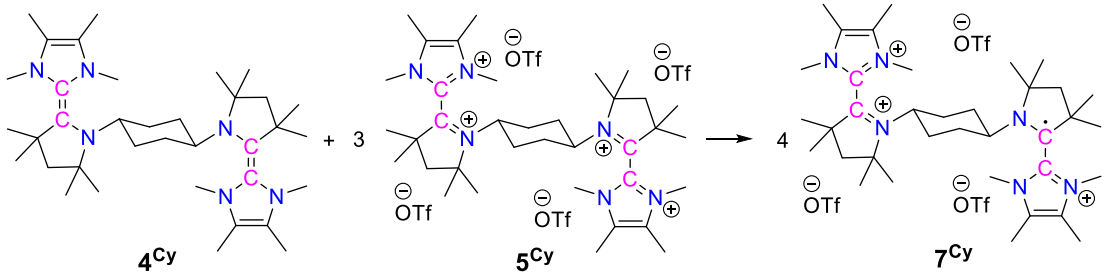
About 6 mL of CH_3CN was added to the mixture of **5^{Cy}** (134 mg, 0.114 mmol) and **6^{Cy}** (100 mg, 0.114 mmol) at −30 °C and then the reaction mixture was warmed to room temperature over 15 minutes. The solvent and other volatiles from the reaction mixture were removed under vacuum and a red colored solid was obtained as compound **7^{Cy}**. **Yield:** 205 mg (88 %). **UV/Vis (CH_3CN):** λ_{max} (nm)= 451, 374, and 308.

Method II



About 6 mL of CH_3CN was added to the mixture of AgOTf (30 mg, 0.117 mmol) and **6^{Cy}** (100 mg, 0.114 mmol) at room temperature. Immediately the formation of the black precipitate of metallic silver was observed. The filtrate was evaporated and the red colored solid of compound **7^{Cy}** was obtained.

Method III



About 4 mL of CH_3CN was added to the mixture of **4^{Cy}** (43 mg, 0.074 mmol) and **5^{Cy}** (262 mg, 0.223 mmol) at −30 °C. The solution of the reaction mixture became dark red colored. It was stirred for 12 hours at room temperature. The filtrate was evaporated and red colored solid of compound **7^{Cy}** was obtained. About 2 mL of THF was added to it and the solution kept for crystallization at −35 °C for 24 hours. In the first fraction we obtained **5^{Cy}**, whereas in the second fraction we obtained red colored crystals of **7^{Cy}**

(minor amount and suitable for single-crystal X-ray diffraction study) along with colorless crystals of **5**^{Cy} (major amount).

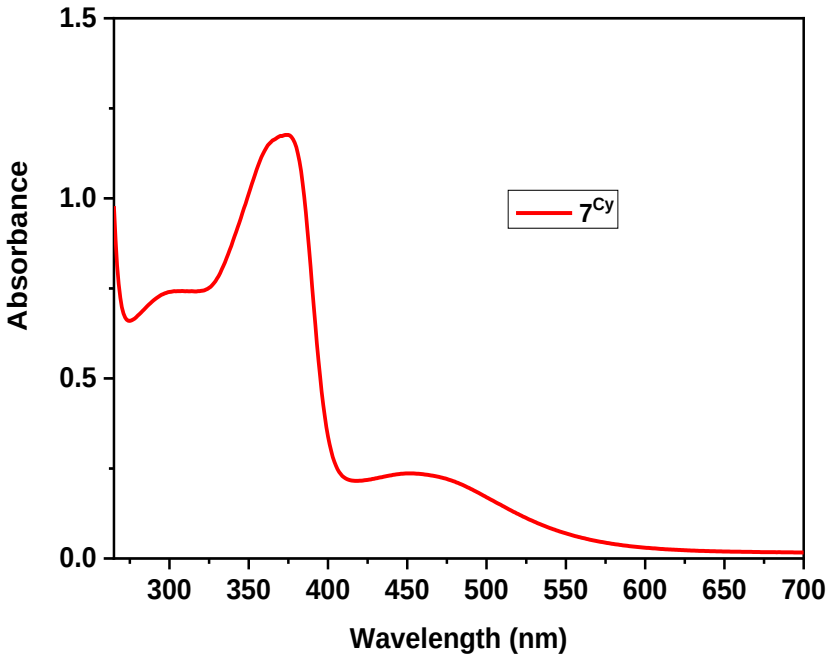
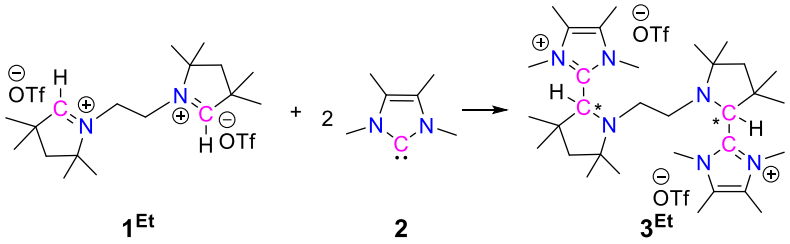


Fig. S15 UV/Vis spectra of **7**^{Cy} in acetonitrile at room temperature.

Synthesis of 3^{Et}



1^{Et} 2 3^{Et}

About 250 mL of THF was added to a 500 mL Schlenk flask containing $\mathbf{1^{Et}}$ (10 g, 17.343 mmol) and **2** (5 g, 40.260 mmol) at 0 °C. After stirring for 24 hrs at room temperature, about 150 mL of diethyl ether was added to the reaction mixture and then the reaction mixture was filtered. The white solid residue was washed with about 50 mL of diethyl ether and dried under vacuum. ^{1}H NMR spectrum of the solid residue showed the formation of a mixture of two diastereomers (*dll*- and *meso*-) of $\mathbf{3^{Et}}$ in ca. 60:40 ratio. These two are diastereomers of each other. **Yield:** 13.2 g (92 %). **M.P.:** > 180 °C. The pure major diastereomer of $\mathbf{3^{Et}}$ was obtained through fractional crystallization by layering diethyl ether over a saturated CH_3CN solution of the crude compound. The obtained crystals were suitable for a single crystal X-ray diffraction study and the analysis of single crystal data showed that it was the *meso*-isomer of $\mathbf{3^{Et}}$. The pure major diastereomer of $\mathbf{3^{Et}}$ was obtained up to the third consecutive fraction of fractional crystallization. In the fourth fraction of fractional crystallization we obtained mostly the minor diastereomer along with small amounts of the major diastereomer. It was not possible to isolate the pure minor diastereomer. We used the mixture of diastereomers for the next reaction. **NMR data of the major diastereomer: ^{1}H NMR** (CD_3CN, 25 °C, 300 MHz): δ = 4.24 (s, 2H, C*H*), 3.94 (s, 6H, CH_3-N), 3.68 (s, 6H, CH_3-N), 2.24 (s, 6H, CH_3-C=C), 2.21 (s, 6H, CH_3-C=C), 2.14-2.00 (m, 4H, CH_2CH_2), 1.87-1.76 (m, 4H, CH_2), 1.31 (s, 6H, CH_3), 1.01 (s, 6H, CH_3), 0.94 (s, 6H, CH_3), 0.78 (s, 6H, CH_3) ppm. **^{13}C{^{1}H} NMR** (CD_3CN, 25 °C, 75 MHz): δ = 144.68 (*C*=N-CH_3), 128.97 (CH_3-*C*=*C*), 128.15 (CH_3-*C*=*C*), 122.11 (q, $^1J_{C\text{-}F}$ = 320.02 Hz, *C*$F_3SO_3^-$), 71.58 (*C*H), 62.90 (*C*(CH_3)$_2$), 55.94 (*C*H_2), 48.95 (*C*H_2CH_2), 43.33 (*C*(CH_3)$_2$), 35.14 (*C*H_3-N), 33.43 (*C*H_3-N), 31.65 (C(*C*H_3)$_2$), 29.58 (C(*C*H_3)$_2$), 27.72 (C(*C*H_3)$_2$), 22.18 (C(*C*H_3)$_2$), 9.03 (*C*H_3-C=C), 8.68 (*C*H_3-C=C) ppm. **^{19}F{^{1}H} NMR:** (CD_3CN, 25 °C, 282 MHz): δ = −79.23 ppm. **NMR data of the minor diastereomer: ^{1}H NMR:** (CD_3CN, 25 °C, 300 MHz): δ = 4.18 (s, 2H, C*H*), 3.96 (s, 6H, CH_3-N), 3.60 (s, 6H, CH_3-N), 2.23 (s, 6H, CH_3-C=C), 2.20 (s, 6H, CH_3-C=C), 1.76-1.87 (m, 4H, CH_2CH_2), 1.66-1.73 (m, 4H, CH_2), 1.29 (s, 6H, CH_3), 1.15 (s, 6H, CH_3), 1.00 (s, 6H, CH_3), 0.74 (s, 6H, CH_3) ppm. **Elemental analysis:** Calculated (%) for $C_{34}H_{58}F_6N_6O_6S_2$: C, 49.50; H, 7.09; N, 10.19; S, 7.77; Found: C, 49.84; H, 6.87; N, 10.08; S, 7.60. **HRMS-ESI (m/z):** Calculated for $C_{33}H_{58}N_6F_3SO_3$ $[M-OTf]^+$: 675.4238; Found: 675.4218.

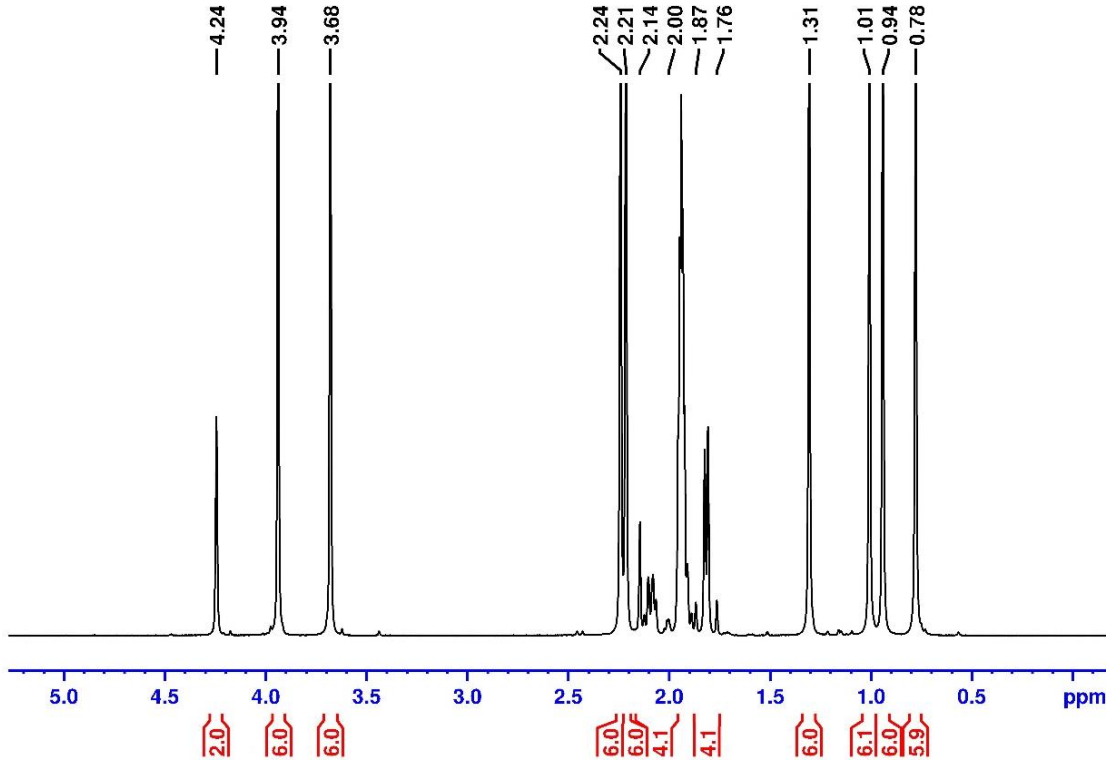


Fig. S16 ^{1}H NMR spectrum of the major diastereomer of **3^{Et}** in CD_3CN at RT.

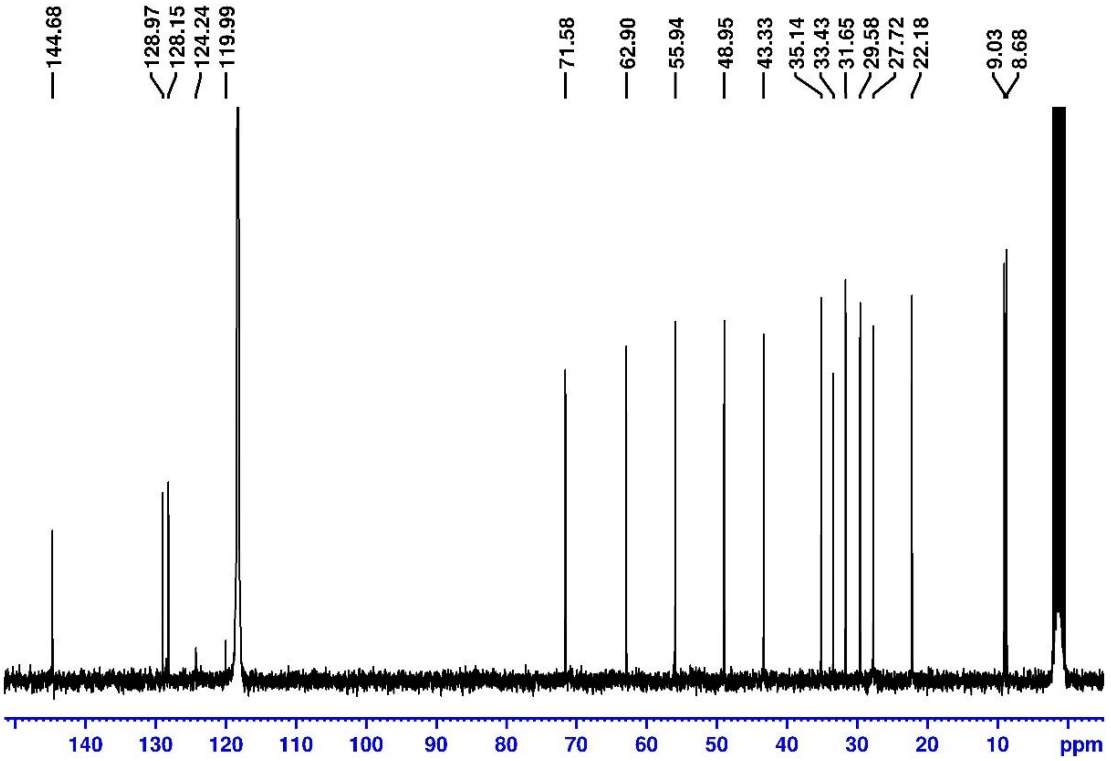


Fig. S17 $^{13}C\{^{1}H\}$ NMR spectrum of the major diastereomer of **3^{Et}** in CD_3CN at RT.

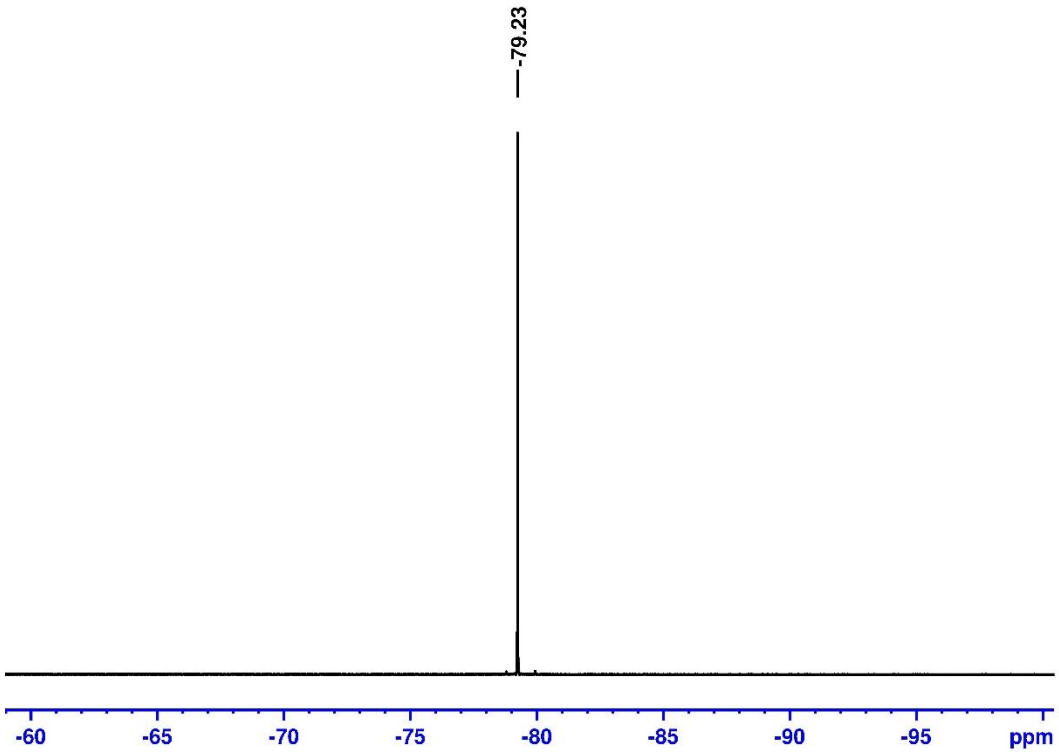


Fig. S18 $^{19}F\{^{1}H\}$ spectrum of the major diastereomer **3^{Et}** in CD_3CN at RT.

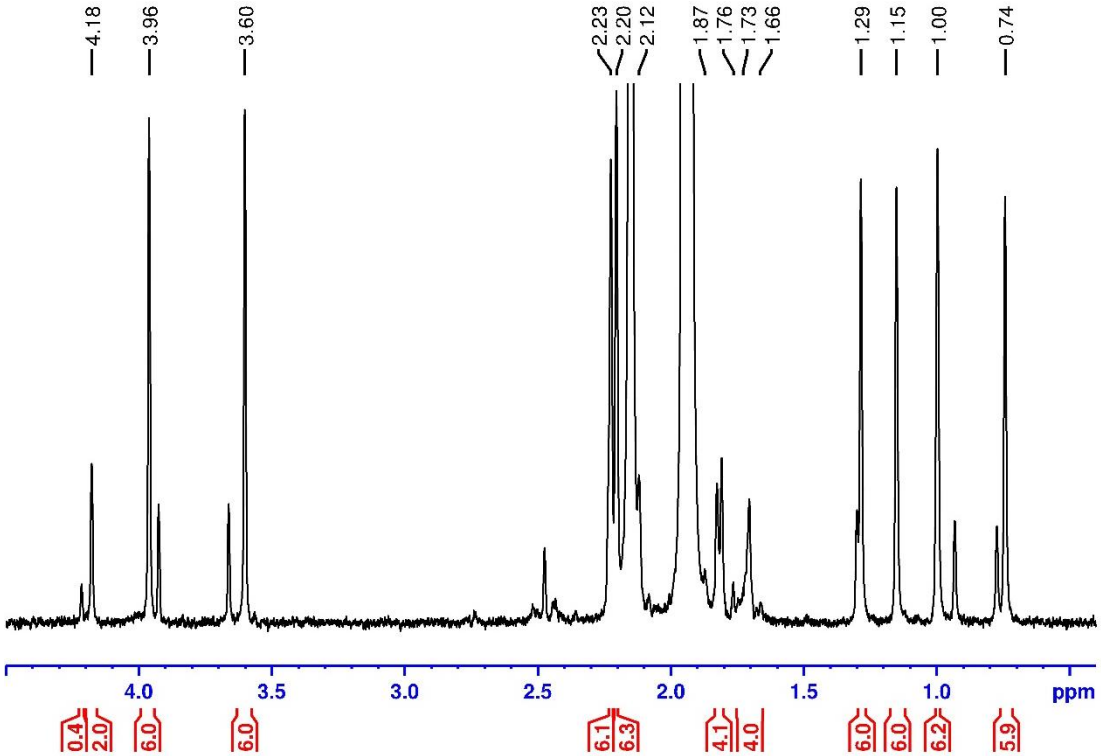


Fig. S19 ^{1}H NMR spectrum of the minor diastereomer of **3^{Et}** with small amounts of the major diastereomer in CD_3CN at RT.

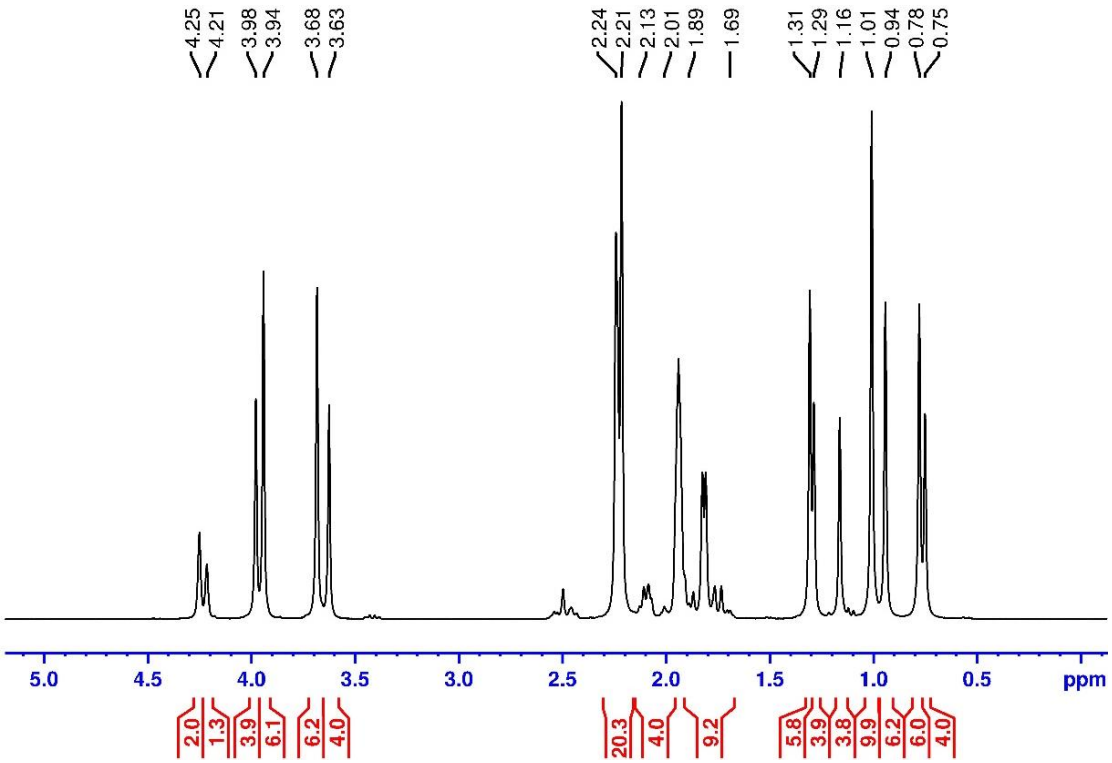


Fig. S20 ^{1}H NMR spectrum of the crude compound of **3^{Et}** (after work up) in CD_3CN at RT.

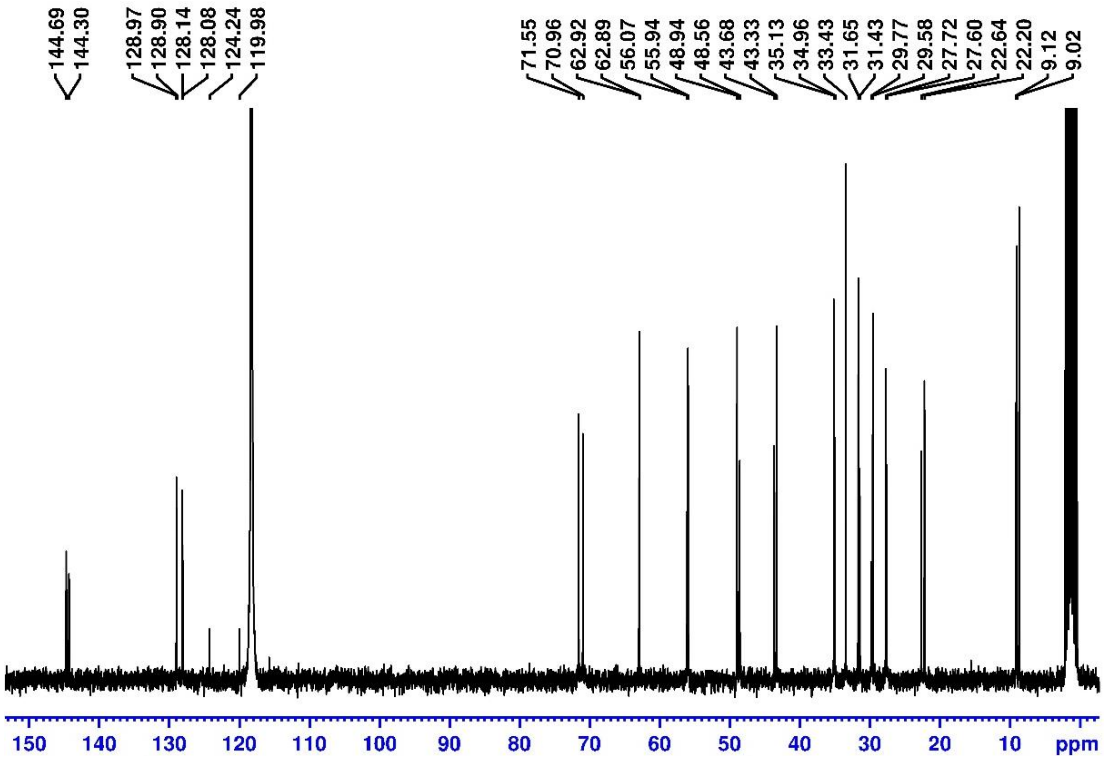


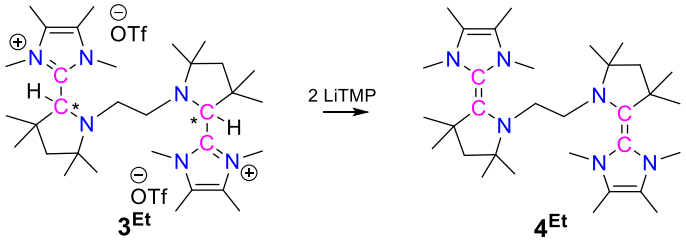
Fig. S21 $^{13}C\{^{1}H\}$ NMR spectrum of the crude compound of **3^{Et}** (after workup) in CD_3CN at RT.

Synthesis of LiTMP

Solid LiTMP (lithium 2,2,6,6-tetramethylpiperidide) was prepared based on the literature procedure.[S4] *n*BuLi (50.5 mL, 80.80 mmol, 1.6 M in hexane) was added to the pentane solution of 2,2,6,6-tetramethylpiperidine (15 mL, 88.89 mmol) at 0 °C. After 2 hours, it was warmed to room temperature and stirred for another 12 hours. The solid residue was filtered and dried. The filtrate was concentrated and kept at −35 °C for crystallization. Both solid residues were collected after drying and stored inside a glove box. **Yield:** 11.8 g (99 %).

Synthesis of 4^{Et}

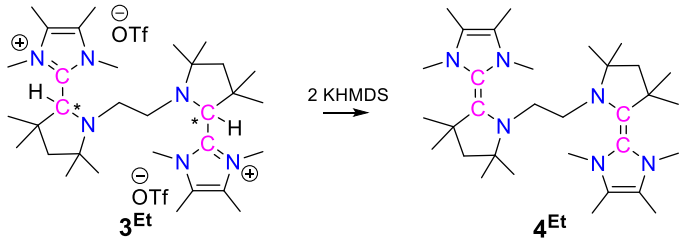
Method I



3^{Et} 4^{Et}

About 30 mL of toluene was added into a 50 mL Schlenk flask containing $\mathbf{3^{Et}}$ (327 mg, 0.395 mmol) and LiTMP (168 mg, 1.141 mmol) at room temperature with stirring. Then the reaction mixture was stirred for 12 hours at room temperature. After that the reaction mixture was filtered while heated to boiling temperature (compound $\mathbf{4^{Et}}$ is poorly soluble in toluene). Further 10 mL of toluene was added to the residue and filtered at boiling temperature. Both filtrates were combined and kept at −35 °C for crystallization. Light yellow colored crystals were obtained after 12 hours which were suitable for a single crystal X-ray diffraction study. Subsequently, the mother liquor was concentrated and kept at −35 °C to get a second crop of crystals. The combined crystals were washed with a small amount of pentane giving pure compound $\mathbf{4^{Et}}$. **Yield:** 130 mg (63 %).

Method II



3^{Et} 4^{Et}

About 80 mL of toluene was added into a 250 mL Schlenk flask containing $\mathbf{3^{Et}}$ (4 g, 4.836 mmol) and KHMDS (2.485 g, 12.457 mmol) at room temperature while stirring. The reaction mixture turned into a yellow colour and the reaction mixture was stirred for 72 hours at 90 °C. After that it was stirred for overnight at room temperature. Then the reaction mixture was filtered while heated to boiling temperature (compound $\mathbf{4^{Et}}$ is poor soluble in toluene). Further 20 mL of toluene was added to the residue and filtered

at boiling temperature. Both filtrates were combined and kept at −35 °C for crystallization. Light yellow colored crystals were obtained after 12 hours and collected. Subsequently, the mother liquor was concentrated and kept at −35 °C to get a second crop of crystals. The combined crystals were washed with a small amount of pentane giving pure compound **4^{Et}**. **Yield:** 2.31 g (91 %). **M.P.:** 162 °C (decomposed). **^{1}H NMR** (THF-D$_8$, 25 °C, 300 MHz): δ = 2.69 (br, 4H, C*H*$_2$C*H*$_2$), 2.67 (s, 6H, C*H*$_3$-N), 2.46 (s, 6H, C*H*$_3$-N), 1.74 (s, 6H, C*H*$_3$-C=C), 1.71 (s, 6H, C*H*$_3$-C=C), 1.61 (s, 4H, C*H*$_2$), 1.26 (s, 12H, C*H*$_3$), 1.10 (s, 12H, C*H*$_3$) ppm. **^{13}C{^{1}H} NMR** (THF-D$_8$, 25 °C, 75 MHz): δ = 138.76 (NC=*C*NN), 122.75 (CH$_3$-*C*=*C*), 122.70 (CH$_3$-*C*=*C*), 112.80 (N*C*=CNN), 60.15 (*C*H$_2$), 59.46 (*C*(CH$_3$)$_2$), 41.94 (*C*H$_3$-N), 39.55 (*C*(CH$_3$)$_2$), 38.91 (*C*H$_2$*C*H$_2$), 33.72 (*C*H$_3$-N), 28.93 (C(*C*H$_3$)$_2$), 27.96 (C(*C*H$_3$)$_2$), 9.99 (*C*H$_3$-C=C), 9.75 (*C*H$_3$-C=C) ppm. Compound **4^{Et}** is not well soluble in THF. For the UV/Vis measurement 2 mg of compound **4^{Et}** was heated to reflux in THF to dissolve it and allowed to cool down to room temperature. Then the resulting solution was subsequently used for the UV/Vis study. **UV/Vis (THF):** λ_{max} (ε) = 290 (31879) nm (L mol^{-1} cm^{-1}). **Elemental analysis:** Calculated (%) for C$_{32}$H$_{56}$N$_6$: C, 73.23; H, 10.76; N, 16.01; Found: C, 72.98; H, 10.825; N, 15.48. **HRMS-ASAP (m/z):** Calculated for C$_{32}$H$_{57}$N$_6$ [M+H]$^+$: 525.4639, Found: 525.4625.

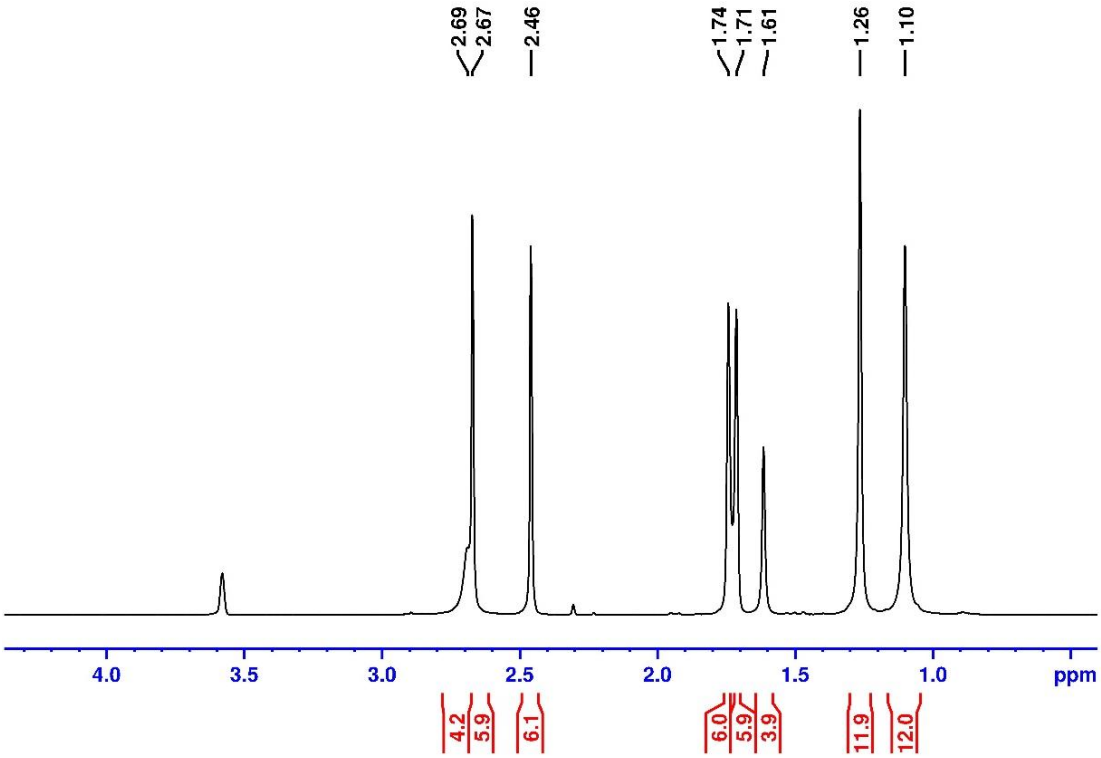


Fig. S22 ^{1}H NMR spectrum of **4^{Et}** in THF-D$_8$ at RT.

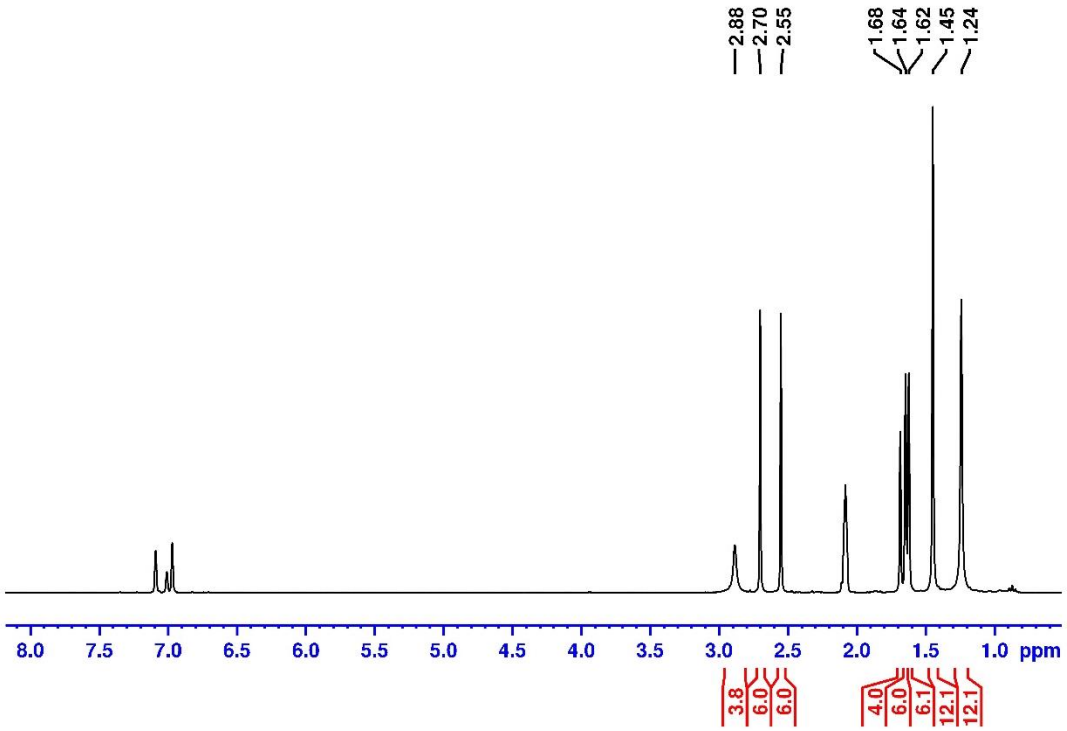


Fig. S23 ^{1}H NMR spectrum of **4^{Et}** in toluene-D_8 at RT.

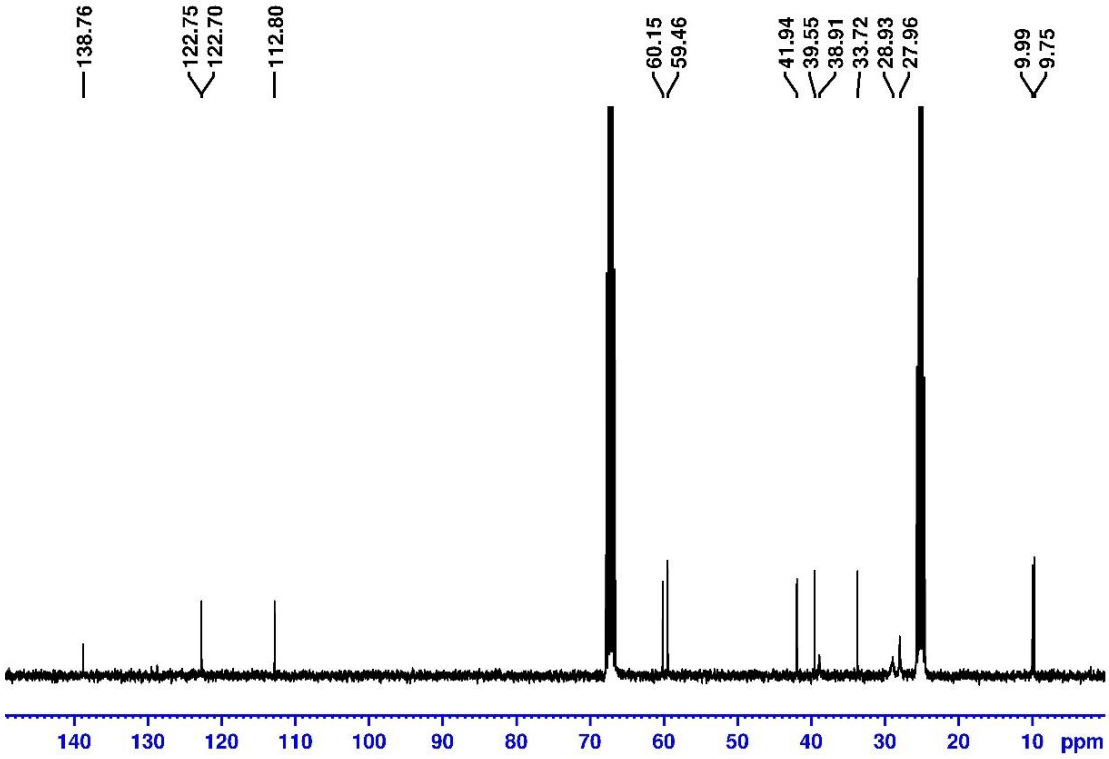
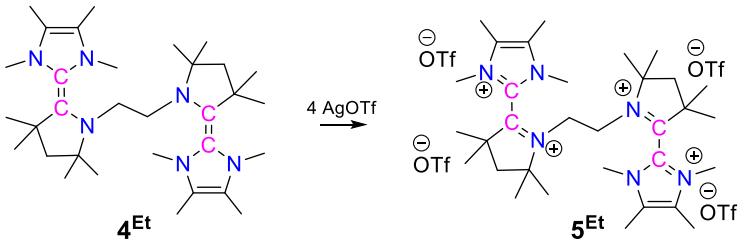


Fig. S24 ^{13}C{^{1}H} NMR spectrum of **4^{Et}** in THF-D_8 at RT.

Synthesis of 5^{Et}



4^{Et} 5^{Et}

40 mL THF solution of **4^{Et}** (210 mg, 0.4 mmol) was added dropwise to a 10 mL THF solution of AgOTf (511 mg, 1.989 mmol) at room temperature while stirring. Immediately, black colored metallic silver precipitated out. After 12 hours all volatiles were removed under vacuum and the residue was dissolved in acetonitrile (50 mL) and filtered. The yellowish green colored filtrate was concentrated and kept for crystallization with diethyl ether diffusion at room temperature for 24 hours and then kept at −30 °C. Yellow colored crystals of **5^{Et}** were obtained after 12 hours which were also suitable for X-ray structural analysis. The obtained crystals were washed with diethyl ether to give pure compound **5^{Et}**. The mother liquor was concentrated and again stored for crystallization. **Yield:** 340 mg (76 %). **M.P.: >** 180 °C. **^{1}H NMR** (CD_3CN, 25 °C, 300 MHz): δ = 4.21 (s, 4H, CH_2CH_2), 3.87 (s, 12H, CH_3-N), 2.51 (s, 4H, CH_2), 2. 41 (s, 12H, CH_3-C=C), 1.67 (s, 12H, CH_3), 1.56 (s, 12H, CH_3) ppm. **^{13}C{^{1}H} NMR** (CD_3CN, 25 °C, 75 MHz): δ = 186.43 (*C*=N^+), 136.12 (CH_3-*C*=*C*), 124.32 (*C*NN^+), 121.7 (q, $^{1}J_{C\text{-}F}$ = 320.05 Hz, *C*$F_3SO_3^-$), 86.18 (*C*$(CH_3)_2$), 57.19 (*C*$(CH_3)_2$), 47.77 (*C*H_2CH_2), 47.34 (*C*H_2), 36.77 (*C*H_3-N), 27.56 (C(*C*$H_3)_2$), 27.01 (C(*C*$H_3)_2$), 9.47 (*C*H_3-C=C) ppm. **^{19}F{^{1}H} NMR** (CD_3CN, 25 °C, 282 MHz): δ = −79.25 ppm. **UV/Vis** (CH_3CN): λ_{max} (ε) = 350 (3474), 243 (23303) nm (L mol^{-1} cm^{-1}). **Elemental analysis:** Calculated (%) for $C_{36}H_{56}N_6F_{12}O_{12}S_4$: C, 38.57; H, 5.04; N, 7. 50; S, 11.44; Found: C, 38.93; H, 5.07; N, 8.04; S, 11.20. **HRMS-ESI (m/z):** Calculated for $C_{34}H_{56}N_6F_6S_3O_6$ $[M-2OTf]^{2+}$: 411.1798, Found: 411.1788.

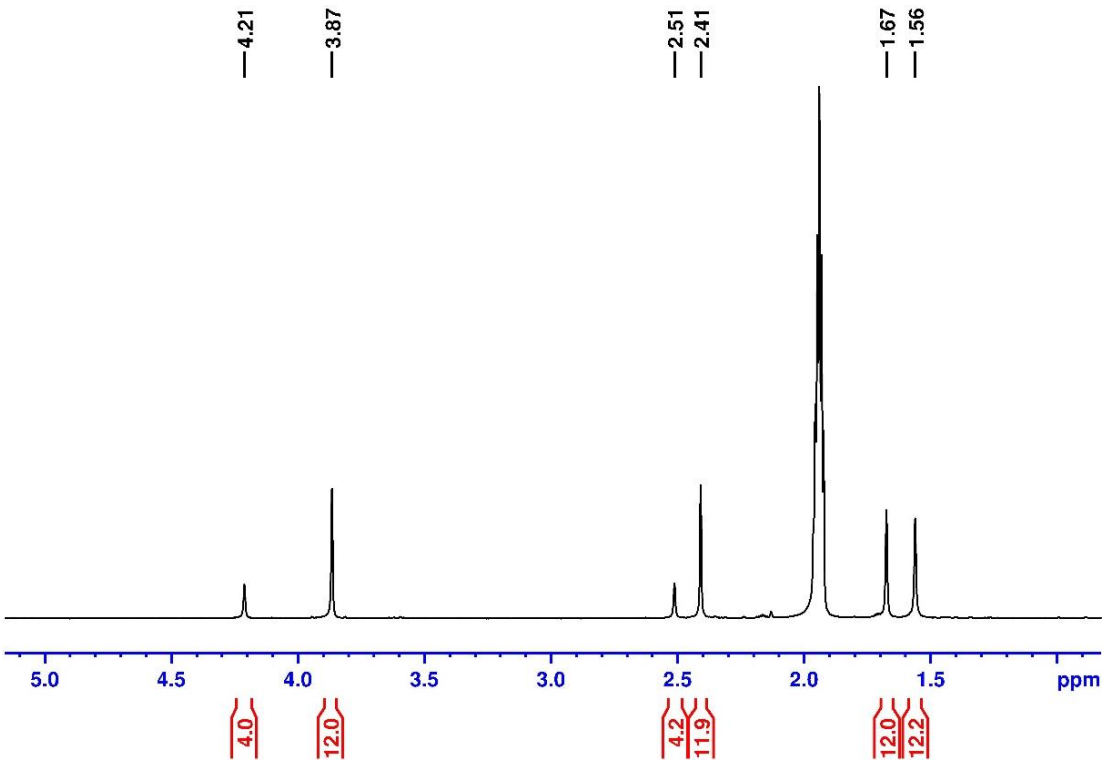


Fig. S25 ^{1}H NMR spectrum of **5^{Et}** in CD_3CN at RT.

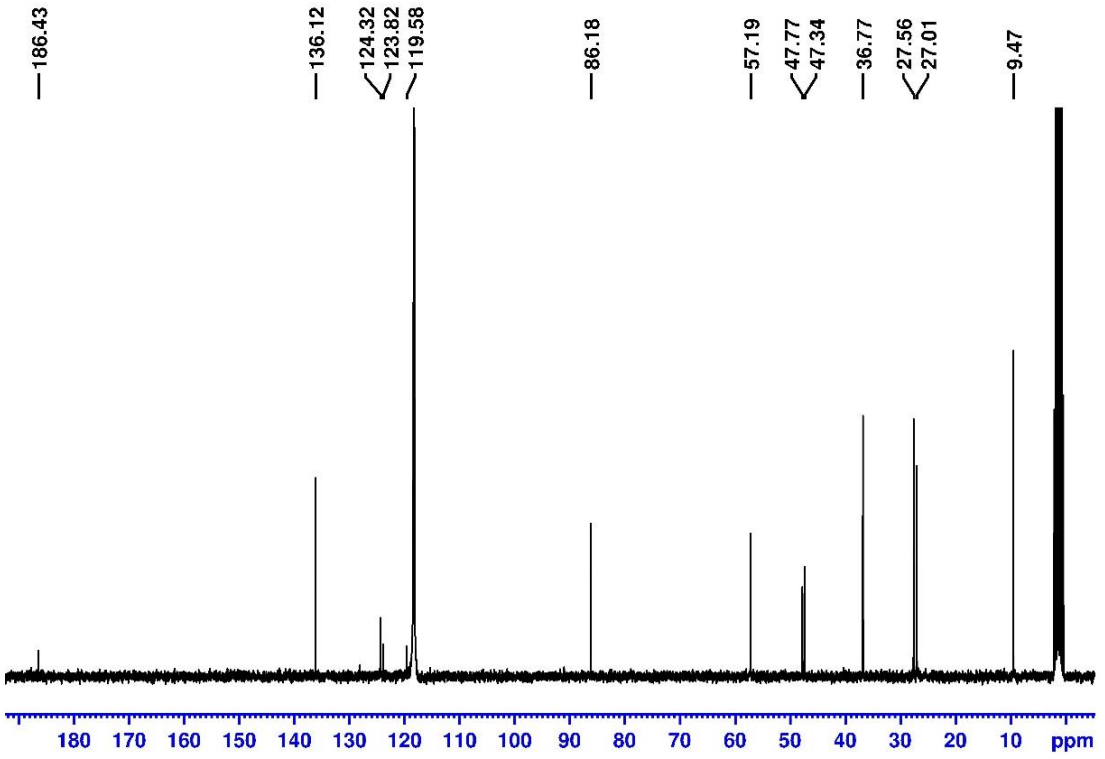


Fig. S26 $^{13}C\{^{1}H\}$ NMR spectrum of **5^{Et}** in CD_3CN at RT.

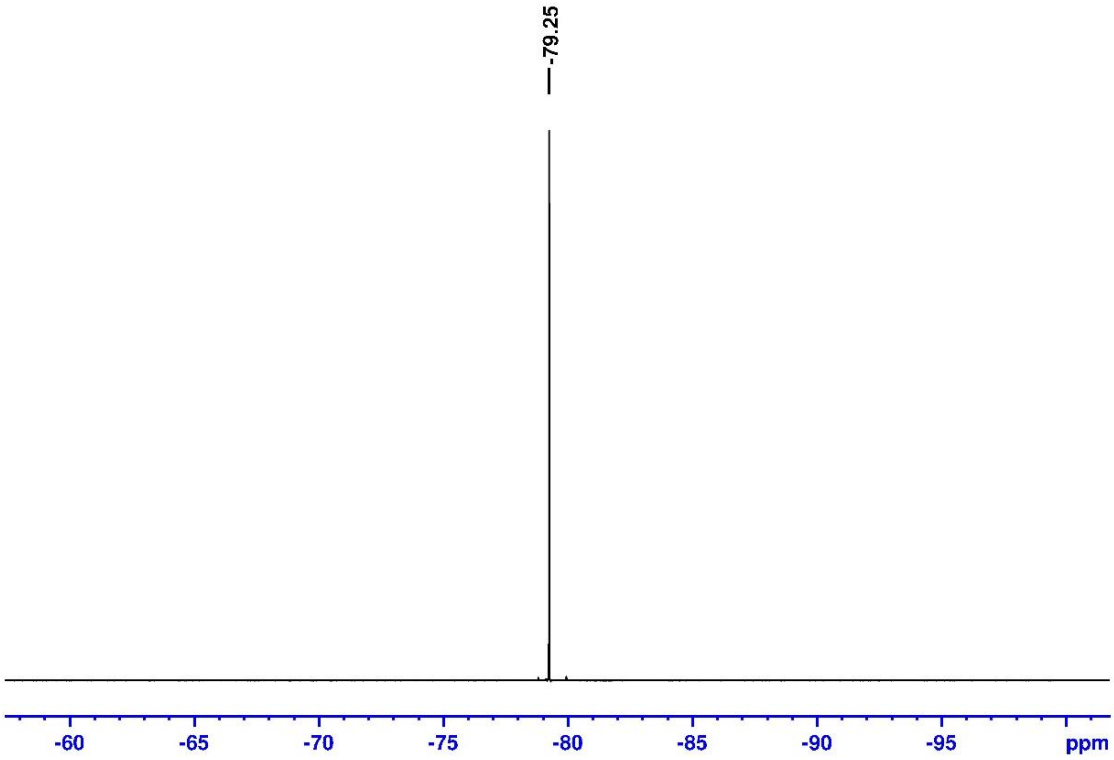
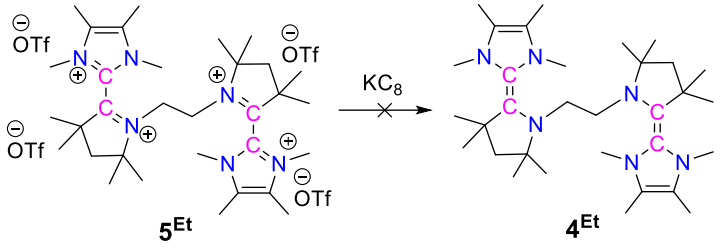


Fig. S27 $^{19}F\{^{1}H\}$ spectrum of **5^{Et}** in CD_3CN at RT.

Reaction of 5^{Et} and KC_8



THF was added to the mixture of **5^{Et}** (104 mg, 0.093 mmol) and KC_8 (150 mg, 1.109 mmol) at room temperature with stirring. After 4 hours stirring at room temperature, solvent and other volatiles were removed under vacuum and a ^{1}H NMR spectrum of the reaction mixture in C_6D_6 was measured. There was no clear evidence of formation of **4^{Et}** in the ^{1}H NMR spectrum of the reaction mixture.

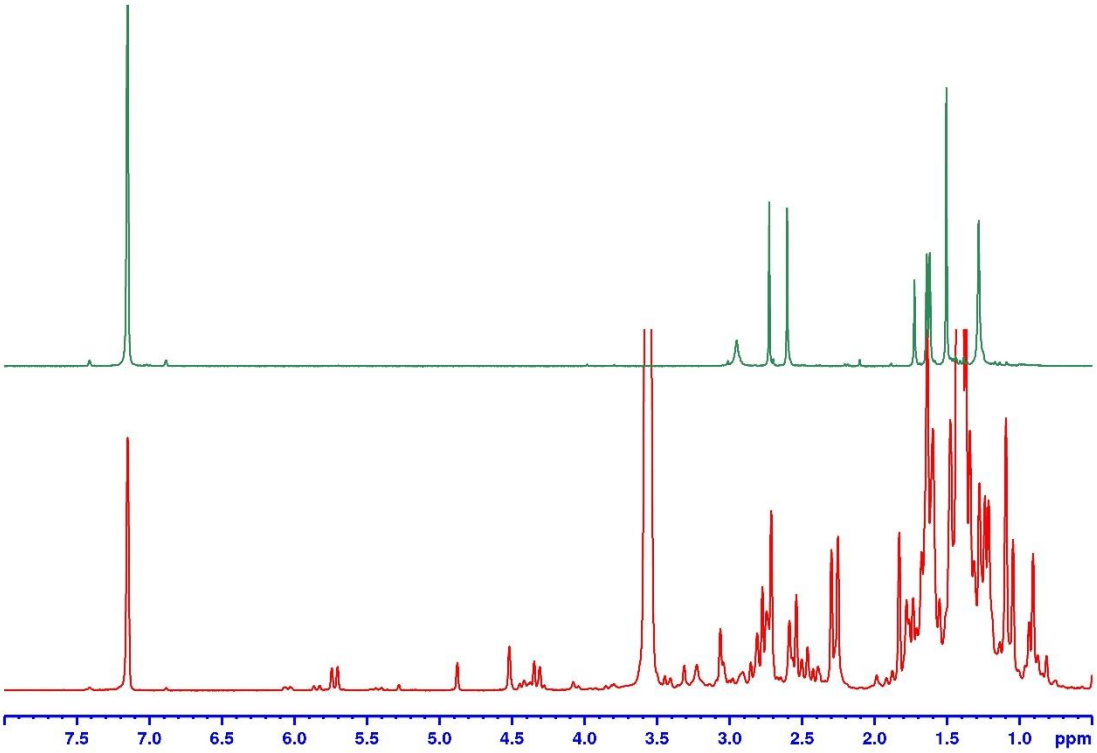
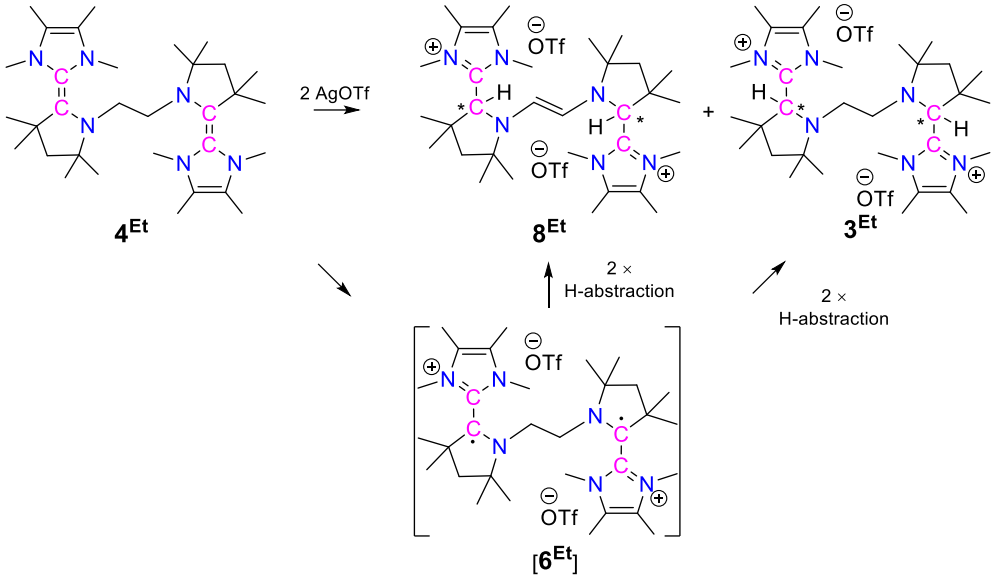


Fig. S28 Overlay of the ^{1}H NMR spectra of reaction mixture of **5^{Et}** and KC_8 (red) and **4^{Et}** (green) in C_6D_6 at RT.

Synthesis of 8^{Et}

Method I



4^{Et} 8^{Et} 3^{Et} $[6^{Et}]$

20 mL of THF was added to the mixture of $\mathbf{4^{Et}}$ (200 mg, 0.381 mmol) and AgOTf (196 mg, 0.763 mmol) at room temperature while stirring. After 6 hours of stirring, all volatiles were removed under vacuum. Then about 10 mL of acetonitrile was added into the residue, and the silver particles allowed to settle down for overnight. The clear yellow supernatant solution was collected with a pipette. Again 10 mL acetonitrile was added to the residue, shaken well, allowed to stand for 10 minutes and supernatant solution was taken out. Alternatively, THF solution of AgOTf (196 mg, 0.763 mmol, in 15 mL of THF) was added to a THF solution of $\mathbf{4^{Et}}$ (200 mg, 0.381 mmol, in 30 mL of THF) dropwise at 0 °C. After 6 hours all volatiles were evaporated under reduced pressure. After that the workup was carried out as in the previous procedure. The ^{1}H NMR spectrum of the filtrate after extraction with CH_3CN showed the formation of two diastereomers of $\mathbf{8^{Et}}$ (56 % & 19 %) along with the compound $\mathbf{3^{Et}}$ (24 %). Then the combined supernatant solution was concentrated to about 4 mL and diethyl ether was added dropwise until a slightly yellow precipitate appeared. This was kept at −30 °C for 12 hours to obtain crystals/more precipitate. The ^{1}H NMR spectrum of the collected precipitate (90 mg) showed that it was the major diastereomer of $\mathbf{8^{Et}}$. Suitable single crystals for a single crystal X-ray diffraction study were obtained for the major diastereomer of $\mathbf{8^{Et}}$ by diffusing diethyl ether into the concentrated CH_3CN/THF (1:2) solution. The analysis of the single crystal X-ray diffraction data showed that it was the *meso*-isomer. After collecting the first crop, diethyl ether was added to the mother liquor again dropwise until further precipitate appeared. The ^{1}H NMR spectrum of the collected precipitate shows that it was the major diastereomers of $\mathbf{8^{Et}}$ along with compound $\mathbf{3^{Et}}$. Subsequently, after collecting the second crop, about 5 mL diethyl ether was added to the mother liquor and kept at −30 °C. After 7 days red colored small crystals formed. The ^{1}H NMR spectrum of the collected red colored crystalline compound (25 mg) showed that it was the minor diastereomer of $\mathbf{8^{Et}}$. We were unable to obtain single crystals suitable for XRD of the minor diastereomer

of **8^{Et}**. **Yield:** 115 mg (36 %). **M.P.:** > 180 °C. **NMR data of the major diastereomer: ^{1}H NMR** (CD_3CN, 25 °C, 300 MHz): δ = 4.66 (s, 2H, C*H*=C*H*), 4.48 (s, 2H, C*H*), 3.78 (s, 6H, C*H*$_3$-N), 3.76 (s, 6H, C*H*$_3$-N), 2.25 (s, 6H, C*H*$_3$-C=C), 2.14 (s, 6H, C*H*$_3$-C=C), 1.89-1.78 (m, 4H, C*H*$_2$), 1.30 (s, 6H, C*H*$_3$), 1.10 (s, 6H, C*H*$_3$), 0.86 (s, 6H, C*H*$_3$), 0.64 (s, 6H, C*H*$_3$) ppm. **^{13}C{^{1}H} NMR** (CD_3CN, 25 °C, 75 MHz): δ = 142.89 (*C*=N-CH_3), 128.92 (CH_3-*C*=*C*), 128.23 (CH_3-*C*=*C*), 122.08 (q, $^{1}J_{C\text{-}F}$ = 320.95 Hz, *C*$F_3SO_3^-$), 116.36 (H*C*=*C*H), 65.73 (*C*H), 62.69 (*C*(CH_3)$_2$), 54.85 (*C*H$_2$), 43.74 (*C*(CH_3)$_2$), 34.18 (*C*H$_3$-N), 33.61 (*C*H$_3$-N), 30.43 (C(*C*H$_3$)$_2$), 27.96 (C(*C*H$_3$)$_2$), 27.32 (C(*C*H$_3$)$_2$), 25.05 (C(*C*H$_3$)$_2$), 8.99 (*C*H$_3$-C=C), 8.70 (*C*H$_3$-C=C) ppm. **^{19}F{^{1}H} NMR** (CD_3CN, 25 °C, 282 MHz): δ = −79.33 ppm. **NMR data of the minor diastereomer: ^{1}H NMR** (CD_3CN, 25 °C, 300 MHz): δ = 4.88 (s, 2H, C*H*=C*H*), 4.39 (s, 2H, C*H*), 3.85 (s, 6H, C*H*$_3$-N), 3.68 (s, 6H, C*H*$_3$-N), 2.23 (s, 6H, C*H*$_3$-C=C), 2.17 (s, 6H, C*H*$_3$-C=C), 1.87-1.80 (m, 4H, C*H*$_2$), 1.28 (s, 6H, C*H*$_3$), 1.22 (s, 6H, C*H*$_3$), 0.85 (s, 6H, C*H*$_3$), 0.76 (s, 6H, C*H*$_3$) ppm. **^{13}C{^{1}H} NMR** (CD_3CN, 25 °C, 75 MHz): δ = 143.01 (*C*=N-CH_3), 128.54 (CH_3-*C*=*C*), 128.30 (CH_3-*C*=*C*), 121.33 (H*C*=*C*H), 68.02 (*C*H), 63.25 (*C*(CH_3)$_2$), 55.14 (*C*H$_2$), 43.55 (*C*(CH_3)$_2$), 34.40 (*C*H$_3$-N), 33.57 (*C*H$_3$-N), 30.71 (C(*C*H$_3$)$_2$), 28.90 (C(*C*H$_3$)$_2$), 27.41 (C(*C*H$_3$)$_2$), 24.39 (C(*C*H$_3$)$_2$), 9.08 (*C*H$_3$-C=C), 8.68 (*C*H$_3$-C=C) ppm. **^{19}F{^{1}H} NMR** (CD_3CN, 25 °C, 282 MHz): δ = −79.33 ppm. **UV/Vis (CH_3CN):** λ_{max} (ε) = 233 (31673) nm (L mol^{-1} cm^{-1}). **Elemental analysis:** Calculated (%) for $C_{34}H_{56}N_6F_6O_6S_2$: C, 49.62; H, 6.86; N, 10.21; S, 7.79; Found: C, 49.71; H, 6.86; N, 10.11; S, 7.53. **HRMS-LIFDI (m/z):** Calculated for $C_{33}H_{56}N_6F_3SO_3$ [M−OTf]$^{+}$: 673.4081, Found: 673.4067.

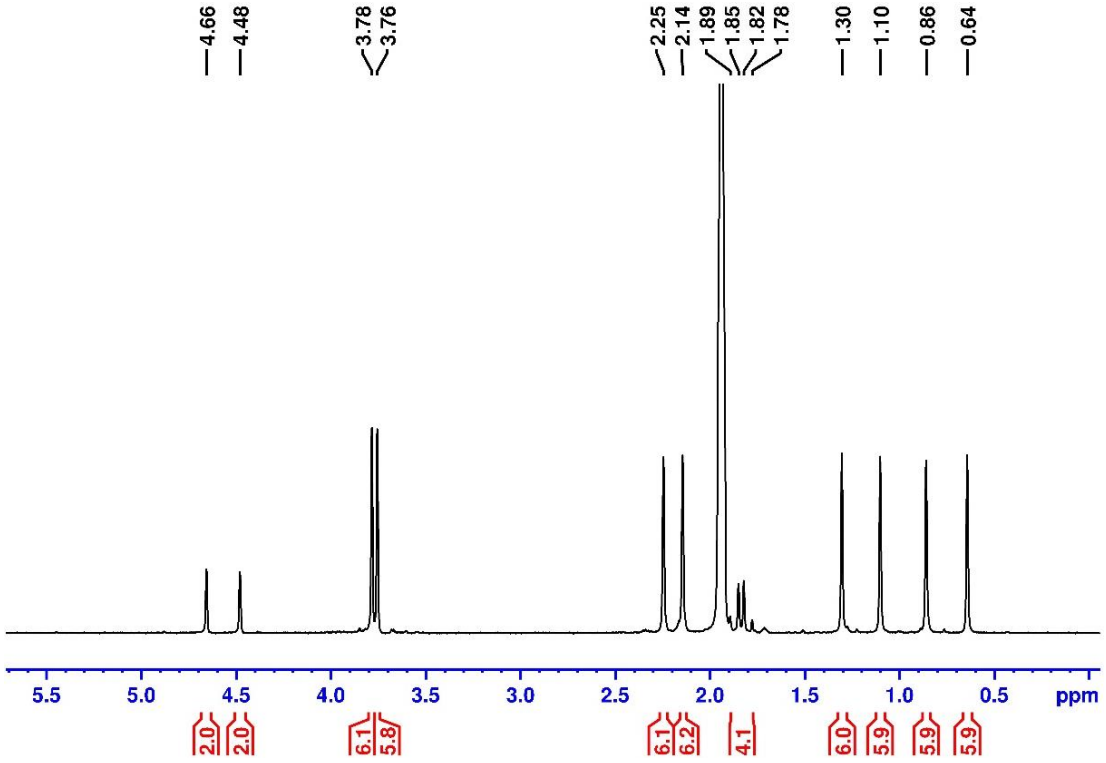


Fig. S29 ^{1}H NMR spectrum of the major diastereomer of **8^{Et}** in CD_3CN at RT.

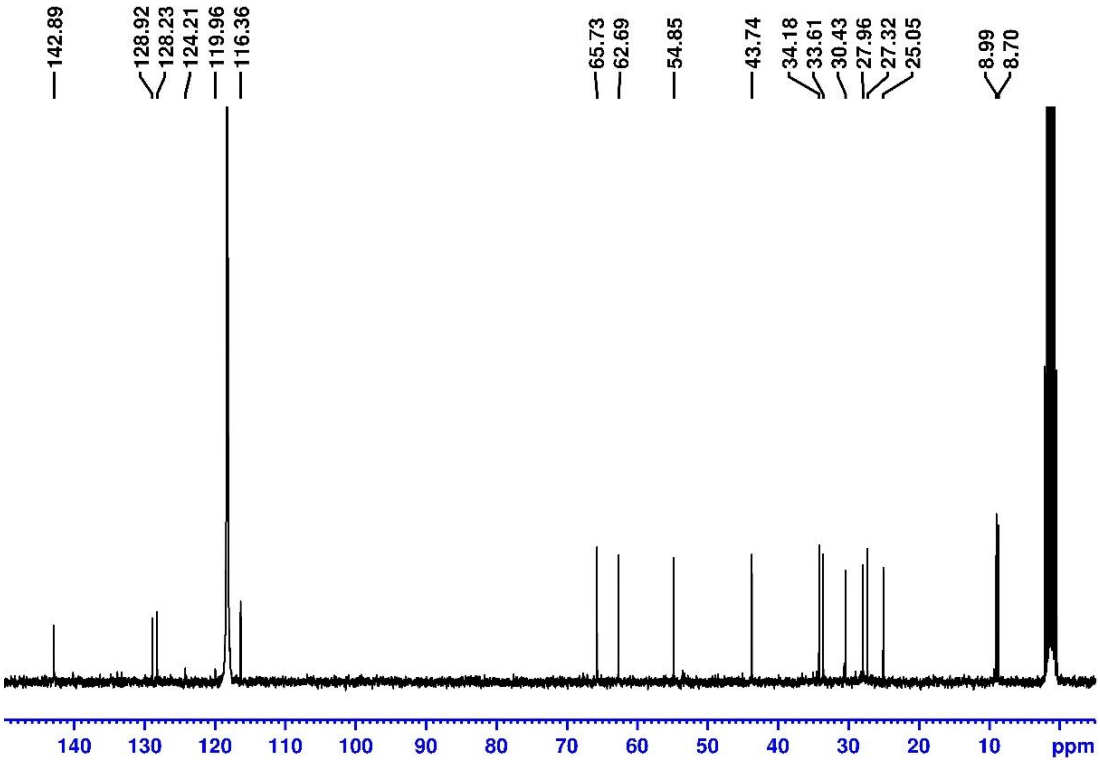


Fig. S30 $^{13}C\{^{1}H\}$ NMR spectrum of the major diastereomer of $\mathbf{8^{Et}}$ in CD_3CN at RT.

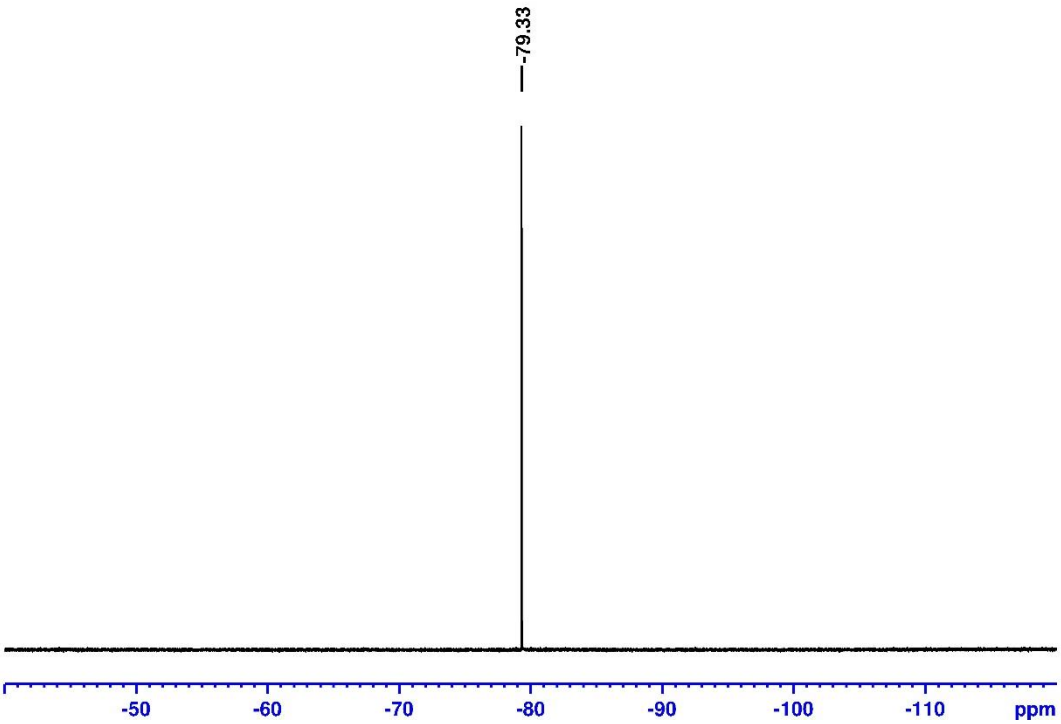


Fig. S31 $^{19}F\{^{1}H\}$ spectrum of the major diastereomer of $\mathbf{8^{Et}}$ in CD_3CN at RT.

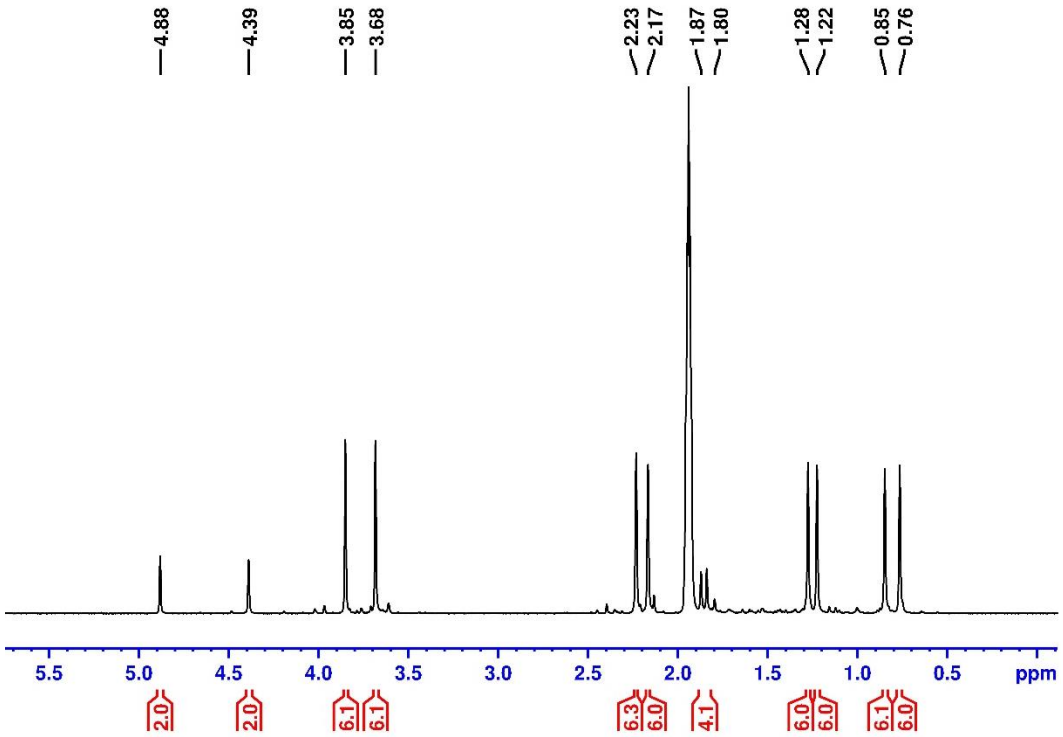


Fig. S32 ^{1}H NMR spectrum of the minor diastereomer of **8^{Et}** in CD_3CN at RT.

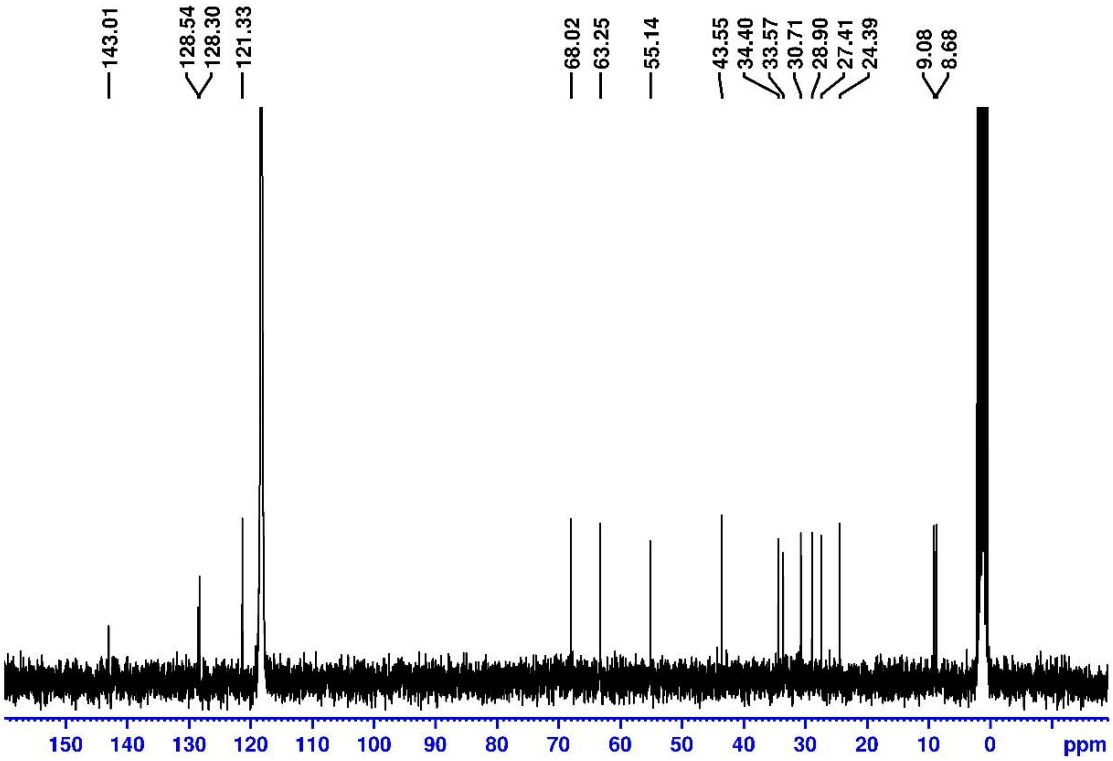


Fig. S33 $^{13}C\{^{1}H\}$ NMR spectrum of the minor diastereomer of **8^{Et}** in CD_3CN at RT.

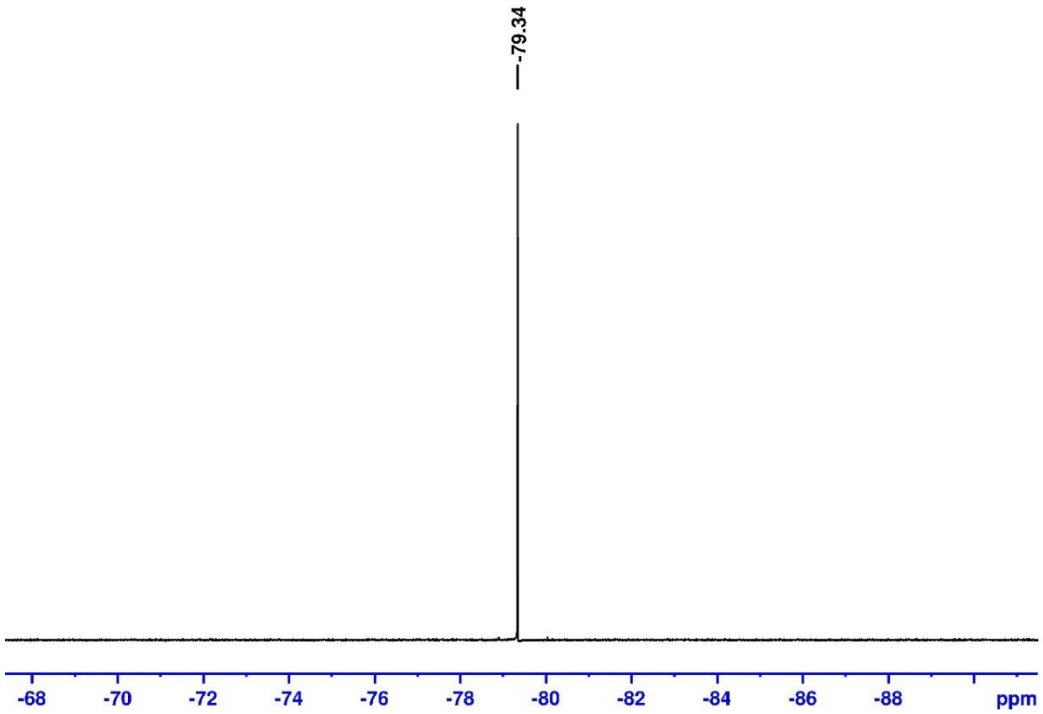


Fig. S34 $^{19}F\{^{1}H\}$ spectrum of the minor diastereomer of **8^{Et}** in CD_3CN at RT.

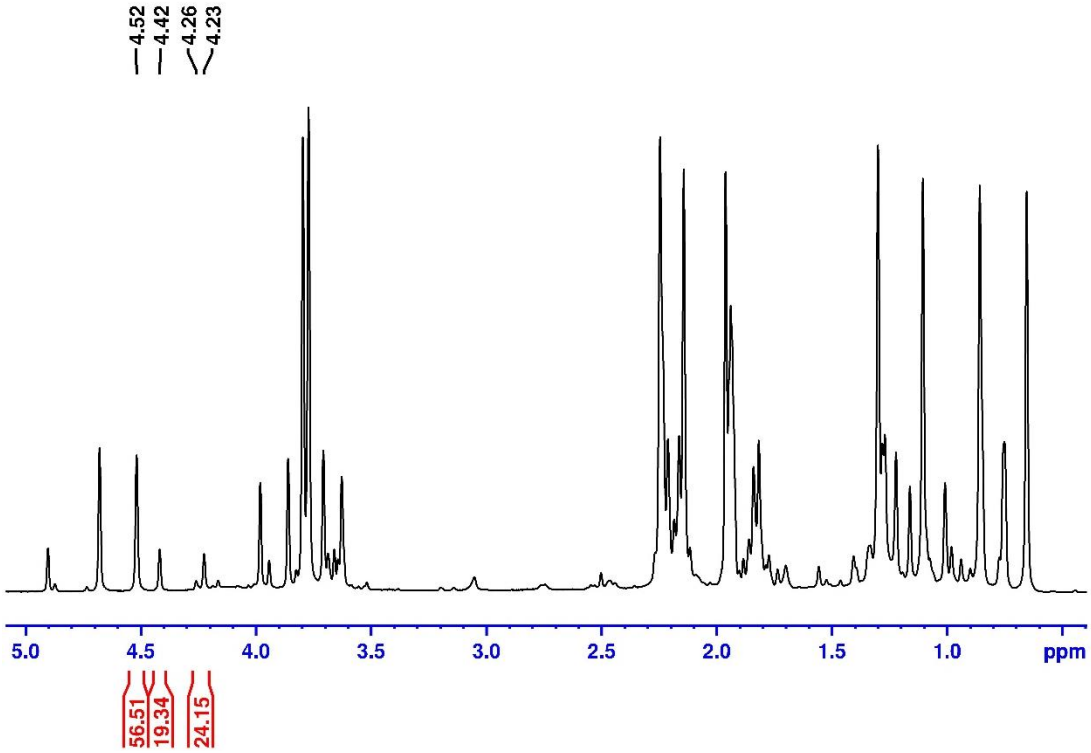


Fig. S35 ^{1}H NMR spectrum of the crude reaction mixture of **8^{Et}** (containing both diastereomers of **8^{Et}** along with compound **3^{Et}** which has also two diastereomers) in CD_3CN at RT.

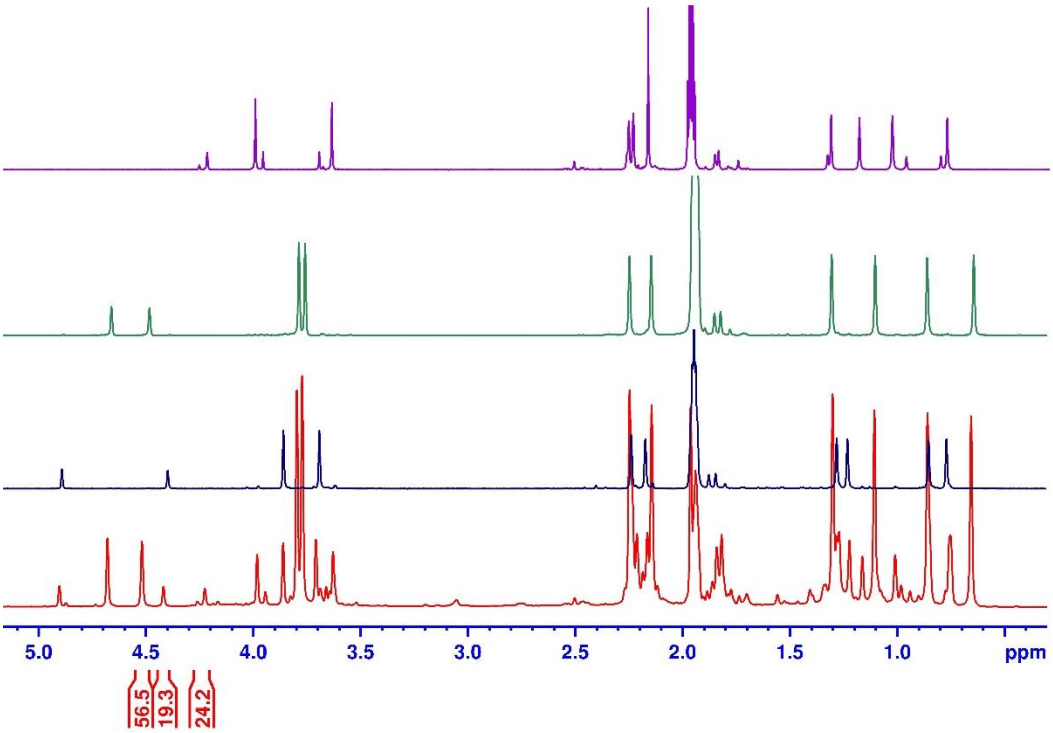
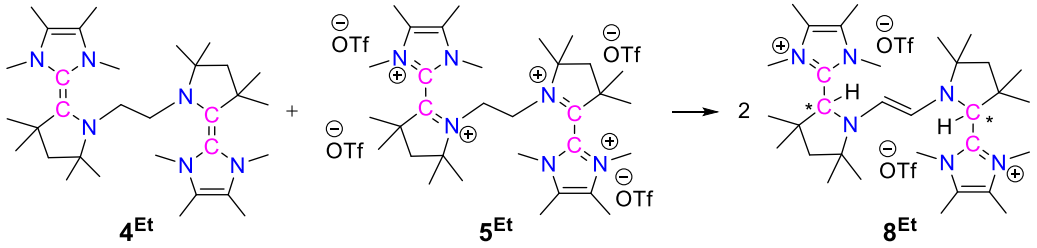


Fig. S36 Overlay of the ^{1}H NMR spectra of the crude reaction mixture of **8^{Et}** (red), minor diastereomer of **8^{Et}** (navy), major diastereomer of **8^{Et}** (green), and two diastereomers **3^{Et}** (purple) in CD_3CN at RT.

Method II



$\mathbf{4^{Et}}$ $\mathbf{5^{Et}}$ $\mathbf{8^{Et}}$

4^{Et} (14 mg, 0.027 mmol) and **5**^{Et} (30 mg, 0.027 mmol) were taken into an NMR tube and about 0.6 mL of CD_3CN was added. The ^1H NMR spectrum of the reaction mixture was measured which showed the formation of two diastereomers of compound **8**^{Et}.

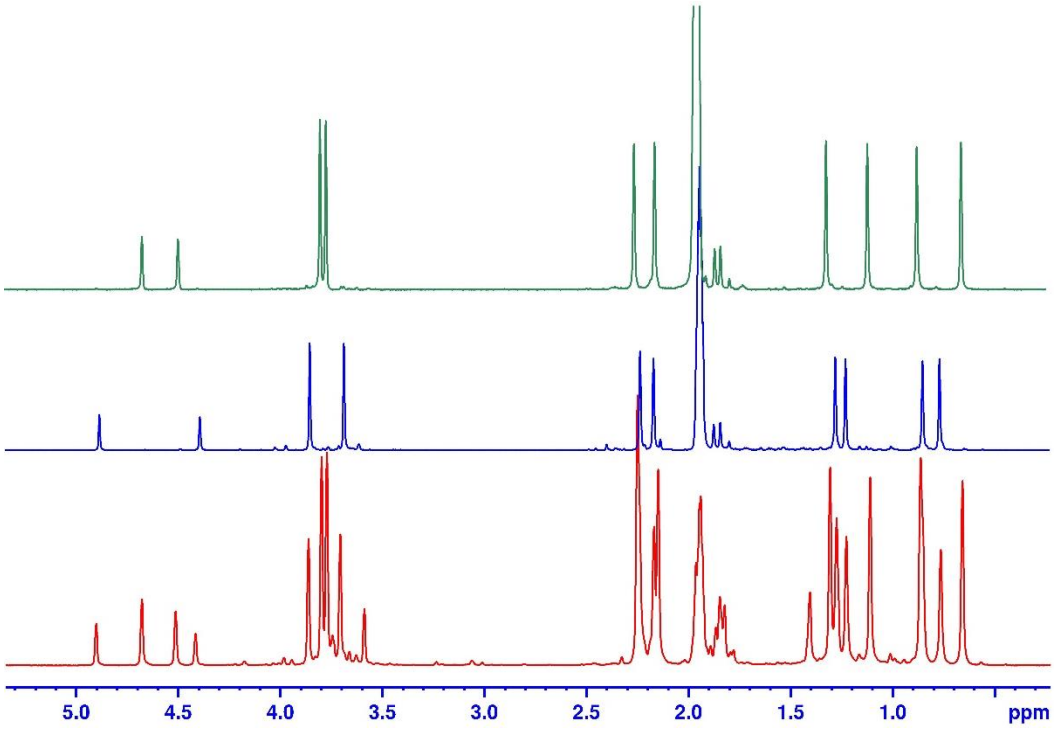
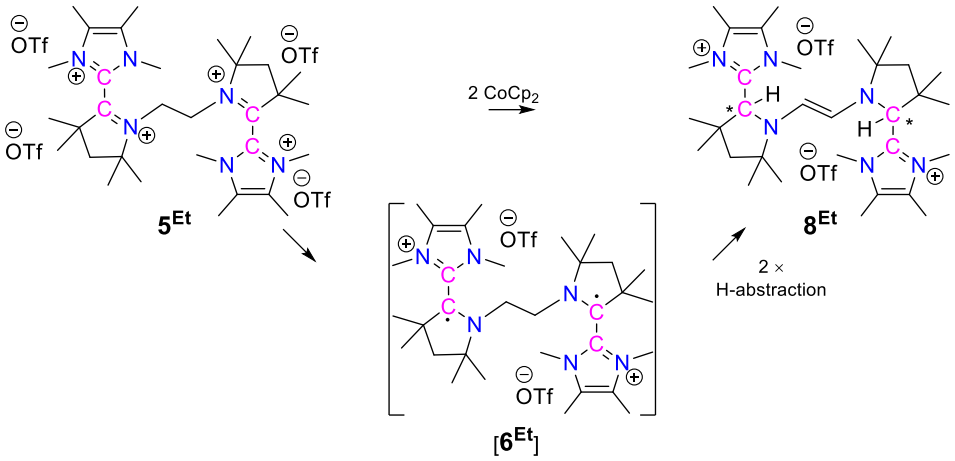


Fig. S37 Overlay of the ^1H NMR spectra of the crude reaction mixture of 1:1 reaction of **4**^{Et} and **5**^{Et} (red) with minor diastereomer of **8**^{Et} (blue) and major diastereomer of **8**^{Et} (green) in CD_3CN at RT.

Method III



An acetonitrile (15 mL) solution of $Co(Cp)_2$ (27 mg, 0.143 mmol) was added dropwise to the acetonitrile solution (15 mL) of **5^{Et}** (80 mg, 0.071 mmol) at room temperature with stirring. After 12 hours, solvent and other volatiles were removed under vacuum and the residue was washed with THF (15 ml) and dried. Then the ^{1}H NMR spectrum of the remaining residue in CD_3CN showed the formation of two diastereomers of **8^{Et}** in ca. 89:11 ratio along with the cobaltocenium cation. The same outcome was obtained when we performed the reaction of **5^{Et}** with four equivalents of $Co(Cp)_2$ in a similar reaction condition.

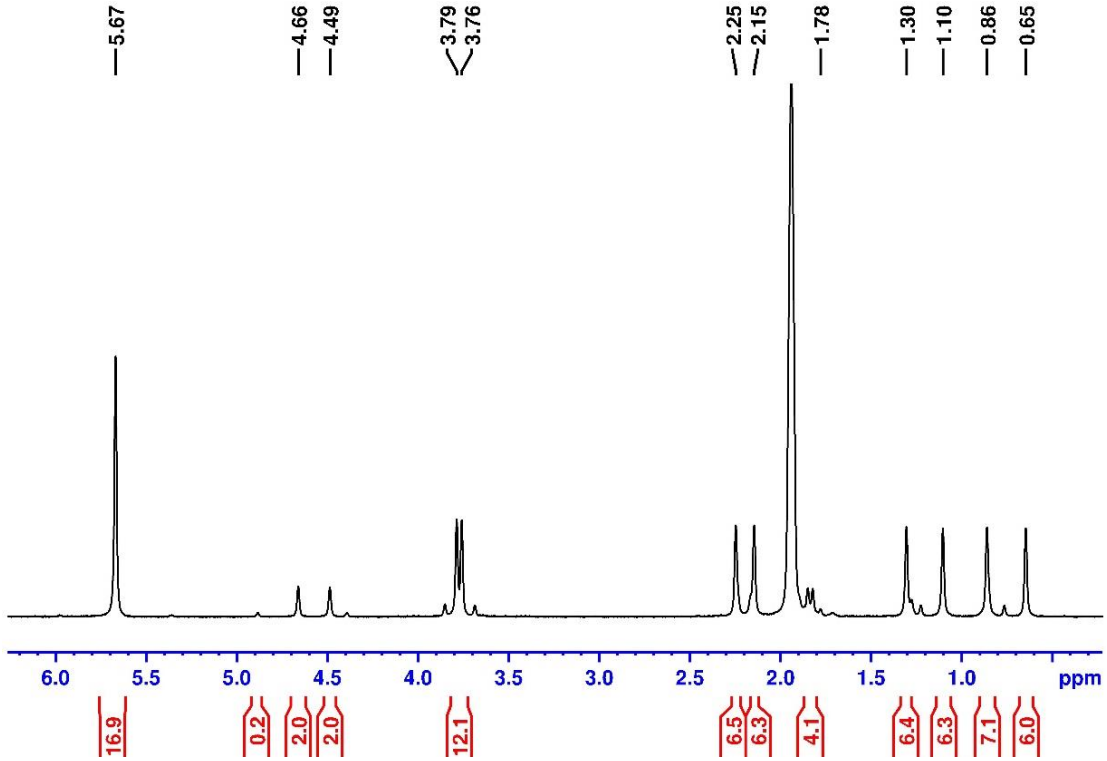


Fig. S38 ^{1}H NMR spectrum after work up of the 1:2 reaction of **5^{Et}** and $Co(Cp)_2$ in CD_3CN at RT.

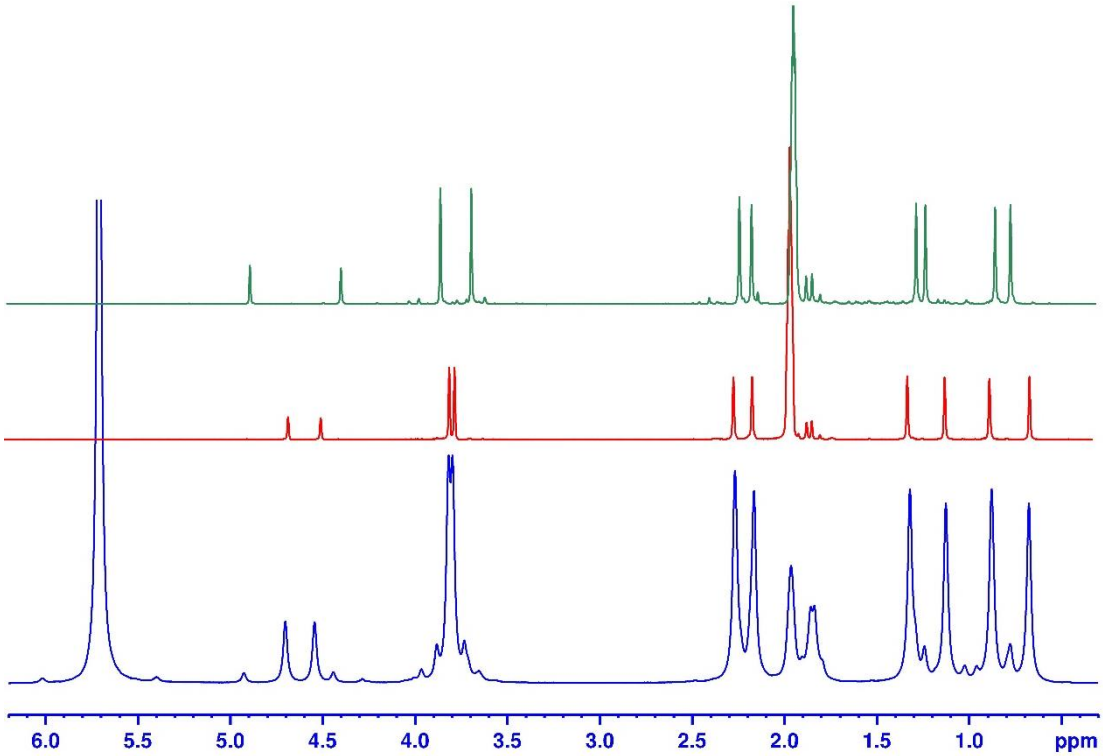
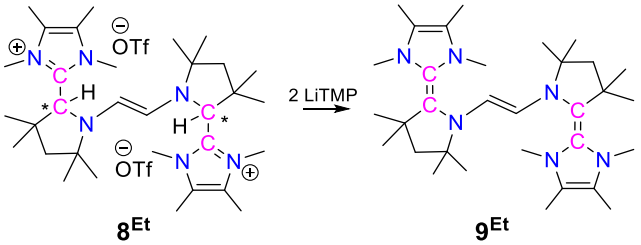


Fig. S39 Overlay of the ^{1}H NMR spectra of the product of the 1:4 reaction of **5^{Et}** and $Co(Cp)_2$ (blue), major diastereomer of **8^{Et}** (red), minor diastereomer of **8^{Et}** (green) in CD_3CN at RT.

Synthesis of 9^{Et}

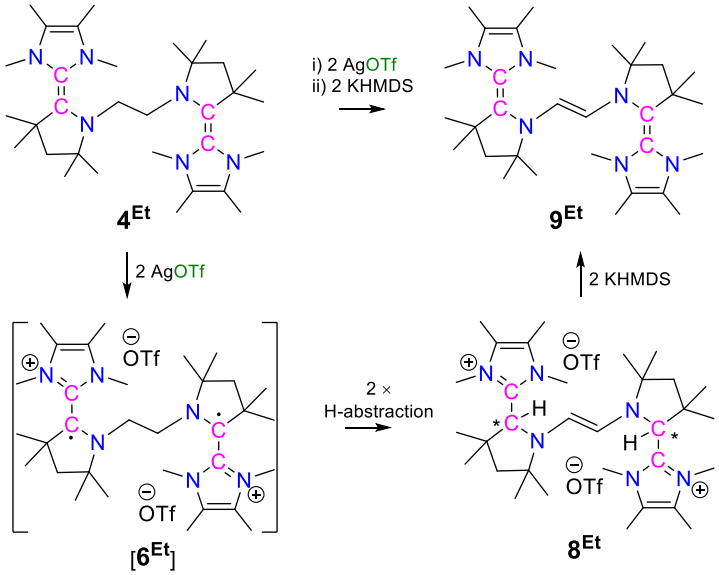
Method I



8^{Et} 9^{Et}

Toluene (25mL) was added to the mixture of the major diastereomer of 8^{Et} (213 mg, 0.258 mmol) and LiTMP (95 mg, 0.645 mmol) at room temperature and stirred for twelve hours. Then the reaction mixture was filtered while heated to boiling temperature. The resulting filtrate was concentrated to about 5 mL and kept at −35 °C for crystallization. After 12 hrs dark yellow crystals of 9^{Et} were obtained which were suitable for an X-ray diffraction study. The obtained single crystals were washed with a small amount of pentane and the mother liquor was concentrated and again kept at −35 °C for crystallization. **Yield:** 56 mg (41 %).

Method II



4^{Et} 9^{Et} $[6^{Et}]$ 8^{Et}

A THF solution of AgOTf (196 mg, 0.763 mmol, in 15 mL of THF) was added to a THF solution of 4^{Et} (200 mg, 0.381 mmol, in 30 mL of THF) dropwise at 0 °C. After 6 hours all volatiles were removed under vacuum and then CH_3CN (10 mL) was added and stirred for 5 minutes. The filtrate was evaporated to dryness to obtain a solid residue which was dried at 80 °C under vacuum for 4 hrs. Then KHMDS (170 mg, 0.852 mmol) and toluene (30 mL) were added to it at room temperature and stirred for 12 hours. The ^1H NMR spectrum of the crude reaction mixture showed the formation of compound 9^{Et} along with a small amount of 4^{Et}. The reaction mixture was filtered while heated to boiling temperature and the resulting

filtrate was concentrated to about 10 mL and kept at −30 °C for crystallization. After 12 hours, orange crystals were obtained and collected. Subsequently, the mother liquor was concentrated and kept again for crystallization at −30 °C. The ^{1}H NMR spectrum of the obtained crystals showed the presence of compound **4^{Et}** (6 %) along with compound **9^{Et}**. **Yield:** 90 mg (45 %). **M.P.:** 162 °C. **^{1}H NMR** (C_6D_6, 25 °C, 300 MHz): δ = 4.91 (s, 2H, C*H*=C*H*), 2.79 (s, 6H, CH_3-N), 2.57 (s, 6H, CH_3-N), 1.80 (s, 4H, CH_2), 1.69 (s, 6H, CH_3-C=C), 1.65 (s, 6H, CH_3-C=C), 1.50 (s, 12H, CH_3), 1.37 (s, 12H, CH_3) ppm. **^{13}C{^{1}H} NMR** (C_6D_6, 25 °C, 75 MHz): δ = 140.77 (NC=*C*NN), 122.13 (CH_3-*C*=*C*), 120.16 (CH_3-*C*=*C*), 108.06 (N*C*=CNN), 105.87 (*C*H=*C*H), 59.91 (CH_2), 59.74 ($C(CH_3)_2$), 43.26 (CH_3-N), 40.11 ($C(CH_3)_2$), 31.75 (CH_3-N), 28.85 ($C(CH_3)_2$), 27.83 ($C(CH_3)_2$), 10.31 (CH_3-C=C), 9.60 (CH_3-C=C) ppm. **UV/Vis** (THF): λ_{max} (ε) = 320 (13087), 236 (26347) nm (L mol^{-1} cm^{-1}). **Elemental analysis:** Calculated (%) for $C_{32}H_{54}N_6$: C, 73.51; H, 10.41; N, 16.07; Found: C, 71.81; H, 10.439; N, 15.32. Most likely due to high air and moisture sensitivity we were not able to get satisfactory elemental analysis data even after repeating measurements. **HRMS-ASAP (m/z):** Calculated for $C_{32}H_{55}N_6$ $[M+H]^+$: 523.4483, Found: 523.4455.

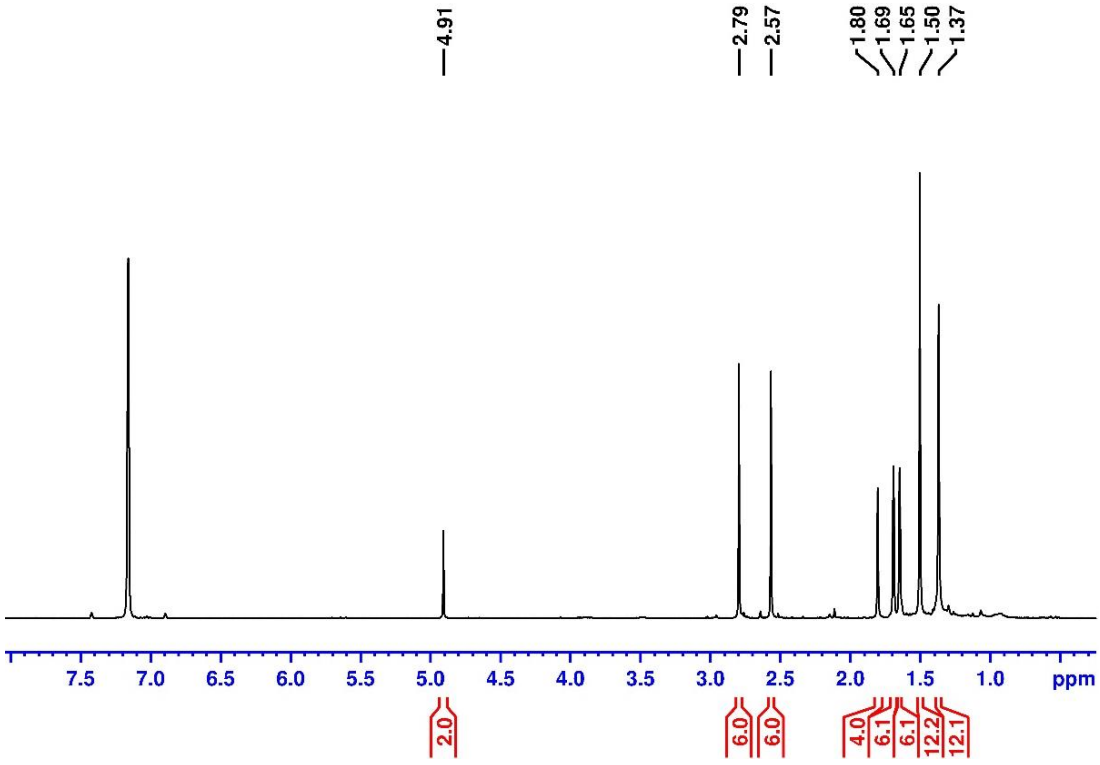


Fig. S40 ^{1}H NMR spectrum of **9^{Et}** in C_6D_6 at RT.

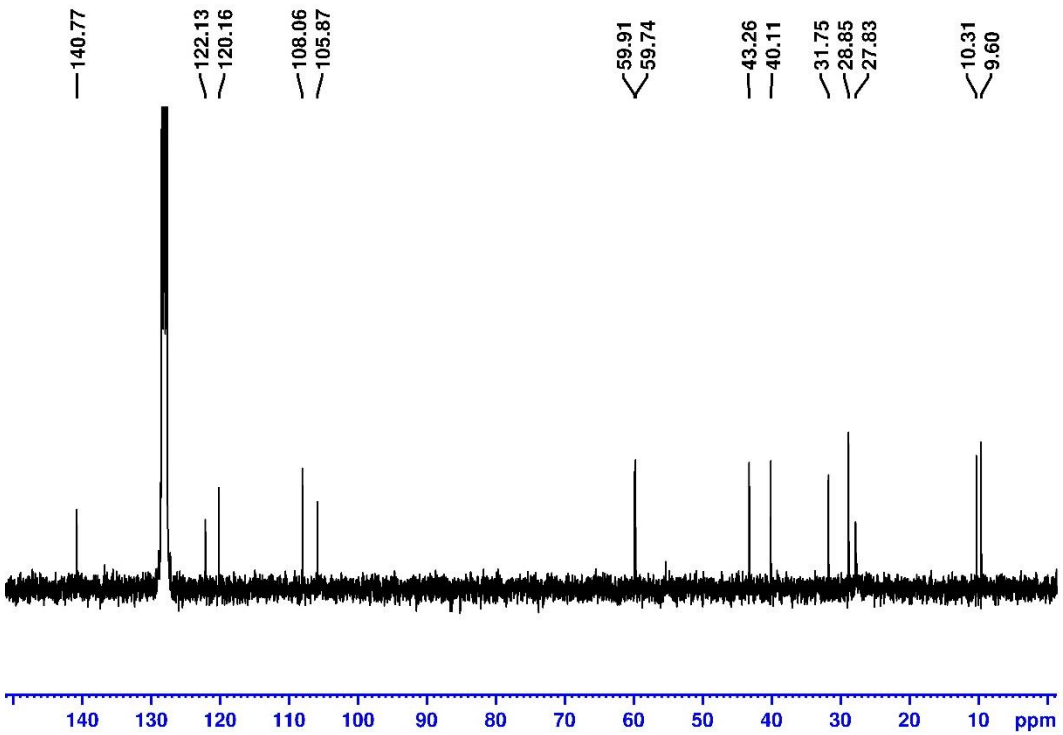


Fig. S41 $^{13}C\{^{1}H\}$ NMR spectrum of **9^{Et}** in C_6D_6 at RT.

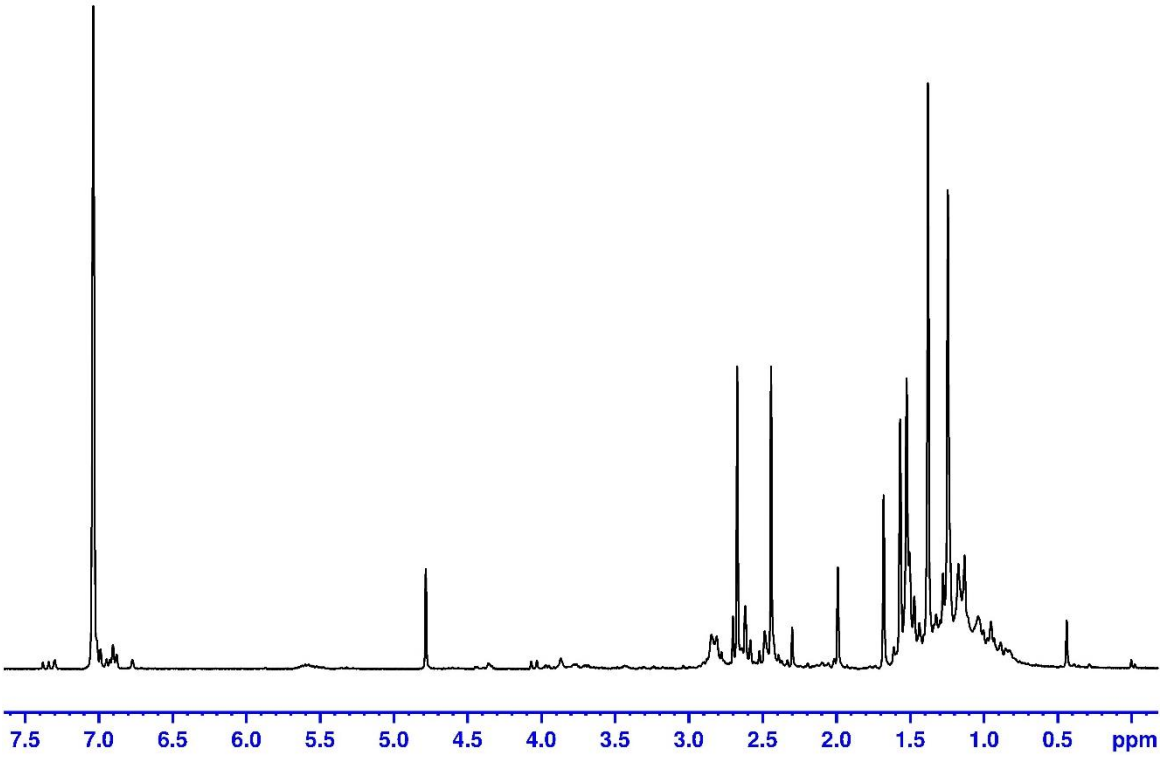
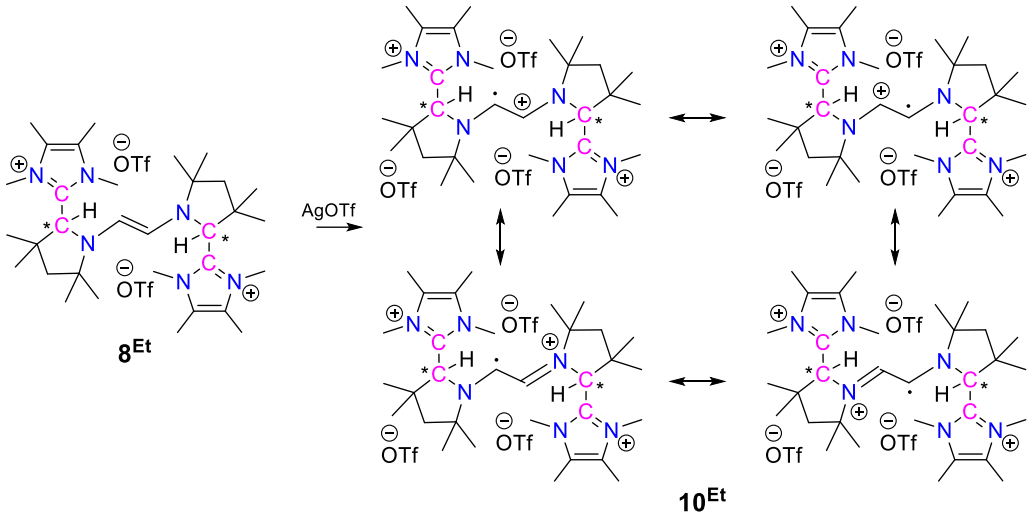


Fig. S42 ^{1}H NMR spectrum of the crude reaction mixture of **9^{Et}** in C_6D_6 at RT (indicating the formation of only *E*-isomer).

Oxidation of 8^{Et}



5 mL CH_3CN was added to the mixture of **8^{Et}** (56 mg, 0.068 mmol) and AgOTf (18 mg, 0.07 mmol) at room temperature. After 10 minutes of stirring the reaction mixture, all volatiles were removed under vacuum. Then about 10 mL of CH_3CN was added to the residue and filtered. The orange colored filtrate was concentrated to about 2 mL and then 3 mL of THF was added into it. The resulting solution was kept for crystallization with diethyl ether diffusion at room temperature. Orange colored crystalline compound **10^{Et}** was obtained after 24 hours. The ^1H NMR spectrum of crystals showed the presence of compound **8^{Et}** also. **Amount of crystalline solids:** 50 mg. Quantitative EPR measurement indicates a radical concentration of ca. 54% in the crystalline crude products considering TEMPO as standard. **HRMS-ESI (m/z):** Calculated for $C_{33}H_{56}N_6F_3SO_3$ $[M-2OTf]^+$: 673.4081; Found: 673.4065.

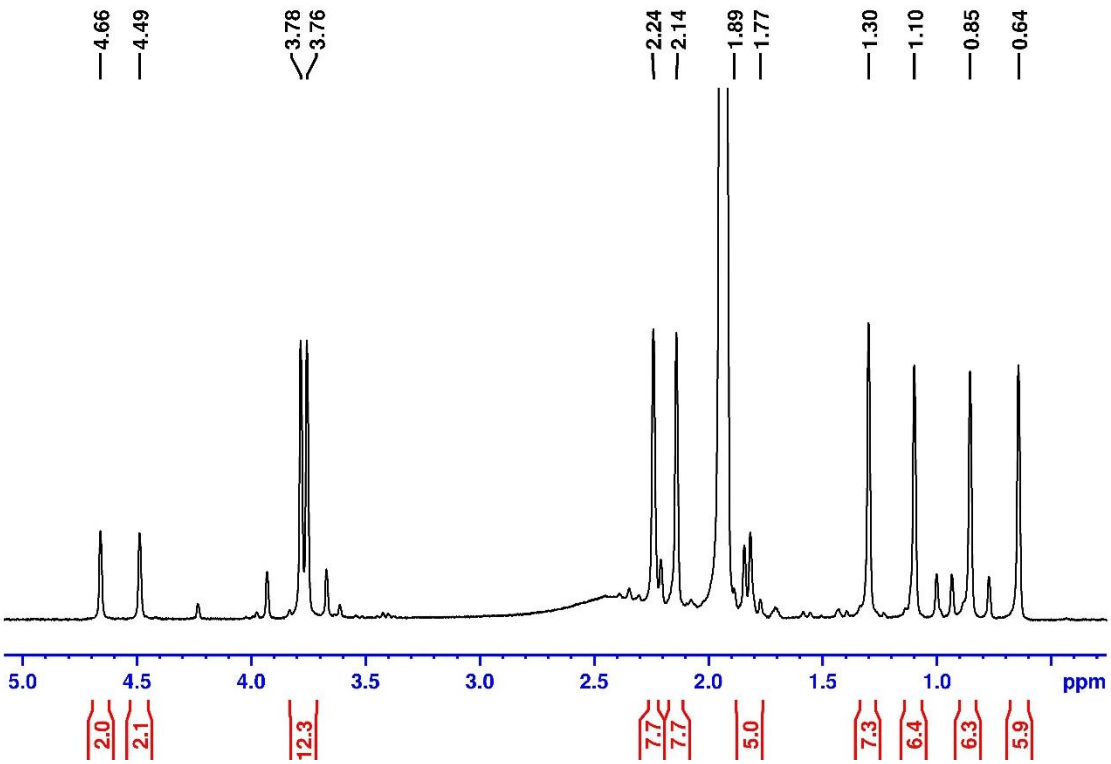


Fig. S43 ^{1}H NMR spectrum of red crystals containing a mixture of **8^{Et}** and **10^{Et}** from the 1:1 reaction of **8^{Et}** and AgOTf in CD_3CN at RT.

UV/Vis spectra

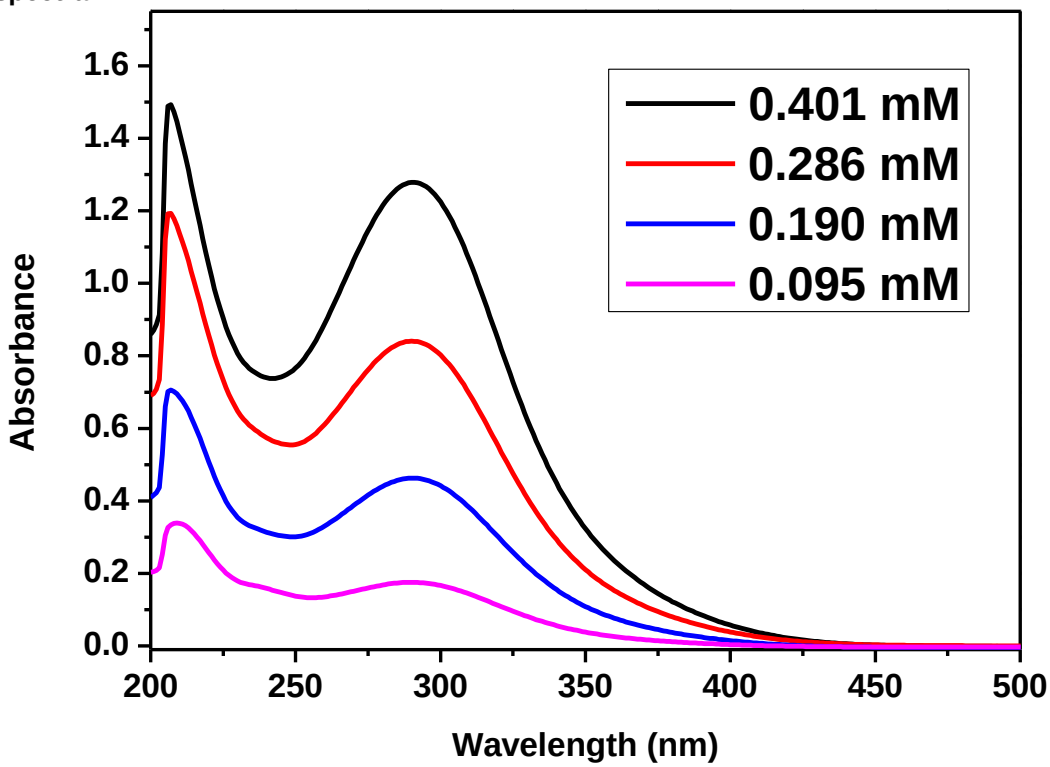


Fig. S44 UV/Vis spectra of $\mathbf{4^{Et}}$ in THF at different concentrations.

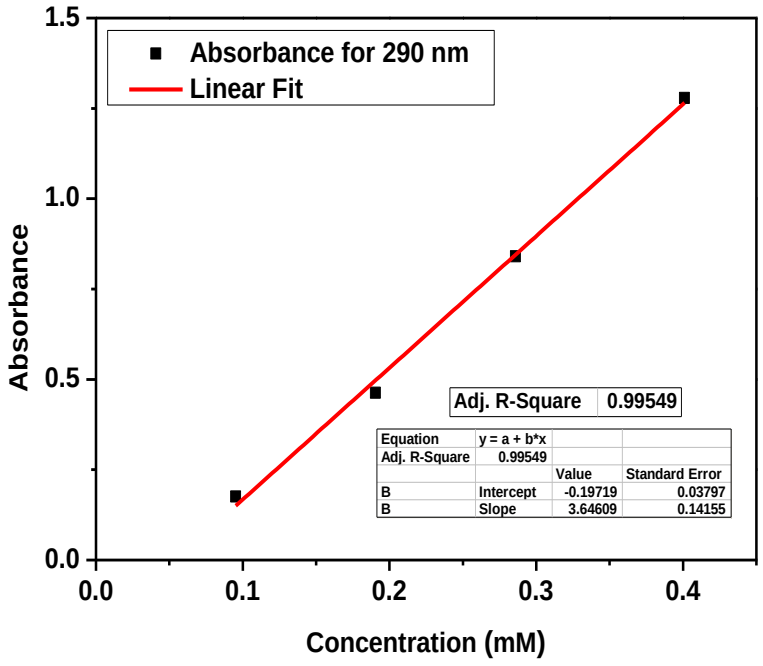


Fig. S45 Linear regression of the concentration dependent absorbance of $\mathbf{4^{Et}}$ at 290 nm.

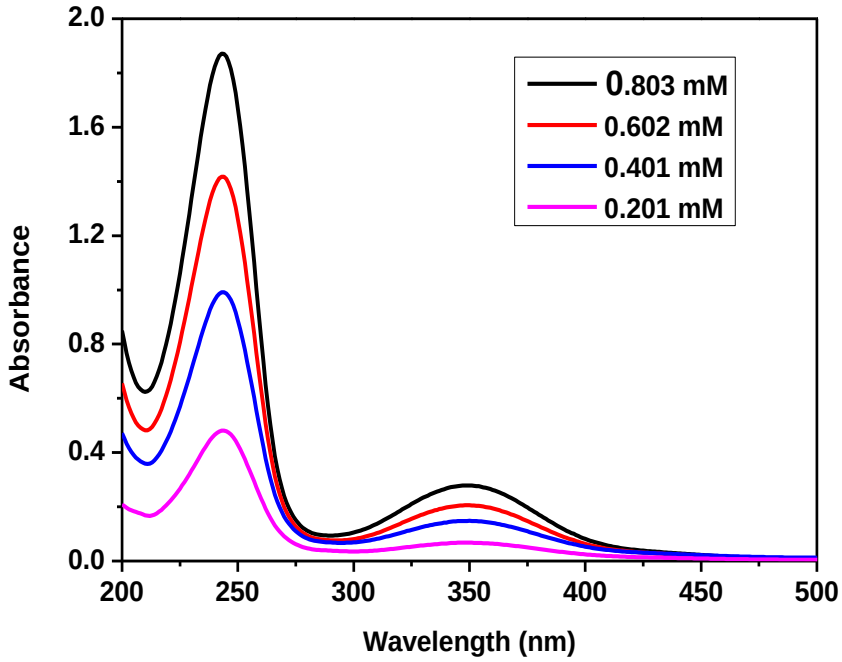


Fig. S46 UV/Vis spectra of **5**^{Et} in acetonitrile at different concentrations.

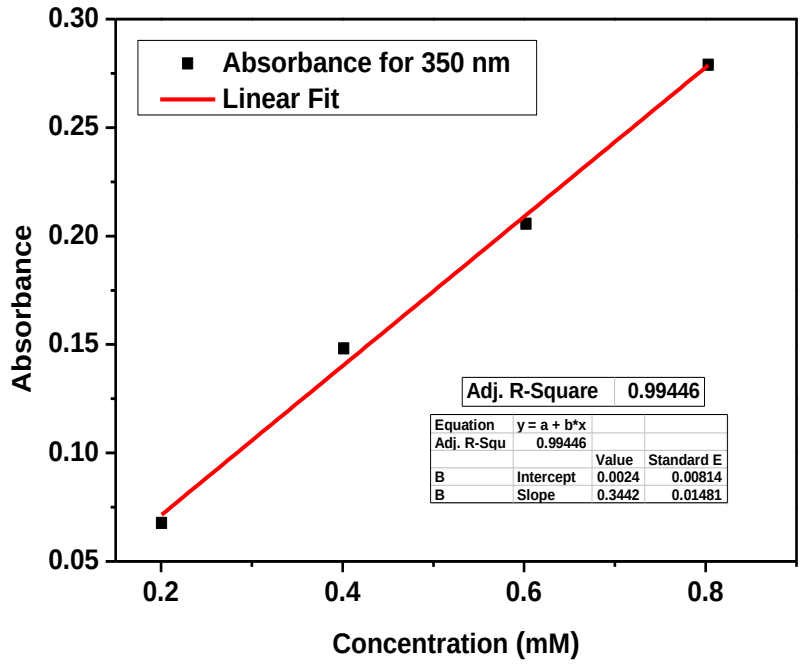


Fig. S47 Linear regression of the concentration dependent absorbance of **5**^{Et} at 350 nm.

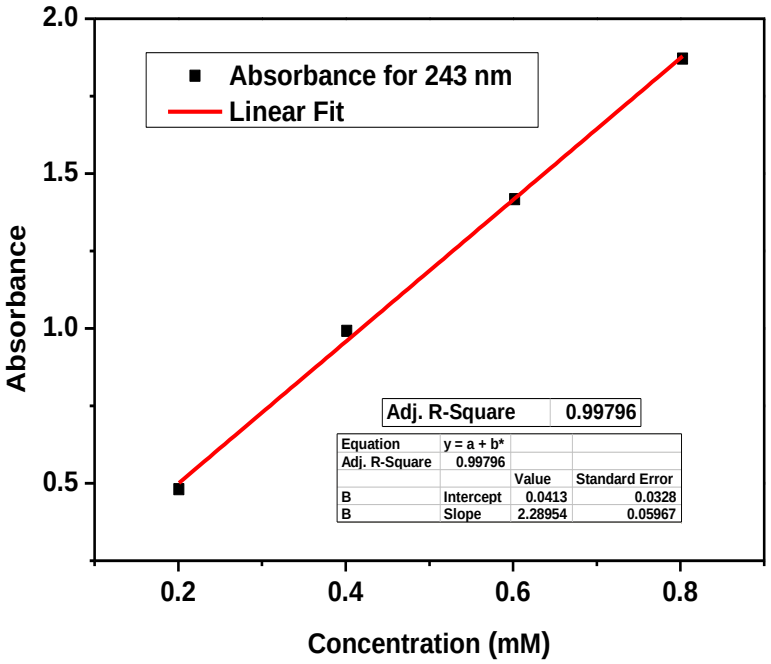


Fig. S48 Linear regression of the concentration dependent absorbance of **5**^{Et} at 243 nm

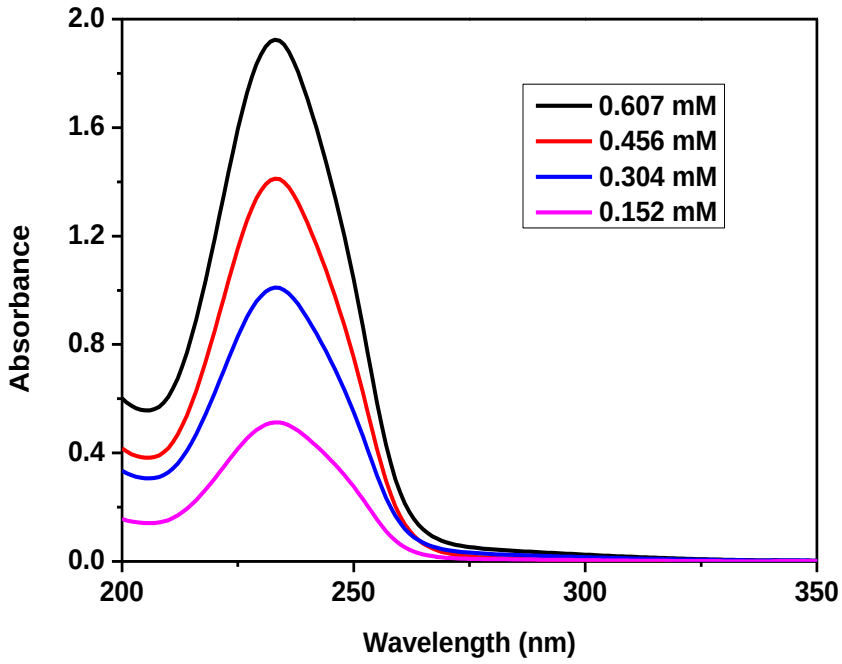


Fig. S49 UV/Vis spectra of the major diastereomer of **8**^{Et} in acetonitrile in different concentrations at RT.

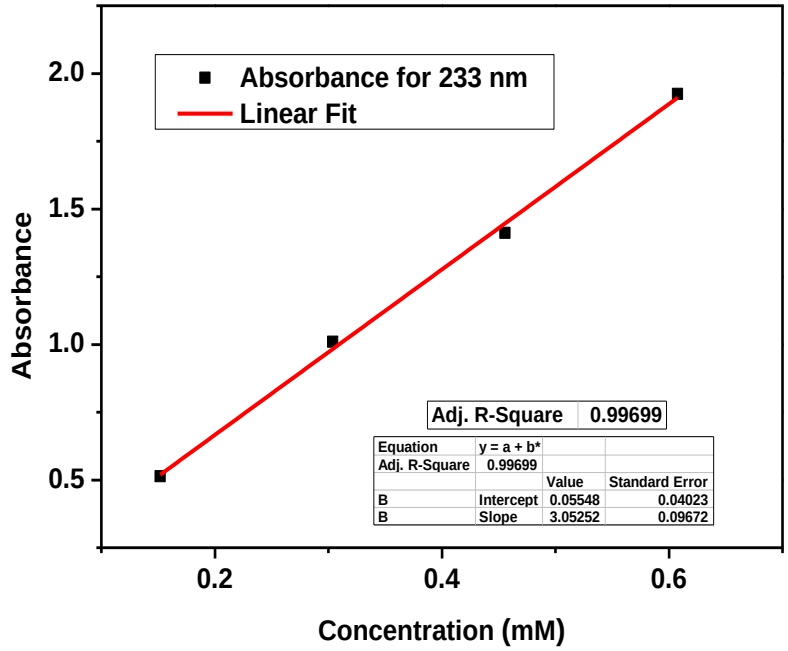


Fig. S50 Linear regression of the concentration dependent absorbance of $\mathbf{8}^{Et}$ at 233 nm.

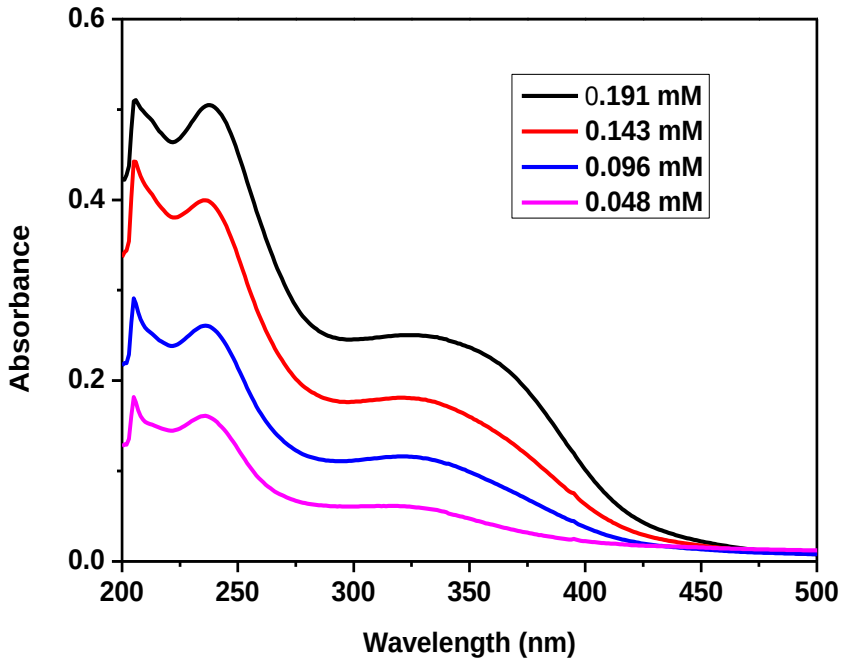


Fig. S51 UV/Vis spectra of $\mathbf{9}^{Et}$ in THF at different concentrations.

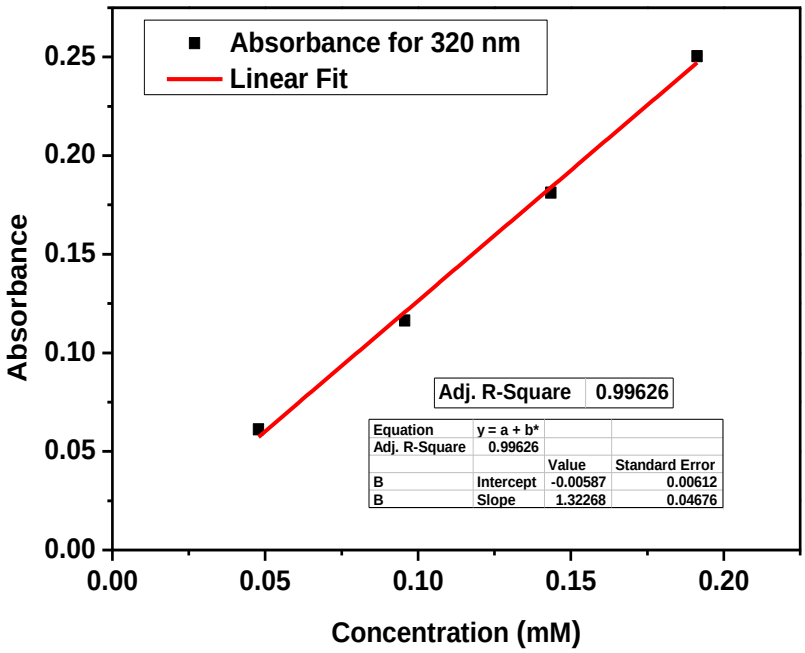


Fig. S52 Linear regression of the concentration dependent absorbance of **9**^{Et} at 320 nm.

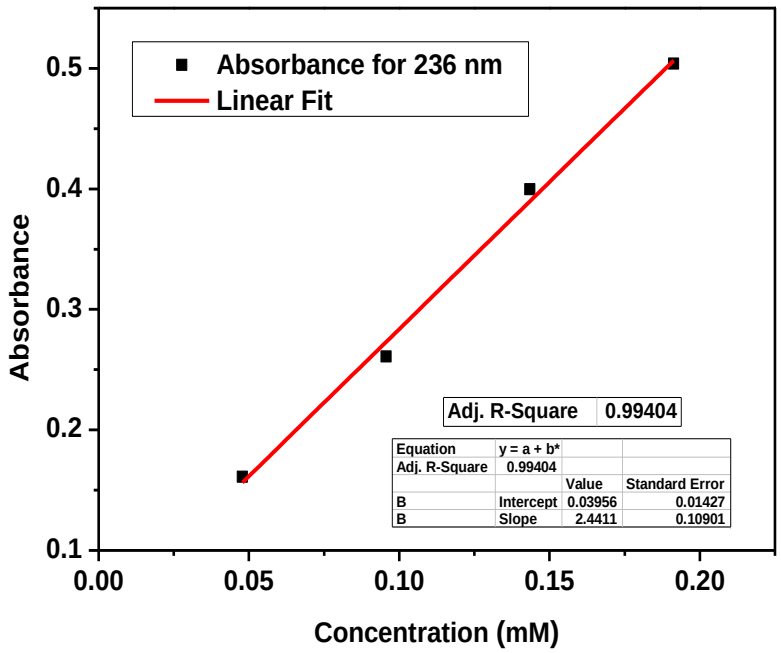
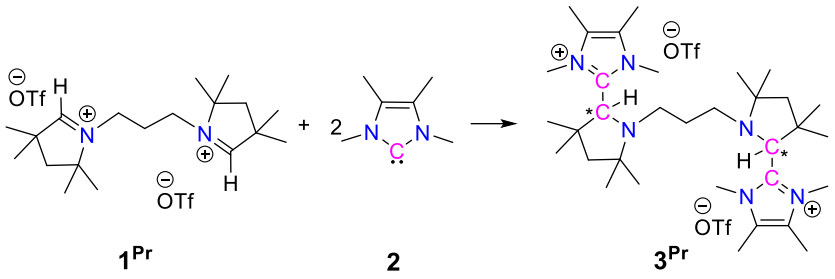


Fig. S53 Linear regression of the concentration dependent absorbance of **9**^{Et} at 236 nm.

Synthesis of 3^{Pr}



1^{Pr} 2 3^{Pr}

For the synthesis of $\mathbf{3^{Pr}}$ we have used $\mathbf{1^{Pr}}$ which contained LiOTf instead of crystalline $\mathbf{1^{Pr}}$. About 90 mL THF was added to the mixture of $\mathbf{1^{Pr}}$ (considering the presence of two molecules of LiOTf) (6g, 6.647 mmol) and **2** (2.1 g, 16.91 mmol) at 0 °C with stirring. After two hours the reaction mixture was warmed to room temperature and stirred for 24 hours. After that the reaction mixture was filtered and the ^{1}H NMR spectrum was recorded for both residue and filtrate. The product $\mathbf{3^{Pr}}$ was present in the residue as well as in the filtrate. The residue was isolated as colorless powder of pure $\mathbf{3^{Pr}}$ of 2.1 g (37 %). The yellow colored filtrate was concentrated up to 30 mL and then about 60 mL of diethylether was added to it and left for 24 hours. Then 3.9 g of a separated sticky material of $\mathbf{3^{Pr}}$ was isolated which contained LiOTf and trace amounts of **2**·HOTf. **M.P.:** > 180 °C (sample from residue). **Note:** In compound $\mathbf{3^{Pr}}$, there are two chiral centers and we see the formation of two diastereomers: the residue contains one diastereomer as major component, while the filtrate contains another diastereomer as major component. Here we are providing the NMR data of the major diastereomer from the residue. **^{1}H NMR** (CD_3CN, 25 °C, 300 MHz): δ = 4.25 (s, 2H, C*H*), 4.00 (s, 6H, CH_3-N), 3.65 (s, 6H, CH_3-N), 2.56-2.47 (m, 2H, CH_2-CH_2-CH_2), 2.21 (s, 6H, CH_3-C=C), 2.20 (s, 6H, CH_3-C=C), 2.15-2.05 (m, 2H, CH_2-CH_2-CH_2), 1.87-1.77 (m, 4H, CH_2), 1.26 (s, 6H, CH_3), 1.14 (s, 6H, CH_3), 1.10 (s, 6H, CH_3), 1.10-1.01 (m, 2H, CH_2-CH_2-CH_2), 0.80 (s, 6H, CH_3) ppm; **^{13}C{^{1}H} NMR** (CD_3CN, 25 °C, 75 MHz): δ = 144.08 (*C*=N-CH_3), 128.82 (CH_3-*C*=*C*), 127.96 (CH_3-*C*=*C*), 122.08 (q, $^1J_{C\text{-}F}$ = 321.03 Hz, *C*$F_3SO_3^-$), 71.37 (*C*H), 62.12 (*C*$(CH_3)_2$), 56.88 (*C*H_2), 47.60 (*C*H_2-CH_2-*C*H_2), 43.41 (*C*$(CH_3)_2$), 34.59 (*C*H_3-N), 33.43 (*C*H_3-N), 30.94 (C(*C*$H_3)_2$), 30.42 (C(*C*$H_3)_2$), 29.40 (CH_2-*C*H_2-CH_2), 27.31 (C(*C*$H_3)_2$), 22.47 (C(*C*$H_3)_2$), 9.00 (*C*H_3-C=C), 8.68 (*C*H_3-C=C) ppm; **^{19}F{^{1}H} NMR** (CD_3CN, 25 °C, 282 MHz): δ = −79.24 ppm. **Elemental analysis:** Calculated (%) for $C_{35}H_{60}N_6F_6O_6S_2$: C, 50.10; H, 7.21; N, 10.02; S, 7.64; Found: C, 49.84; H, 7.23; N, 9.70; S, 7.70. **HRMS-ESI (m/z):** Calculated for $C_{34}H_{60}N_6F_3SO_3$ $[M\text{-}1OTf]^+$: 689.4395, Found: 689.4397.

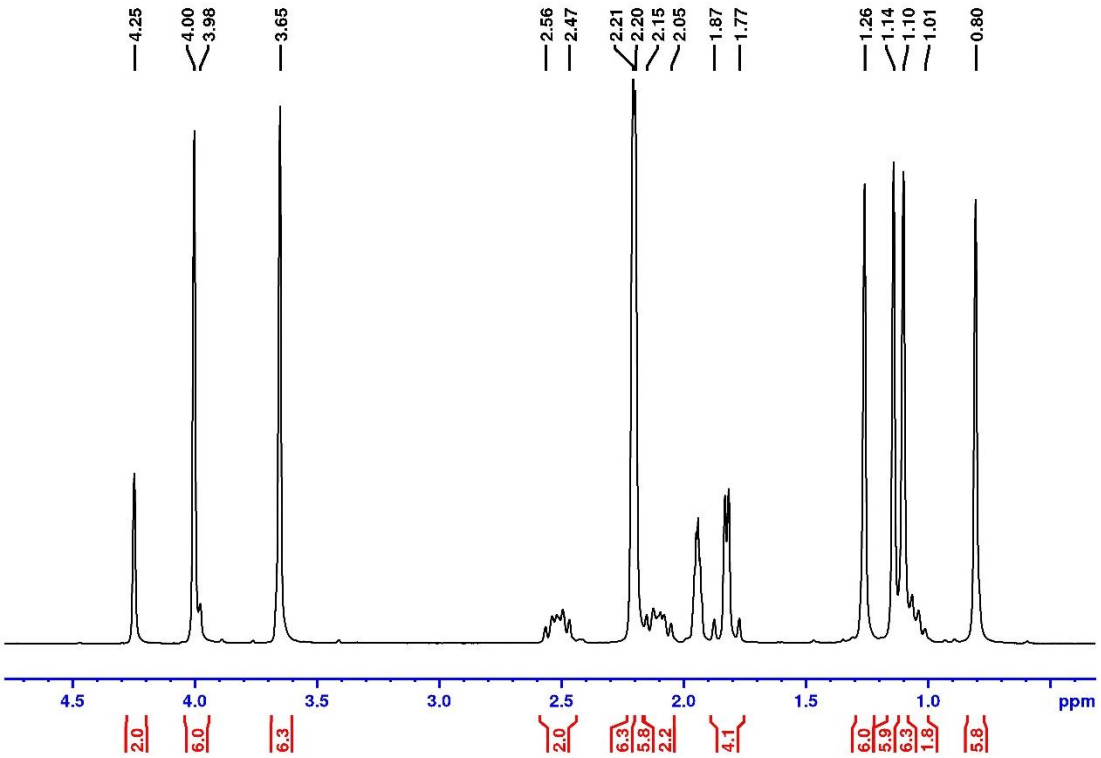


Fig. S54 ^{1}H NMR spectrum of the residue of the reaction mixture yielding **3^{Pr}** in CD_3CN at RT.

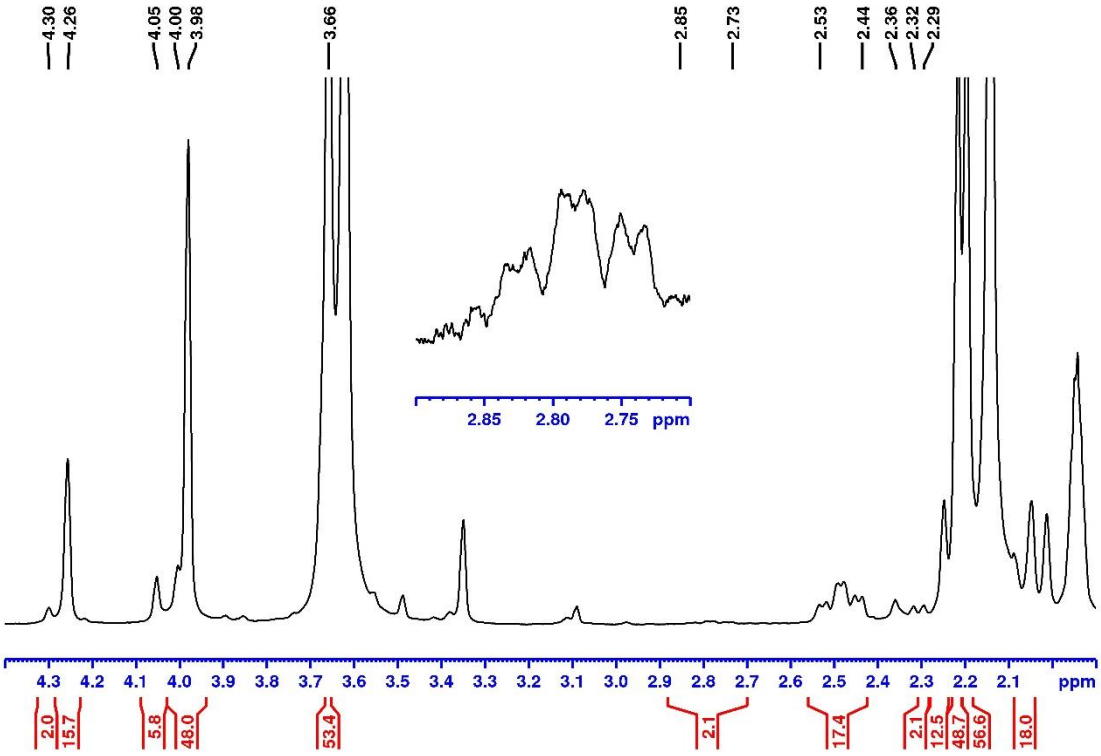


Fig. S55 ^{1}H NMR spectrum of the filtrate of the reaction mixture yielding **3^{Pr}** in CD_3CN at RT.

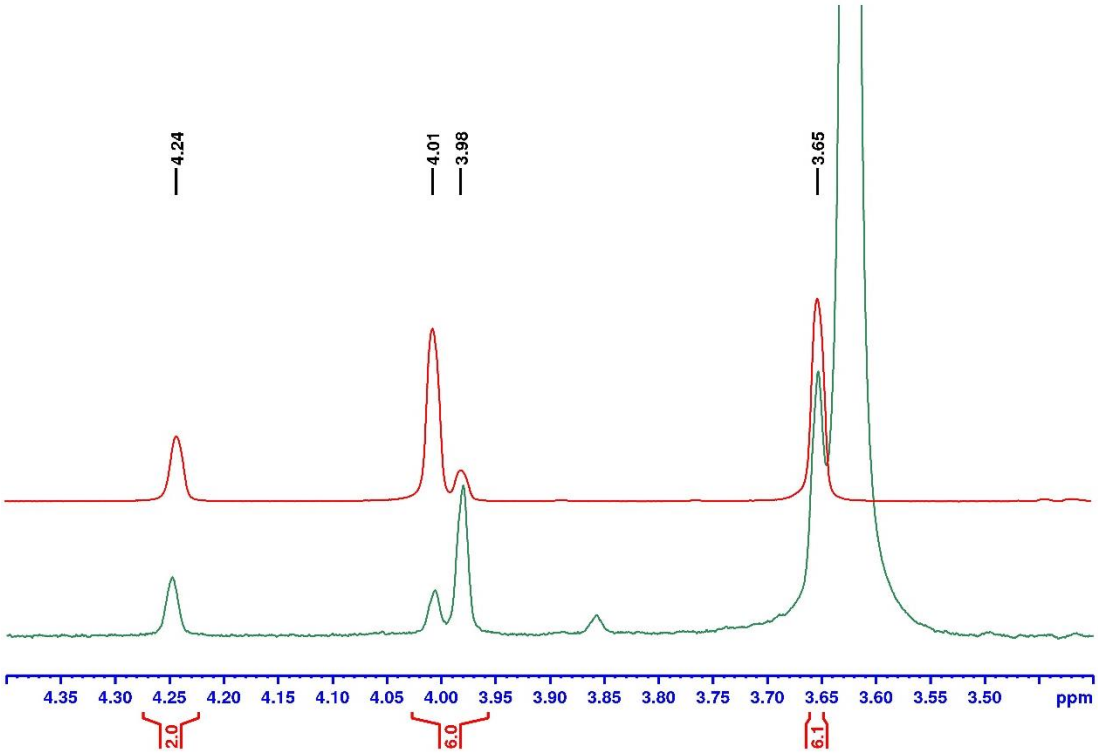


Fig. S56 Overlay of ^{1}H NMR spectra (selected region) of residue (red) and filtrate (green) of the reaction mixture yielding **3^{Pr}** in CD_3CN at RT.

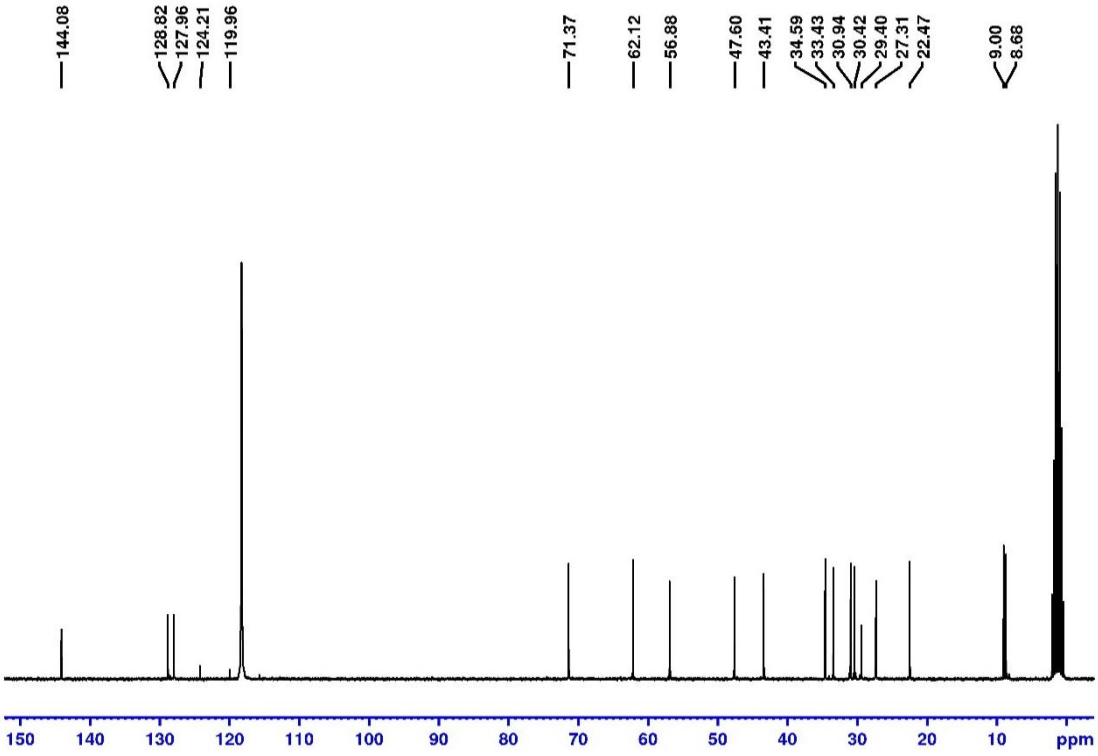


Fig. S57 $^{13}C\{^{1}H\}$ NMR spectrum of the residue of the reaction mixture yielding **3^{Pr}** in CD_3CN at RT.

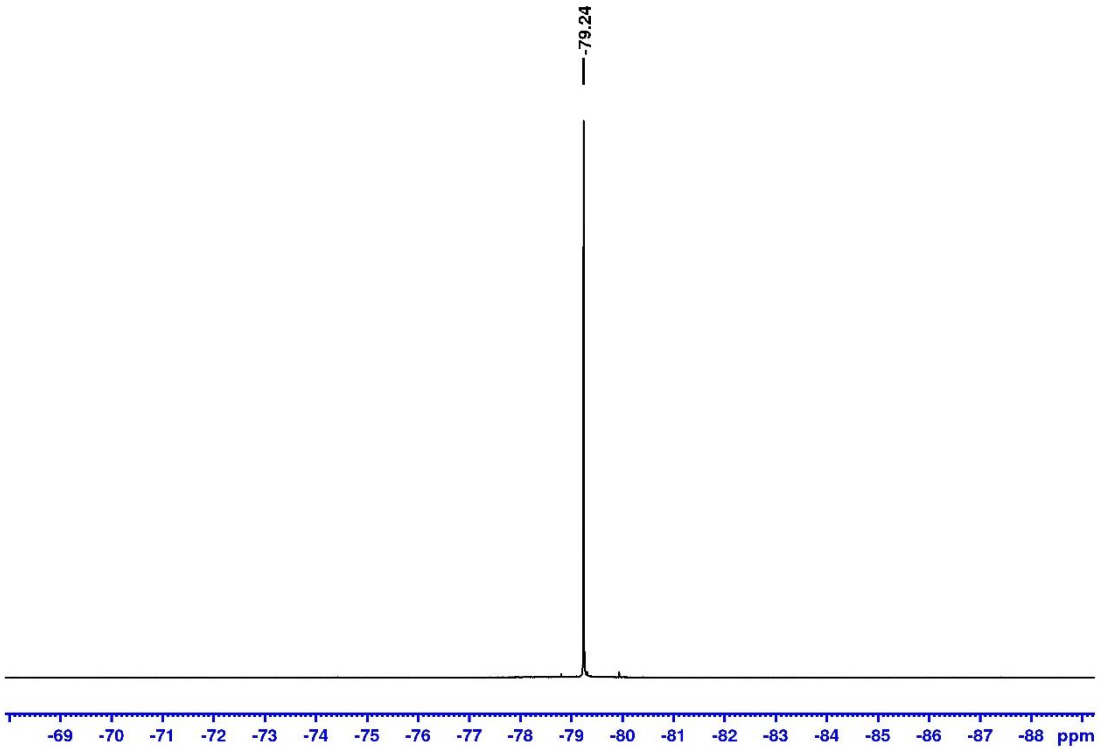
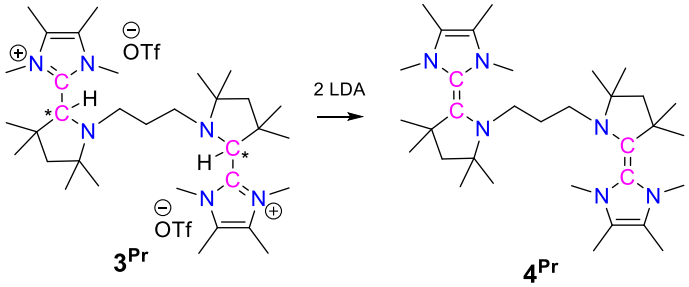


Fig. S58 $^{19}F\{^{1}H\}$ NMR spectrum of the residue of the reaction mixture yielding **3^{Pr}** in CD_3CN at RT.

Synthesis of 4^{Pr}



About 40 mL of toluene was added into a 50 mL of Schlenk flask containing **3^{Pr}** (2.04 g, 2.43 mmol) and LDA (662 mg, 6.18 mmol) at room temperature with stirring. The reaction mixture turned into a yellow color. After 24 hours stirring at room temperature the reaction mixture was filtered under hot condition and the filtrate was evaporated to yield a reddish brown oily type of liquid. Then pentane (30 mL) was added to it, stirred well and filtered and the filtrate was evaporated to yield a brownish oily liquid which transformed into crystalline solids after some time. The crystalline solid (875 mg) was collected and the filtrate was evaporated. The ^{1}H NMR spectra of crystalline solids and filtrate were measured which showed the presence of **4^{Pr}** as pure compound. **Yield:** 1.15 g (88 %). **M.P.:** 105 °C. Compound **4^{Pr}** can be obtained in a satisfactory yield using **3^{Pr}** which contains LiOTf and traces of **2**·HOTf in a similar procedure. **^{1}H NMR** (C_6D_6, 25 °C, 300 MHz): δ = 2.84 (t, 4H, 7.62 Hz, C*H*$_2$-CH$_2$-C*H*$_2$), 2.73 (s, 6H, C*H*$_3$-N), 2.66 (s, 6H, C*H*$_3$-N), 1.84-1.75 (CH$_2$-C*H*$_2$-CH$_2$), 1.72 (s, 4H, C*H*$_2$), 1.63 (s, 12H, C*H*$_3$-C=C), 1.46 (s, 12H, C*H*$_3$), 1.25 (s, 12H, C*H*$_3$) ppm. **^{13}C{^{1}H} NMR** (C_6D_6, 25 °C, 75 MHz): δ = 140.03 (NC=*C*NN), 122.50 (CH$_3$-*C*=*C*), 121.92 (CH$_3$-*C*=*C*), 112.56 (N*C*=CNN), 59.95 (*C*H$_2$), 59.56 (*C*(CH$_3$)$_2$), 42.13 (*C*H$_3$-N), 40.85 (*C*H$_2$-CH$_2$-*C*H$_2$), 39.77 (*C*(CH$_3$)$_2$), 33.42 (*C*H$_3$-N), 29.05 (C(*C*H$_3$)$_2$), 28.29 (C(*C*H$_3$)$_2$), 10.21 (*C*H$_3$-C=C), 9.98 (*C*H$_3$-C=C) ppm. **Elemental analysis:** Calculated (%) for $C_{33}H_{58}N_6$: C, 73.55; H, 10.85; N, 15.60; Found: C, 70.22; H, 10.88; N, 15.35.

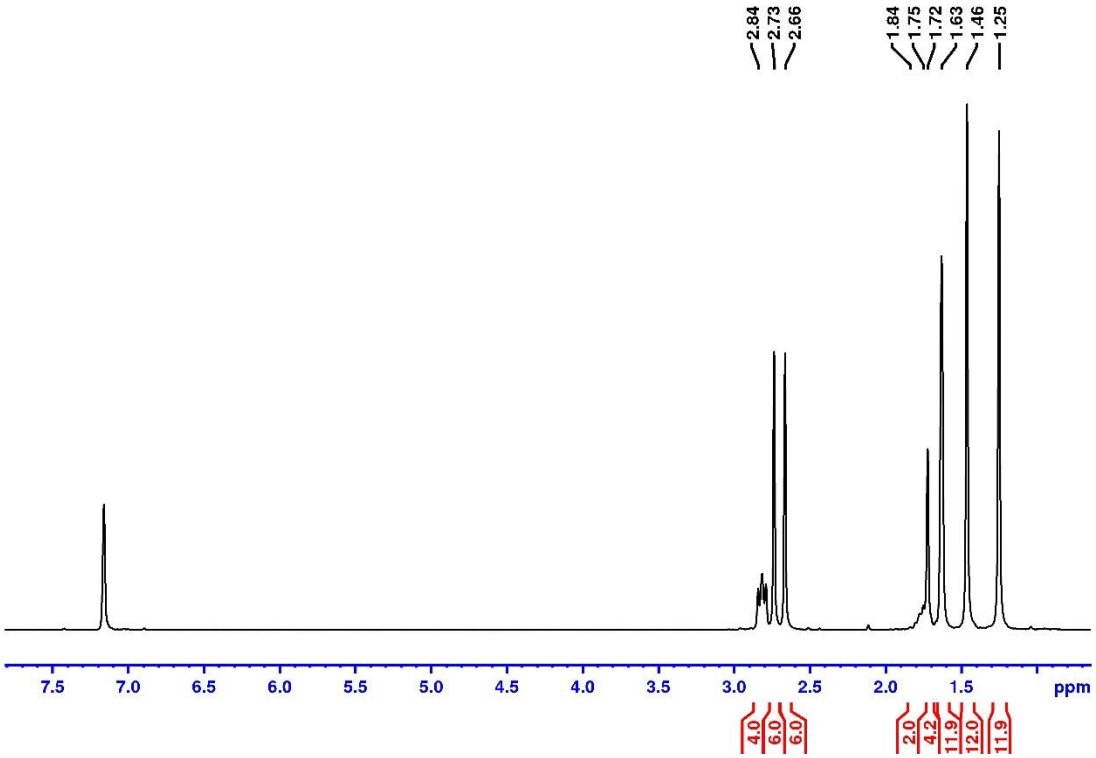


Fig. S59 ^{1}H NMR spectrum of crystals of **4^{Pr}** in C_6D_6 at RT.

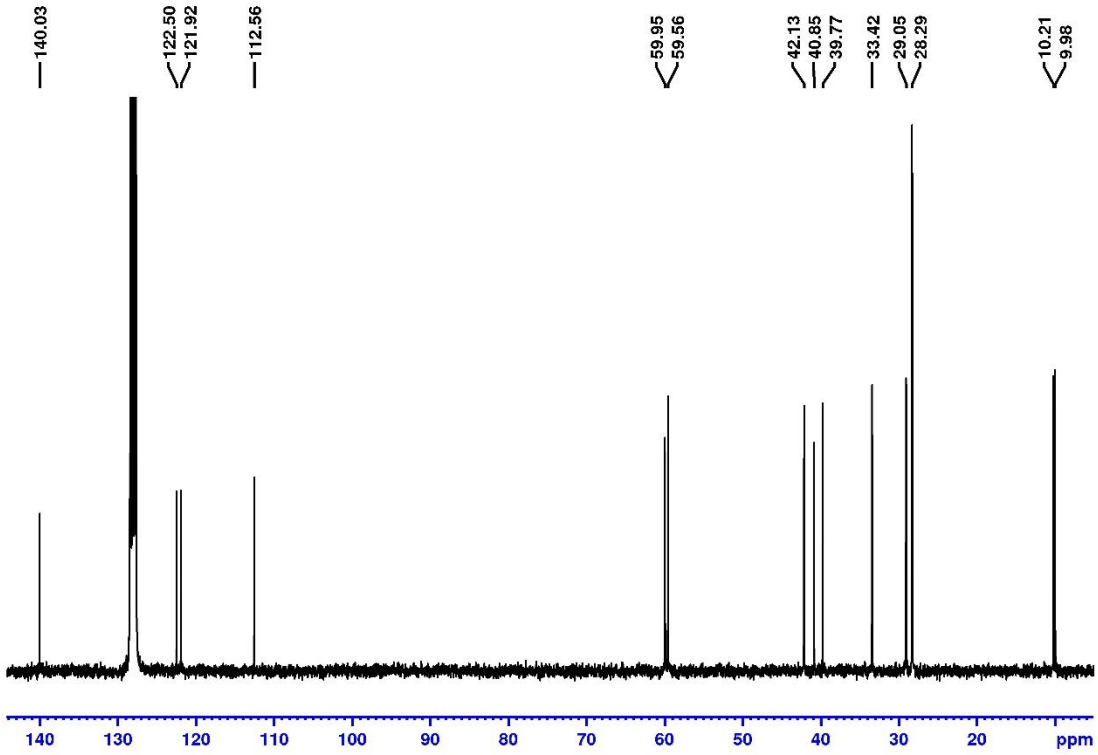
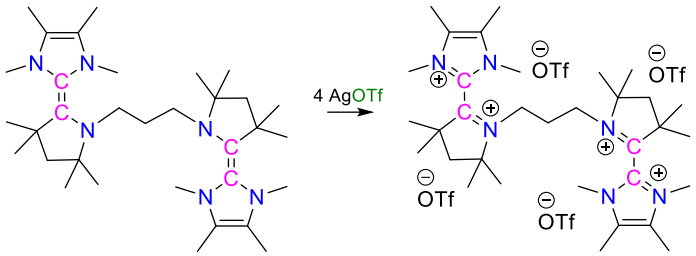


Fig. S60 $^{13}C\{^{1}H\}$ NMR spectrum of crystals of **4^{Pr}** in C_6D_6 at RT.

Synthesis of 5^{Pr}



4^{Pr} 5^{Pr}

10 mL THF solution of **4^{Pr}** (217 mg, 0.403 mmol) was added dropwise to 10 mL THF solution of AgOTf (524 mg, 2.039 mmol) at room temperature while stirring. Immediately, black colored metallic silver precipitated out. After 4 hours all volatiles were removed under vacuum and the residue was dissolved in about 7 mL acetonitrile and decanted from dropper (first part). Again about 50 mL acetonitrile was added to the residue, stirred well and allowed to stand for settling down the black particles and then filtered (second part). The filtrate (second part) was evaporated to obtain a precipitate of **5^{Pr}**. The acetonitrile solution (first part) was evaporated to obtain a precipitate of **5^{Pr}** and this precipitate was washed with 10 mL of THF to remove excess silver triflate. Finally, **5^{Pr}** was washed with ether and dried under vacuum. The ^{1}H NMR spectrum of the precipitate was measured, which showed the formation of pure **5^{Pr}**. **Yield:** 406 mg (89 %). A concentrated solution of **5^{Pr}** in acetonitrile was kept for crystallization with diethyl ether diffusion at room temperature. Colorless crystals of **5^{Pr}** were obtained after 6 hours which were suitable for X-ray structural analysis. **5^{Pr}** is an air stable compound. **M.P.:** > 180 °C. **^{1}H NMR** (CD_3CN, 25 °C, 300 MHz): δ = 4.24-4.19 (t, 4H, 8.20 Hz, C*H*$_2$-CH$_2$-C*H*$_2$), 3.72 (s, 12H, C*H*$_3$-N), 2.47 (s, 4H, C*H*$_2$), 2.33 (s, 12H, C*H*$_3$-C=C), 2.33 (br. 2H, CH$_2$-C*H*$_2$-CH$_2$), 1.84 (s, 12H, C*H*$_3$), 1.49 (s, 12H, C*H*$_3$) ppm. **^{13}C{^{1}H} NMR** (CD_3CN, 25 °C, 75 MHz): δ = 182.44 (*C*=N$^+$), 134.87 (CH$_3$-*C*=*C*), 124.90 (*C*NN$^+$), 121.69 (q, $^{1}J_{C\text{-}F}$ = 320.43 Hz, *C*F$_3$SO$_3^-$), 85.07 (*C*(CH$_3$)$_2$), 55.90 (*C*(CH$_3$)$_2$), 48.33 (*C*H$_2$-CH$_2$-*C*H$_2$), 47.81 (*C*H$_2$), 36.09 (*C*H$_3$-N), 31.21 (CH$_2$-*C*H$_2$-CH$_2$), 27.93 (C(*C*H$_3$)$_2$), 26.80 (C(*C*H$_3$)$_2$), 9.37 (*C*H$_3$-C=C) ppm. **^{19}F{^{1}H} NMR** (CD_3CN, 25 °C, 282 MHz): δ = −79.21 ppm. **Elemental analysis:** Calculated (%) for $C_{37}H_{58}N_6F_{12}O_{12}S_4$: C, 39.15; H, 5.15; N, 7. 40; S, 11.30; Found: C, 39.37; H, 5.23; N, 7.70; S, 11.29. **HRMS-ESI (m/z):** Calculated for $C_{36}H_{58}N_6F_9O_9S_3$ [M-1OTf]$^{3+}$: 985.3279, Found: 985.3246.

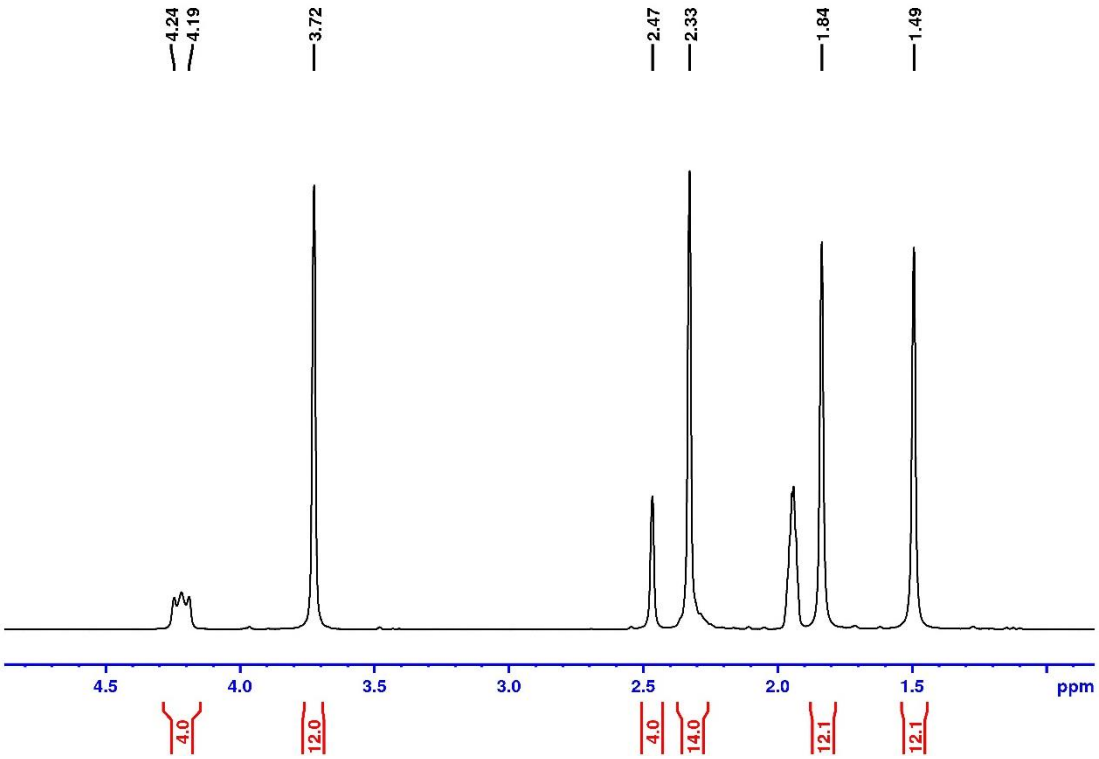


Fig. S61 ^{1}H NMR spectrum of compound **5^{Pr}** in CD_3CN at RT.

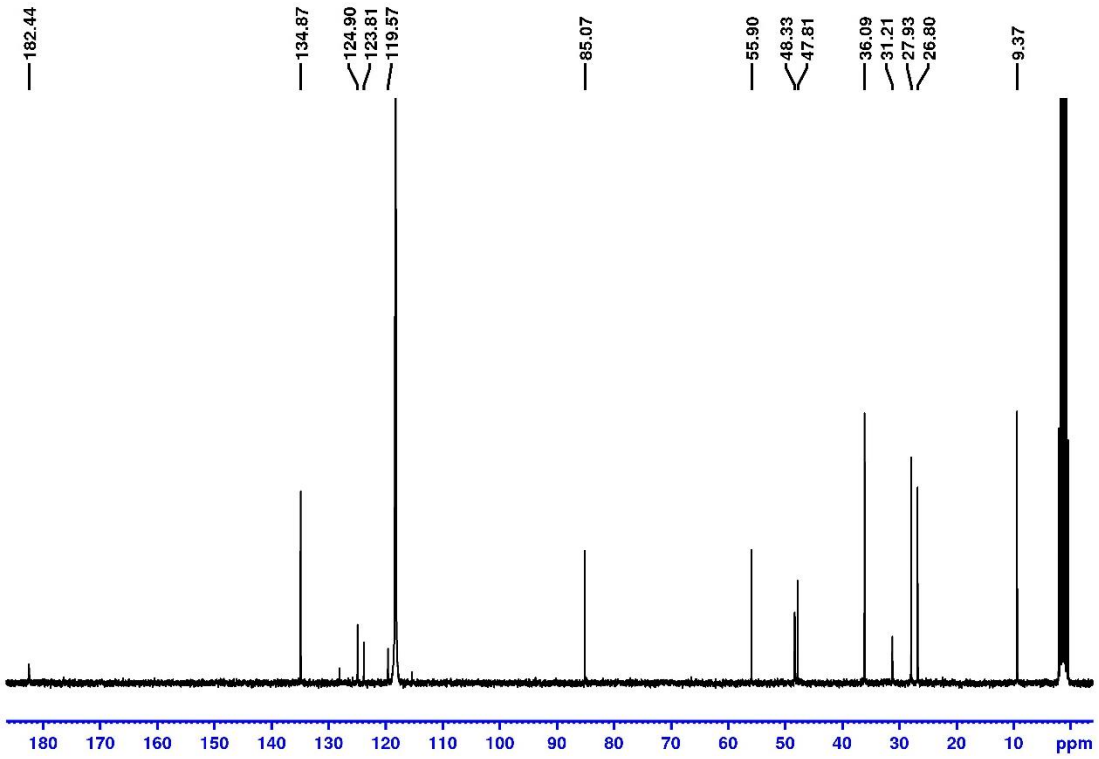


Fig. S62 $^{13}C\{^{1}H\}$ NMR spectrum of compound **5^{Pr}** in CD_3CN at RT.

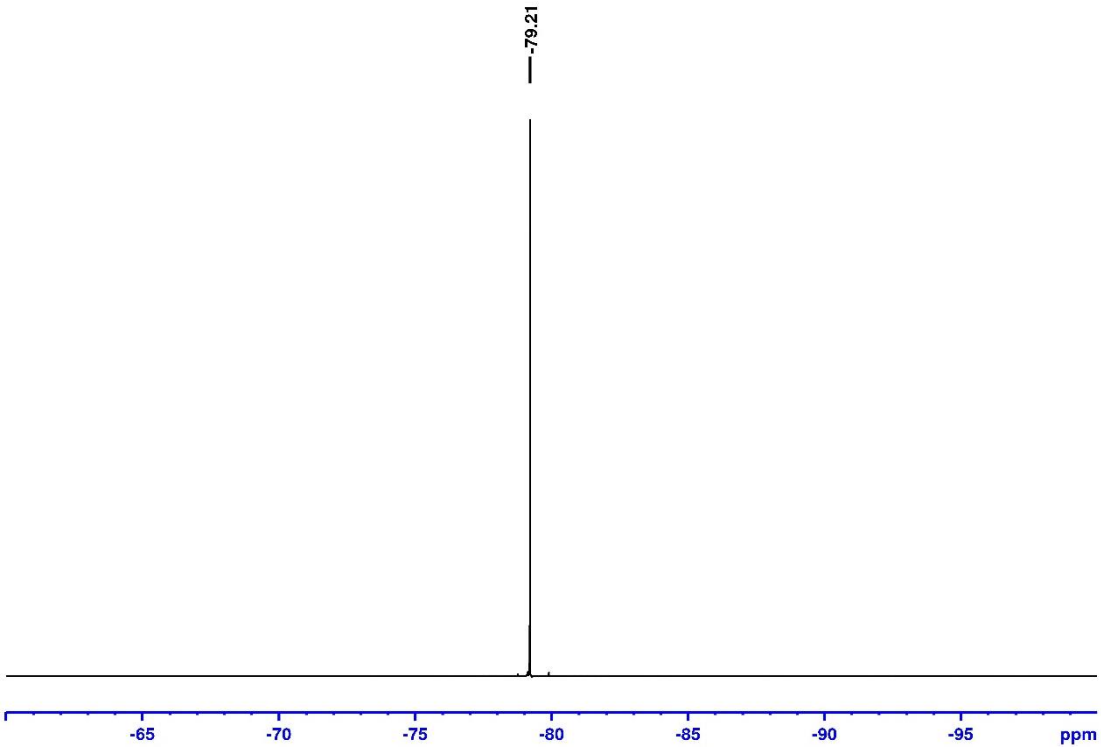
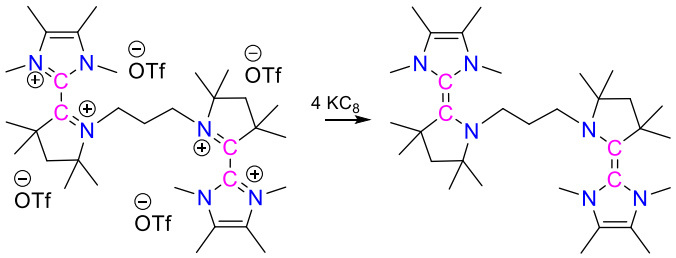


Fig. S63 $^{19}F\{^{1}H\}$ NMR spectrum of compound **5^{Pr}** in CD_3CN at RT.

Reduction of 5^{Pr}



5^{Pr} 4^{Pr}

THF was added to the mixture of $\mathbf{5^{Pr}}$ (75 mg, 0.066 mmol) and KC_8 (72 mg, 0.532 mmol) at −30 °C with stirring. After 6 hours stirring at room temperature, solvent and other volatiles were removed under vacuum and the ^1H NMR spectrum of the reaction mixture in C_6D_6 was measured which showed the formation of mostly $\mathbf{4^{Pr}}$ along with the residual THF solvent.

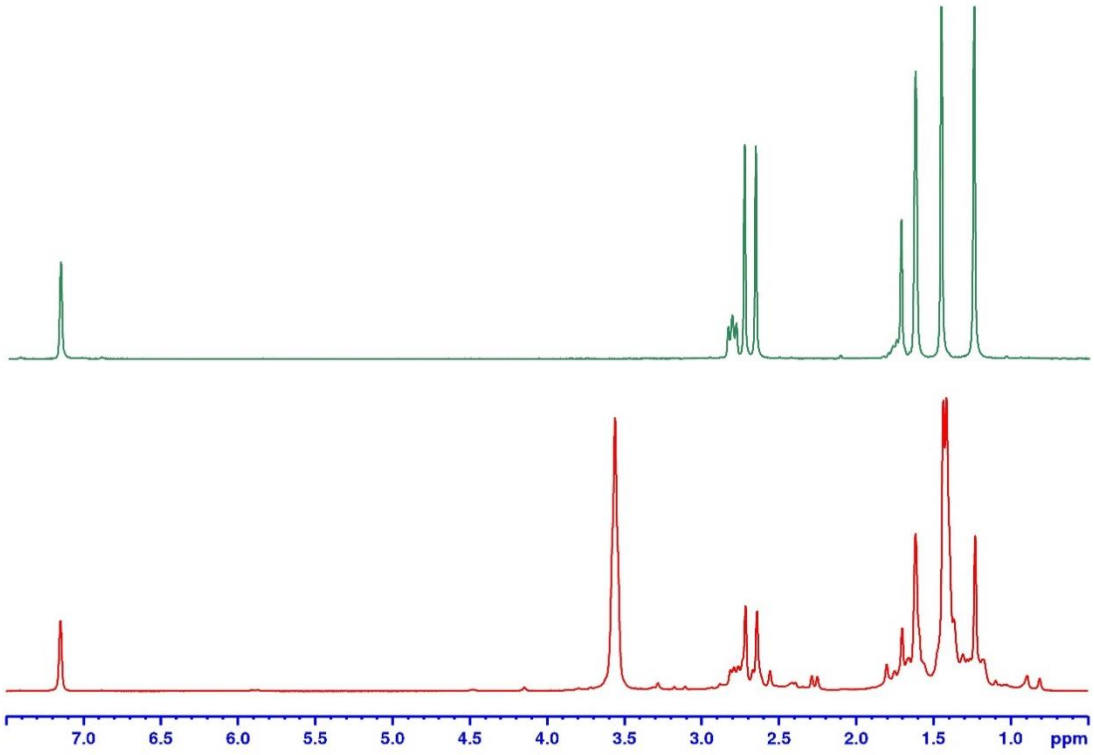
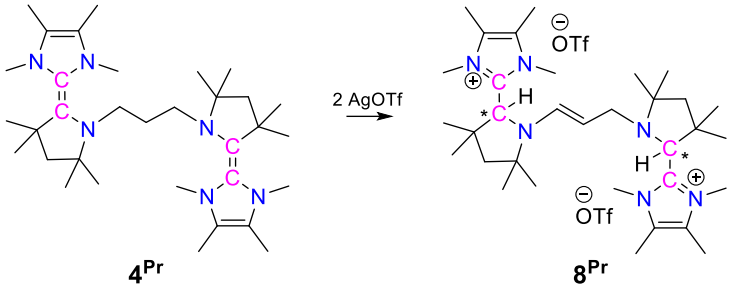


Fig. S64 Overlay of the ^1H NMR spectra of the reaction mixture of $\mathbf{5^{Pr}}$ and KC_8 (red) and $\mathbf{4^{Pr}}$ (green) in C_6D_6 at RT.

Synthesis of 8^{Pr}

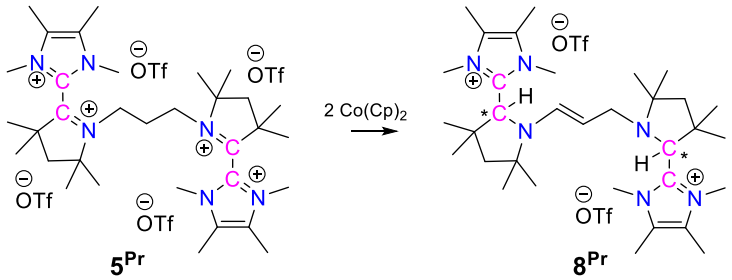
Method I



4^{Pr} 8^{Pr}

A THF (15 mL) solution of AgOTf (100 mg, 0.389 mmol) was added to the THF (30 mL) solution of $\mathbf{4}^{Pr}$ (95 mg, 0.176 mmol) dropwise with stirring at 0 °C. After 2 hours the ^{1}H NMR spectrum of reaction mixture was measured which showed the formation of $\mathbf{8}^{Pr}$ along with the starting dication $\mathbf{3}^{Pr}$. This NMR spectrum was overlapping with the NMR spectrum of the comproportionation reaction between $\mathbf{4}^{Pr}$ and $\mathbf{5}^{Pr}$. Solvent and other volatiles of the reaction mixture were removed under vacuum and acetonitrile (10 mL) was added to the residue, stirred and allowed to stand for six hours to settle down the black silver particles. Then the solution was decanted and then evaporated under vacuum to obtain $\mathbf{8}^{Pr}$. **Yield:** 106 mg (72%).

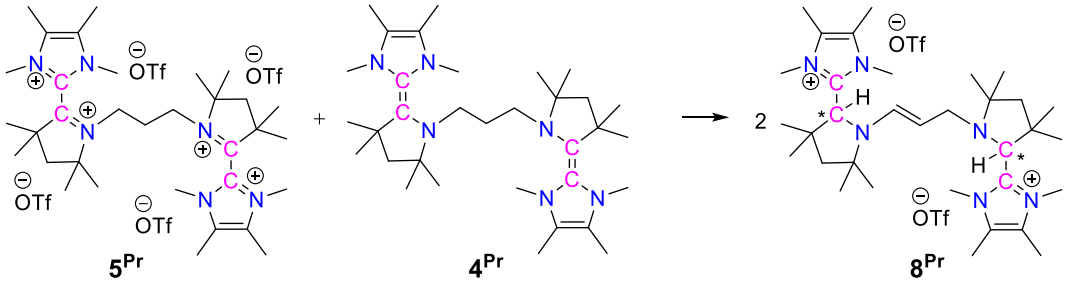
Method II



5^{Pr} 8^{Pr}

An acetonitrile solution of $Co(Cp)_2$ (15 mg, 0.079 mmol) was added dropwise to the acetonitrile solution (15 mL) of $\mathbf{5}^{Pr}$ (46 mg, 0.040 mmol) at room temperature with stirring. After 12 hours, solvent and other volatiles were removed under vacuum and the ^{1}H NMR spectrum of the reaction mixture was measured in CD_3CN which showed the formation of $\mathbf{8}^{Pr}$ along with cobaltocenium triflate. It was not possible to separate the cobaltocenium triflate and, hence, impossible to calculate the yield of the formation of $\mathbf{8}^{Pr}$.

Method III



Acetonitrile was added to the mixture of **4^{Pr}** (80 mg, 0.148 mmol) and **5^{Pr}** (160 mg, 0.141 mmol) at room temperature and stirred for 12 hours. After that the solvent and other volatiles were evaporated and a foam like solid residue was obtained. The ^{1}H NMR spectrum of this residue was measured which showed the formation of two diastereomers of compound **8^{Pr}**. **Yield:** 210 mg (87 %). Due to its complex nature we were not able to assign the NMR spectra unambiguously. **^{1}H NMR** (CD_3CN, 25 °C, 300 MHz): δ = 6.08-6.12 (d, 14.0 Hz, 1H, C*H*=CH-CH_2 of one diastereomer), 5.99-6.04 (d, 14.0 Hz, 1H, C*H*=CH-CH_2 of another diastereomer), 4.62, 4.52, 4.43, 4.33, 4.31, 4.26, 4.24, 4.19, 4.10, 3.99, 3.95, 3.85, 3.76, 3.71, 3.69, 3.66, 3.65, 3.63, 3.46, 3.08, 2.94, 2.91, 2.64, 2.63, 2.51, 2.24, 2.22, 1.86, 1.82, 1.81, 1.78, 1.76, 1.43, 1.39, 1.37, 1.34, 1.31, 1.26, 1.22, 1.15, 1.13, 1.11, 1.02, 1.00, 0.84, 0.82, 0.80, 0.77, 0.72 ppm. **^{13}C{^{1}H} NMR** (CD_3CN, 25 °C, 75 MHz): δ = 144.43, 143.05, 142.83, 133.26 (*C*H=CH-CH_2 of one diastereomer), 132.99 (*C*H=CH-CH_2 of another diastereomer), 128.96, 128.86, 128.56, 128.39, 128.27, 127.94, 127.76, 127.72, 124.21, 119.96, 102.58 (CH=*C*H-CH_2 of one diastereomer), 102.13 (CH=*C*H-CH_2 of another diastereomer), 70.38, 68.61, 66.48, 65.95, 65.00, 63.42, 63.09, 62.07, 61.41, 56.96, 56.87, 56.82, 56.54, 55.29, 55.24, 49.53, 47.61, 43.78, 43.65, 43.39, 43.33, 43.27, 43.18, 35.00, 34.74, 34.55, 34.51, 33.97, 33.93, 33.80, 33.69, 33.42, 31.76, 31.42, 31.12, 31.03, 30.55, 30.25, 29.62, 27.94, 27.87, 27.50, 27.44, 27.28, 27.22, 27.13, 23.81, 22.85, 22.41, 9.10, 9.05, 8.99, 8.97, 8.84, 8.78, 8.75, 8.72, 8.67 ppm. **^{19}F{^{1}H} NMR** (CD_3CN, 25 °C, 282 MHz): δ = −79.23 ppm. **Elemental analysis:** Calculated (%) for $C_{35}H_{58}N_6F_6O_6S_2$: C, 50.23; H, 6.98; N, 10.04; S, 7.66; Found: C, 50.08; H, 6.81; N, 10.34; S, 7.17. **HRMS-ESI (m/z):** Calculated for $C_{33}H_{58}N_6$ [M-2OTf]: 269.2356, Found: 269.2359.

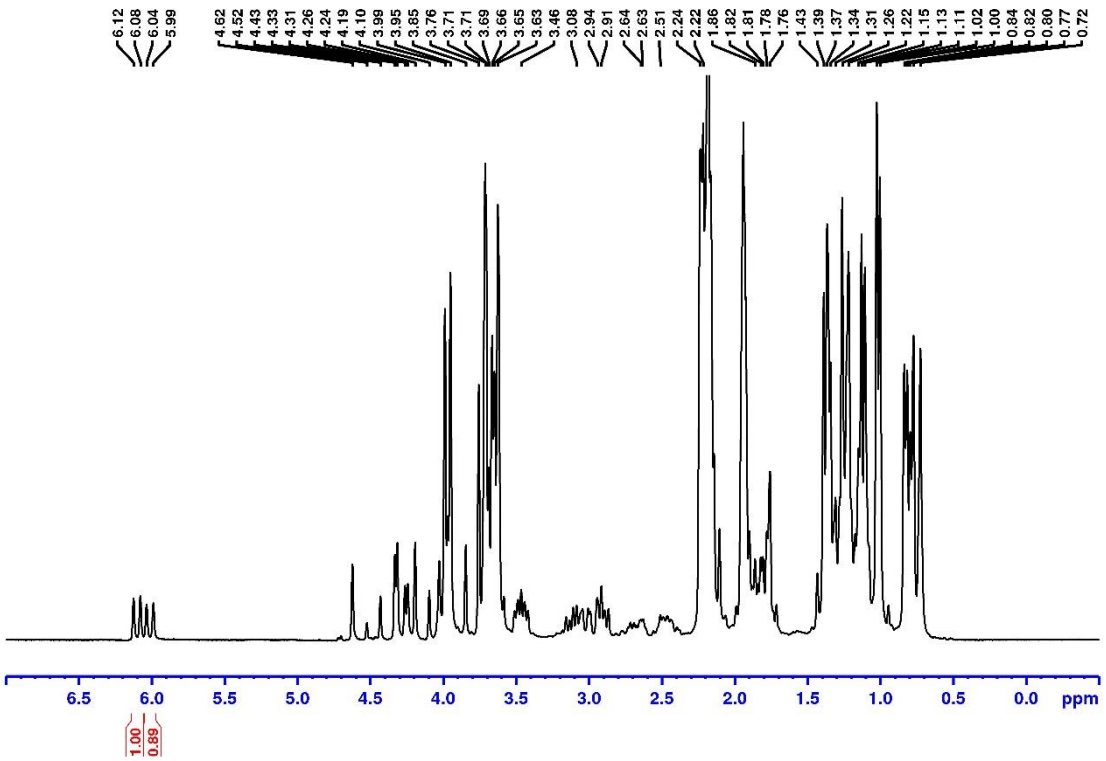


Fig. S65 ^{1}H NMR spectrum of **8^{Pr}** in its crude reaction mixture in CD_3CN at RT.

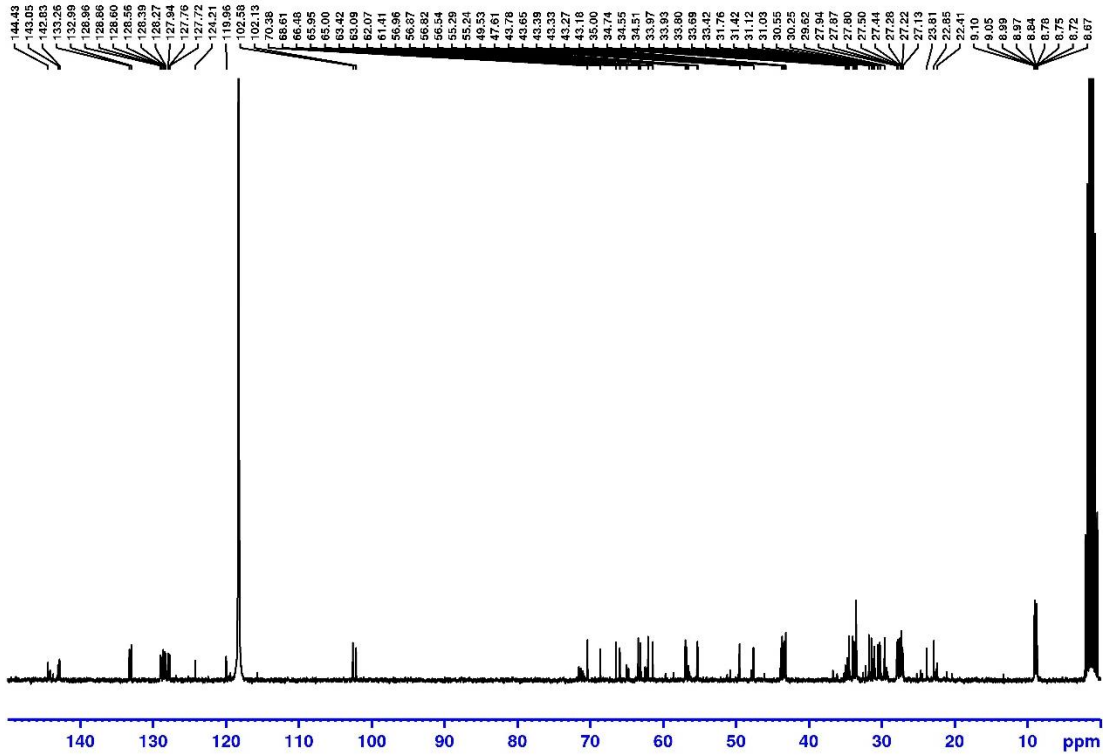


Fig. S66 $^{13}C\{^{1}H\}$ NMR spectrum of **8^{Pr}** in its crude reaction mixture in CD_3CN at RT.

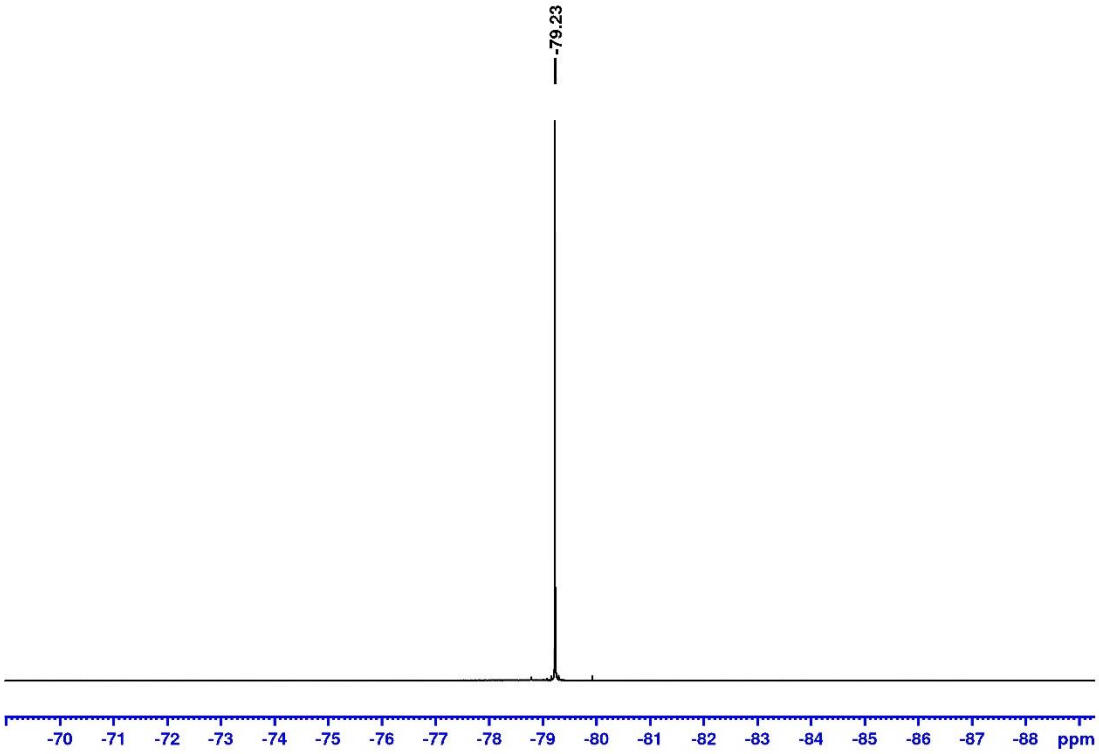
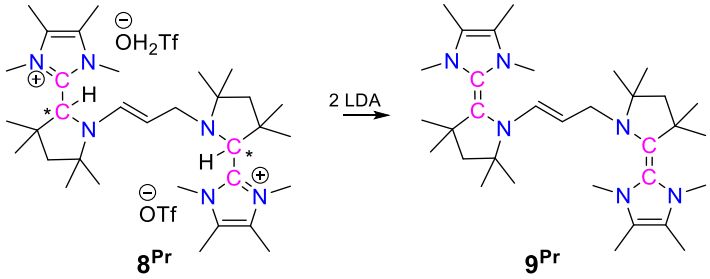


Fig. S67 $^{19}F\{^{1}H\}$ NMR spectrum of **8^{Pr}** in its crude reaction mixture in CD_3CN at RT.

Synthesis of 9^{Pr}



8^{Pr} 9^{Pr}

About 40 mL of toluene was added into a 50 mL Schlenk flask containing $\mathbf{8^{Pr}}$ (prepared by comproportionation reaction between $\mathbf{5^{Pr}}$ and $\mathbf{4^{Pr}}$) (630 mg, 0.753 mmol) and solid LDA (200 mg, 1.864 mmol) at room temperature with stirring. After 18 hours stirring at room temperature the reaction mixture was filtered and the filtrate was evaporated to obtain a reddish brown oily type of liquid. The ^{1}**H**, ^{7}**Li** and ^{19}**F** NMR spectrum of this oily compound showed the presence of $\mathbf{9^{Pr}}$ along with lithium triflate compound. Then pentane (2 x 20 mL) was added to it, stirred well and filtered and the filtrate was concentrated up to 5 mL and kept for crystallization at −35 °C. After 24 hours, colorless crystals (150 mg + 70 mg) were collected which were suitable for single crystal X-ray diffraction. **Yield:** 220 mg (54 %). **M.P.:** 121 °C. ^{1}**H NMR** (C_6D_6, 25 °C, 300 MHz): δ = 6.15-6.19 (d, 1H, 12.90 Hz, C*H*=CH-CH_2), 3.80-3.89 (m, 1H, CH=C*H*-CH_2), 3.68-3.70 (d, 2H, 5.50 Hz, CH=CH-CH_2), 2.80 (s, 3H, CH_3-N), 2.78 (s, 3H, CH_3-N), 2.76 (s, 3H, CH_3-N), 2.44 (s, 3H, CH_3-N), 1.78 (s, 2H, CH_2), 1.68 (s, 2H, CH_2), 1.68 (s, 3H, CH_3-C=C), 1.66 (s, 3H, CH_3-C=C), 1.63 (s, 3H, CH_3-C=C), 1.60 (s, 3H, CH_3-C=C), 1.50 (s, 6H, C(CH_3)$_2$), 1.40 (s, 6H, C(CH_3)$_2$), 1.38 (s, 6H, C(CH_3)$_2$), 1.28 (s, 6H, C(CH_3)$_2$) ppm. ^{13}**C{^{1}H} NMR** (C_6D_6, 25 °C, 75 MHz): δ = 143.06 (NC=*C*NN), 140.01 (NC=*C*NN), 127.41 (*C*H=CH-CH_2), 122.40 (CH_3-*C*=*C*), 121.87 (CH_3-*C*=*C*), 121.25 (CH_3-*C*=*C*), 119.73 (CH_3-*C*=*C*), 114.47 (N*C*=CNN), 102.80 (N*C*=CNN), 97.68 (CH=*C*H-CH_2), 60.85 (CH_2), 60.16 (CH_2), 59.85 (*C*(CH_3)$_2$), 59.29 (*C*(CH_3)$_2$), 44.88 (CH=CH-*C*H_2), 42.59 (*C*H_3-N), 42.31 (*C*H_3-N), 39.93 (*C*(CH_3)$_2$), 39.89 (*C*(CH_3)$_2$), 32.74 (*C*H_3-N), 32.21 (*C*H_3-N), 29.55 (C(*C*H_3)$_2$), 28.33 (C(*C*H_3)$_2$), 10.30 (*C*H_3-C=C), 10.06 (*C*H_3-C=C), 10.02 (*C*H_3-C=C), 9.56 (*C*H_3-C=C) ppm. Most likely due to high air and moisture sensitivity we were not able to get satisfactory elemental analysis data even after repeating measurements.

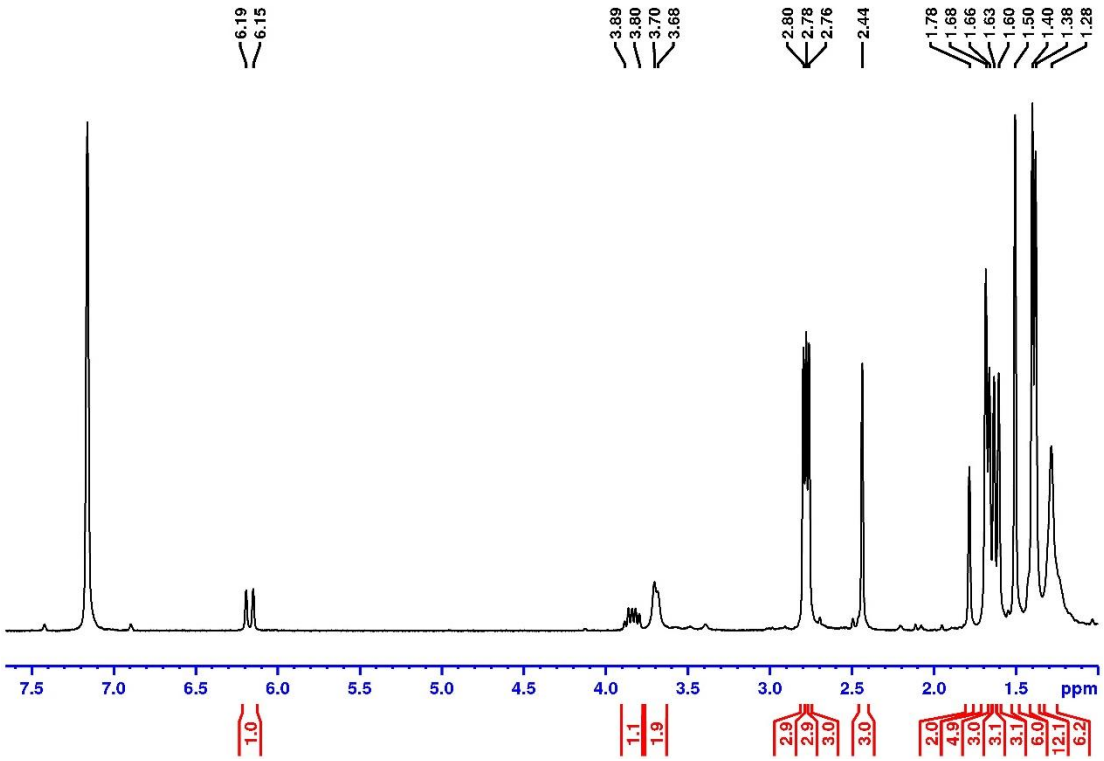


Fig. S68 ^{1}H NMR spectrum of compound $\mathbf{9^{Pr}}$ in C_6D_6 at RT.

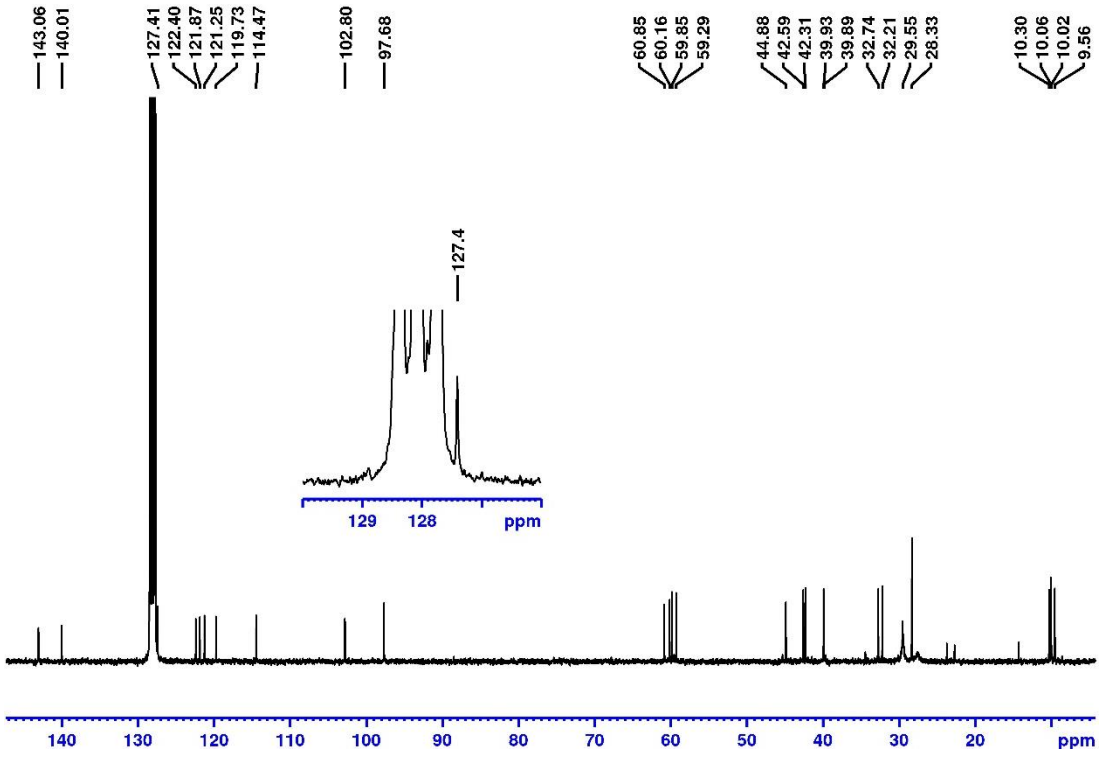


Fig. S69 $^{13}C\{^{1}H\}$ NMR spectrum of compound $\mathbf{9^{Pr}}$ in C_6D_6 at RT.

Molecular Structures of 3^{Cy}, 5^{Cy}, 3^{Et}, 4^{Et}, 5^{Et}, 8^{Et}, 9^{Et}, 10^{Et}, 3^{Pr}, 4^{Pr}, 5^{Pr}, and 9^{Pr}

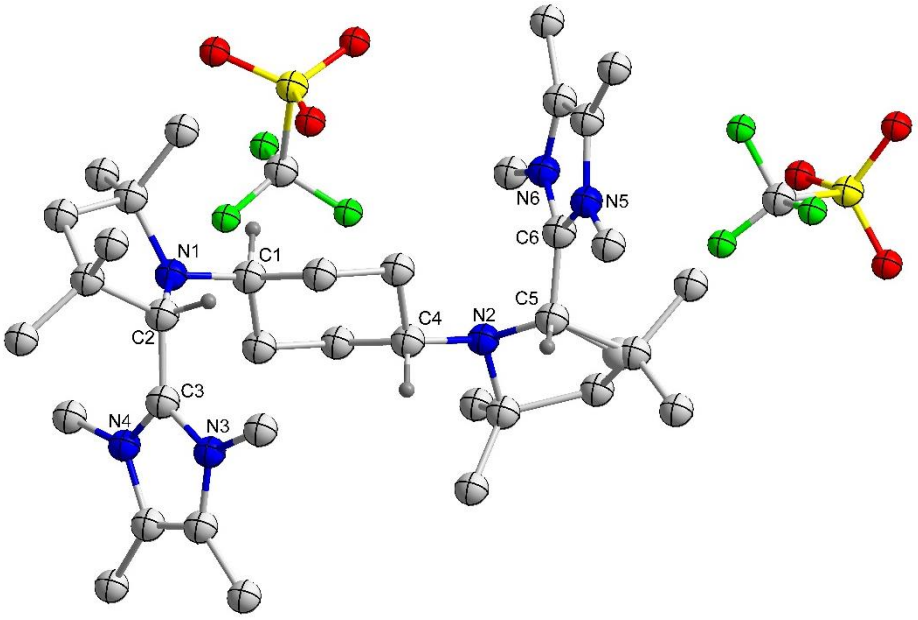


Fig. S70 Molecular structure of 3^{Cy} (*meso*-isomer) in the solid state with thermal ellipsoids at the 50 % probability level. All hydrogen atoms except on C1, C2, C4 and C5 are omitted for clarity.

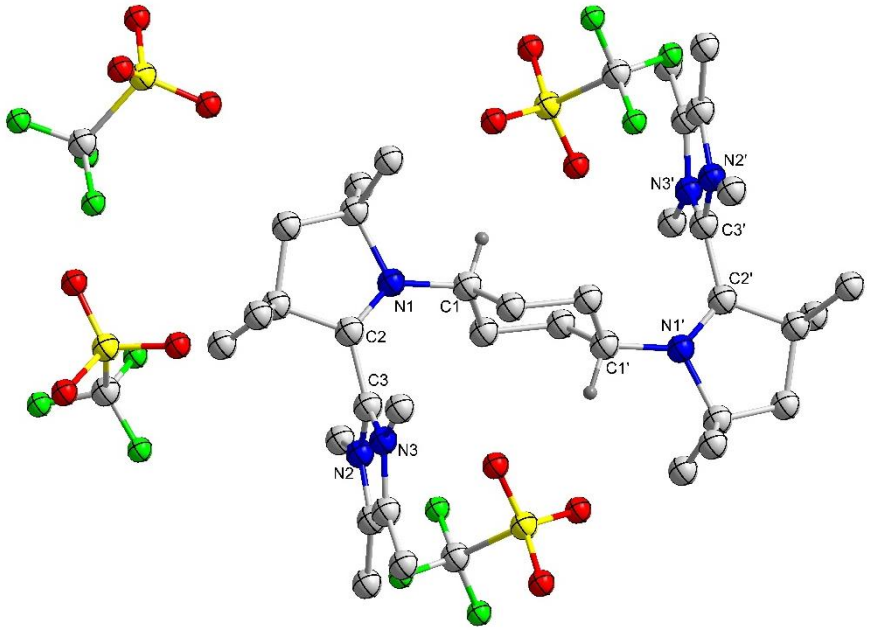


Fig. S71 Molecular structure of 5^{Cy} in the solid state with thermal ellipsoids at the 50 % probability level. All hydrogen atoms except on C1, and C1' are omitted for clarity.

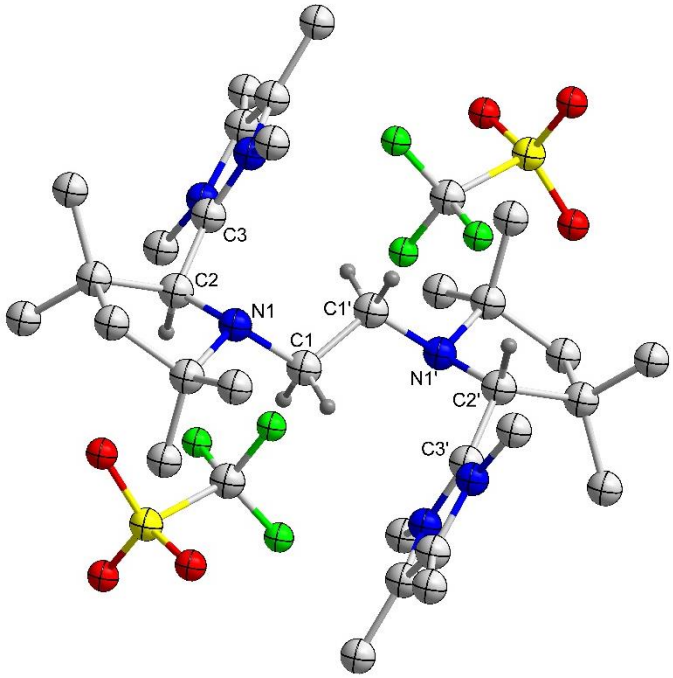


Fig. S72 Molecular structure of **3^{Et}** (*meso*-isomer) in the solid state with thermal ellipsoids at the 50 % probability level. All hydrogen atoms except on C1, C1', C2 and C2' are omitted for clarity.

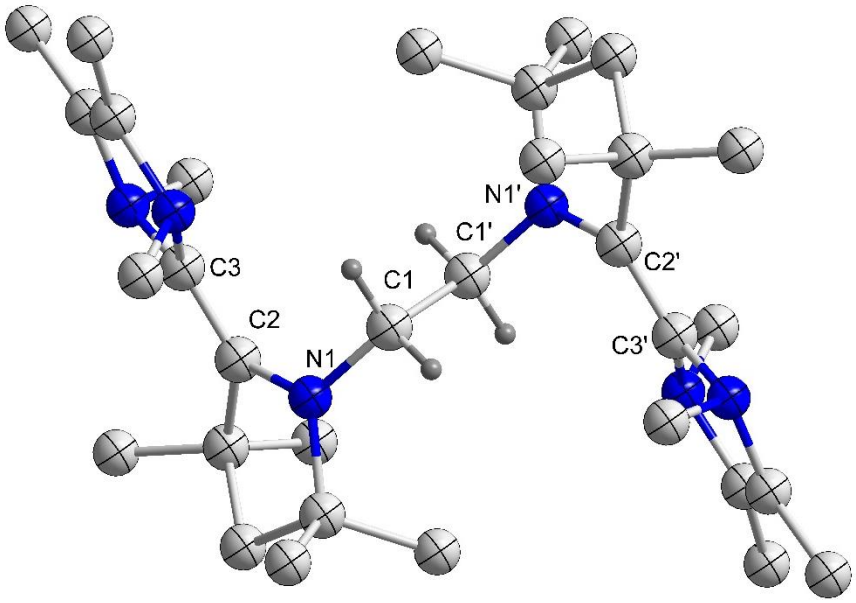


Fig. S73 Molecular structure of **4^{Et}** in the solid state with thermal ellipsoids at the 50 % probability level. All hydrogen atoms except on C1 and C1' are omitted for clarity.

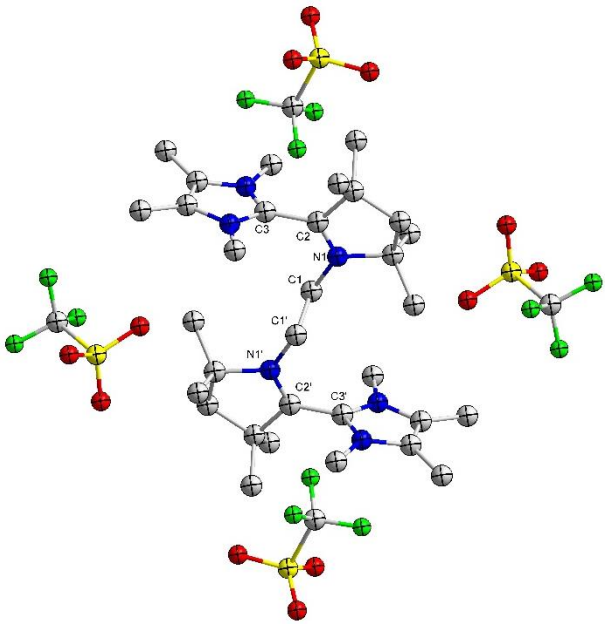


Fig. S74 Molecular structure of **5**^{Et} in the solid state with thermal ellipsoids at the 50 % probability level. All hydrogen atoms are omitted for clarity.

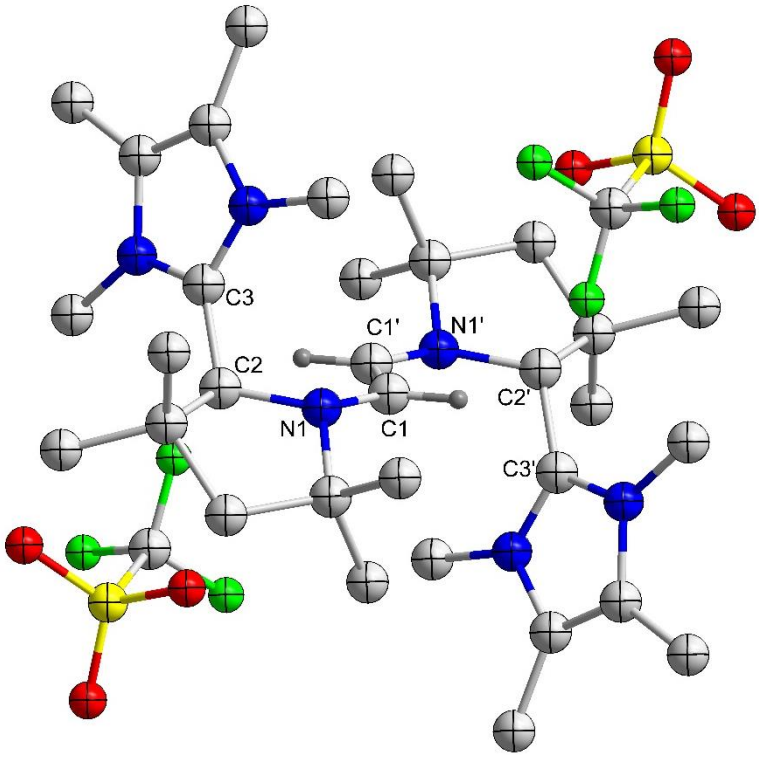


Fig. S75 Molecular structure of **8**^{Et} (*meso*-isomer) in the solid state with thermal ellipsoids at the 50 % probability level. All hydrogen atoms except on C1 and C1'are omitted for clarity.

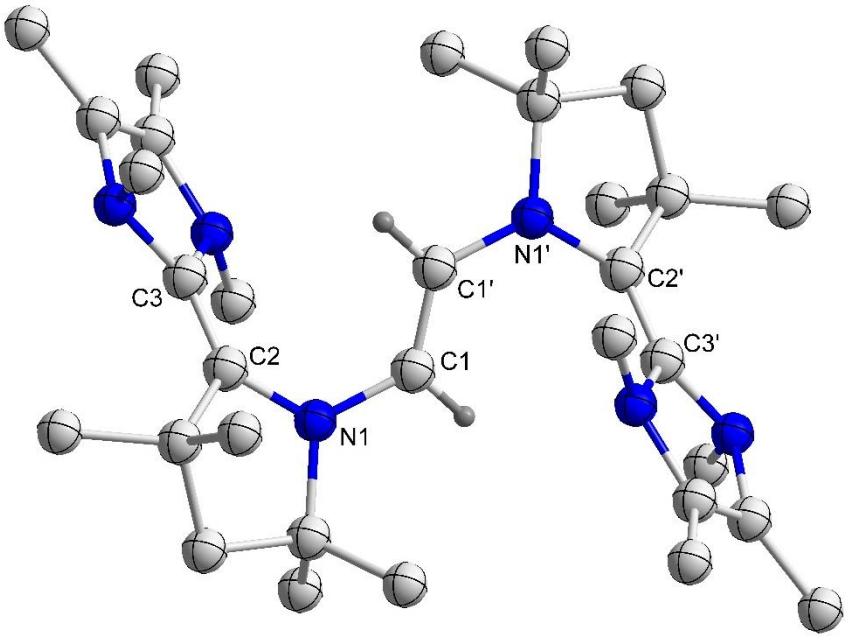


Fig. S76 Molecular structure of **9^{Et}** in the solid state with thermal ellipsoids at the 50 % probability level. All hydrogen atoms except on C1 and C1' are omitted for clarity.

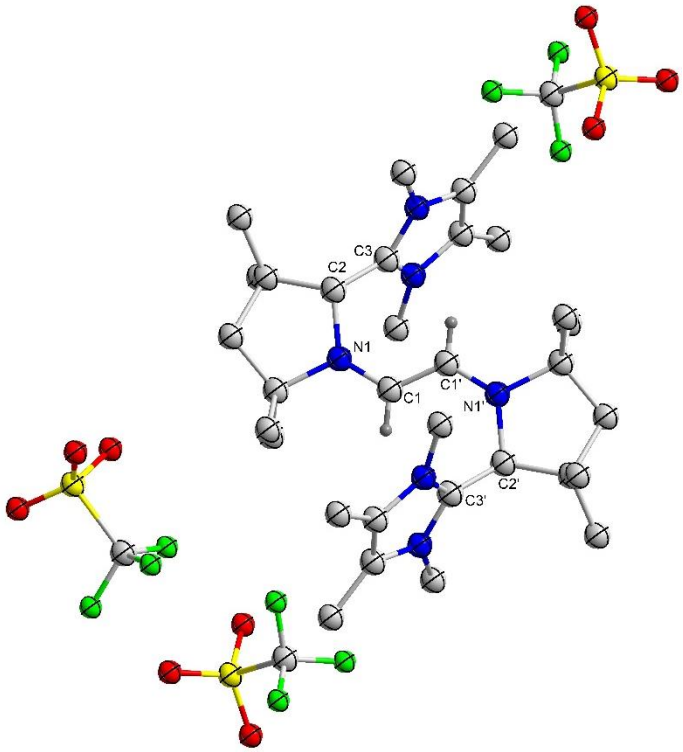


Fig. S77 Molecular structure of **10^{Et}** (*meso*-isomer) in the solid state with thermal ellipsoids at the 50 % probability level. All hydrogen atoms except on C1 and C1'are omitted for clarity.

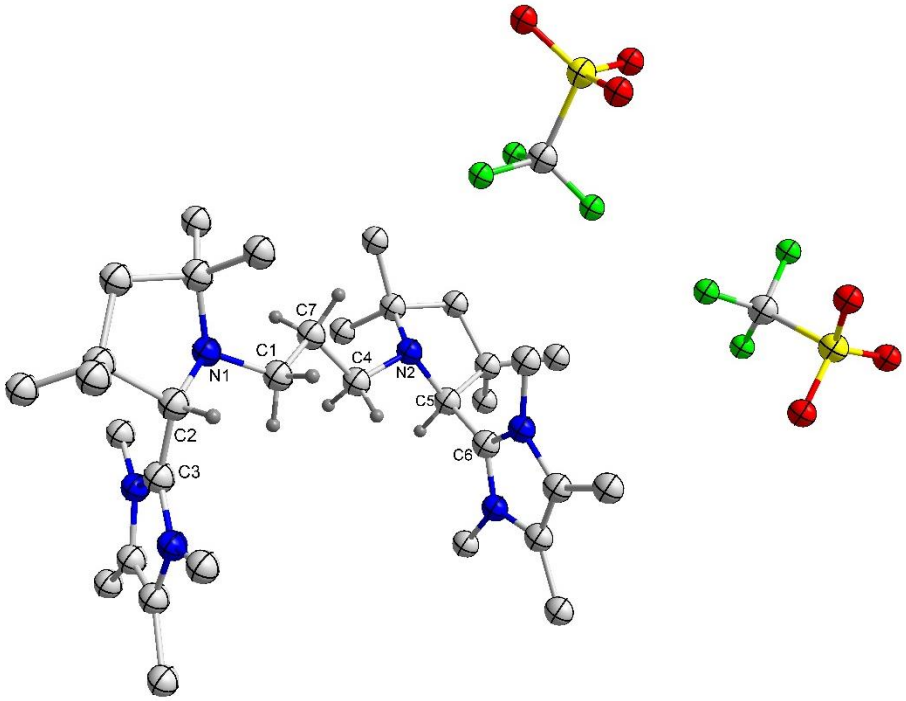


Fig. S78 Molecular structure of **3^{Pr}** (*meso*-isomer) in the solid state with thermal ellipsoids at the 50 % probability level. All hydrogen atoms except on C1, C2, C4, C5 and C7 are omitted for clarity.

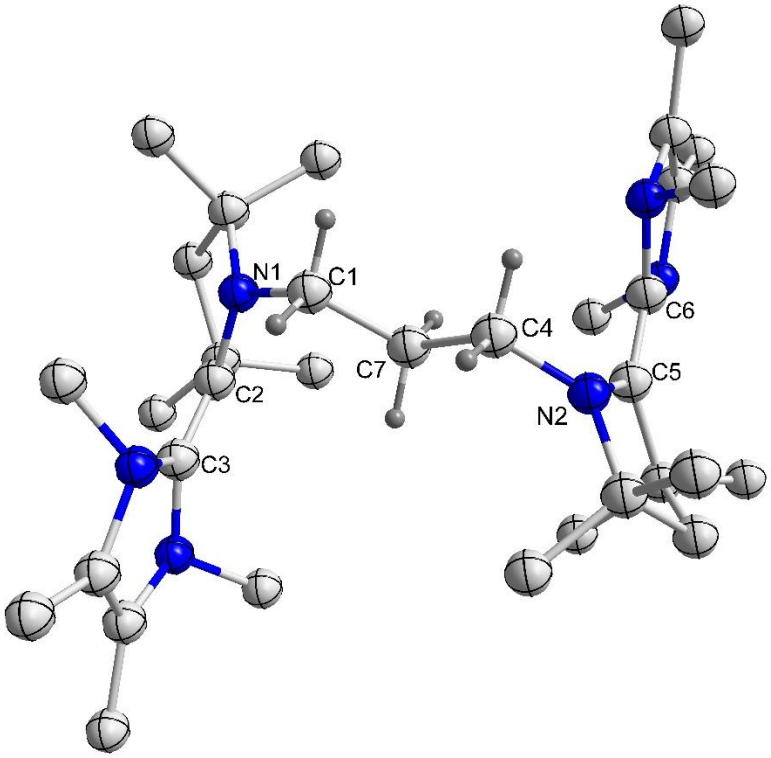


Fig. S79 Molecular structure of **4^{Pr}** in the solid state with thermal ellipsoids at the 50 % probability level. All hydrogen atoms except on C1, C4 and C7 are omitted for clarity.

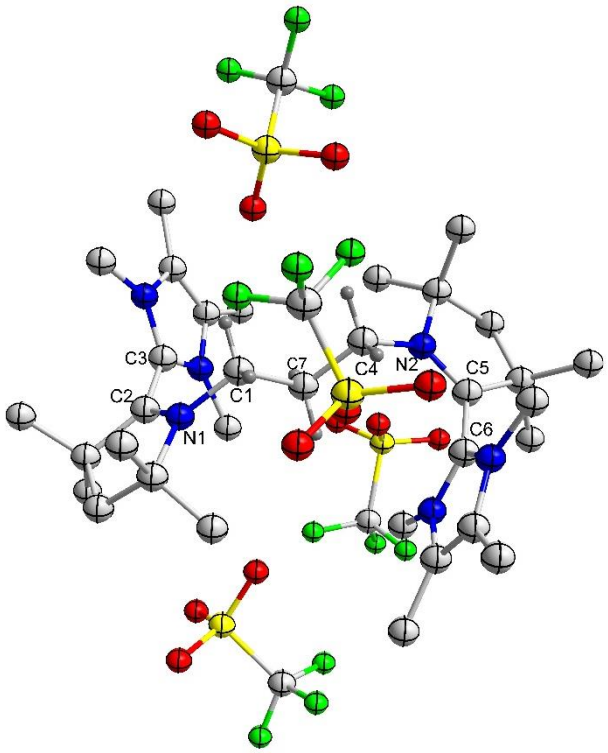


Fig. S80 Molecular structure of **5^{Pr}** in the solid state with thermal ellipsoids at the 50 % probability level. All hydrogen atoms except on C1, C4 and C7 are omitted for clarity.

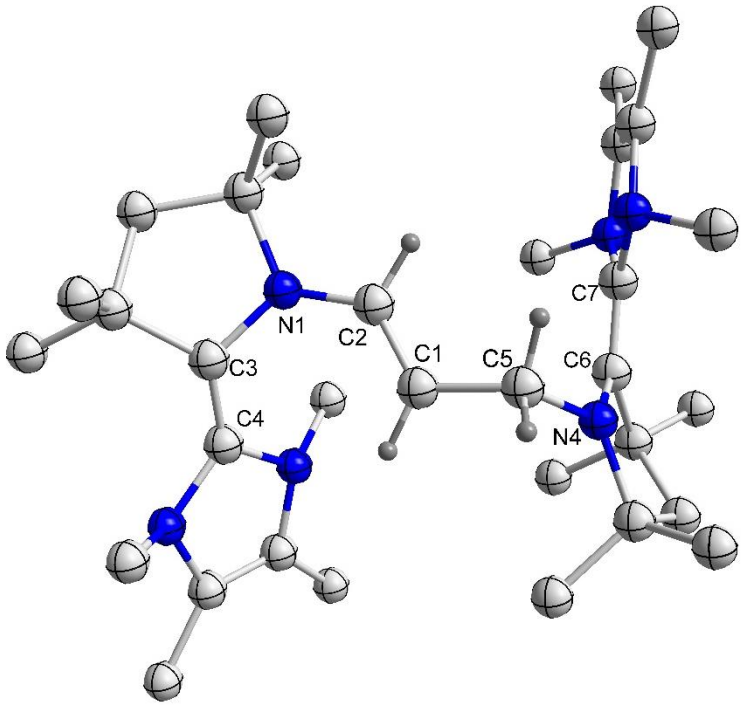


Fig. S81 Molecular structure of **9^{Pr}** in the solid state with thermal ellipsoids at the 50 % probability level. All hydrogen atoms except on C1, C2 and C5 are omitted for clarity.

Crystallographic Details

Single-crystal X-ray diffraction data of $\mathbf{3^{Cy}}$, $\mathbf{5^{Cy}}$, $\mathbf{6^{Cy}}$, $\mathbf{7^{Cy}}$, $\mathbf{3^{Et}}$, $\mathbf{4^{Et}}$, $\mathbf{5^{Et}}$, $\mathbf{8^{Et}}$, $\mathbf{9^{Et}}$, $\mathbf{10^{Et}}$, $\mathbf{3^{Pr}}$, $\mathbf{4^{Pr}}$, and $\mathbf{9^{Pr}}$ were collected using a Rigaku diffractometer with graphite-monochromated molybdenum *Kα* radiation, λ = 0.71073 Å. For $\mathbf{5^{Pr}}$ diffraction data was collected using a STOE-IPDS 2T diffractometer with graphite-monochromated molybdenum *Kα* radiation, λ = 0.71073 Å. Data integration and reduction were processed with CrysAlisPro (Rigaku) or XArea (STOE) software.[S5] An empirical absorption correction was applied to the collected reflections with SCALE3 ABSPACK integrated with CrysAlisPro. The applied absorption correction for the STOE measurement was numerical (face indexed) using X-Shape and X-Red32 as implemented in XArea. The structures were solved by direct methods using SHELXT[S6] and refined by full matrix least-squares method based on F^2 by using SHELXL[S7] through the Olex2[S8] interface. All non-hydrogen-atoms were refined with anisotropic displacement parameters. The hydrogen atoms, unless stated otherwise, were refined isotropically on calculated positions using a riding model with their U_{iso} values constrained to 1.5 U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for the aromatic carbon atoms. Crystal and structure refinement data of all these compounds are summarized in Tables S1-S14. Individual reflexes which were clear outliers were removed from the refinements with OMIT instructions. The crystal of $\mathbf{3^{Cy}}$ was of minor quality (weak diffraction, some thermal motion). This results in some reflexes missing from the data set and generating a B-alert. One pyrrolidine moiety is disordered comprising one iPr and a methylene group. For the pyrrolidine disorder only SAME was used as constraint; occupancies are 52% and 48%. One of the triflate anions is also disordered, which was modelled with SAME, SIMU and DELU constraints; occupancies are 77% and 23%. There is also some motion in the second triflate and in the imidazol moiety. Modelling this as disorder did not improve the refinement and was abandoned. In the structure of $\mathbf{5^{Cy}}$ approximately ten very mobile water molecules per formula are co-crystallized. The respective diffuse electron density was SQUEEZED[S9] from the refinement. The two triflate anions in the asymmetric unit are disordered entirely over two orientations. Occupancies are 66% vs. 34% and 77% vs. 23%. These disorders were treated with SAME, SIMU and DELU constraints. In addition there is a disorder of a methylene carbon in the non-aromatic fivefold ring (ring pucker). Occupancies are 54% vs. 46%. The model was refined without any constraints or restraints. In the structure of $\mathbf{6^{Cy}}$ one $C(CH_3)_2$ moiety is disordered over two orientations. This was modelled with three SADI constraints plus SIMU and DELU. Occupancies are 80% vs. 20%. The two triflate anions are disordered entirely. This was modelled with SAME, SIMU and DELU constraints. Occupancies are 65% vs. 35% for one and 63% vs. 37% for the other anion. The two iso-propyl hydrogen atoms were found and refined freely. The structure was further refined as inversion twin with roughly 26% of the minor domain being part of the data set. In the structure of $\mathbf{7^{Cy}}$ two of the triflates are disordered entirely with occupancies of 62% and 38% and of 51% and 49%, respectively. One triflate has a disorder only in the SO_3 moiety with occupancies of 65% and 35%. All disorders were modelled with SAME, SIMU and DELU constraints. In the structure of $\mathbf{3^{Et}}$ the triflate anion is disordered over two positions which are both well refined and have occupancies of 89% and 11%. Only for the CF_3 moiety of

the minor occupancy constraints had to be used (SIMU and DELU). All other atoms of the disorder are refined freely. Half of the cation is refined in the asymmetric unit. The second half is generated by symmetry operation (inversion centre). This renders the diastereomer necessarily to be the meso-isomer. Symmetry generation and meso-isomer form are the same also for the structures of **8^{Et}** and **10^{Et}**. The refinements of **4^{Et}**, **4^{Pr}** and **5^{Et}** were unremarkable. In the structure of **8^{Et}** two disorder problems are present. The triflate anion is disordered by a rotation over two orientations with occupancies of 70% and 30%. The disorder was treated with SAME, SIMU and DELU constraints for all atoms of this disorder. Secondly the CAAC rings are disordered with a distinct ring pucker which extends to all of the associated methyl substituents with occupancies of 79% and 21%. This disorder was treated only with a SAME constraint; i.e. thermal displacement parameters are refined freely. The H-atom of the ethenyl bridge was located and refined freely (no constraints or restraints) proving that it is indeed an ethenyl bridge (only one H was refined, the second is symmetry generated). In the structure of **10^{Et}** also two disorder problems are present. One of the two triflate anions is located directly on a two-fold rotoinversion axis (this axis and the C-S molecule axis are aligned). Therefore, all respective occupancies are fixed at 50% while all else was refined freely. PART -1 was used for all O and F atoms so that they do not bind their symmetry generated direct neighbors. The CAAC ring exhibits the exact same disorder as found for **8^{Et}**. For **10^{Et}** occupancies of 50% and 50% were observed. The disorder was treated again only with a SAME constraint. The H-atom of the ethenyl bridge (similar to **8^{Et}**) and the methine H-atom on the CAAC carbon atom bound to the NHC ring were both located and refined freely (no constraints or restraints). In the refinement of **9^{Et}** the H-atom of the ethenyl bridge was located and refined freely (no constraints or restraints; similar to the structures of **8^{Et}** and **10^{Et}**). In the structure of **3^{Pr}** two triflate anions are disordered; one in its entirely with occupancies of 60% and 40%, the other only with its O and F atoms (while C and S are not disordered) and occupancies of 54% and 46%. All atoms of the entirely disordered anion are constrained with SAME, SIMU and DELU commands. For the second anion only SAME was used for the O and F atoms. The methane hydrogen atoms on C4 and C19 were found and refined freely. The refinement of the data for **9^{Pr}** was unremarkable. The hydrogen atoms on the central ene-moiety (C1 and C17) were found and refined freely. The checkcif-file for the structure of **5^{Pr}** contains one B-alert. This refers to the proximity of one O and one N without them being in a hydrogen bond interaction for the absence of H. Based on spectroscopic data it is certain that the N is not protonated and neither is the triflate. The proximity therefore goes back to crystal packing. Isolated electron density indicative of an actual atom site was refined as half a molecule (fixed to 0.5) of water per formula after the electron count was established using the SQUEEZE routine in PLATON. The reported structure is unsqueezed. The hydrogen atoms were located but had to be constrained. All O-H and H-H distances are fixed to the ideal water geometry (DFIX). The displacement factors of H were constrained to the parent oxygen atom with a factor of 1.2. One fivefold ring is slightly disordered with a small ring pucker. This was modelled with SADI, SIMU and DELU constraints. Occupancies are 84% and 16%. One of the triflate anions is disordered entirely, which was modelled with SAME, SIMU and DELU constraints. Occupancies are 75% and 25%.

Table S1. Crystal data and structure refinement for **3^{Cy}** (CCDC 2161956)

Identification code	aj1925r
Empirical formula	$C_{38}H_{64}N_6O_6F_6S_2$
Formula weight	879.07
Temperature/K	250(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	9.1161(4)
b/Å	46.1464(16)
c/Å	11.2799(6)
α/°	90
β/°	105.642(5)
γ/°	90
Volume/Å^3	4569.4(4)
Z	4
ρ_{calc}g/cm^3	1.278
μ/mm^{-1}	0.189
F(000)	1872.0
Crystal size/mm^3	0.106 × 0.094 × 0.092
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.344 to 52.744
Index ranges	-11 ≤ h ≤ 11, -57 ≤ k ≤ 47, -12 ≤ l ≤ 14
Reflections collected	32348
Independent reflections	9288 [R_{int} = 0.0469, R_{sigma} = 0.0557]
Data/restraints/parameters	9288/579/651
Goodness-of-fit on F^2	1.054
Final R indexes [I>=2σ (I)]	R_1 = 0.0756, wR_2 = 0.2015
Final R indexes [all data]	R_1 = 0.1226, wR_2 = 0.2238
Largest diff. peak/hole / e Å^{-3}	0.88/-0.56

Table S2. Crystal data and structure refinement for **5^{Cy}** (CCDC2161957).

Identification code	aj1944r_sq
Empirical formula	$C_{40}H_{82}N_6O_{22}F_{12}S_4$
Formula weight	1355.35
Temperature/K	293(2)
Crystal system	triclinic
Space group	P-1
a/Å	11.1305(3)
b/Å	11.4290(3)
c/Å	13.7220(4)
α/°	92.322(2)
β/°	99.653(2)
γ/°	113.256(2)
Volume/Å^3	1570.03(8)
Z	1
ρ_{calc}g/cm^3	1.433
μ/mm^{-1}	0.260
F(000)	712.0
Crystal size/mm^3	0.376 × 0.237 × 0.219
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.088 to 57.844
Index ranges	-13 ≤ h ≤ 14, -14 ≤ k ≤ 13, -17 ≤ l ≤ 18
Reflections collected	27333
Independent reflections	7324 [R_{int} = 0.0336, R_{sigma} = 0.0350]
Data/restraints/parameters	7324/1180/498
Goodness-of-fit on F^2	1.043
Final R indexes [I>=2σ (I)]	R_1 = 0.0636, wR_2 = 0.1887
Final R indexes [all data]	R_1 = 0.0937, wR_2 = 0.2043
Largest diff. peak/hole / e Å^{-3}	0.37/-0.24

Table S3. Crystal data and structure refinement for **6^{Cy}** (CCDC 2161958)

Identification code	aj2007
Empirical formula	$C_{42}H_{68}N_8O_6F_6S_2$
Formula weight	959.16
Temperature/K	297(2)
Crystal system	orthorhombic
Space group	$Pna2_1$
a/Å	27.5528(14)
b/Å	8.4292(5)
c/Å	22.0477(12)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	5120.5(5)
Z	4
ρ_{calc}g/cm^3	1.244
μ/mm^{-1}	0.176
F(000)	2040.0
Crystal size/mm^3	0.518 × 0.357 × 0.21
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.174 to 54.204
Index ranges	-35 ≤ h ≤ 35, -10 ≤ k ≤ 10, -28 ≤ l ≤ 22
Reflections collected	62744
Independent reflections	10191 [R_{int} = 0.0555, R_{sigma} = 0.0426]
Data/restraints/parameters	10191/1525/780
Goodness-of-fit on F^2	1.026
Final R indexes [I>=2σ (I)]	R_1 = 0.0741, wR_2 = 0.2041
Final R indexes [all data]	R_1 = 0.1046, wR_2 = 0.2258
Largest diff. peak/hole / e Å^{-3}	0.53/-0.31
Flack parameter	0.26(19)

Table S4. Crystal data and structure refinement for **7^{Cy}** (CCDC 2161959).

Identification code	aj2030
Empirical formula	$C_{41}H_{65}F_9N_7O_9S_3$
Formula weight	1067.18
Temperature/K	250(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	13.7065(5)
b/Å	11.8374(5)
c/Å	32.3229(16)
α/°	90
β/°	91.669(4)
γ/°	90
Volume/Å^3	5242.1(4)
Z	4
ρ_{calc}g/cm^3	1.352
μ/mm^{-1}	0.229
F(000)	2244.0
Crystal size/mm^3	0.058 × 0.037 × 0.022
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.044 to 50.052
Index ranges	-15 ≤ h ≤ 16, -14 ≤ k ≤ 14, -34 ≤ l ≤ 38
Reflections collected	39048
Independent reflections	9249 [R_{int} = 0.1234, R_{sigma} = 0.0948]
Data/restraints/parameters	9249/1296/822
Goodness-of-fit on F^2	1.068
Final R indexes [I>=2σ (I)]	R_1 = 0.0641, wR_2 = 0.1779
Final R indexes [all data]	R_1 = 0.1031, wR_2 = 0.1938
Largest diff. peak/hole / e Å^{-3}	0.80/-0.39

Table SS5. Crystal data and structure refinement for **3^{Et}** (CCDC 2047110).

Identification code	AJ0064
Empirical formula	$C_{34}H_{58}F_6N_6O_6S_2$
Formula weight	824.98
Temperature/K	127.15
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	9.4465(5)
b/Å	20.4280(8)
c/Å	11.4500(7)
α/°	90
β/°	112.936(7)
γ/°	90
Volume/Å^3	2034.9(2)
Z	2
ρ_{calc}g/cm^3	1.346
μ/mm^{-1}	0.208
F(000)	876.0
Crystal size/mm^3	0.44 × 0.37 × 0.10
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.17 to 53
Index ranges	-11 ≤ h ≤ 11, -25 ≤ k ≤ 25, -13 ≤ l ≤ 14
Reflections collected	17318
Independent reflections	4206 [R_{int} = 0.0350, R_{sigma} = 0.0300]
Data/restraints/parameters	4206/24/325
Goodness-of-fit on F^2	1.047
Final R indexes [I>=2σ (I)]	R_1 = 0.0410, wR_2 = 0.1081
Final R indexes [all data]	R_1 = 0.0487, wR_2 = 0.1127
Largest diff. peak/hole / e Å^{-3}	0.95/-0.32

Table S6. Crystal data and structure refinement for **4^{Et}** (CCDC 2047111).

Identification code	AJ0381
Empirical formula	$C_{32}H_{56}N_6$
Formula weight	524.82
Temperature/K	120(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	7.9568(4)
b/Å	18.1921(10)
c/Å	11.2323(7)
α/°	90
β/°	107.697(6)
γ/°	90
Volume/Å^3	1548.94(16)
Z	2
ρ_{calc}g/cm^3	1.125
μ/mm^{-1}	0.067
F(000)	580.0
Crystal size/mm^3	0.316 × 0.142 × 0.127
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.562 to 52.726
Index ranges	-8 ≤ h ≤ 9, -21 ≤ k ≤ 22, -14 ≤ l ≤ 12
Reflections collected	10872
Independent reflections	3153 [R_{int} = 0.0332, R_{sigma} = 0.0358]
Data/restraints/parameters	3153/0/180
Goodness-of-fit on F^2	1.051
Final R indexes [I>=2σ (I)]	R_1 = 0.0473, wR_2 = 0.1096
Final R indexes [all data]	R_1 = 0.0611, wR_2 = 0.1146
Largest diff. peak/hole / e Å^{-3}	0.23/-0.20

Table SS7. Crystal data and structure refinement for **5^{Et}** (CCDC 2047114).

Identification code	AJ1406
Empirical formula	$C_{36}H_{56}F_{12}N_6O_{12}S_4$
Formula weight	1121.10
Temperature/K	101.15
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	12.7027(3)
b/Å	13.3266(3)
c/Å	14.3241(3)
α/°	90
β/°	93.044(2)
γ/°	90
Volume/Å^3	2421.42(9)
Z	2
ρ_{calc}g/cm^3	1.538
μ/mm^{-1}	0.306
F(000)	1164.0
Crystal size/mm^3	0.32 × 0.23 × 0.15
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.696 to 52.744
Index ranges	-15 ≤ h ≤ 15, -16 ≤ k ≤ 16, -17 ≤ l ≤ 17
Reflections collected	29135
Independent reflections	4938 [R_{int} = 0.0288, R_{sigma} = 0.0189]
Data/restraints/parameters	4938/0/324
Goodness-of-fit on F^2	1.030
Final R indexes [I>=2σ (I)]	R_1 = 0.0309, wR_2 = 0.0763
Final R indexes [all data]	R_1 = 0.0338, wR_2 = 0.0778
Largest diff. peak/hole / e Å^{-3}	0.38/-0.42

Table S8. Crystal data and structure refinement for **8^{Et}** (CCDC 2047112).

Identification code	AJ1408
Empirical formula	$C_{42}H_{72}F_6N_6O_8S_2$
Formula weight	967.17
Temperature/K	100.15
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	10.2368(4)
b/Å	11.7148(5)
c/Å	20.4531(8)
α/°	90
β/°	92.856(3)
γ/°	90
Volume/Å^3	2449.73(17)
Z	2
ρ_{calc}g/cm^3	1.311
μ/mm^{-1}	0.186
F(000)	1032.0
Crystal size/mm^3	0.24 × 0.19 × 0.15
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.292 to 52.746
Index ranges	-11 ≤ h ≤ 12, -13 ≤ k ≤ 14, -25 ≤ l ≤ 25
Reflections collected	18267
Independent reflections	5003 [R_{int} = 0.0643, R_{sigma} = 0.0556]
Data/restraints/parameters	5003/381/424
Goodness-of-fit on F^2	1.028
Final R indexes [I>=2σ (I)]	R_1 = 0.0607, wR_2 = 0.1635
Final R indexes [all data]	R_1 = 0.0734, wR_2 = 0.1747
Largest diff. peak/hole / e Å^{-3}	0.75/-0.55

Table S9. Crystal data and structure refinement for **9^{Et}** (2047115).

Identification code	AJ1445
Empirical formula	$C_{32}H_{54}N_6$
Formula weight	522.81
Temperature/K	120.15
Crystal system	triclinic
Space group	P-1
a/Å	8.4164(4)
b/Å	9.9098(3)
c/Å	10.3761(4)
α/°	101.120(3)
β/°	111.201(4)
γ/°	93.802(3)
Volume/Å^3	782.89(6)
Z	1
ρ_{calc}g/cm^3	1.109
μ/mm^{-1}	0.066
F(000)	288.0
Crystal size/mm^3	0.26 × 0.21 × 0.19
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.378 to 52.738
Index ranges	-10 ≤ h ≤ 10, -12 ≤ k ≤ 10, -11 ≤ l ≤ 12
Reflections collected	14448
Independent reflections	3204 [R_{int} = 0.0414, R_{sigma} = 0.0321]
Data/restraints/parameters	3204/0/184
Goodness-of-fit on F^2	1.064
Final R indexes [I>=2σ (I)]	R_1 = 0.0441, wR_2 = 0.1144
Final R indexes [all data]	R_1 = 0.0518, wR_2 = 0.1189
Largest diff. peak/hole / e Å^{-3}	0.38/-0.19

Table S10. Crystal data and structure refinement for **10^{Et}** (CCDC 2047113).

Identification code	AJ1512
Empirical formula	$C_{35}H_{56}F_9N_6O_9S_3$
Formula weight	972.03
Temperature/K	100.15
Crystal system	monoclinic
Space group	*I*2/*a*
a/Å	11.2729(4)
b/Å	20.2466(7)
c/Å	19.5699(6)
α/°	90
β/°	92.742(3)
γ/°	90
Volume/Å^3	4461.5(3)
Z	4
ρ_{calc}g/cm^3	1.447
μ/mm^{-1}	0.261
F(000)	2036.0
Crystal size/mm^3	0.23 × 0.19 × 0.14
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.736 to 52.742
Index ranges	-13 ≤ h ≤ 14, -25 ≤ k ≤ 19, -24 ≤ l ≤ 24
Reflections collected	28001
Independent reflections	4552 [R_{int} = 0.0328, R_{sigma} = 0.0239]
Data/restraints/parameters	4552/6/374
Goodness-of-fit on F^2	1.064
Final R indexes [I>=2σ (I)]	R_1 = 0.0477, wR_2 = 0.1245
Final R indexes [all data]	R_1 = 0.0542, wR_2 = 0.1281
Largest diff. peak/hole / e Å^{-3}	0.61/-0.50

Table S11. Crystal data and structure refinement for **3^{Pr}** (CCDC 2161952).

Identification code	aj0161rt
Empirical formula	$C_{35}H_{60}N_6O_6F_6S_2$
Formula weight	839.01
Temperature/K	190(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	16.4086(4)
b/Å	22.9375(7)
c/Å	11.3222(3)
α/°	90
β/°	97.679(2)
γ/°	90
Volume/Å^3	4223.1(2)
Z	4
ρ_{calc}g/cm^3	1.320
μ/mm^{-1}	0.201
F(000)	1784.0
Crystal size/mm^3	0.42 × 0.307 × 0.269
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.004 to 57.886
Index ranges	-21 ≤ h ≤ 19, -25 ≤ k ≤ 30, -15 ≤ l ≤ 15
Reflections collected	56617
Independent reflections	9882 [R_{int} = 0.0868, R_{sigma} = 0.0483]
Data/restraints/parameters	9882/567/648
Goodness-of-fit on F^2	1.035
Final R indexes [I>=2σ (I)]	R_1 = 0.0577, wR_2 = 0.1588
Final R indexes [all data]	R_1 = 0.0775, wR_2 = 0.1709
Largest diff. peak/hole / e Å^{-3}	0.35/-0.33

Table S12. Crystal data and structure refinement for **4^{Pr}** (CCDC 2161953).

Identification code	aj1872
Empirical formula	$C_{33}H_{58}N_6$
Formula weight	538.85
Temperature/K	250(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	11.5251(10)
b/Å	28.9745(15)
c/Å	11.6064(9)
α/°	90
β/°	119.306(11)
γ/°	90
Volume/Å^3	3379.7(5)
Z	4
ρ_{calc}g/cm^3	1.059
μ/mm^{-1}	0.063
F(000)	1192.0
Crystal size/mm^3	0.27 × 0.23 × 0.18
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.83 to 58.088
Index ranges	-14 ≤ h ≤ 15, -37 ≤ k ≤ 38, -15 ≤ l ≤ 15
Reflections collected	58618
Independent reflections	8242 [R_{int} = 0.0388, R_{sigma} = 0.0295]
Data/restraints/parameters	8242/0/368
Goodness-of-fit on F^2	1.046
Final R indexes [I>=2σ (I)]	R_1 = 0.0529, wR_2 = 0.1333
Final R indexes [all data]	R_1 = 0.0805, wR_2 = 0.1449
Largest diff. peak/hole / e Å^{-3}	0.29/-0.20

Table S13. Crystal data and structure refinement for **5^{Pr}** (CCDC 2204009)

Identification code	mk645
Empirical formula	$C_{37}H_{59}F_{12}N_6O_{12.5}S_4$
Formula weight	1144.14
Temperature/K	170(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	14.521(3)
b/Å	11.291(2)
c/Å	30.821(6)
α/°	90
β/°	93.80(3)
γ/°	90
Volume/Å^3	5042.4(18)
Z	4
ρ_{calc}g/cm^3	1.507
μ/mm^{-1}	0.296
F(000)	2380.0
Crystal size/mm^3	0.31 × 0.102 × 0.057
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.988 to 59.022
Index ranges	-20 ≤ h ≤ 20, -15 ≤ k ≤ 13, -42 ≤ l ≤ 42
Reflections collected	56832
Independent reflections	13960 [R_{int} = 0.1030, R_{sigma} = 0.0738]
Data/restraints/parameters	13960/423/755
Goodness-of-fit on F^2	1.040
Final R indexes [I>=2σ (I)]	R_1 = 0.0548, wR_2 = 0.1153
Final R indexes [all data]	R_1 = 0.1276, wR_2 = 0.1442
Largest diff. peak/hole / e Å^{-3}	0.41/-0.53

Table S14. Crystal data and structure refinement for **9^{Pr}** (CCDC 2161955).

Identification code	aj1992
Empirical formula	$C_{33}H_{56}N_6$
Formula weight	536.83
Temperature/K	297(2)
Crystal system	triclinic
Space group	P-1
a/Å	8.4000(5)
b/Å	10.3658(7)
c/Å	20.0368(13)
α/°	78.183(5)
β/°	79.823(5)
γ/°	82.783(5)
Volume/Å^3	1673.56(19)
Z	2
ρ_{calc}g/cm^3	1.065
μ/mm^{-1}	0.064
F(000)	592.0
Crystal size/mm^3	0.423 × 0.352 × 0.274
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.066 to 57.788
Index ranges	-11 ≤ h ≤ 10, -13 ≤ k ≤ 13, -26 ≤ l ≤ 22
Reflections collected	29087
Independent reflections	7703 [R_{int} = 0.0721, R_{sigma} = 0.0687]
Data/restraints/parameters	7703/0/376
Goodness-of-fit on F^2	1.082
Final R indexes [I>=2σ (I)]	R_1 = 0.0602, wR_2 = 0.1675
Final R indexes [all data]	R_1 = 0.0873, wR_2 = 0.1818
Largest diff. peak/hole / e Å^{-3}	0.24/-0.28

EPR Spectroscopy

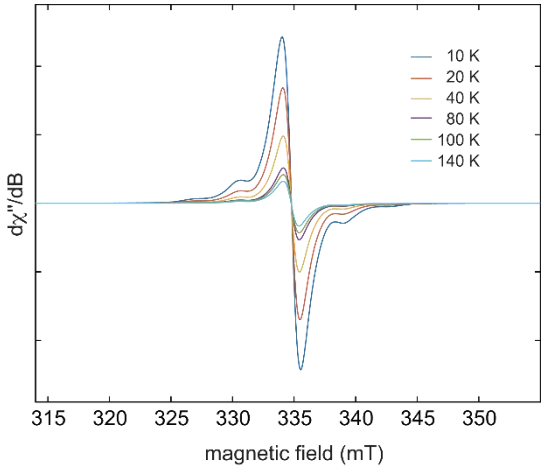


Fig. S82 Variable temperature X-band EPR spectra of **6^{Cy}** in a 1:1 toluene/acetonitrile mixture between 10 and 140 K for the *g* = 2.

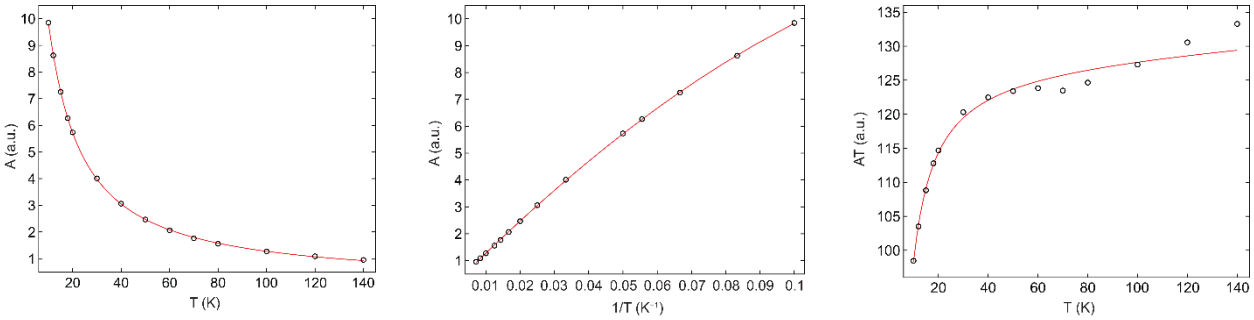


Fig. S83 Three different representations of the temperature dependence of the double integral EPR intensity (*A*) of **6^{Cy}** in a 1:1 toluene/acetonitrile mixture. Circles (○) represent the experimental results and the red line corresponds to the fit with the Bleaney-Bowers equation.

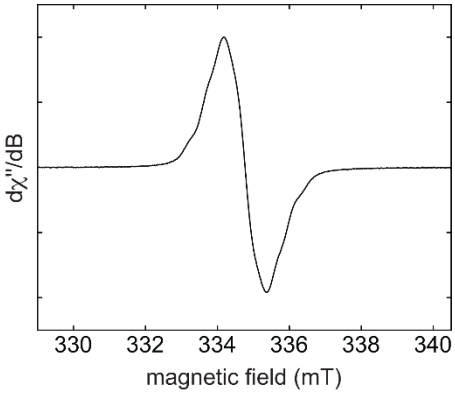


Fig. S84 Experimental EPR spectrum of **6^{Cy}** in acetonitrile. The signal is centered around g_{iso} = 2.0029.

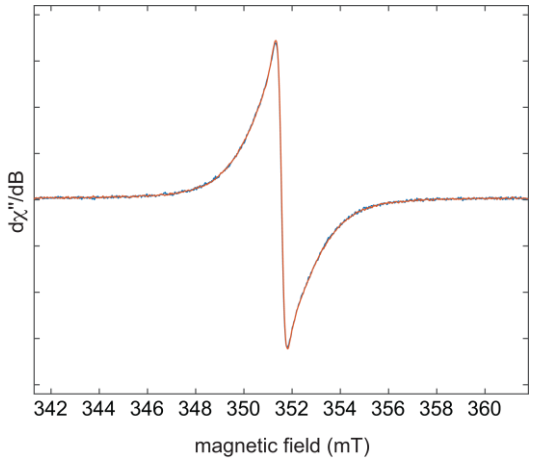


Fig. S85 EPR spectra of a solid sample of **6^{Cy}**, before (blue) and after heating at 80 °C for 1 h (red).

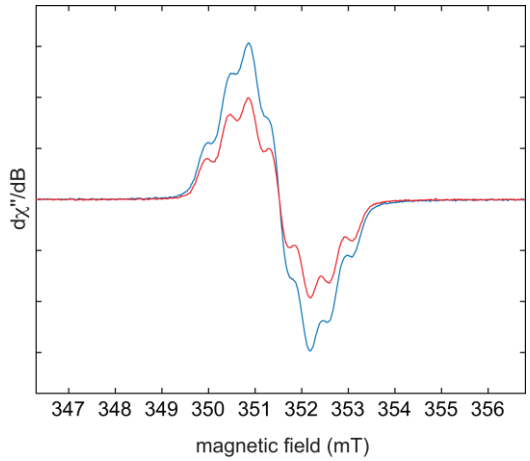


Fig. S86 EPR spectra of **6^{Cy}** in a mixture of acetonitrile and toluene, before (blue) and after heating at 80 °C for 1 h (red).

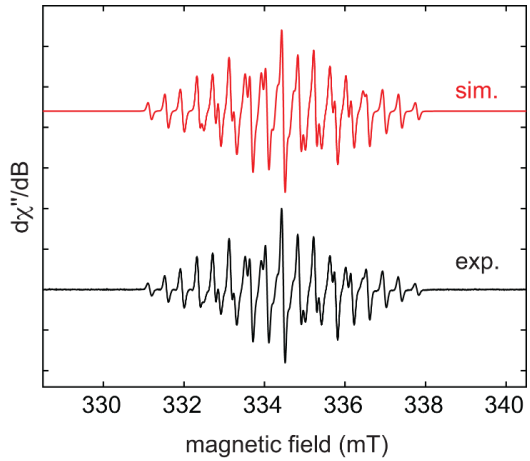


Fig. S87 Experimental (black) and simulated (red) X-band EPR spectra of **10^{Et}** in acetonitrile. The simulation parameters are: g_{iso} = 2.0034, a(^{14}N) = 22.3 MHz (2N), a(^{1}H) = 36.7 MHz (2H), and a(^{1}H) = 11.7 MHz (2H).

Magnetic Study of 6^{Cy}

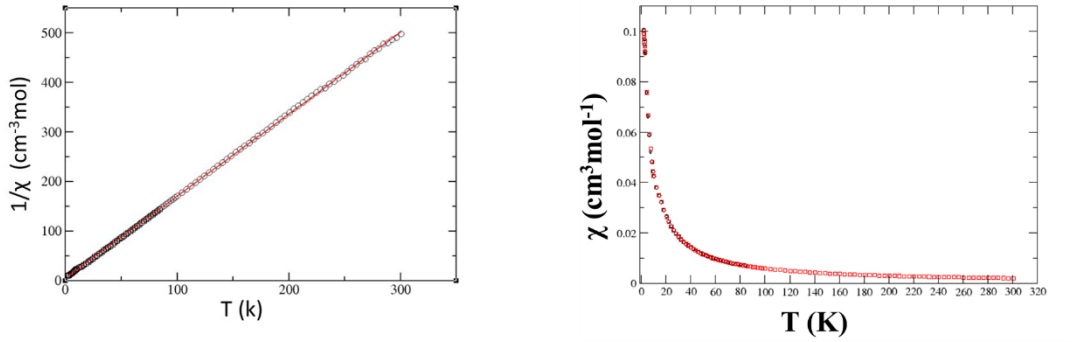


Fig. S88 Plot of magnetic susceptibility versus temperature for **6^{Cy}**.

As we know curie Weiss law: $1/\chi = \theta/C - T/C$

From the plot: $y = 1.65765*x + 5.0814$

$1/C = -1.65765$, $C = -0.6033$, $\theta/C = 5.0814$, $\theta = -3.065$

Cyclic Voltammetry

All electrochemical measurements were carried out using a conventional three-electrode cell system, with an METROHM PGStat 204 potentiostat/galvanostat apparatus controlled by the software NOVA 2.1.4 in an argon glove box. A glassy carbon disc electrode (d = 3 mm) served as working electrode and a platinum wire was used as pseudo-reference and auxiliary electrode respectively. 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). All voltammograms were referenced against Fc/Fc^{+} = 0 V. The electrochemical measurements were undertaken at room temperature by dissolving ca. 1.0 x 10^{-5} mol of analyte in 30 mL acetonitrile containing 0.1 mol l^{-1} Bu_4NPF_6 electrolyte.

Table S15. Summary of the electrochemical data relative to the potential of Fc/Fc^{+}.

Compounds	*Epk* (100 mV/s) [V]	*Epa* (100 mV/s) [V]	$E_{1/2}$ (100 mV/s) [V]	*Epk* (1000 mV/s) [V]	*Epa* (1000 mV/s) [V]	$E_{1/2}$ (1000 mV/s) [V]
5^{Cy}	−0.950 (shoulder), −1.071, −1.663	−0.908, −1.002 (shoulder), −1.556	−0.929, −1.036, −1.609	−0.898 (shoulder), −1.018, −1.622	−0.855, −0.956 (shoulder), −1.525	−0.876, −0.957, −1.573
6^{Cy}	−0.893 (shoulder), −1.013, −1.605	−0.843, −0.956 (shoulder), −1.505	−0.868, −0.984, −1.555	−0.881 (shoulder), −1.013, −1.613	−0.856, −0.943, −1.518	−0.868, −0.978, −1.565
7^{Cy}	−0.895 (shoulder), −1.021, −1.614	−0.857, −0.958 (shoulder), −1.520	−0.876, −0.989, −1.567	−0.884 (shoulder), −1.022, −1.621	−0.852, −0.953 (shoulder), −1.521	−0.868, −0.987, −1.571
5^{Et}	−0.613, −0.722, −0.865	−0.553, −0.682	−0.583, −0.702	−0.588, −0.720, −0.872	−0.538, −0.677, −0.798	−0.563, −0.698, −0.835
5^{Pr}	−0.826 (shoulder), −0.976, −1.532	−0.753, −0.901 (shoulder), −1.411	−0.789, −0.938, −1.471	−0.827, −0.977, −1.562	−0-776, −0.908, −1.453	−0.801, −0.942, −1.507

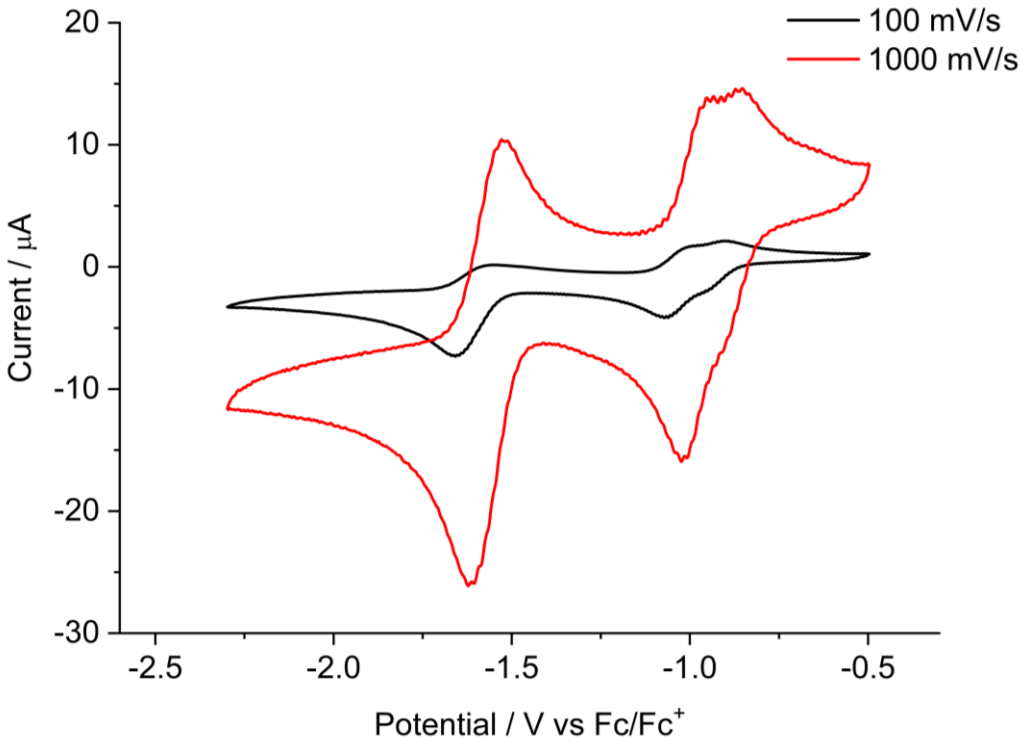


Fig. S89 Cyclic voltammograms of **5**^{cy} in CH_3CN (0.1 M Bu_4NPF_6) at different scan rates.

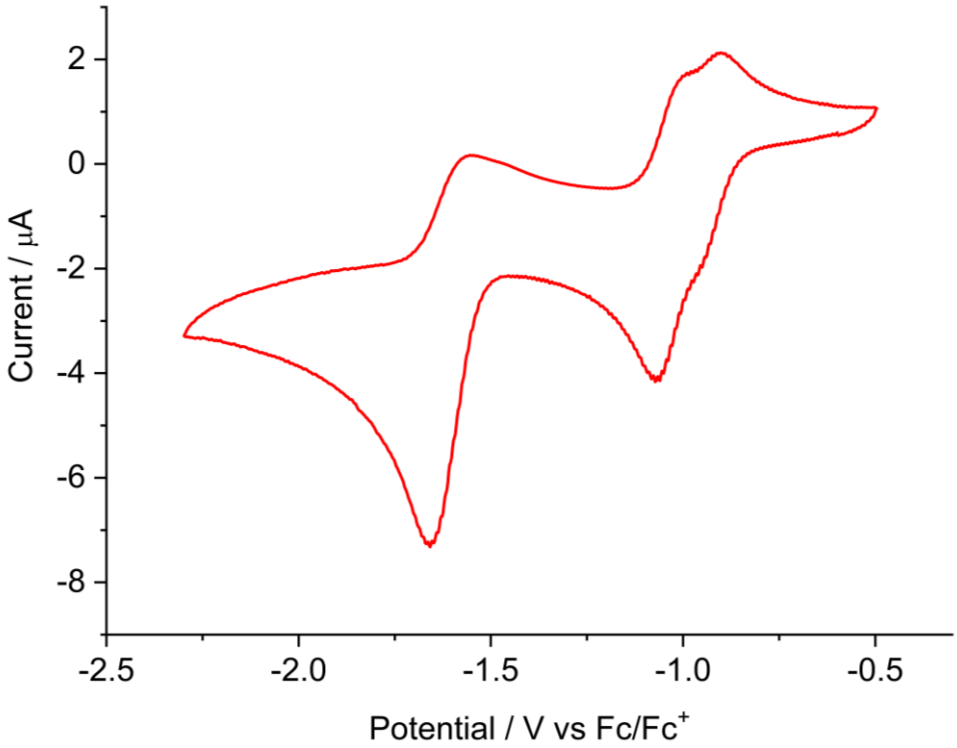


Fig. S90 Cyclic voltammogram of **5**^{cy} in CH_3CN (0.1 M Bu_4NPF_6) at scan rate of 100 mV/s.

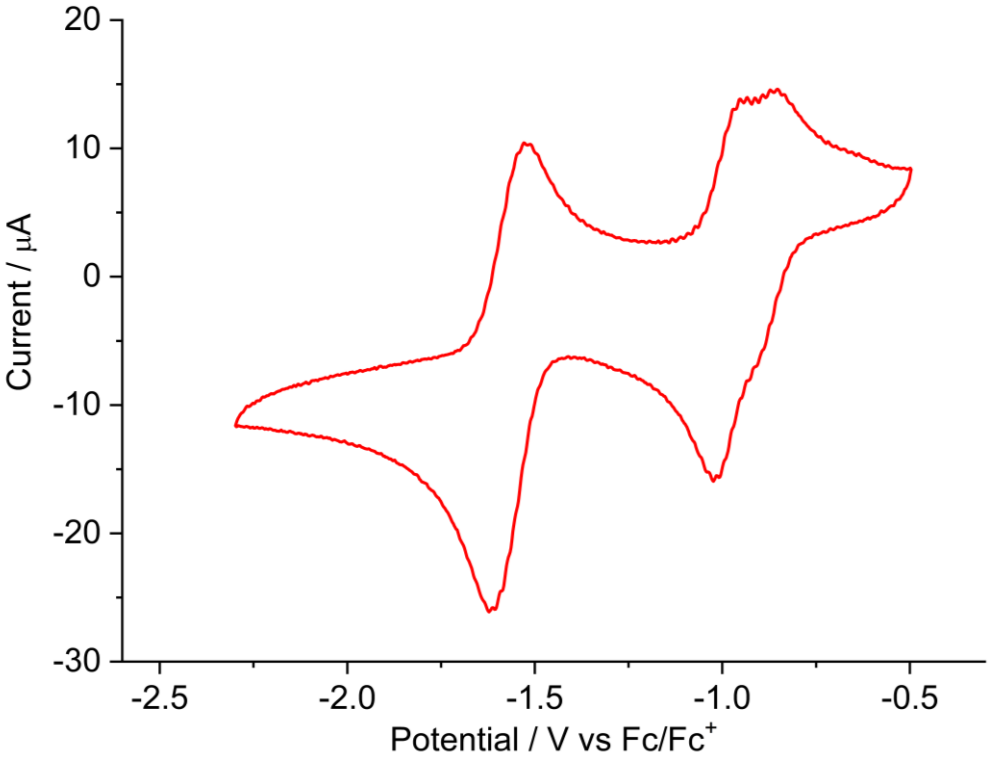


Fig. S91 Cyclic voltammogram of **5**^{cy} in CH_3CN (0.1 M Bu_4NPF_6) at scan rate of 1000 mV/s.

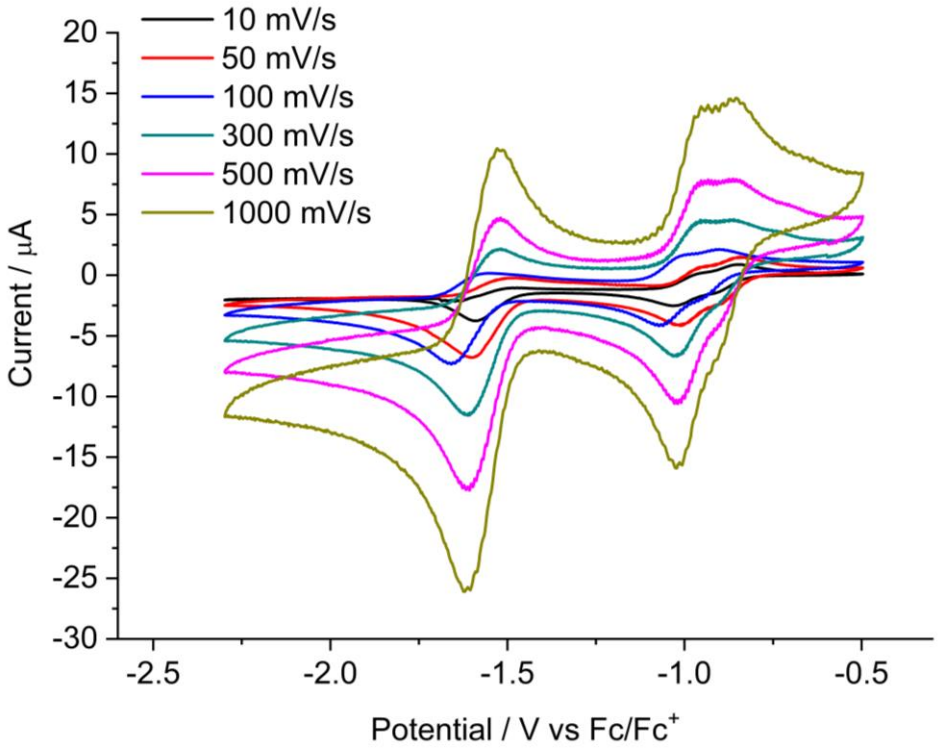


Fig. S92 Cyclic voltammograms of **5**^{cy} in CH_3CN (0.1 M Bu_4NPF_6) at different scan rates.

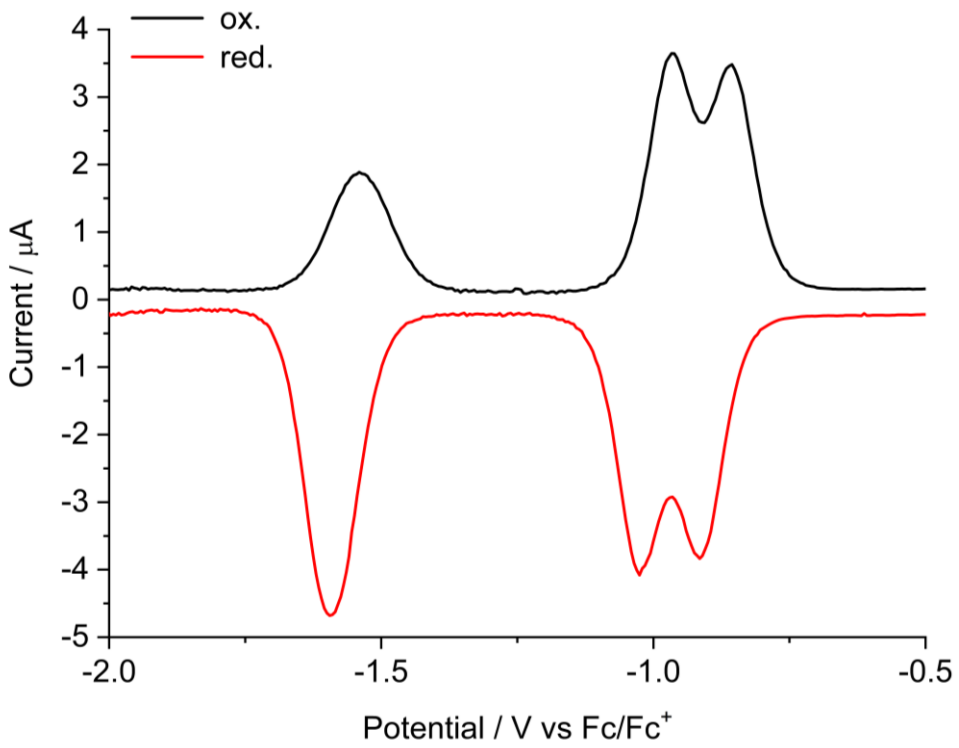


Fig. S93 Differential pulse voltammograms (DPVs) of **5**^{cy} in CH_3CN at scan rate of 10 mV/s with 0.1 M Bu_4NPF_6.

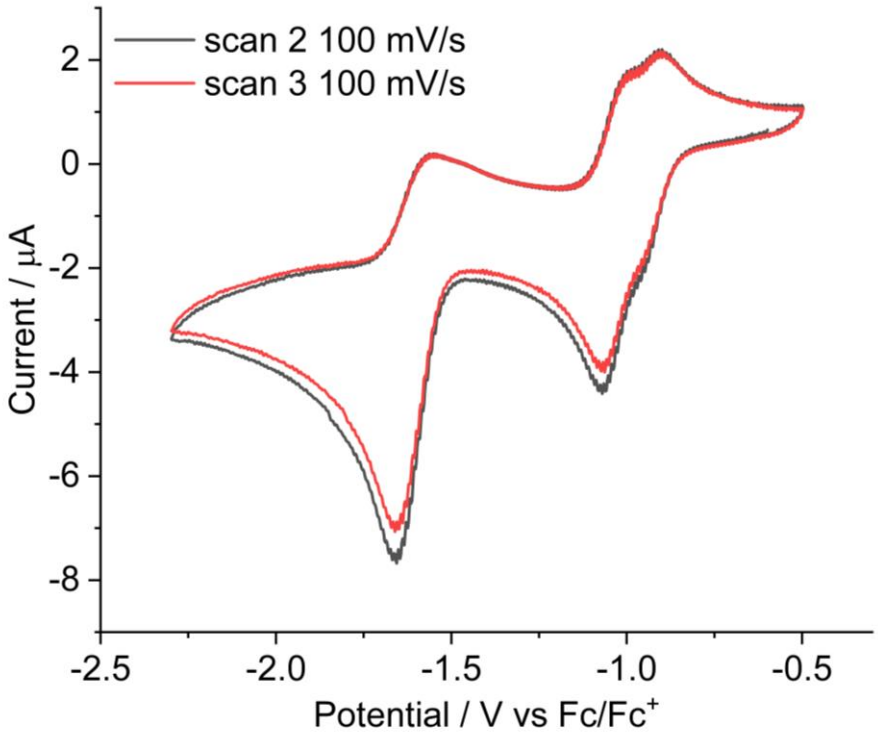


Fig. S94 Cyclic voltammograms of **5**^{Cy} in CH_3CN (0.1 M Bu_4NPF_6) at scan rate of 100 mV/s, considering second and third scans.

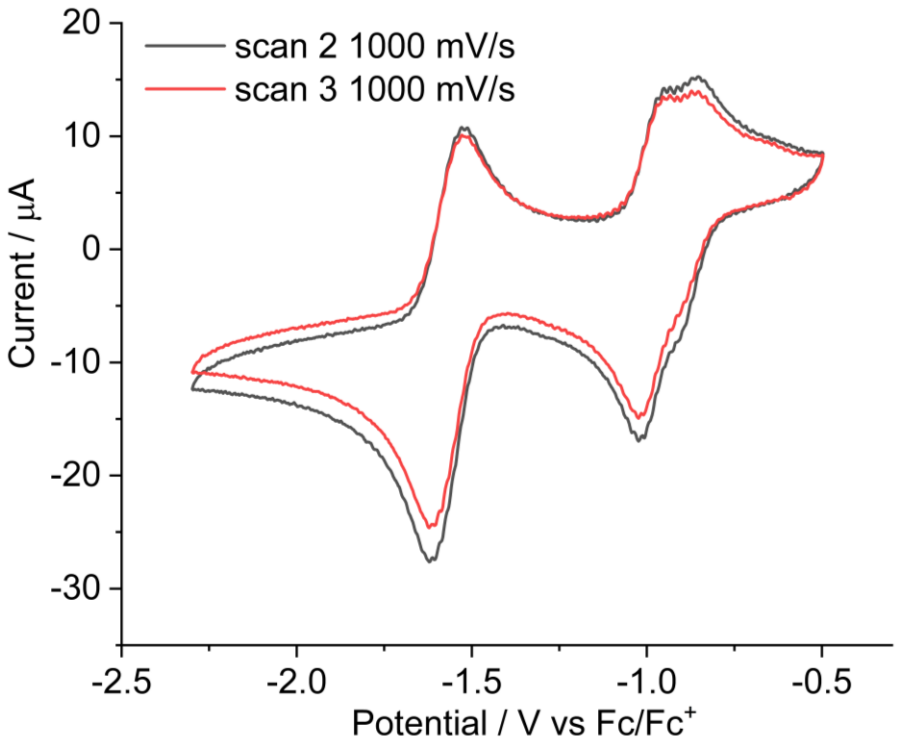


Fig. S95 Cyclic voltammograms of **5**^{cy} in CH_3CN (0.1 M Bu_4NPF_6) at scan rate of 1000 mV/s, considering second and third scans.

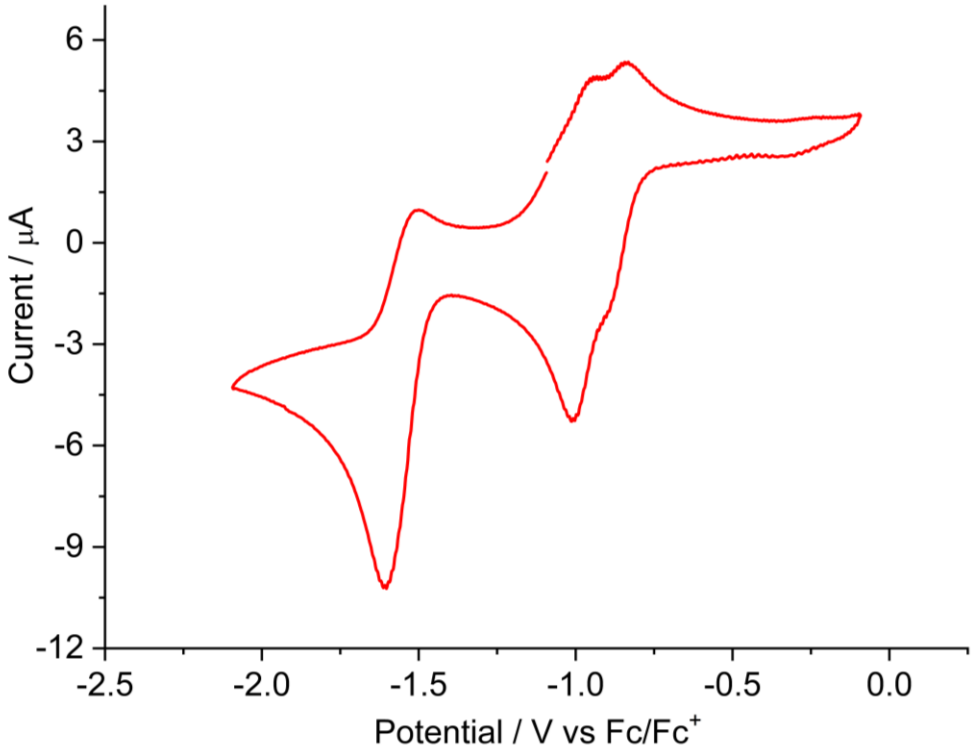


Fig. S96 Cyclic voltammogram of **6**^{cy} in CH_3CN (0.1 M Bu_4NPF_6) at scan rate of 100 mV/s.

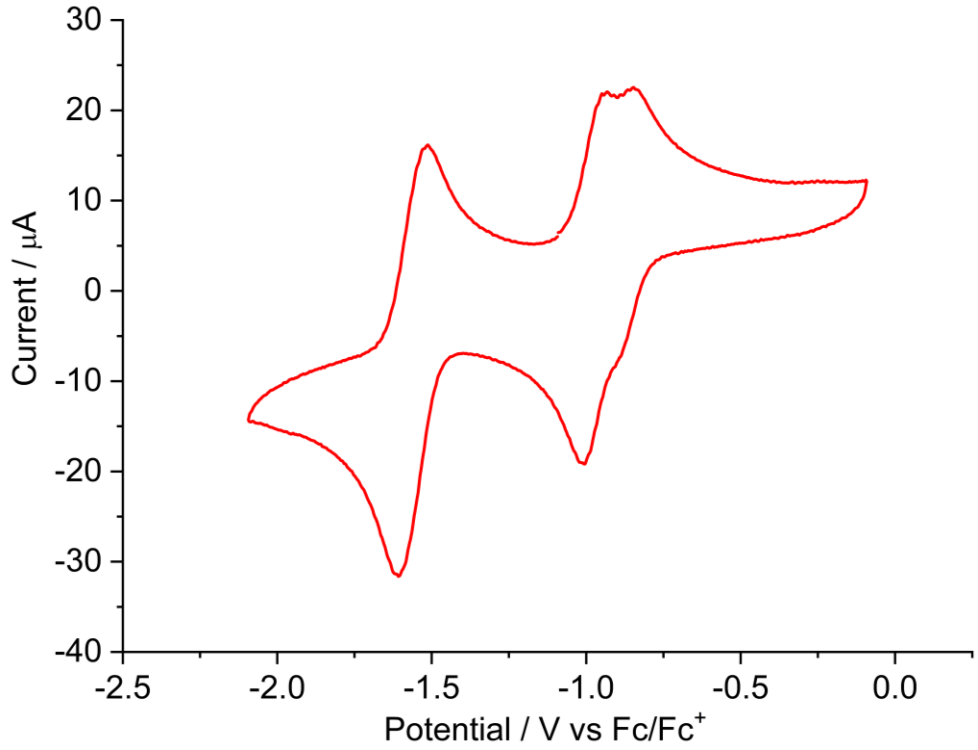


Fig. S97 Cyclic voltammogram of **6^{cy}** in CH_3CN (0.1 M Bu_4NPF_6) at scan rate of 1000 mV/s.

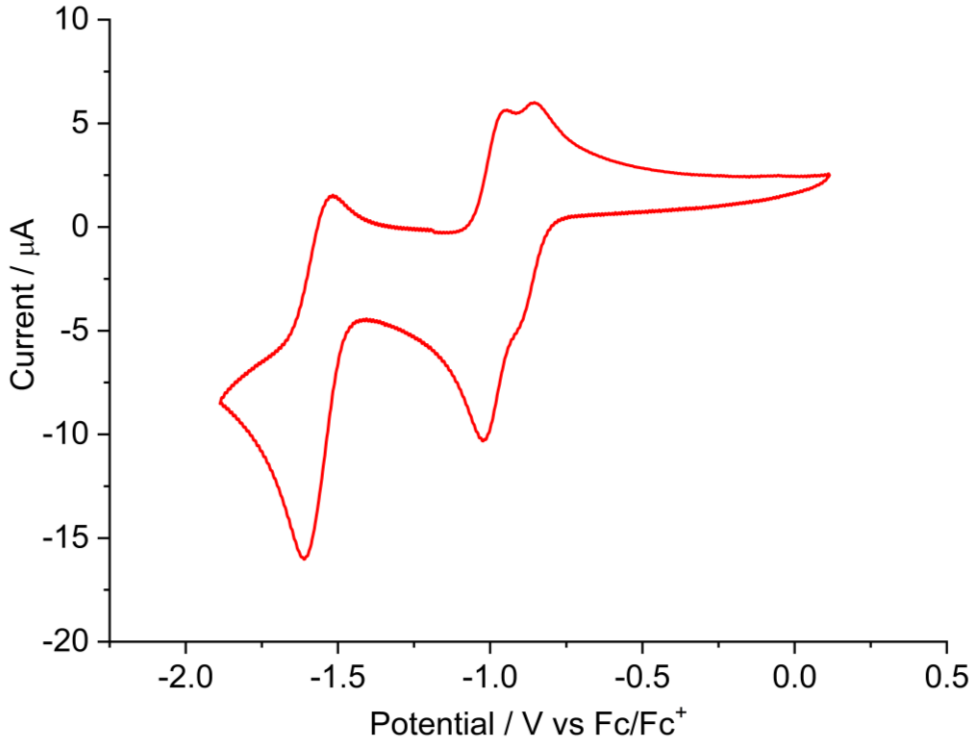


Fig. S98 Cyclic voltammogram of **7^{cy}** in CH_3CN (0.1 M Bu_4NPF_6) at scan rate of 100 mV/s.

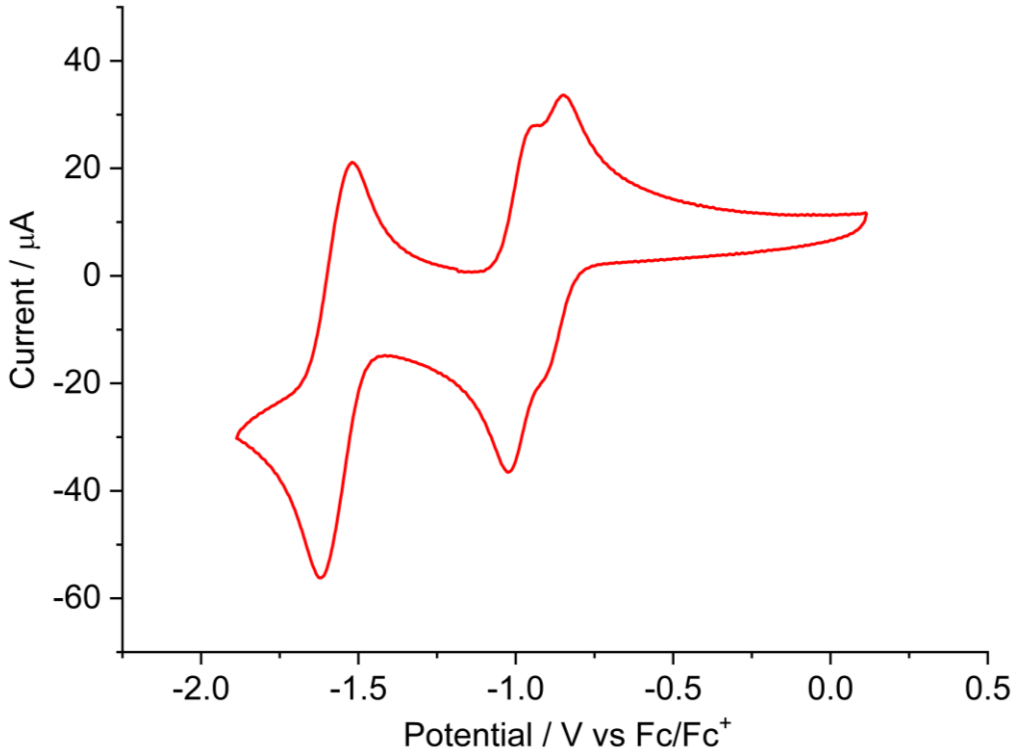


Fig. S99 Cyclic voltammogram of **7^{cy}** in CH_3CN (0.1 M Bu_4NPF_6) at scan rate of 1000 mV/s.

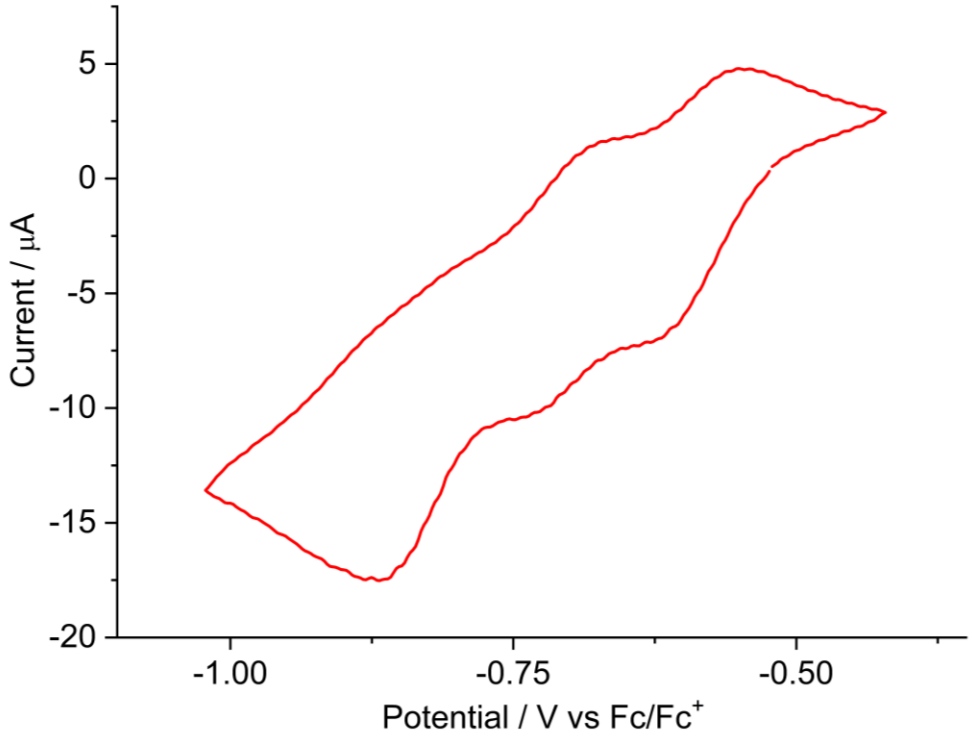


Fig. S100 Cyclic voltammogram of **5^{Et}** in CH_3CN (0.1 M Bu_4NPF_6) at scan rate of 100 mV/s.

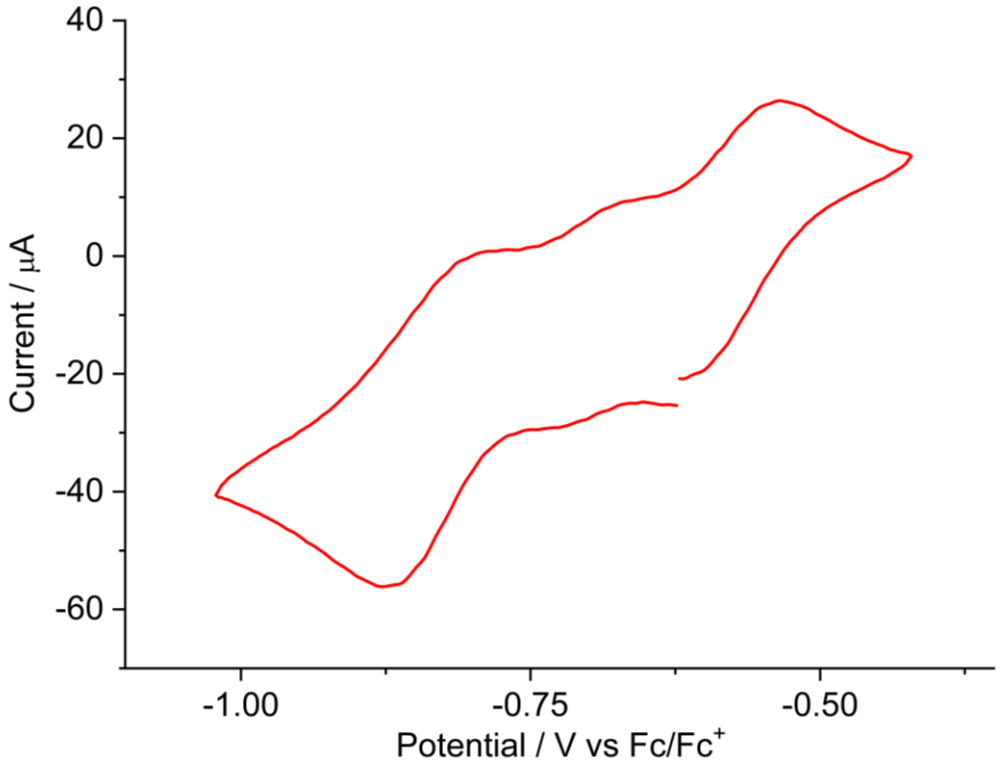


Fig. S101 Cyclic voltammogram of **5^{Et}** in CH_3CN (0.1 M Bu_4NPF_6) at scan rate of 1000 mV/s.

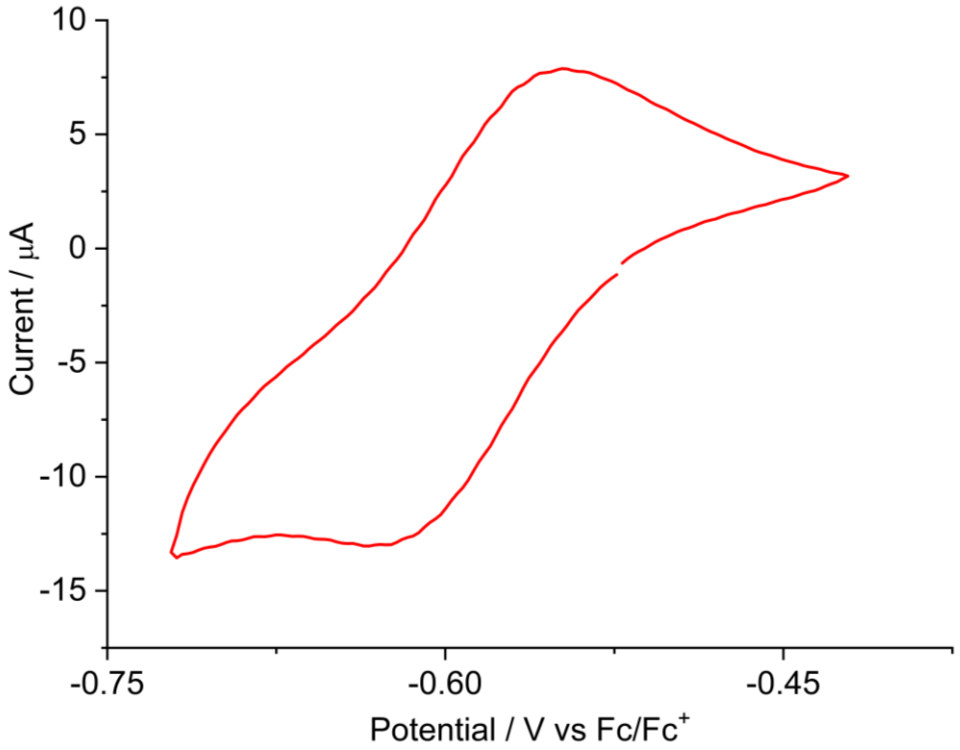


Fig. S102 Cyclic voltammogram of **5^{Et}** in CH_3CN (0.1 M Bu_4NPF_6) at scan rate of 100 mV/s, considering only the first reduction.

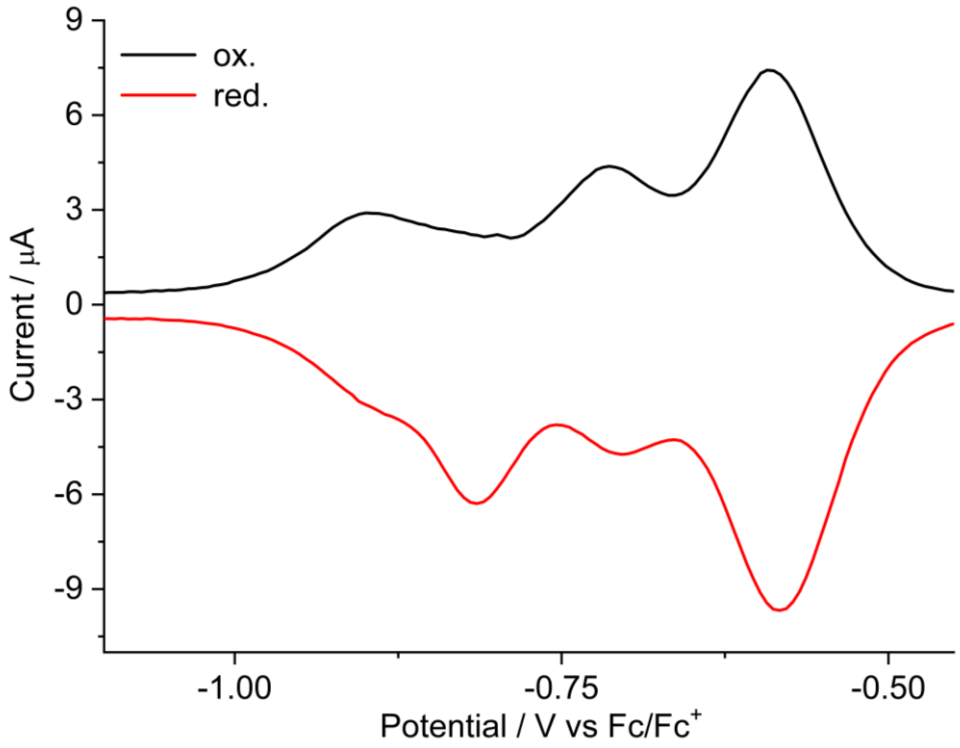


Fig. S103 Differential pulse voltammograms (DPVs) of **5^{Et}** in CH_3CN at scan rate of 10 mV/s with 0.2 M Bu_4NPF_6.

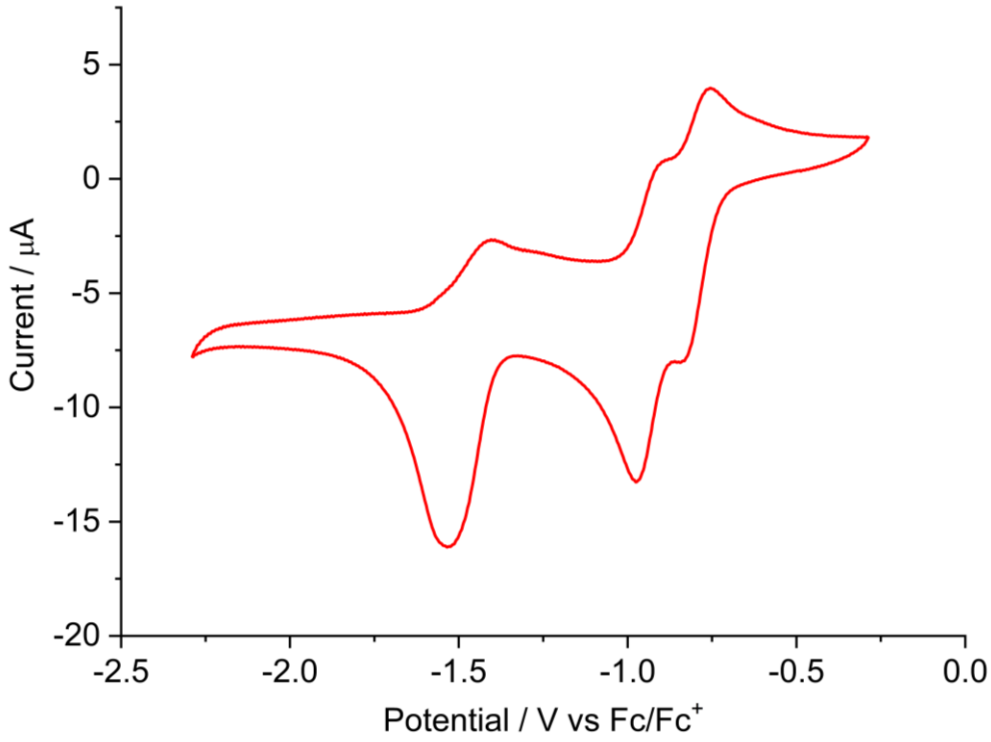


Fig. S104 Cyclic voltammogram of **5^{Pr}** in CH_3CN (0.1 M Bu_4NPF_6) at scan rate of 100 mV/s.

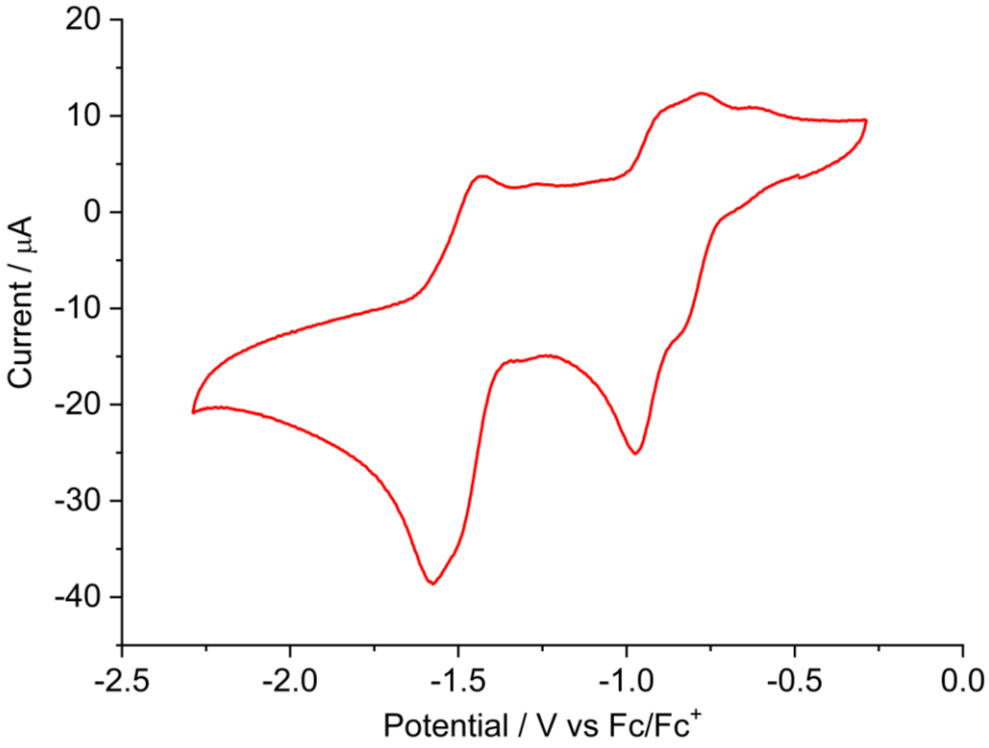


Fig. S105 Cyclic voltammogram of **5^{Pr}** in CH_3CN (0.1 M Bu_4NPF_6) at scan rate of 1000 mV/s.

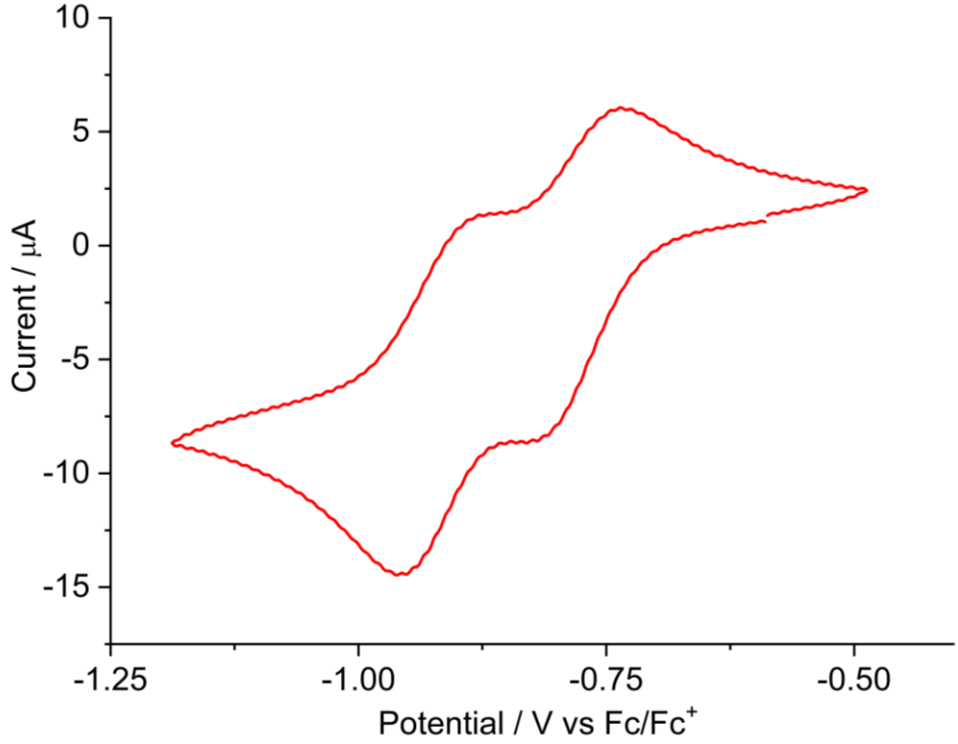


Fig. S106 Cyclic voltammogram of **5^{Pr}** in CH_3CN (0.1 M Bu_4NPF_6) at scan rate of 100 mV/s, considering only the first and second reduction.

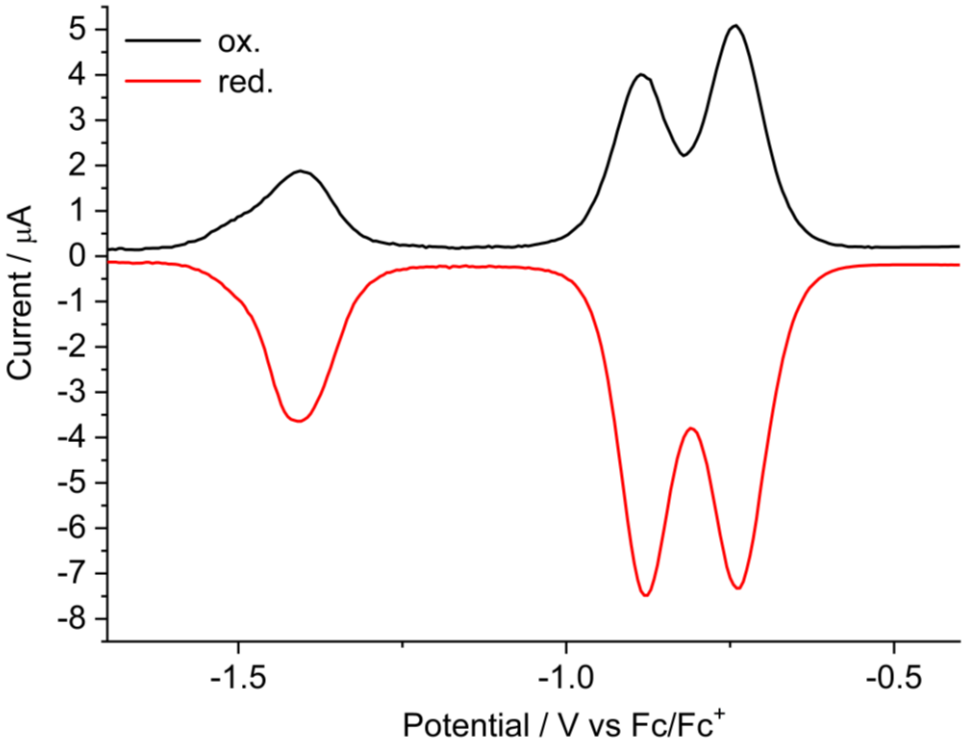


Fig. S107 Differential pulse voltammograms (DPVs) of **5^{Pr}** in CH_3CN at scan rate of 10 mV/s with 0.1 M Bu_4NPF_6.

Quantum Chemical Calculations

The DFT calculations were performed using Gaussian 16 (Revision C.01) suite[S10] of electronic structure Programs. The multireference CASSCF calculations were performed using ORCA–4.2.1.[S11] The geometries of **6^{Cy}** was optimized in the gas phase with ωB97XD, MN12SX, B3LYP-D3, and PBE0 (PBE1PBE) functional and Def2SVP basis-set. To verify the stationary point and to obtain zero-point vibrational energy (ZPVE) corrections, frequency analysis was performed on optimized geometries. The singlet geometries were optimized with spin-unrestricted broken-symmetry (BS) wavefunctions. TD-DFT calculations were performed at MN12SX/Def2SV level on (U)MN12SX/Def2SV optimized geometry. The solvent effect was accounted with polarizable continuum model (PCM) including acetonitrile as the solvent. Multi-reference CASSCF(2,2)/NEVPT2/def2-TZVP provided the adiabatic singlet-triplet energy gap (–0.037 kJmol^{-1}).

Table S16. Summary of calculated exchange coupling for **6^{Cy}**.

DFT[a] functional	E_T[b] / Hartree	S^2(T)	E_{BS}[b] / Hartree	S^2(BS)	J[c] (cm^{-1})	ΔE_{ST}[d] / kJmol^{-1}
ωB97XD	–3656.452216	2.011	–3656.452196	1.010	4.39	0.105
MN12SX	–3654.542102	2.009	–3654.542118	1.008	–3.51	–0.084
B3LYP-D3	–3657.402097	2.008	–3657.402100	1.008	–0.66	–0.015
PBE0	–3653.797912	2.011	–3653.797924	1.008	–2.63	–0.063

[a]Def2SVP basis-set. [b]ZPVE corrections are included. [c]The exchange coupling constant $J = (E_{BS}–E_T)/(S^2(T)–S^2(BS))$. S^2(BS) and S^2(T) are the eigenvalues of the spin operator for broken-symmetry singlet and triplet states, respectively. [d]Energy difference between singlet and triplet state $\Delta E_{ST} = 2J$.[S12]

Table S17. Summary of TD-DFT calculated key low energy transitions of **6^{Cy}**.

Excited singlet state	Wavelength (nm)	Energy (eV)	Major transtions	Contribution	oscillator strength (*f*)
1	680.48	1.8220	233A -> 234A	0.99993	0.0008
2	542.41	2.2858	233B -> 234B	0.99986	0.0005
3	488.16	2.5398	233A -> 235A	0.99545	0.0304
4	414.31	2.9925	232A -> 234A	0.18233	0.0517
			233B -> 236B	0.96927	
HOMO: 133, LUMO: 134					

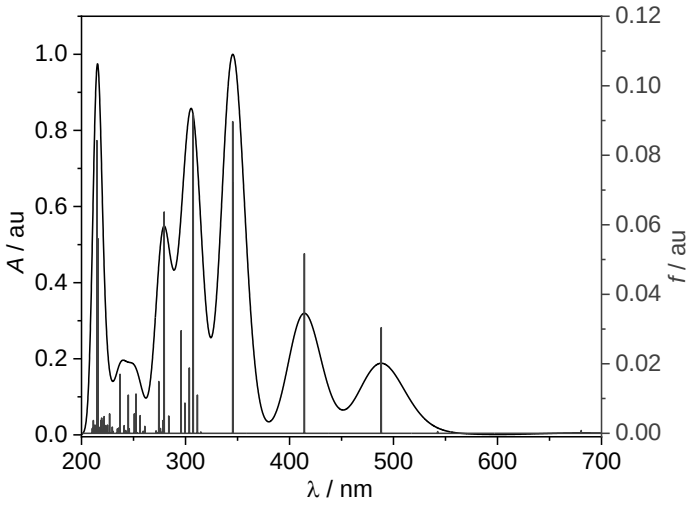


Fig. S108 TD-DFT calculated electronic absorption spectra of **6**^{Cy}. *f* = oscillator strength

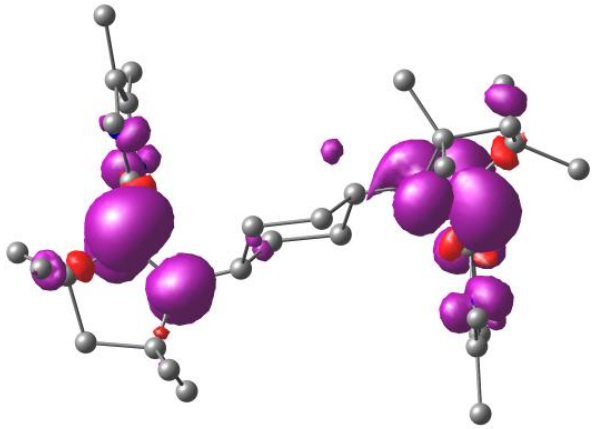


Fig. S109 Spin-density plot of **6^{Cy}** (at isovalue of 0.012 and hydrogens are omitted for clarity).

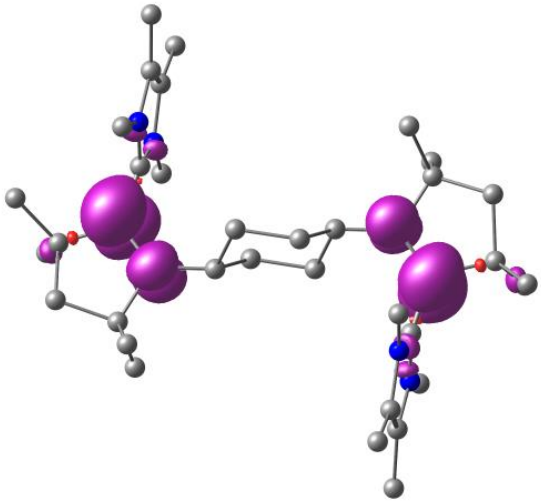


Fig. S110 Spin-density plot of **7^{Cy}** (at isovalue of 0.012 and hydrogens are omitted for clarity).

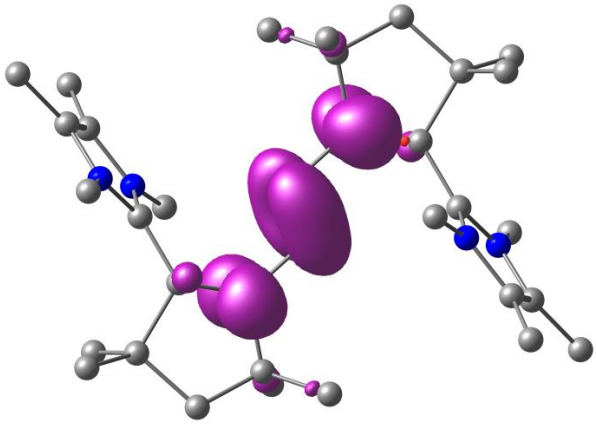


Fig. S111 Spin-density plot of **10^{Et}** (at isovalue of 0.012 and hydrogens are omitted for clarity).

Table S18. Selected frontier molecular orbitals of **4**^{Cy}, **5**^{Cy}, and **7**^{Cy}.

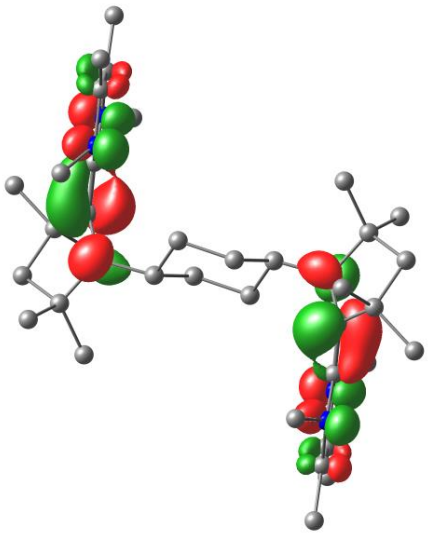
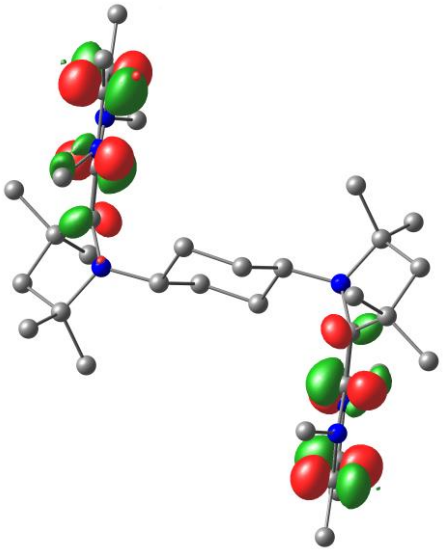
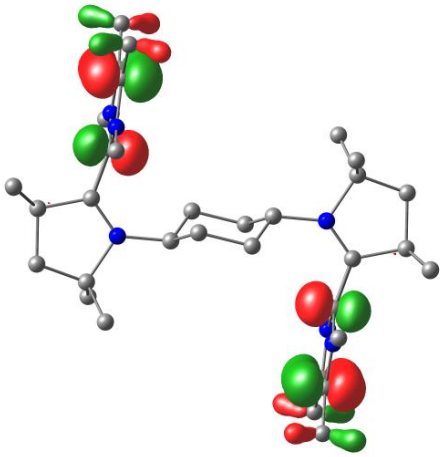
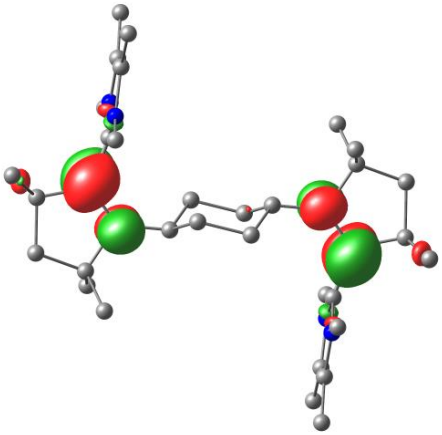
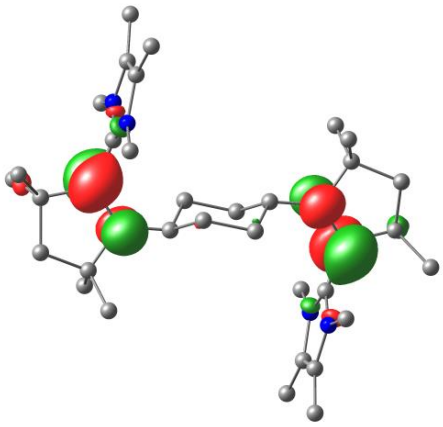
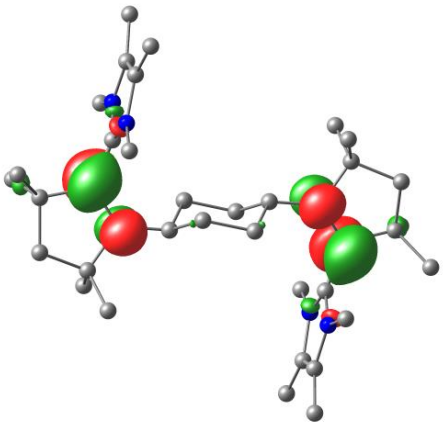
Compound	HOMO	LUMO
4^{Cy}		
5^{Cy}		
7^{Cy}		

Table S19. Selected frontier molecular orbitals of $\mathbf{4}^{Et}$, $\mathbf{5}^{Et}$, $\mathbf{8}^{Et}$, and $\mathbf{9}^{Et}$.

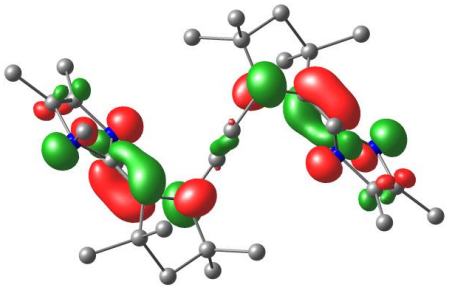
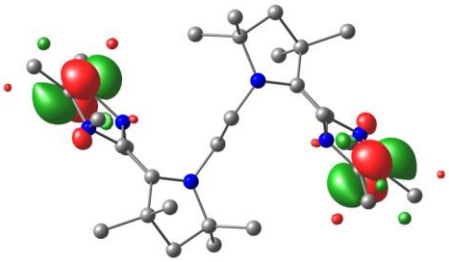
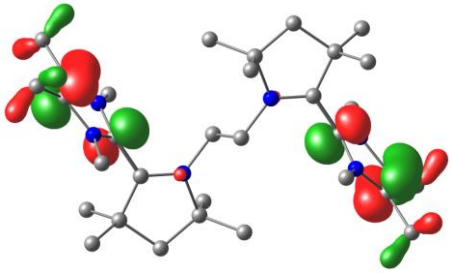
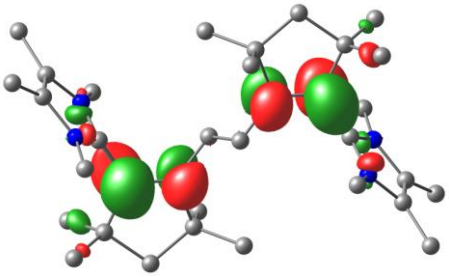
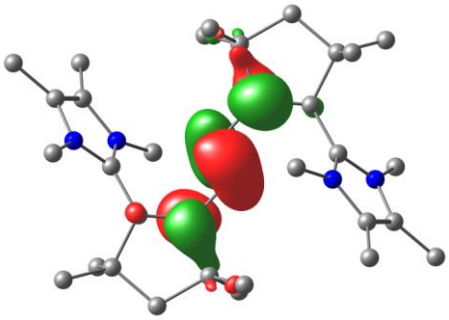
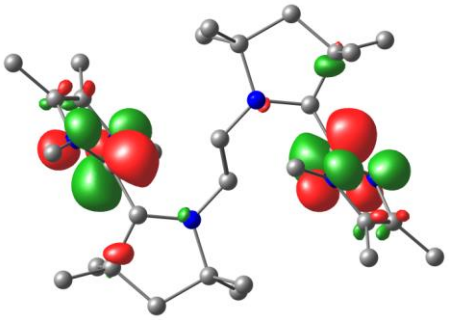
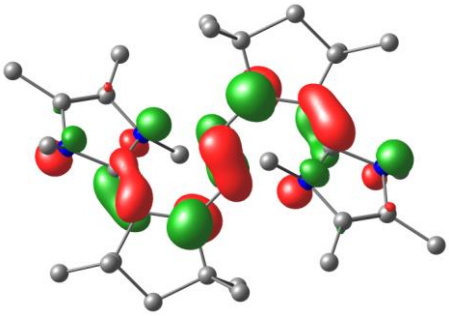
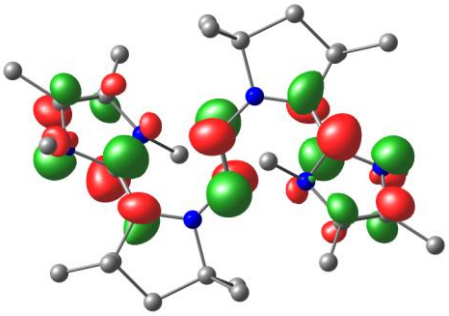
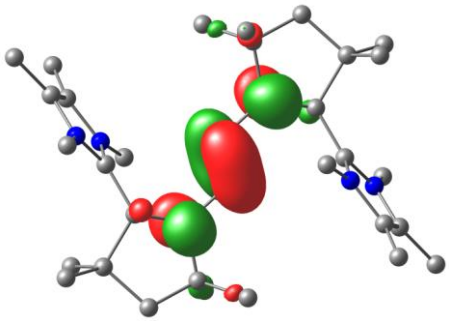
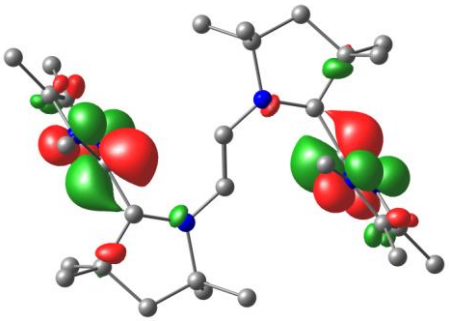
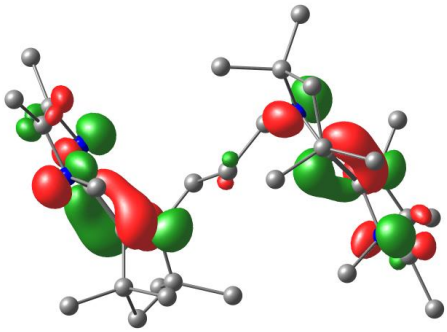
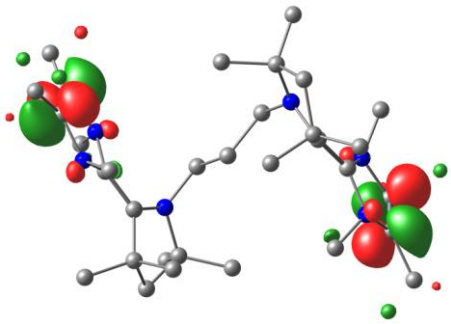
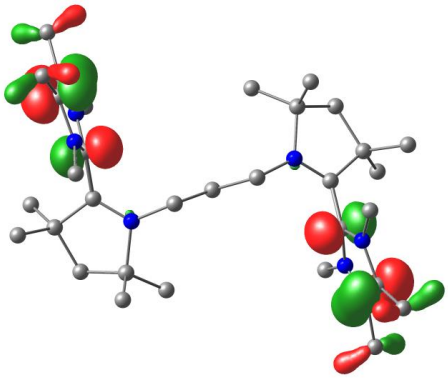
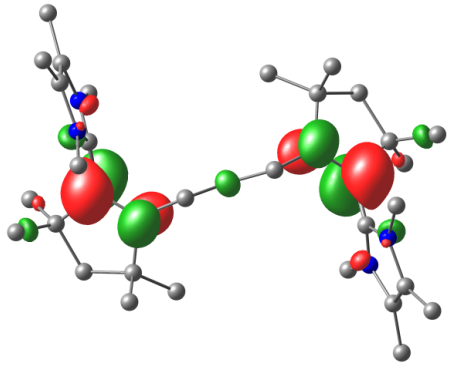
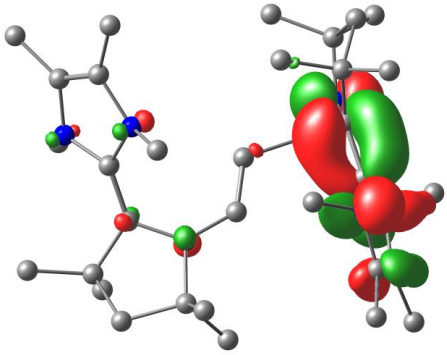
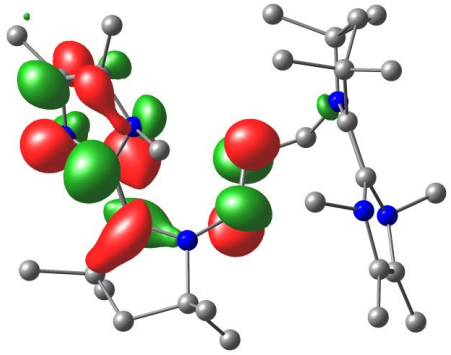
Compound	HOMO	LUMO
$\mathbf{4}^{Et}$		
$\mathbf{5}^{Cy}$		
$\mathbf{8}^{Et}$		
$\mathbf{9}^{Et}$		
$\mathbf{10}^{Et}$		

Table S20. Selected frontier molecular orbitals of $\mathbf{4}^{Pr}$, $\mathbf{5}^{Pr}$, and $\mathbf{9}^{Pr}$.

Compound	HOMO	LUMO
$\mathbf{4}^{Pr}$		
$\mathbf{5}^{Pr}$		
$\mathbf{9}^{Pr}$		

Cartesian Coordinates

6^{Cy}-Broken Symmetry Singlet			
N	-1.652415000	2.551899000	0.527361000
N	-3.982643000	0.380925000	1.223394000
N	-4.449585000	0.727728000	-0.854704000
N	1.820758000	-1.704411000	-1.272195000
N	3.912278000	-0.743569000	0.808133000
N	3.065824000	-2.303463000	2.055533000
C	-0.596989000	1.626481000	0.130070000
C	-0.572143000	0.339516000	0.940552000
H	-1.474720000	-0.266286000	0.746973000
H	-0.559531000	0.574807000	2.019809000
C	0.658297000	-0.487395000	0.601069000
H	0.622038000	-1.413606000	1.195475000
H	1.550389000	0.100767000	0.875934000
C	0.686925000	-0.839171000	-0.884497000
C	0.603141000	0.436069000	-1.723886000
H	0.538085000	0.195336000	-2.794532000
H	1.521030000	1.034959000	-1.578997000
C	-0.614390000	1.274593000	-1.353986000
H	-0.636148000	2.195051000	-1.966529000
H	-1.537043000	0.701493000	-1.584803000
C	-2.973559000	2.438065000	0.171952000
C	-2.667640000	4.557854000	1.141951000
H	-2.896028000	4.433526000	2.216894000
H	-2.691416000	5.639982000	0.928584000
C	-1.288716000	3.948135000	0.856112000
C	-0.568019000	4.631456000	-0.306733000
H	0.420360000	4.181749000	-0.477881000
H	-0.382415000	5.689403000	-0.059047000
H	-1.145816000	4.590666000	-1.242935000
C	-0.384257000	3.986269000	2.085196000
H	-0.836084000	3.429675000	2.924532000
H	-0.235277000	5.031872000	2.402649000
H	0.618538000	3.579971000	1.868331000
C	-3.709169000	1.191636000	0.177315000
C	-5.198618000	-0.362364000	-0.455309000
C	-4.894173000	-0.588987000	0.858852000
C	-3.449414000	0.528419000	2.558141000
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H	-2.852807000	-0.363786000	2.812181000
H	-4.276232000	0.643452000	3.278838000
C	-4.369116000	1.199057000	-2.214657000
H	-3.551148000	1.932647000	-2.283482000
H	-5.312036000	1.675858000	-2.531850000
H	-4.154384000	0.351789000	-2.887167000
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H	-6.640894000	-1.874098000	-0.857729000
H	-5.482555000	-1.619540000	-2.172793000
H	-6.792254000	-0.437092000	-1.898956000
C	-5.382864000	-1.622212000	1.800282000
H	-6.153782000	-2.239717000	1.318884000
H	-5.830018000	-1.169716000	2.702323000
H	-4.557432000	-2.283542000	2.113395000
C	2.524161000	-2.460693000	-0.362654000
C	2.948081000	-3.808770000	-0.921639000
C	2.884076000	-3.464536000	-2.416515000
H	3.870301000	-3.073985000	-2.728984000
H	2.666204000	-4.341234000	-3.050591000
C	1.835392000	-2.352154000	-2.612034000
C	2.011414000	-4.977167000	-0.581691000
H	0.950728000	-4.733137000	-0.727060000
H	2.125049000	-5.292102000	0.468238000
H	2.272683000	-5.848237000	-1.208749000
C	4.369710000	-4.176947000	-0.500728000
H	4.701773000	-5.095770000	-1.014039000
H	4.432538000	-4.371460000	0.584732000
H	5.087967000	-3.373348000	-0.741228000
C	2.356222000	-1.427125000	-3.720846000
H	1.596220000	-0.747192000	-4.130426000

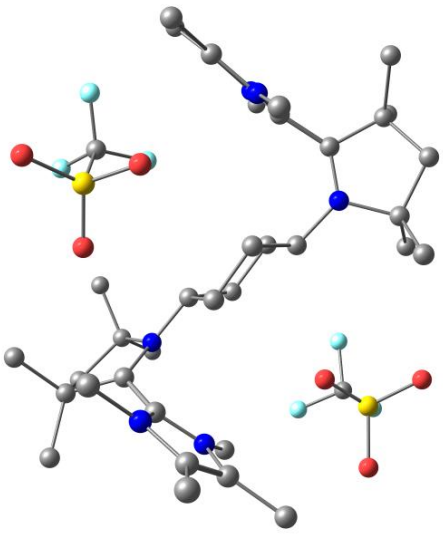
DFT level: UMN12SX/def2SVP

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 1.006427
(Hartree/Particle)
Thermal correction to Energy= 1.069835
Thermal correction to Enthalpy= 1.070780
Thermal correction to Gibbs Free Energy= 0.910995
Sum of electronic and zero-point Energies= -3654.542118
Sum of electronic and thermal Energies= -3654.478709
Sum of electronic and thermal Enthalpies= -3654.477765
Sum of electronic and thermal Free Energies= -3654.637550

Charge = 0 Multiplicity = 1



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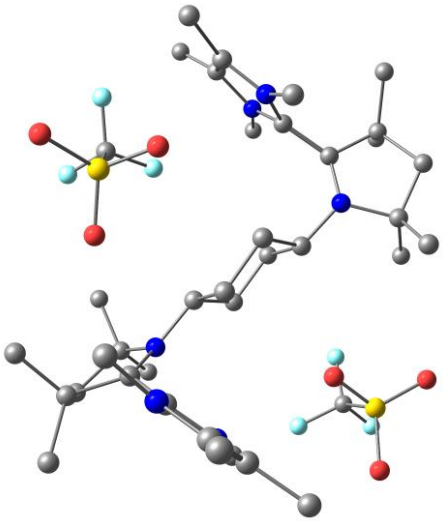
H	3.207923000	-0.823897000	-3.363745000	
C	0.458894000	-2.899342000	-2.990959000	
H	0.028428000	-3.528171000	-2.195431000	
H	0.539305000	-3.497808000	-3.913243000	
H	-0.257307000	-2.085207000	-3.195990000	
C	3.148540000	-1.858669000	0.782500000	
C	4.296784000	-0.465211000	2.104999000	
C	3.773208000	-1.455988000	2.891270000	
C	4.367579000	-0.039679000	-0.370858000	
H	5.098183000	-0.661851000	-0.918836000	
H	4.825257000	0.915840000	-0.079051000	
H	3.516240000	0.182213000	-1.027520000	
C	2.209348000	-3.381928000	2.489017000	
H	2.769932000	-4.327233000	2.598193000	
H	1.393223000	-3.518903000	1.756602000	
H	1.765975000	-3.126871000	3.463820000	
C	5.130181000	0.706386000	2.455796000	
H	6.142015000	0.636764000	2.019372000	
H	5.240025000	0.784135000	3.546250000	
H	4.681431000	1.639626000	2.077155000	
C	3.854800000	-1.672981000	4.354251000	
H	2.876556000	-1.547877000	4.852231000	
H	4.547206000	-0.949821000	4.807340000	
H	4.222396000	-2.684794000	4.598315000	
C	-3.707651000	3.767093000	0.322169000	
C	-5.014951000	3.610598000	1.101280000	
H	-5.487692000	4.593086000	1.273789000	
H	-4.845923000	3.142037000	2.086378000	
H	-5.744337000	2.989837000	0.549491000	
C	-4.030902000	4.440011000	-1.019565000	
H	-3.159389000	4.491842000	-1.689805000	
H	-4.394784000	5.470214000	-0.856504000	
H	-4.831958000	3.897420000	-1.550568000	
H	0.354802000	2.148823000	0.327866000	
H	-0.233789000	-1.430653000	-1.064184000	
S	3.336327000	3.428534000	0.188949000	
O	2.671317000	4.670941000	0.552661000	
O	4.771480000	3.337366000	0.448460000	
O	2.590018000	2.201737000	0.527999000	
C	3.269354000	3.445233000	-1.662421000	
F	3.892757000	4.497889000	-2.155892000	
F	3.836343000	2.352212000	-2.174187000	
F	2.008873000	3.470465000	-2.099339000	
S	-1.932579000	-3.425016000	0.862818000	
O	-2.290289000	-2.270420000	1.695571000	
O	-2.467885000	-4.702713000	1.289982000	
O	-0.542897000	-3.421973000	0.391857000	
C	-2.869176000	-3.090900000	-0.703999000	
F	-2.500397000	-3.908120000	-1.677157000	
F	-2.679709000	-1.837245000	-1.142065000	
F	-4.178198000	-3.243626000	-0.517599000	
6^{Cy}-Triplet				DFT level: UMN12SX/def2SVP
N	-1.652064000	2.552174000	0.527845000	- Thermochemistry -
N	-3.982843000	0.381539000	1.223230000	----------
N	-4.449125000	0.728477000	-0.854989000	Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
N	1.820404000	-1.704918000	-1.272015000	
N	3.912310000	-0.743905000	0.808007000	Zero-point correction= 1.006428
N	3.065578000	-2.303482000	2.055614000	(Hartree/Particle)
C	-0.596699000	1.626573000	0.130517000	Thermal correction to Energy= 1.069836
C	-0.572433000	0.339414000	0.940604000	Thermal correction to Enthalpy= 1.070780
H	-1.475028000	-0.266168000	0.746414000	Thermal correction to Gibbs Free Energy= 0.909965
H	-0.560309000	0.574346000	2.019951000	Sum of electronic and zero-point Energies= -3654.542102
C	0.658028000	-0.487625000	0.601420000	Sum of electronic and thermal Energies= -3654.478693
H	0.621510000	-1.413836000	1.195780000	Sum of electronic and thermal Enthalpies= -3654.477749
H	1.550114000	0.100441000	0.876557000	Sum of electronic and thermal Free Energies= -3654.638564
C	0.686878000	-0.839226000	-0.884184000	
C	0.603836000	0.436276000	-1.723252000	Charge = 0 Multiplicity = 3
H	0.539299000	0.196035000	-2.794039000	
H	1.521799000	1.034811000	-1.577563000	

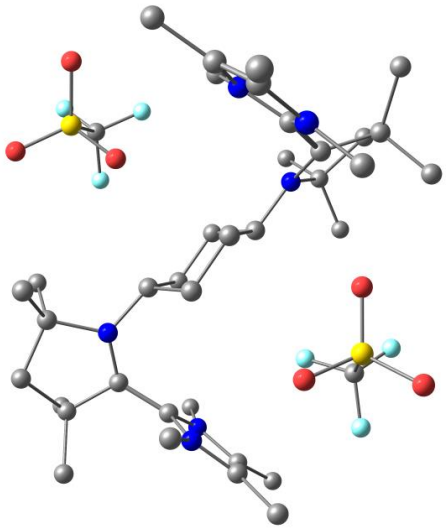
C	-0.613577000	1.275172000	-1.353656000
H	-0.634645000	2.195821000	-1.965925000
H	-1.536333000	0.702547000	-1.585177000
C	-2.973182000	2.438590000	0.172197000
C	-2.666960000	4.558412000	1.142039000
H	-2.895307000	4.434256000	2.217010000
H	-2.690579000	5.640515000	0.928529000
C	-1.288146000	3.948454000	0.856213000
C	-0.567498000	4.631431000	-0.306860000
H	0.420714000	4.181407000	-0.478163000
H	-0.381535000	5.689355000	-0.059342000
H	-1.145519000	4.590690000	-1.242928000
C	-0.383592000	3.986788000	2.085216000
H	-0.835388000	3.430362000	2.924677000
H	-0.234549000	5.032446000	2.402453000
H	0.619177000	3.580428000	1.868365000
C	-3.708950000	1.192250000	0.177263000
C	-5.198301000	-0.361621000	-0.455896000
C	-4.894347000	-0.588270000	0.858376000
C	-3.449876000	0.528843000	2.558103000
H	-2.811672000	1.423492000	2.588607000
H	-2.853409000	-0.363455000	2.812157000
H	-4.276828000	0.643875000	3.278647000
C	-4.368243000	1.199873000	-2.214897000
H	-3.550429000	1.933661000	-2.283390000
H	-5.311159000	1.676453000	-2.532429000
H	-4.153052000	0.352672000	-2.887348000
C	-6.070510000	-1.101818000	-1.394840000
H	-6.640409000	-1.873367000	-0.858821000
H	-5.481758000	-1.618632000	-2.173586000
H	-6.791573000	-0.436272000	-1.899951000
C	-5.383458000	-1.621432000	1.799659000
H	-6.154169000	-2.238966000	1.317968000
H	-5.830991000	-1.168867000	2.701477000
H	-4.558154000	-2.282747000	2.113138000
C	2.524012000	-2.461082000	-0.362536000
C	2.947697000	-3.809307000	-0.921321000
C	2.883160000	-3.465440000	-2.416245000
H	3.869264000	-3.074923000	-2.729139000
H	2.665091000	-4.342283000	-3.050051000
C	1.834410000	-2.353120000	-2.611675000
C	2.011178000	-4.977629000	-0.580725000
H	0.950433000	-4.733609000	-0.725673000
H	2.125311000	-5.292381000	0.469206000
H	2.272142000	-5.848824000	-1.207737000
C	4.369470000	-4.177363000	-0.500789000
H	4.701346000	-5.096361000	-1.013910000
H	4.432654000	-4.371512000	0.584718000
H	5.087646000	-3.373845000	-0.741799000
C	2.354760000	-1.428555000	-3.721103000
H	1.594381000	-0.749207000	-4.130958000
H	2.710277000	-2.048723000	-4.562388000
H	3.206277000	-0.824767000	-3.364511000
C	0.457742000	-2.900389000	-2.989869000
H	0.027490000	-3.528847000	-2.193937000
H	0.537811000	-3.499233000	-3.911939000
H	-0.258442000	-2.086270000	-3.195032000
C	3.148477000	-1.858946000	0.782495000
C	4.296769000	-0.465385000	2.104844000
C	3.773043000	-1.455982000	2.891244000
C	4.367883000	-0.040276000	-0.371042000
H	5.099042000	-0.662323000	-0.918417000
H	4.824993000	0.915560000	-0.079380000
H	3.516760000	0.180964000	-1.028200000
C	2.208836000	-3.381678000	2.489270000
H	2.769271000	-4.327020000	2.598885000
H	1.392851000	-3.518788000	1.756727000
H	1.765288000	-3.126220000	3.463889000
C	5.130332000	0.706138000	2.455493000
H	6.142210000	0.636214000	2.019221000



H	5.240037000	0.784119000	3.545943000
H	4.681812000	1.639369000	2.076561000
C	3.854620000	-1.672813000	4.354253000
H	2.876399000	-1.547536000	4.852232000
H	4.547124000	-0.949688000	4.807248000
H	4.222091000	-2.684649000	4.598413000
C	-3.707128000	3.767696000	0.322416000
C	-5.014344000	3.611320000	1.101708000
H	-5.486987000	4.593849000	1.274258000
H	-4.845213000	3.142765000	2.086790000
H	-5.743845000	2.990604000	0.550020000
C	-4.030534000	4.440594000	-1.019286000
H	-3.159111000	4.492399000	-1.689650000
H	-4.394360000	5.470811000	-0.856187000
H	-4.831689000	3.898026000	-1.550164000
H	0.355147000	2.148641000	0.328785000
H	-0.234046000	-1.430331000	-1.064050000
S	3.336769000	3.428315000	0.188521000
O	2.671793000	4.670783000	0.552087000
O	4.771916000	3.337131000	0.448076000
O	2.590419000	2.201563000	0.527670000
C	3.269836000	3.444843000	-1.662856000
F	3.893588000	4.497241000	-2.156437000
F	3.836473000	2.351577000	-2.174484000
F	2.009363000	3.470453000	-2.099783000
S	-1.933100000	-3.424865000	0.862979000
O	-2.291044000	-2.270181000	1.695518000
O	-2.468241000	-4.702576000	1.290301000
O	-0.543395000	-3.421727000	0.392071000
C	-2.869610000	-3.091056000	-0.703934000
F	-2.500993000	-3.908640000	-1.676849000
F	-2.679849000	-1.837581000	-1.142361000
F	-4.178676000	-3.243445000	-0.517493000

6^{Cy}-Broken Symmetry Singlet				DFT level: UwB97XD/def2SVP
N	1.726536000	2.537535000	-0.505644000	- Thermochemistry -
N	4.017361000	0.315122000	-1.172605000	----------
N	4.437354000	0.646055000	0.919379000	Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
N	-1.873257000	-1.626386000	1.286176000	
N	-3.928779000	-0.674621000	-0.832141000	Zero-point correction= 1.010443
N	-3.070236000	-2.249279000	-2.055685000	(Hartree/Particle)
C	0.653768000	1.633258000	-0.100634000	Thermal correction to Energy= 1.073751
C	0.566775000	0.366381000	-0.944199000	Thermal correction to Enthalpy= 1.074695
H	1.451314000	-0.271902000	-0.803084000	Thermal correction to Gibbs Free Energy= 0.914396
H	0.522828000	0.634179000	-2.010649000	Sum of electronic and zero-point Energies= -3656.452196
C	-0.679875000	-0.437783000	-0.587563000	Sum of electronic and thermal Energies= -3656.388888
H	-0.667923000	-1.353356000	-1.188305000	Sum of electronic and thermal Enthalpies= -3656.387944
H	-1.560436000	0.169657000	-0.835144000	Sum of electronic and thermal Free Energies= -3656.548243
C	-0.695383000	-0.814969000	0.895924000	
C	-0.540320000	0.439696000	1.762292000	Charge = 0 Multiplicity = 1
H	-0.448226000	0.168697000	2.820568000	
H	-1.438850000	1.065263000	1.660411000	
C	0.695641000	1.253104000	1.377846000	
H	0.749522000	2.160699000	1.998860000	
H	1.599701000	0.653014000	1.581687000	
C	3.049891000	2.405864000	-0.155647000	
C	2.789114000	4.501297000	-1.205051000	
H	3.015934000	4.343038000	-2.271482000	
H	2.832095000	5.584131000	-1.019185000	
C	1.394000000	3.925834000	-0.901784000	
C	0.682978000	4.676533000	0.231391000	
H	-0.319198000	4.270541000	0.406732000	
H	0.544521000	5.729975000	-0.050930000	
H	1.252678000	4.637947000	1.169880000	
C	0.497556000	3.922607000	-2.142385000	
H	0.950969000	3.327158000	-2.950206000	
H	0.359933000	4.953232000	-2.501627000	
H	-0.502649000	3.528094000	-1.913007000	
C	3.751840000	1.136084000	-0.135754000	
C	5.150111000	-0.479253000	0.543002000	
C	4.878791000	-0.692331000	-0.779708000	

C	3.498665000	0.466256000	-2.519295000
H	2.864019000	1.358034000	-2.550141000
H	2.903512000	-0.424193000	-2.762962000
H	4.332663000	0.576954000	-3.225933000
C	4.353306000	1.152001000	2.272810000
H	3.578921000	1.927542000	2.300950000
H	5.313215000	1.581652000	2.591539000
H	4.075731000	0.335293000	2.952625000
C	5.973070000	-1.254822000	1.509017000
H	6.516244000	-2.050764000	0.986731000
H	5.341445000	-1.735158000	2.271647000
H	6.708922000	-0.616025000	2.020565000
C	5.345103000	-1.752721000	-1.712057000
H	6.061093000	-2.412275000	-1.208235000
H	5.839441000	-1.319522000	-2.594934000
H	4.486065000	-2.355013000	-2.041739000
C	-2.583895000	-2.387077000	0.381872000
C	-3.026864000	-3.721202000	0.959654000
C	-2.993194000	-3.351894000	2.454095000
H	-3.982618000	-2.964523000	2.743622000
H	-2.779374000	-4.216612000	3.099219000
C	-1.945538000	-2.232765000	2.646023000
C	-2.064025000	-4.883684000	0.650454000
H	-1.012331000	-4.593490000	0.755879000
H	-2.187538000	-5.235328000	-0.383440000
H	-2.282452000	-5.734044000	1.316072000
C	-4.442058000	-4.106081000	0.516057000
H	-4.772913000	-5.017402000	1.037711000
H	-4.480523000	-4.313960000	-0.564719000
H	-5.166808000	-3.305741000	0.732595000
C	-2.492977000	-1.250013000	3.694131000
H	-1.754339000	-0.512210000	4.028271000
H	-2.815623000	-1.815544000	4.582389000
H	-3.363162000	-0.706617000	3.298638000
C	-0.590478000	-2.791634000	3.096207000
H	-0.179197000	-3.495733000	2.361720000
H	-0.710761000	-3.316016000	4.055460000
H	0.150989000	-1.994168000	3.247068000
C	-3.174489000	-1.794092000	-0.789387000
C	-4.286227000	-0.398967000	-2.139979000
C	-3.755861000	-1.397626000	-2.909812000
C	-4.374573000	0.053748000	0.342237000
H	-5.132500000	-0.536993000	0.878027000
H	-4.784081000	1.023496000	0.041345000
H	-3.520780000	0.236403000	0.999772000
C	-2.223451000	-3.352956000	-2.468112000
H	-2.802545000	-4.284263000	-2.552212000
H	-1.407436000	-3.482239000	-1.740440000
H	-1.780547000	-3.120987000	-3.444180000
C	-5.113647000	0.779063000	-2.515048000
H	-6.146138000	0.677316000	-2.145880000
H	-5.151374000	0.883548000	-3.606214000
H	-4.704559000	1.704235000	-2.083089000
C	-3.813124000	-1.620440000	-4.380816000
H	-2.822399000	-1.513033000	-4.850281000
H	-4.482260000	-0.886410000	-4.845761000
H	-4.193811000	-2.624525000	-4.622567000
C	3.813254000	3.713396000	-0.356249000
C	5.126815000	3.509405000	-1.122941000
H	5.610166000	4.478328000	-1.322293000
H	4.956824000	3.012599000	-2.090006000
H	5.838991000	2.897288000	-0.545856000
C	4.133475000	4.424062000	0.971843000
H	3.242207000	4.535950000	1.603189000
H	4.543942000	5.428552000	0.781285000
H	4.888320000	3.864548000	1.545239000
H	-0.284144000	2.180927000	-0.261363000
H	0.187357000	-1.457410000	1.046285000
S	-3.212649000	3.474984000	-0.200799000
O	-2.596740000	4.737743000	-0.596519000



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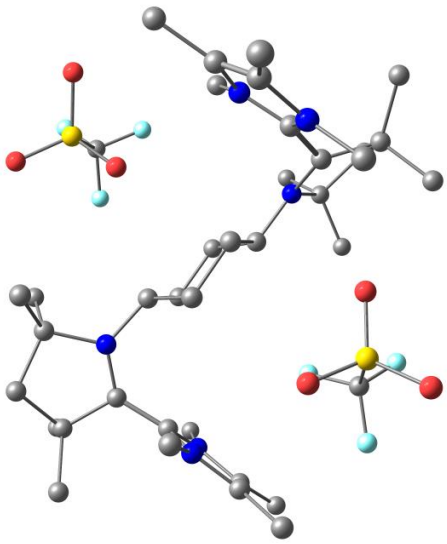
C	-3.161216000	3.539211000	1.659501000	
F	-3.814104000	4.594047000	2.121014000	
F	-3.708515000	2.444815000	2.201563000	
F	-1.900119000	3.605735000	2.102939000	
S	1.828866000	-3.461382000	-0.941522000	
O	2.279107000	-2.269411000	-1.682281000	
O	2.313207000	-4.736320000	-1.447083000	
O	0.414479000	-3.413821000	-0.535445000	
C	2.704655000	-3.289932000	0.695056000	
F	2.250136000	-4.169729000	1.579641000	
F	2.542241000	-2.065146000	1.225550000	
F	4.017427000	-3.486509000	0.559809000	
6^{Cy}-Triplet				DFT level: UwB97XD/def2SVP
N	1.726539000	2.537574000	-0.505802000	- Thermochemistry -
N	4.017541000	0.315303000	-1.172531000	----------
N	4.437265000	0.646236000	0.919505000	Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
N	-1.873178000	-1.626496000	1.286177000	
N	-3.928966000	-0.674843000	-0.831979000	Zero-point correction= 1.010415
N	-3.070210000	-2.249331000	-2.055596000	(Hartree/Particle)
C	0.653786000	1.633230000	-0.100780000	Thermal correction to Energy= 1.073737
C	0.567014000	0.366248000	-0.944159000	Thermal correction to Enthalpy= 1.074681
H	1.451528000	-0.272001000	-0.802724000	Thermal correction to Gibbs Free Energy= 0.913275
H	0.523353000	0.633853000	-2.010670000	Sum of electronic and zero-point Energies= -3656.452216
C	-0.679718000	-0.437900000	-0.587711000	Sum of electronic and thermal Energies= -3656.388895
H	-0.667654000	-1.353483000	-1.188419000	Sum of electronic and thermal Enthalpies= -3656.387950
H	-1.560247000	0.169531000	-0.835446000	Sum of electronic and thermal Free Energies= -3656.549356
C	-0.695396000	-0.814948000	0.895810000	
C	-0.540622000	0.439869000	1.762026000	Charge = 0 Multiplicity = 3
H	-0.448797000	0.169105000	2.820384000	
H	-1.439155000	1.065348000	1.659732000	
C	0.695371000	1.253336000	1.377766000	
H	0.748979000	2.161035000	1.998652000	
H	1.599454000	0.653402000	1.581954000	
C	3.049885000	2.406013000	-0.155713000	
C	2.788925000	4.501499000	-1.204994000	
H	3.015699000	4.343368000	-2.271453000	
H	2.831827000	5.584318000	-1.019023000	
C	1.393872000	3.925904000	-0.901712000	
C	0.682854000	4.676416000	0.231598000	
H	-0.319229000	4.270236000	0.407061000	
H	0.544164000	5.729841000	-0.050668000	
H	1.252688000	4.637916000	1.170008000	
C	0.497354000	3.922772000	-2.142263000	
H	0.950695000	3.327340000	-2.950134000	
H	0.359758000	4.953419000	-2.501449000	
H	-0.502859000	3.528303000	-1.912845000	
C	3.751900000	1.136271000	-0.135728000	
C	5.150121000	-0.479036000	0.543201000	
C	4.878958000	-0.692123000	-0.779540000	
C	3.498864000	0.466357000	-2.519240000	
H	2.864308000	1.358197000	-2.550160000	
H	2.903619000	-0.424065000	-2.762806000	
H	4.332867000	0.576922000	-3.225891000	
C	4.352990000	1.152121000	2.272942000	
H	3.578538000	1.927599000	2.301006000	
H	5.312816000	1.581845000	2.591821000	
H	4.075399000	0.335357000	2.952683000	
C	5.972963000	-1.254599000	1.509320000	
H	6.516287000	-2.050473000	0.987088000	
H	5.341231000	-1.735026000	2.271804000	
H	6.708678000	-0.615780000	2.021039000	
C	5.345413000	-1.752505000	-1.711830000	
H	6.061285000	-2.412093000	-1.207888000	
H	5.839933000	-1.319300000	-2.594603000	
H	4.486424000	-2.354776000	-2.041672000	
C	-2.583846000	-2.387227000	0.381927000	
C	-3.026624000	-3.721430000	0.959691000	
C	-2.992805000	-3.352178000	2.454127000	



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C	-2.063721000	-4.883821000	0.650329000	
H	-1.012035000	-4.593527000	0.755557000	
H	-2.187393000	-5.235488000	-0.383536000	
H	-2.281932000	-5.734199000	1.315997000	
C	-4.441840000	-4.106422000	0.516265000	
H	-4.772538000	-5.017793000	1.037928000	
H	-4.480439000	-4.314264000	-0.564514000	
H	-5.166634000	-3.306158000	0.732935000	
C	-2.492539000	-1.250449000	3.694336000	
H	-1.753777000	-0.512886000	4.028742000	
H	-2.815339000	-1.816173000	4.582415000	
H	-3.362600000	-0.706772000	3.298957000	
C	-0.590005000	-2.791792000	3.095896000	
H	-0.178748000	-3.495761000	2.361276000	
H	-0.710090000	-3.316290000	4.055109000	
H	0.151385000	-1.994250000	3.246741000	
C	-3.174535000	-1.794229000	-0.789272000	
C	-4.286479000	-0.399205000	-2.139796000	
C	-3.755950000	-1.397740000	-2.909683000	
C	-4.374923000	0.053424000	0.342406000	
H	-5.133056000	-0.537284000	0.877938000	
H	-4.784228000	1.023272000	0.041554000	
H	-3.521248000	0.235864000	1.000156000	
C	-2.223344000	-3.352930000	-2.468077000	
H	-2.802372000	-4.284277000	-2.552193000	
H	-1.407292000	-3.482161000	-1.740436000	
H	-1.780497000	-3.120896000	-3.444154000	
C	-5.114082000	0.778704000	-2.514819000	
H	-6.146530000	0.676841000	-2.145562000	
H	-5.151922000	0.883155000	-3.605985000	
H	-4.705070000	1.703945000	-2.082931000	
C	-3.813176000	-1.620486000	-4.380699000	
H	-2.822456000	-1.512967000	-4.850149000	
H	-4.482373000	-0.886492000	-4.845613000	
H	-4.193773000	-2.624591000	-4.622502000	
C	3.813173000	3.713593000	-0.356316000	
C	5.126666000	3.509680000	-1.123134000	
H	5.609929000	4.478632000	-1.322559000	
H	4.956592000	3.012832000	-2.090163000	
H	5.838944000	2.897624000	-0.546112000	
C	4.133496000	4.424235000	0.971773000	
H	3.242362000	4.535744000	1.603374000	
H	4.543569000	5.428889000	0.781227000	
H	4.888692000	3.864923000	1.544902000	
H	-0.284123000	2.180818000	-0.261777000	
H	0.187423000	-1.457248000	1.046322000	
S	-3.212855000	3.474802000	-0.200845000	
O	-2.596895000	4.737473000	-0.596761000	
O	-4.645997000	3.319124000	-0.479865000	
O	-2.414188000	2.268034000	-0.508931000	
C	-3.161498000	3.539331000	1.659443000	
F	-3.814595000	4.594122000	2.120764000	
F	-3.708633000	2.444912000	2.201629000	
F	-1.900435000	3.606143000	2.102914000	
S	1.829060000	-3.461290000	-0.941671000	
O	2.279320000	-2.269312000	-1.682406000	
O	2.313429000	-4.736223000	-1.447215000	
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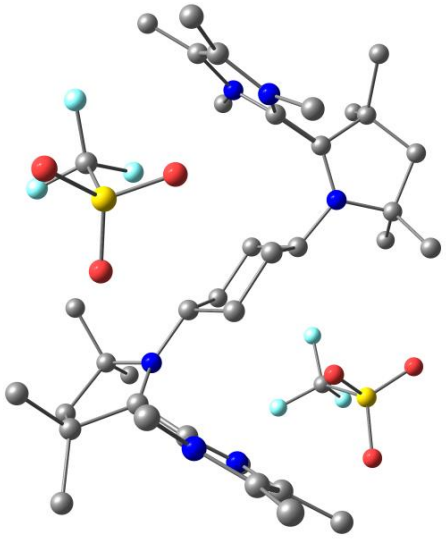
C	2.704815000	-3.289811000	0.694919000	
F	2.250461000	-4.169751000	1.579449000	
F	2.542186000	-2.065097000	1.225499000	
F	4.017624000	-3.486135000	0.559638000	
6^{Cy}-Broken Symmetry Singlet				DFT level: uB3LYP/Def2SVP
N	-1.855770000	2.467317000	0.495979000	- Thermochemistry -
N	-4.004654000	0.103886000	1.226215000	----------
N	-4.500755000	0.403829000	-0.865240000	Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
N	1.968299000	-1.542976000	-1.286788000	

N	3.948703000	-0.479660000	0.854842000
N	3.197610000	-2.131174000	2.069147000
C	-0.728180000	1.614327000	0.097366000
C	-0.585524000	0.347885000	0.941927000
H	-1.441089000	-0.322950000	0.794384000
H	-0.559285000	0.614540000	2.009606000
C	0.699298000	-0.407961000	0.591501000
H	0.720055000	-1.323598000	1.190516000
H	1.551166000	0.230955000	0.847849000
C	0.744163000	-0.780920000	-0.897727000
C	0.532354000	0.469869000	-1.766507000
H	0.456856000	0.195090000	-2.825509000
H	1.399284000	1.136120000	-1.664367000
C	-0.744932000	1.229308000	-1.386091000
H	-0.835894000	2.133522000	-2.008369000
H	-1.622053000	0.591523000	-1.591132000
C	-3.178851000	2.247318000	0.169776000
C	-3.030508000	4.392475000	1.156352000
H	-3.248629000	4.241637000	2.225753000
H	-3.136694000	5.467291000	0.948982000
C	-1.600132000	3.890740000	0.861960000
C	-0.935920000	4.660138000	-0.294264000
H	0.084354000	4.307622000	-0.474823000
H	-0.853646000	5.724579000	-0.028280000
H	-1.513386000	4.576606000	-1.225227000
C	-0.698751000	3.967113000	2.102966000
H	-1.115041000	3.362482000	2.924856000
H	-0.624195000	5.012654000	2.440069000
H	0.323839000	3.631118000	1.880469000
C	-3.808347000	0.943007000	0.174438000
C	-5.142169000	-0.762382000	-0.463773000
C	-4.820115000	-0.957308000	0.855622000
C	-3.486562000	0.300403000	2.572437000
H	-2.912079000	1.231729000	2.596930000
H	-2.834452000	-0.545769000	2.824673000
H	-4.323388000	0.361732000	3.283505000
C	-4.453164000	0.878179000	-2.236992000
H	-3.716636000	1.687462000	-2.298291000
H	-5.435645000	1.253039000	-2.559540000
H	-4.145082000	0.054799000	-2.897140000
C	-5.940174000	-1.592207000	-1.407643000
H	-6.449495000	-2.399359000	-0.866733000
H	-5.293544000	-2.065877000	-2.163884000
H	-6.702535000	-0.993848000	-1.932184000
C	-5.193641000	-2.050843000	1.794275000
H	-5.899618000	-2.740048000	1.314314000
H	-5.667080000	-1.654642000	2.707414000
H	-4.294491000	-2.615657000	2.081829000
C	2.718767000	-2.270863000	-0.381856000
C	3.222103000	-3.587736000	-0.966958000
C	3.182246000	-3.211658000	-2.466222000
H	4.154767000	-2.778254000	-2.747392000
H	3.012735000	-4.082715000	-3.116306000
C	2.080861000	-2.137711000	-2.660374000
C	2.309286000	-4.801696000	-0.678163000
H	1.249527000	-4.572861000	-0.831692000
H	2.408308000	-5.135098000	0.364228000
H	2.603136000	-5.645005000	-1.325156000
C	4.653201000	-3.916138000	-0.512746000
H	5.029558000	-4.807421000	-1.039876000
H	4.690299000	-4.130887000	0.567018000
H	5.343586000	-3.081324000	-0.713659000
C	2.589886000	-1.112711000	-3.694118000
H	1.819348000	-0.401577000	-4.015026000
H	2.937496000	-1.648766000	-4.592320000
H	3.434572000	-0.537115000	-3.287520000
C	0.753854000	-2.756652000	-3.131026000
H	0.370575000	-3.492707000	-2.413503000
H	0.907507000	-3.257077000	-4.099258000
H	-0.026178000	-1.995096000	-3.273702000

Zero-point correction= 1.000098
(Hartree/Particle)
Thermal correction to Energy= 1.063898
Thermal correction to Enthalpy= 1.064843
Thermal correction to Gibbs Free Energy= 0.904076
Sum of electronic and zero-point Energies= -3657.402100
Sum of electronic and thermal Energies= -3657.338299
Sum of electronic and thermal Enthalpies= -3657.337355
Sum of electronic and thermal Free Energies= -3657.498122

Charge = 0 Multiplicity = 1



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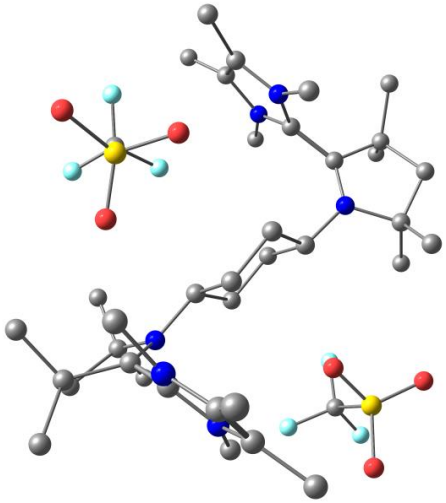
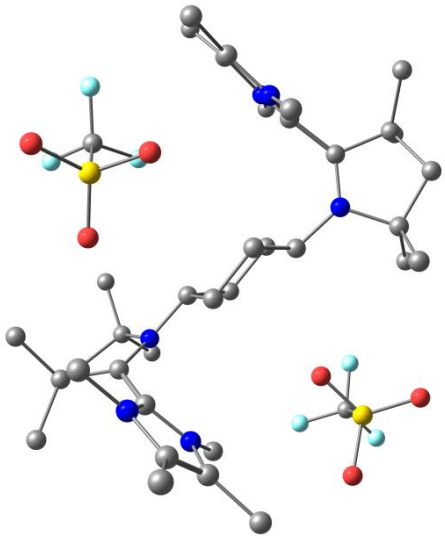
C	3.824507000	-1.236088000	2.934319000	
C	4.362228000	0.281669000	-0.316984000	
H	5.124023000	-0.286387000	-0.873973000	
H	4.754701000	1.255092000	-0.009704000	
H	3.499111000	0.458909000	-0.960988000	
C	2.415541000	-3.289037000	2.480115000	
H	3.047558000	-4.187283000	2.556812000	
H	1.605085000	-3.462260000	1.757264000	
H	1.964389000	-3.090917000	3.460767000	
C	5.016838000	1.045942000	2.562255000	
H	6.047452000	1.048574000	2.169593000	
H	5.069922000	1.128477000	3.655727000	
H	4.521618000	1.941307000	2.158627000	
C	3.897546000	-1.464579000	4.405499000	
H	2.901389000	-1.430571000	4.879129000	
H	4.515974000	-0.690978000	4.878794000	
H	4.342480000	-2.445168000	4.641981000	
C	-4.010940000	3.526226000	0.321030000	
C	-5.322803000	3.278213000	1.086658000	
H	-5.851077000	4.228430000	1.266006000	
H	-5.135807000	2.804613000	2.062800000	
H	-6.002442000	2.623080000	0.517148000	
C	-4.356441000	4.187175000	-1.032401000	
H	-3.467627000	4.319188000	-1.663533000	
H	-4.809669000	5.179363000	-0.870544000	
H	-5.084791000	3.581252000	-1.593042000	
H	0.175840000	2.210363000	0.265564000	
H	-0.101511000	-1.466055000	-1.058128000	
S	3.009819000	3.610434000	0.214263000	
O	2.288092000	4.840023000	0.581430000	
O	4.464234000	3.574861000	0.485107000	
O	2.304758000	2.341729000	0.560543000	
C	2.939674000	3.623938000	-1.668475000	
F	3.525310000	4.708735000	-2.168034000	
F	3.549957000	2.542188000	-2.191625000	
F	1.663238000	3.600857000	-2.102395000	
S	-1.621212000	-3.521088000	0.914201000	
O	-2.094443000	-2.353556000	1.701773000	
O	-2.094956000	-4.830985000	1.372185000	
O	-0.197255000	-3.436525000	0.503804000	
C	-2.511059000	-3.305956000	-0.738162000	
F	-1.996365000	-4.105912000	-1.675713000	
F	-2.425469000	-2.034957000	-1.201915000	
F	-3.817834000	-3.591471000	-0.621839000	
6^{Cy}-Triplet				DFT level: uB3LYP/Def2SVP
N	-1.855311000	2.467709000	0.496810000	- Thermochemistry -
N	-4.004015000	0.104121000	1.226276000	----------
N	-4.501199000	0.405393000	-0.864788000	Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
N	1.967504000	-1.543850000	-1.286195000	
N	3.950632000	-0.478608000	0.853634000	Zero-point correction= 1.000088
N	3.196920000	-2.127375000	2.069934000	(Hartree/Particle)
C	-0.727728000	1.614594000	0.097947000	Thermal correction to Energy= 1.063886
C	-0.585385000	0.348169000	0.942581000	Thermal correction to Enthalpy= 1.064831
H	-1.441344000	-0.322120000	0.794934000	Thermal correction to Gibbs Free Energy= 0.903013
H	-0.559072000	0.614799000	2.010261000	Sum of electronic and zero-point Energies= -3657.402097
C	0.698886000	-0.408727000	0.592325000	Sum of electronic and thermal Energies= -3657.338299
H	0.718377000	-1.324625000	1.190995000	Sum of electronic and thermal Enthalpies= -3657.337355
H	1.551477000	0.228958000	0.849437000	Sum of electronic and thermal Free Energies= -3657.499172
C	0.743653000	-0.781459000	-0.896965000	
C	0.532419000	0.469445000	-1.765688000	Charge = 0 Multiplicity = 3
H	0.457035000	0.194844000	-2.824736000	
H	1.399606000	1.135254000	-1.663177000	
C	-0.744690000	1.229429000	-1.385470000	
H	-0.835230000	2.133594000	-2.007889000	
H	-1.622042000	0.591960000	-1.590602000	
C	-3.178467000	2.248061000	0.170558000	
C	-3.029686000	4.393325000	1.156757000	
H	-3.247736000	4.242704000	2.226204000	

H	-3.135651000	5.468143000	0.949255000
C	-1.599418000	3.891265000	0.862208000
C	-0.935460000	4.659993000	-0.294592000
H	0.084804000	4.307440000	-0.475143000
H	-0.853211000	5.724619000	-0.029271000
H	-1.513112000	4.575850000	-1.225392000
C	-0.697674000	3.967835000	2.102906000
H	-1.113923000	3.363663000	2.925162000
H	-0.622699000	5.013509000	2.439550000
H	0.324760000	3.631498000	1.880211000
C	-3.808191000	0.943933000	0.174879000
C	-5.142530000	-0.761066000	-0.463675000
C	-4.819662000	-0.956869000	0.855423000
C	-3.486021000	0.299889000	2.572672000
H	-2.910232000	1.230395000	2.597391000
H	-2.835121000	-0.547251000	2.824807000
H	-4.322989000	0.362324000	3.283492000
C	-4.453198000	0.879865000	-2.236501000
H	-3.716469000	1.688989000	-2.297597000
H	-5.435518000	1.255006000	-2.559245000
H	-4.145169000	0.056473000	-2.896689000
C	-5.940600000	-1.590614000	-1.407734000
H	-6.451577000	-2.396655000	-0.866702000
H	-5.293743000	-2.065697000	-2.162918000
H	-6.701651000	-0.991707000	-1.933549000
C	-5.192825000	-2.050847000	1.793717000
H	-5.898334000	-2.740301000	1.313428000
H	-5.666634000	-1.655068000	2.706863000
H	-4.293480000	-2.615355000	2.081273000
C	2.718950000	-2.270417000	-0.380938000
C	3.224106000	-3.587044000	-0.965063000
C	3.181445000	-3.213113000	-2.464772000
H	4.152841000	-2.778405000	-2.747880000
H	3.012492000	-4.085234000	-3.113587000
C	2.078092000	-2.141169000	-2.658847000
C	2.314642000	-4.802740000	-0.673151000
H	1.254195000	-4.576945000	-0.826287000
H	2.415592000	-5.134015000	0.369754000
H	2.610016000	-5.646533000	-1.318854000
C	4.656551000	-3.911642000	-0.512138000
H	5.034208000	-4.802956000	-1.038320000
H	4.695349000	-4.124603000	0.567951000
H	5.344913000	-3.075669000	-0.715193000
C	2.583436000	-1.117918000	-3.696144000
H	1.810711000	-0.409676000	-4.018254000
H	2.931109000	-1.655792000	-4.593244000
H	3.427303000	-0.539093000	-3.292389000
C	0.750725000	-2.762663000	-3.125130000
H	0.369445000	-3.496852000	-2.404641000
H	0.902805000	-3.265690000	-4.092275000
H	-0.030171000	-2.002055000	-3.268389000
C	3.270086000	-1.655961000	0.796083000
C	4.286843000	-0.188465000	2.169360000
C	3.824798000	-1.232029000	2.934136000
C	4.365368000	0.280648000	-0.319138000
H	5.130131000	-0.286885000	-0.872628000
H	4.754504000	1.255881000	-0.013365000
H	3.503380000	0.453789000	-0.965839000
C	2.413681000	-3.284022000	2.482102000
H	3.045510000	-4.182038000	2.563037000
H	1.605244000	-3.459328000	1.757510000
H	1.959818000	-3.083067000	3.460959000
C	5.021368000	1.047368000	2.559238000
H	6.052318000	1.046745000	2.167395000
H	5.073796000	1.131533000	3.652620000
H	4.528687000	1.943320000	2.153758000
C	3.896519000	-1.458509000	4.405685000
H	2.900090000	-1.421698000	4.878558000
H	4.516257000	-0.685471000	4.878218000
H	4.339256000	-2.439670000	4.643930000



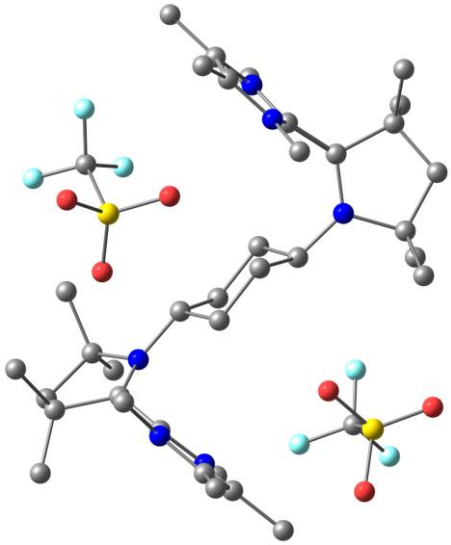
C	-4.010331000	3.527094000	0.321598000
C	-5.322153000	3.279204000	1.087452000
H	-5.850345000	4.229472000	1.266844000
H	-5.135021000	2.805607000	2.063576000
H	-6.001888000	2.624120000	0.518003000
C	-4.356004000	4.187936000	-1.031820000
H	-3.467319000	4.319836000	-1.663178000
H	-4.809084000	5.180196000	-0.869944000
H	-5.084536000	3.582060000	-1.592304000
H	0.176355000	2.210628000	0.265871000
H	-0.102264000	-1.466283000	-1.057293000
S	3.010047000	3.608535000	0.212113000
O	2.288163000	4.837745000	0.580124000
O	4.464870000	3.573981000	0.481035000
O	2.306440000	2.339419000	0.559376000
C	2.938070000	3.622208000	-1.670527000
F	3.524007000	4.706660000	-2.170471000
F	3.547185000	2.540033000	-2.194238000
F	1.661233000	3.600050000	-2.103490000
S	-1.621138000	-3.521669000	0.913752000
O	-2.092505000	-2.353530000	1.701533000
O	-2.095190000	-4.831027000	1.372823000
O	-0.197646000	-3.438299000	0.501588000
C	-2.512785000	-3.306558000	-0.737655000
F	-1.999998000	-4.107336000	-1.675456000
F	-2.426616000	-2.035732000	-1.202082000
F	-3.819713000	-3.590890000	-0.619811000

6^{Cy} -Broken Symmetry Singlet				DFT level: PBE1PBE/def2SVP
N	-1.551830000	2.662897000	0.459278000	
N	-4.036543000	0.689260000	1.182993000	- Thermochemistry -
N	-4.487093000	1.045431000	-0.901094000	----------
N	1.722622000	-1.759722000	-1.380674000	Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
N	3.885562000	-1.068865000	0.776271000	
N	2.902855000	-2.616167000	1.942143000	Zero-point correction= 1.003205
C	-0.558853000	1.667948000	0.054630000	(Hartree/Particle)
C	-0.555990000	0.387788000	0.883223000	Thermal correction to Energy= 1.067975
H	-1.485160000	-0.188609000	0.750391000	Thermal correction to Enthalpy= 1.068919
H	-0.481981000	0.638399000	1.952785000	Thermal correction to Gibbs Free Energy= 0.902876
C	0.633886000	-0.493175000	0.508480000	Sum of electronic and zero-point Energies= -3653.797924
H	0.565787000	-1.413072000	1.101419000	Sum of electronic and thermal Energies= -3653.733154
H	1.557216000	0.050119000	0.757276000	Sum of electronic and thermal Enthalpies= -3653.732210
C	0.618742000	-0.854696000	-0.976125000	Sum of electronic and thermal Free Energies= -3653.898254
C	0.559888000	0.421550000	-1.820144000	
H	0.461893000	0.177694000	-2.885981000	Charge = 0 Multiplicity = 1
H	1.497562000	0.986735000	-1.696243000	
C	-0.621247000	1.306666000	-1.427147000	
H	-0.614156000	2.222394000	-2.039821000	
H	-1.565407000	0.773716000	-1.641136000	
C	-2.884468000	2.662006000	0.113154000	
C	-2.414393000	4.735673000	1.116980000	
H	-2.698809000	4.607073000	2.173971000	
H	-2.331608000	5.816580000	0.930391000	
C	-1.082807000	4.010636000	0.869352000	
C	-0.241145000	4.680103000	-0.222254000	
H	0.710603000	4.155636000	-0.369924000	
H	0.018083000	5.702302000	0.089634000	
H	-0.771203000	4.736021000	-1.182929000	
C	-0.244481000	3.917694000	2.144441000	
H	-0.788579000	3.381978000	2.938182000	
H	-0.010009000	4.930087000	2.506767000	
H	0.717968000	3.420082000	1.955509000	
C	-3.720376000	1.478553000	0.129266000	
C	-5.292559000	-0.002221000	-0.492593000	
C	-5.002979000	-0.230307000	0.826775000	
C	-3.479439000	0.796953000	2.514209000	
H	-2.763763000	1.625478000	2.529147000	
H	-2.966430000	-0.144380000	2.757318000	
H	-4.283533000	0.988231000	3.239275000	
C	-4.401128000	1.526097000	-2.259283000	
H	-3.524264000	2.179929000	-2.337735000	



H	-5.301515000	2.091832000	-2.540720000
H	-4.283295000	0.675910000	-2.945297000
C	-6.206132000	-0.716056000	-1.418040000
H	-6.830012000	-1.423414000	-0.858364000
H	-5.644185000	-1.300464000	-2.164429000
H	-6.874332000	-0.024763000	-1.954754000
C	-5.547172000	-1.228077000	1.778936000
H	-6.333809000	-1.822072000	1.298431000
H	-5.980580000	-0.743496000	2.668176000
H	-4.742230000	-1.908028000	2.099062000
C	2.361510000	-2.602257000	-0.490381000
C	2.642463000	-3.972689000	-1.093521000
C	2.649805000	-3.574451000	-2.578614000
H	3.675702000	-3.289353000	-2.861041000
H	2.347692000	-4.401613000	-3.238295000
C	1.729469000	-2.350294000	-2.751851000
C	1.550895000	-5.019220000	-0.805464000
H	0.537196000	-4.605986000	-0.875429000
H	1.648232000	-5.427478000	0.210119000
H	1.652523000	-5.862787000	-1.507532000
C	4.001705000	-4.537909000	-0.678257000
H	4.209878000	-5.470754000	-1.225585000
H	4.031312000	-4.778376000	0.395816000
H	4.818793000	-3.830452000	-0.890046000
C	2.376812000	-1.418880000	-3.786056000
H	1.737101000	-0.577158000	-4.078314000
H	2.597117000	-1.995362000	-4.698758000
H	3.325672000	-1.011951000	-3.406911000
C	0.328999000	-2.754473000	-3.221796000
H	-0.162937000	-3.438566000	-2.517701000
H	0.405941000	-3.259310000	-4.196344000
H	-0.326857000	-1.882385000	-3.356864000
C	3.017020000	-2.106427000	0.692154000
C	4.314681000	-0.914112000	2.080546000
C	3.703958000	-1.897332000	2.814639000
C	4.412347000	-0.323568000	-0.349558000
H	5.297602000	-0.836225000	-0.758277000
H	4.680289000	0.688790000	-0.025613000
H	3.641790000	-0.249070000	-1.122223000
C	1.959829000	-3.639670000	2.341422000
H	2.433555000	-4.632920000	2.362441000
H	1.100613000	-3.648666000	1.652564000
H	1.587616000	-3.410246000	3.347766000
C	5.276617000	0.140113000	2.485398000
H	6.280814000	-0.051047000	2.072528000
H	5.364037000	0.175006000	3.578610000
H	4.965865000	1.133653000	2.120457000
C	3.790576000	-2.206287000	4.263983000
H	2.830777000	-2.044457000	4.781713000
H	4.535286000	-1.556681000	4.740482000
H	4.092598000	-3.250533000	4.442489000
C	-3.486064000	4.063470000	0.232869000
C	-4.848979000	4.062359000	0.929845000
H	-5.205173000	5.094075000	1.077740000
H	-4.799396000	3.579921000	1.917961000
H	-5.610653000	3.536246000	0.331815000
C	-3.637628000	4.776986000	-1.121381000
H	-2.715827000	4.737688000	-1.716968000
H	-3.894713000	5.837628000	-0.967034000
H	-4.447015000	4.330791000	-1.718811000
H	0.418520000	2.143248000	0.223999000
H	-0.316331000	-1.421339000	-1.134096000
S	3.547412000	3.276736000	0.367229000
O	3.079240000	4.573032000	0.855245000
O	4.896365000	2.855847000	0.786357000
O	2.543154000	2.185527000	0.419856000
C	3.755713000	3.537898000	-1.459378000
F	4.621143000	4.507265000	-1.712520000
F	4.194978000	2.422552000	-2.052535000
F	2.592138000	3.858164000	-2.031340000

S	-2.188431000	-3.355598000	1.024103000	
O	-2.585567000	-2.110177000	1.714719000	
O	-2.711289000	-4.590184000	1.596089000	
O	-0.774527000	-3.377416000	0.598051000	
C	-3.075773000	-3.224064000	-0.605596000	
F	-2.713993000	-4.200626000	-1.429463000	
F	-2.813863000	-2.059036000	-1.221366000	
F	-4.398558000	-3.290015000	-0.442165000	
6^{Cy} -Triplet				DFT level: PBE1PBE/def2SVP
N	-1.551742000	2.662981000	0.459394000	- Thermochemistry -
N	-4.036508000	0.689453000	1.183018000	----------
N	-4.487020000	1.045622000	-0.901077000	Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
N	1.722576000	-1.759942000	-1.380627000	
N	3.885568000	-1.069043000	0.776265000	Zero-point correction= 1.003205
N	2.902650000	-2.616166000	1.942188000	(Hartree/Particle)
C	-0.558725000	1.667974000	0.054735000	Thermal correction to Energy= 1.067976
C	-0.556139000	0.387741000	0.883131000	Thermal correction to Enthalpy= 1.068920
H	-1.485290000	-0.188607000	0.749937000	Thermal correction to Gibbs Free Energy= 0.901835
H	-0.482457000	0.638170000	1.952763000	Sum of electronic and zero-point Energies= -3653.797912
C	0.633817000	-0.493244000	0.508619000	Sum of electronic and thermal Energies= -3653.733142
H	0.565610000	-1.413103000	1.101581000	Sum of electronic and thermal Enthalpies= -3653.732198
H	1.557103000	0.050069000	0.757550000	Sum of electronic and thermal Free Energies= -3653.899282
C	0.618831000	-0.854723000	-0.975998000	
C	0.560339000	0.421619000	-1.819903000	Charge = 0 Multiplicity = 3
H	0.462587000	0.177967000	-2.885809000	
H	1.498055000	0.986632000	-1.695639000	
C	-0.620741000	1.306942000	-1.427112000	
H	-0.613231000	2.222758000	-2.039645000	
H	-1.564938000	0.774249000	-1.641545000	
C	-2.884359000	2.662155000	0.113170000	
C	-2.414201000	4.735894000	1.116793000	
H	-2.698625000	4.607408000	2.173796000	
H	-2.331362000	5.816780000	0.930101000	
C	-1.082652000	4.010766000	0.869240000	
C	-0.240986000	4.680060000	-0.222470000	
H	0.710726000	4.155517000	-0.370114000	
H	0.018314000	5.702277000	0.089297000	
H	-0.771068000	4.735908000	-1.183135000	
C	-0.244306000	3.917986000	2.144330000	
H	-0.788399000	3.382368000	2.938140000	
H	-0.009829000	4.930425000	2.506523000	
H	0.718142000	3.420352000	1.955455000	
C	-3.720311000	1.478735000	0.129292000	
C	-5.292512000	-0.002013000	-0.492584000	
C	-5.002955000	-0.230096000	0.826791000	
C	-3.479413000	0.797134000	2.514239000	
H	-2.763675000	1.625605000	2.529164000	
H	-2.966472000	-0.144232000	2.757369000	
H	-4.283500000	0.988481000	3.239294000	
C	-4.400968000	1.526223000	-2.259285000	
H	-3.524147000	2.180114000	-2.337699000	
H	-5.301371000	2.091880000	-2.540830000	
H	-4.283014000	0.676008000	-2.945244000	
C	-6.206098000	-0.715823000	-1.418037000	
H	-6.829991000	-1.423174000	-0.858366000	
H	-5.644165000	-1.300233000	-2.164434000	
H	-6.874286000	-0.024511000	-1.954741000	
C	-5.547180000	-1.227844000	1.778958000	
H	-6.333814000	-1.821838000	1.298447000	
H	-5.980598000	-0.743242000	2.668181000	
H	-4.742254000	-1.907804000	2.099108000	
C	2.361560000	-2.602466000	-0.490393000	
C	2.642412000	-3.972942000	-1.093464000	
C	2.649476000	-3.574819000	-2.578580000	
H	3.675321000	-3.289735000	-2.861213000	
H	2.347246000	-4.402023000	-3.238158000	
C	1.729115000	-2.350668000	-2.751753000	
C	1.550931000	-5.019494000	-0.805132000	
H	0.537204000	-4.606287000	-0.874892000	
H	1.648513000	-5.427730000	0.210437000	

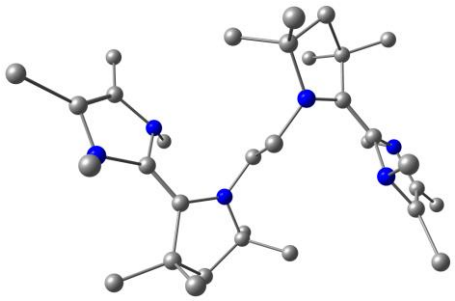


H	1.652427000	-5.863080000	-1.507195000	
C	4.001740000	-4.538083000	-0.678374000	
H	4.209840000	-5.470999000	-1.225609000	
H	4.031534000	-4.778401000	0.395729000	
H	4.818775000	-3.830634000	-0.890397000	
C	2.376266000	-1.419440000	-3.786254000	
H	1.736367000	-0.577953000	-4.078778000	
H	2.596684000	-1.996166000	-4.698776000	
H	3.325044000	-1.012186000	-3.407253000	
C	0.328532000	-2.754841000	-3.221346000	
H	-0.163289000	-3.438818000	-2.517058000	
H	0.405243000	-3.259798000	-4.195851000	
H	-0.327301000	-1.882730000	-3.356386000	
C	3.017002000	-2.106588000	0.692150000	
C	4.314539000	-0.914165000	2.080565000	
C	3.703681000	-1.897278000	2.814697000	
C	4.412517000	-0.323870000	-0.349569000	
H	5.298072000	-0.836362000	-0.757845000	
H	4.680053000	0.688647000	-0.025786000	
H	3.642198000	-0.249823000	-1.122514000	
C	1.959564000	-3.639615000	2.341470000	
H	2.433299000	-4.632856000	2.362705000	
H	1.100451000	-3.648712000	1.652489000	
H	1.587198000	-3.410045000	3.347724000	
C	5.276489000	0.140051000	2.485404000	
H	6.280712000	-0.051200000	2.072638000	
H	5.363815000	0.175045000	3.578620000	
H	4.965820000	1.133572000	2.120338000	
C	3.790111000	-2.206072000	4.264087000	
H	2.830255000	-2.044139000	4.781680000	
H	4.534790000	-1.556443000	4.740602000	
H	4.092065000	-3.250310000	4.442750000	
C	-3.485899000	4.063655000	0.232744000	
C	-4.848809000	4.062648000	0.929732000	
H	-5.204967000	5.094389000	1.077546000	
H	-4.799231000	3.580288000	1.917887000	
H	-5.610507000	3.536512000	0.331752000	
C	-3.637456000	4.777069000	-1.121562000	
H	-2.715675000	4.737673000	-1.717173000	
H	-3.894473000	5.837738000	-0.967290000	
H	-4.446890000	4.330880000	-1.718932000	
H	0.418626000	2.143216000	0.224396000	
H	-0.316310000	-1.421223000	-1.134054000	
S	3.547596000	3.276666000	0.367178000	
O	3.079445000	4.572976000	0.855177000	
O	4.896550000	2.855764000	0.786289000	
O	2.543331000	2.185466000	0.419846000	
C	3.755879000	3.537791000	-1.459437000	
F	4.621348000	4.507117000	-1.712606000	
F	4.195091000	2.422414000	-2.052576000	
F	2.592313000	3.858095000	-2.031392000	
S	-2.188529000	-3.355569000	1.024054000	
O	-2.585592000	-2.110182000	1.714769000	
O	-2.711354000	-4.590184000	1.596007000	
O	-0.774655000	-3.377386000	0.597890000	
C	-3.075976000	-3.223942000	-0.605578000	
F	-2.714304000	-4.200500000	-1.429497000	
F	-2.814045000	-2.058908000	-1.221332000	
F	-4.398754000	-3.289830000	-0.442063000	
4^{Et}				DFT level: RB3LYP-D3/6-31G(d,p)
N	-1.004299000	-1.389584000	-0.811337000	- Thermochemistry -
N	-3.079111000	0.612210000	-1.184823000	----------
N	-4.231047000	-0.132486000	0.661333000	Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
C	-0.173593000	-0.204723000	-0.722646000	
H	-0.671452000	0.644822000	-1.205548000	Zero-point correction= 0.847027
H	0.751616000	-0.381353000	-1.275721000	(Hartree/Particle)
C	-2.246013000	-1.452875000	-0.125919000	Thermal correction to Energy= 0.890626
C	-2.411226000	-2.854858000	0.450191000	Thermal correction to Enthalpy= 0.891571
C	-3.145274000	-0.431549000	-0.217146000	Thermal correction to Gibbs Free Energy= 0.773371
C	-0.438718000	-2.724203000	-1.092659000	Sum of electronic and zero-point Energies= -1580.912385

C	-1.569055000	-3.656255000	-0.589910000
H	-1.175508000	-4.588444000	-0.172311000
H	-2.217580000	-3.923367000	-1.431374000
C	-3.857577000	-3.372368000	0.438737000
H	-4.503269000	-2.828760000	1.131668000
H	-3.883040000	-4.431859000	0.718089000
H	-4.291974000	-3.266313000	-0.559771000
C	0.896626000	-3.000700000	-0.368108000
H	1.673349000	-2.286855000	-0.653680000
H	1.254721000	-4.002228000	-0.629833000
H	0.793171000	-2.952327000	0.716603000
C	-4.778247000	1.111470000	0.217931000
C	-2.911836000	0.209630000	-2.581535000
H	-2.011543000	-0.398210000	-2.673077000
H	-2.801929000	1.097648000	-3.207660000
H	-3.767254000	-0.382374000	-2.942146000
C	-4.123176000	1.528866000	-0.879381000
C	-0.212360000	-2.885710000	-2.607831000
H	-1.140518000	-2.690576000	-3.153230000
H	0.129537000	-3.897719000	-2.854694000
H	0.548115000	-2.180359000	-2.961931000
C	-1.797666000	-3.009992000	1.862200000
H	-0.809764000	-2.548329000	1.916740000
H	-1.697646000	-4.069257000	2.128012000
H	-2.417866000	-2.536649000	2.626591000
C	-4.007842000	-0.282555000	2.095295000
H	-3.959771000	-1.333549000	2.371500000
H	-4.842233000	0.155696000	2.645189000
H	-3.070830000	0.200203000	2.417071000
C	-4.333623000	2.738767000	-1.725161000
H	-3.397049000	3.301332000	-1.822921000
H	-5.079807000	3.400926000	-1.281522000
H	-4.670632000	2.490114000	-2.739574000
C	-5.917466000	1.746067000	0.943416000
H	-6.713728000	1.014076000	1.123488000
H	-6.339817000	2.564455000	0.356685000
H	-5.627149000	2.158331000	1.918570000
N	1.004378000	1.389493000	0.811654000
N	3.079228000	-0.612374000	1.184487000
N	4.230955000	0.132709000	-0.661649000
C	0.173746000	0.204582000	0.722950000
H	0.671667000	-0.644938000	1.205830000
H	-0.751471000	0.381142000	1.276034000
C	2.246016000	1.452932000	0.126108000
C	2.411153000	2.855019000	-0.449773000
C	3.145295000	0.431597000	0.217028000
C	0.438730000	2.724045000	1.093167000
C	1.568984000	3.656227000	0.590473000
H	1.175359000	4.588446000	0.173015000
H	2.217535000	3.923270000	1.431938000
C	3.857485000	3.372585000	-0.438269000
H	4.503187000	2.829110000	-1.131294000
H	3.882901000	4.432120000	-0.717460000
H	4.291905000	3.266395000	0.560215000
C	-0.896669000	3.000553000	0.368722000
H	-1.673354000	2.286664000	0.654289000
H	-1.254783000	4.002047000	0.630547000
H	-0.793289000	2.952258000	-0.715998000
C	4.778184000	-1.111358000	-0.218587000
C	2.912164000	-0.210078000	2.581308000
H	2.011920000	0.397797000	2.673094000
H	2.802282000	-1.098222000	3.207261000
H	3.767670000	0.381792000	2.941932000
C	4.123241000	-1.528981000	0.878716000
C	0.212444000	2.885358000	2.608370000
H	1.140644000	2.690226000	3.153698000
H	-0.129511000	3.897314000	2.855368000
H	-0.547962000	2.179913000	2.962429000
C	1.797564000	3.010348000	-1.861747000
H	0.809665000	2.548686000	-1.916333000

Sum of electronic and thermal Energies= -1580.868786
Sum of electronic and thermal Enthalpies= -1580.867842
Sum of electronic and thermal Free Energies= -1580.986041

Charge = 0 Multiplicity = 1



H	1.697534000	4.069650000	-2.127410000
H	2.417755000	2.537112000	-2.626213000
C	4.007569000	0.283101000	-2.095549000
H	3.959493000	1.334157000	-2.371517000
H	4.841874000	-0.155054000	-2.645650000
H	3.070499000	-0.199555000	-2.417307000
C	4.333759000	-2.739075000	1.724203000
H	3.397178000	-3.301630000	1.821955000
H	5.079869000	-3.401160000	1.280327000
H	4.670902000	-2.490654000	2.738629000
C	5.917302000	-1.745820000	-0.944346000
H	6.713559000	-1.013807000	-1.124352000
H	6.339703000	-2.564346000	-0.357844000
H	5.626862000	-2.157863000	-1.919557000

5^{Et}

DFT level: B3LYP-D3/6-31G(d,p)

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symmetry c1

N	-1.305337000	-1.388687000	0.173299000
N	-3.831434000	0.458703000	1.143553000
N	-3.973877000	0.626760000	-1.029342000
C	-0.418659000	-0.278855000	0.592768000
H	0.243609000	-0.671697000	1.365679000
H	-1.023792000	0.509706000	1.033517000
C	-2.569879000	-1.295368000	-0.142762000
C	-3.356219000	-0.042738000	-0.026604000
C	-3.208659000	-2.635769000	-0.450312000
C	-1.974976000	-3.573002000	-0.498654000
H	-2.188512000	-4.542530000	-0.045015000
H	-1.695766000	-3.755771000	-1.539981000
C	-0.819643000	-2.859148000	0.233822000
C	-4.184600000	-2.960245000	0.723456000
H	-3.696233000	-2.971076000	1.699501000
H	-4.594750000	-3.958366000	0.547090000
H	-5.023509000	-2.259921000	0.749382000
C	-4.012983000	-2.673266000	-1.767234000
H	-4.877043000	-2.005564000	-1.738212000
H	-4.395969000	-3.689168000	-1.896923000
H	-3.395377000	-2.444169000	-2.638678000
C	-0.699632000	-3.248717000	1.715137000
H	0.083835000	-2.688231000	2.233997000
H	-0.427901000	-4.306508000	1.770158000
H	-1.638570000	-3.124680000	2.257297000
C	0.519088000	-3.026745000	-0.484777000
H	0.470849000	-2.690377000	-1.524603000
H	0.760261000	-4.093206000	-0.500957000
H	1.338988000	-2.522758000	0.038414000
C	-4.842326000	1.566655000	-0.497380000
C	-4.762887000	1.450185000	0.879862000
C	-3.540337000	-0.026642000	2.503512000
H	-4.433168000	-0.493496000	2.924095000
H	-3.248588000	0.817079000	3.130354000
H	-2.734710000	-0.757737000	2.473823000
C	-3.718064000	0.497496000	-2.474885000
H	-4.618630000	0.145512000	-2.980050000
H	-2.908952000	-0.210457000	-2.642433000
H	-3.441573000	1.474044000	-2.875526000
C	-5.656465000	2.478440000	-1.349369000
H	-5.026607000	3.135503000	-1.959221000
H	-6.289449000	3.112585000	-0.728185000
H	-6.310218000	1.914830000	-2.023245000
C	-5.499432000	2.166507000	1.959396000
H	-6.103662000	1.474293000	2.556017000
H	-6.176671000	2.904794000	1.529251000
H	-4.818304000	2.693012000	2.636161000
N	1.305347000	1.388709000	-0.173345000
N	3.831440000	-0.458737000	-1.143509000
N	3.973836000	-0.626747000	1.029392000
C	0.418666000	0.278878000	-0.592811000
H	-0.243600000	0.671716000	-1.365727000
H	1.023800000	-0.509686000	-1.033554000

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.851901 (Hartree/Particle)

Thermal correction to Energy= 0.895677

Thermal correction to Enthalpy= 0.896621

Thermal correction to Gibbs Free Energy= 0.776279

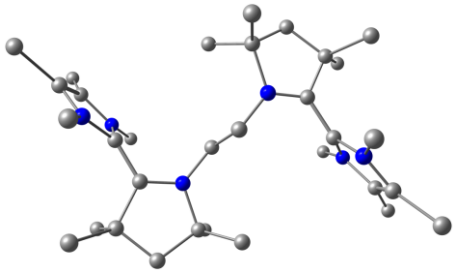
Sum of electronic and zero-point Energies= -1579.657223

Sum of electronic and thermal Energies= -1579.613447

Sum of electronic and thermal Enthalpies= -1579.612502

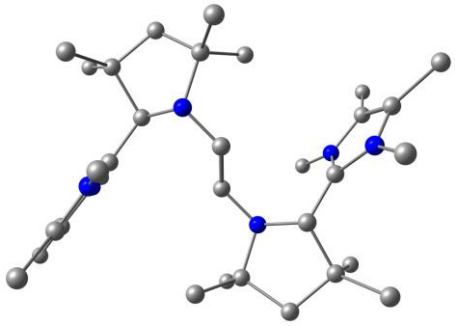
Sum of electronic and thermal Free Energies= -1579.732845

Charge = 4 Multiplicity = 1



C	2.569883000	1.295381000	0.142741000	
C	3.356207000	0.042737000	0.026627000	
C	3.208674000	2.635779000	0.450277000	
C	1.975004000	3.573030000	0.498574000	
H	2.188562000	4.542546000	0.044921000	
H	1.695773000	3.755823000	1.539891000	
C	0.819676000	2.859178000	-0.233913000	
C	4.184644000	2.960216000	-0.723478000	
H	3.696298000	2.971033000	-1.699534000	
H	4.594805000	3.958335000	-0.547124000	
H	5.023544000	2.259880000	-0.749372000	
C	4.012972000	2.673291000	1.767214000	
H	4.877021000	2.005574000	1.738222000	
H	4.395972000	3.689189000	1.896891000	
H	3.395346000	2.444221000	2.638650000	
C	0.699705000	3.248716000	-1.715238000	
H	-0.083761000	2.688234000	-2.234104000	
H	0.427995000	4.306512000	-1.770289000	
H	1.638653000	3.124651000	-2.257375000	
C	-0.519069000	3.026817000	0.484651000	
H	-0.470862000	2.690471000	1.524486000	
H	-0.760221000	4.093283000	0.500802000	
H	-1.338967000	2.522836000	-0.038549000	
C	4.842275000	-1.566673000	0.497468000	
C	4.762867000	-1.450231000	-0.879778000	
C	3.540381000	0.026585000	-2.503485000	
H	4.433228000	0.493420000	-2.924057000	
H	3.248636000	-0.817144000	-3.130316000	
H	2.734763000	0.757692000	-2.473830000	
C	3.718001000	-0.497443000	2.474928000	
H	4.618567000	-0.145468000	2.980099000	
H	2.908902000	0.210533000	2.642445000	
H	3.441481000	-1.473974000	2.875587000	
C	5.656379000	-2.478455000	1.349494000	
H	5.026496000	-3.135491000	1.959350000	
H	6.289361000	-3.112629000	0.728336000	
H	6.310131000	-1.914843000	2.023369000	
C	5.499418000	-2.166593000	-1.959281000	
H	6.103661000	-1.474404000	-2.555917000	
H	6.176646000	-2.904873000	-1.529105000	
H	4.818293000	-2.693115000	-2.636037000	
8^{Et}				DFT level: B3LYP-D3/6-31G(d,p)
N	0.989861000	1.556704000	-0.389055000	- Thermochemistry -
N	3.184872000	-0.427869000	-1.122136000	----------
N	3.730042000	-0.535414000	0.972761000	Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
C	0.003938000	0.559094000	-0.377004000	
C	2.193404000	1.396532000	0.410558000	Zero-point correction= 0.853143
H	1.932387000	1.305340000	1.479926000	(Hartree/Particle)
C	2.998512000	0.164942000	0.074533000	Thermal correction to Energy= 0.896121
C	2.962881000	2.750211000	0.226913000	Thermal correction to Enthalpy= 0.897065
C	0.531776000	2.993108000	-0.334006000	Thermal correction to Gibbs Free Energy= 0.780293
C	1.772782000	3.736998000	0.230975000	Sum of electronic and zero-point Energies= -1580.561525
H	1.570685000	4.056622000	1.258051000	Sum of electronic and thermal Energies= -1580.518547
H	2.001366000	4.638389000	-0.343219000	Sum of electronic and thermal Enthalpies= -1580.517603
C	3.732484000	2.813720000	-1.103368000	Sum of electronic and thermal Free Energies= -1580.634375
H	3.081251000	2.669129000	-1.966797000	
H	4.535264000	2.070302000	-1.144280000	Charge = 2 Multiplicity = 1
H	4.197253000	3.797863000	-1.205801000	
C	3.932991000	3.014272000	1.384614000	
H	4.765150000	2.302104000	1.381348000	
H	3.432283000	2.963014000	2.357326000	
H	4.366199000	4.013769000	1.291011000	
C	-0.664099000	3.166316000	0.620360000	
H	-1.571122000	2.698995000	0.225576000	
H	-0.871688000	4.230453000	0.764764000	
H	-0.448661000	2.726670000	1.600380000	
C	0.147718000	3.456540000	-1.744685000	
H	0.996457000	3.395252000	-2.429698000	
H	-0.198389000	4.493954000	-1.724127000	
H	-0.665070000	2.845581000	-2.153417000	

C	4.393237000	-1.584253000	0.334410000
C	4.045327000	-1.517710000	-0.985635000
C	2.589173000	-0.065733000	-2.413898000
H	1.907541000	0.764586000	-2.265469000
H	2.046263000	-0.928433000	-2.803341000
H	3.382518000	0.212530000	-3.109493000
C	3.871453000	-0.287116000	2.411752000
H	3.188469000	0.494242000	2.730951000
H	4.892941000	0.026971000	2.633705000
H	3.648868000	-1.205621000	2.956859000
C	5.288659000	-2.525490000	1.065640000
H	5.739099000	-3.233055000	0.368986000
H	4.742969000	-3.103173000	1.819396000
H	6.101677000	-1.995373000	1.572350000
C	4.428342000	-2.377087000	-2.141320000
H	5.133622000	-3.144932000	-1.822206000
H	4.905908000	-1.795197000	-2.936078000
H	3.557131000	-2.882552000	-2.571455000
H	-0.796955000	0.754530000	-1.082410000
N	-0.989891000	-1.556757000	0.389147000
N	-3.184897000	0.427934000	1.122092000
N	-3.729934000	0.535414000	-0.972842000
C	-0.003954000	-0.559161000	0.377088000
C	-2.193418000	-1.396576000	-0.410488000
H	-1.932370000	-1.305425000	-1.479852000
C	-2.998498000	-0.164944000	-0.074539000
C	-2.962929000	-2.750238000	-0.226830000
C	-0.531833000	-2.993170000	0.334127000
C	-1.772847000	-3.737047000	-0.230855000
H	-1.570743000	-4.056695000	-1.257922000
H	-2.001457000	-4.638422000	0.343354000
C	-3.732559000	-2.813721000	1.103437000
H	-3.081342000	-2.669134000	1.966878000
H	-4.535328000	-2.070291000	1.144326000
H	-4.197346000	-3.797856000	1.205870000
C	-3.933021000	-3.014306000	-1.384544000
H	-4.765184000	-2.302141000	-1.381290000
H	-3.432301000	-2.963046000	-2.357249000
H	-4.366227000	-4.013804000	-1.290945000
C	0.664048000	-3.166416000	-0.620223000
H	1.571074000	-2.699102000	-0.225437000
H	0.871620000	-4.230559000	-0.764606000
H	0.448627000	-2.726784000	-1.600254000
C	-0.147798000	-3.456585000	1.744817000
H	-0.996543000	-3.395272000	2.429821000
H	0.198291000	-4.494007000	1.724280000
H	0.664998000	-2.845635000	2.153547000
C	-4.393135000	1.584299000	-0.334575000
C	-4.045309000	1.517797000	0.985493000
C	-2.589287000	0.065850000	2.413910000
H	-1.907676000	-0.764502000	2.265571000
H	-2.046373000	0.928553000	2.803339000
H	-3.382686000	-0.212345000	3.109471000
C	-3.871246000	0.287073000	-2.411836000
H	-3.188279000	-0.494332000	-2.730952000
H	-4.892734000	-0.026966000	-2.633856000
H	-3.648569000	1.205547000	-2.956959000
C	-5.288476000	2.525540000	-1.065900000
H	-5.738928000	3.233155000	-0.369303000
H	-4.742717000	3.103167000	-1.819650000
H	-6.101487000	1.995434000	-1.572633000
C	-4.428362000	2.377235000	2.141119000
H	-5.133596000	3.145092000	1.821930000
H	-4.905996000	1.795395000	2.935873000
H	-3.557159000	2.882687000	2.571285000
H	0.796932000	-0.754596000	1.082502000



9^{Et}			
C	-0.061582000	0.558740000	-0.376370000
C	2.265688000	1.419690000	-0.113351000
C	3.016297000	0.283245000	-0.241728000

DFT level: B3LYP-D3/6-31G(d,p)

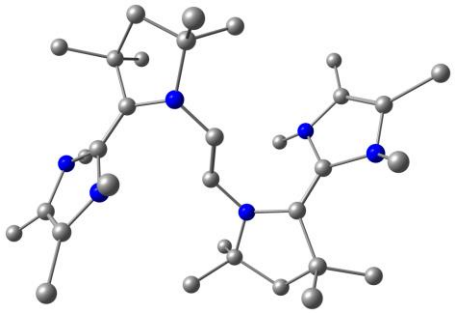
- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

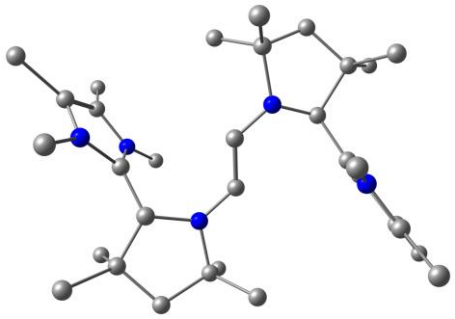
C	2.692091000	2.815791000	0.321483000
C	1.890267000	3.656608000	-0.718865000
H	1.670610000	4.664523000	-0.352339000
H	2.497498000	3.763683000	-1.624048000
C	0.595602000	2.872023000	-1.054110000
C	4.189829000	3.112686000	0.161133000
H	4.809034000	2.556292000	0.867574000
H	4.380067000	4.180237000	0.320178000
H	4.525526000	2.847122000	-0.845750000
C	2.219894000	3.158490000	1.753923000
H	1.177968000	2.864091000	1.900422000
H	2.306342000	4.234310000	1.949432000
H	2.813214000	2.636628000	2.508791000
C	-0.630777000	3.447860000	-0.320758000
H	-1.534928000	2.869299000	-0.524214000
H	-0.805428000	4.478097000	-0.648558000
H	-0.477823000	3.452605000	0.760498000
C	0.323536000	2.865128000	-2.569785000
H	1.171662000	2.424346000	-3.102221000
H	0.165395000	3.881845000	-2.947544000
H	-0.570943000	2.276606000	-2.802171000
C	4.555087000	-1.378785000	0.086214000
C	3.736494000	-1.779503000	-0.905551000
C	4.088679000	0.136716000	1.974951000
H	3.142581000	-0.235007000	2.400203000
H	4.171829000	1.195745000	2.209830000
H	4.924823000	-0.369301000	2.460420000
C	2.161125000	-0.549443000	-2.415411000
H	1.124777000	-0.227302000	-2.318170000
H	2.181809000	-1.470523000	-2.998727000
H	2.724042000	0.228355000	-2.953921000
C	5.736221000	-2.064103000	0.687263000
H	6.594456000	-1.383113000	0.733150000
H	6.026765000	-2.929671000	0.088032000
H	5.550316000	-2.422556000	1.708337000
C	3.774002000	-3.021611000	-1.730232000
H	2.801773000	-3.526964000	-1.713985000
H	4.519313000	-3.718143000	-1.341570000
H	4.022392000	-2.821837000	-2.780506000
N	0.939464000	1.507305000	-0.597900000
N	4.151595000	-0.085148000	0.532868000
N	2.733222000	-0.797824000	-1.101498000
H	-0.975162000	0.738041000	-0.928529000
C	0.061573000	-0.558699000	0.376459000
C	-2.265676000	-1.419692000	0.113378000
C	-3.016313000	-0.283259000	0.241709000
C	-2.692037000	-2.815811000	-0.321446000
C	-1.890212000	-3.656604000	0.718921000
H	-1.670513000	-4.664512000	0.352401000
H	-2.497467000	-3.763698000	1.624086000
C	-0.595584000	-2.871978000	1.054208000
C	-4.189771000	-3.112736000	-0.161114000
H	-4.808979000	-2.556350000	-0.867558000
H	-4.379988000	-4.180291000	-0.320166000
H	-4.525484000	-2.847184000	0.845767000
C	-2.219817000	-3.158516000	-1.753877000
H	-1.177904000	-2.864072000	-1.900378000
H	-2.306215000	-4.234344000	-1.949368000
H	-2.813158000	-2.636694000	-2.508755000
C	0.630845000	-3.447770000	0.320905000
H	1.534961000	-2.869166000	0.524392000
H	0.805528000	-4.477997000	0.648723000
H	0.477936000	-3.452534000	-0.760357000
C	-0.323571000	-2.865069000	2.569892000
H	-1.171733000	-2.424318000	3.102298000
H	-0.165405000	-3.881780000	2.947659000
H	0.570879000	-2.276514000	2.802307000
C	-4.555111000	1.378747000	-0.086328000
C	-3.736556000	1.779498000	0.905454000
C	-4.088636000	-0.136811000	-1.975008000

Zero-point correction= 0.822460
(Hartree/Particle)
Thermal correction to Energy= 0.866130
Thermal correction to Enthalpy= 0.867074
Thermal correction to Gibbs Free Energy= 0.748532
Sum of electronic and zero-point Energies= -1579.718522
Sum of electronic and thermal Energies= -1579.674852
Sum of electronic and thermal Enthalpies= -1579.673907
Sum of electronic and thermal Free Energies= -1579.792450

Charge = 0 Multiplicity = 1

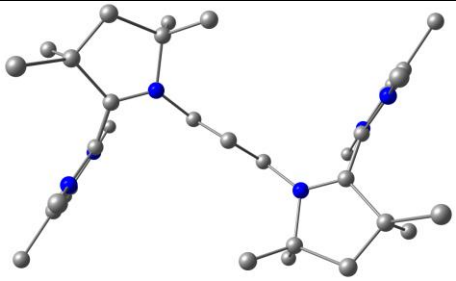


H	-3.142486000	0.234815000	-2.400228000	
H	-4.171871000	-1.195840000	-2.209861000	
H	-4.924713000	0.369267000	-2.460527000	
C	-2.161204000	0.549506000	2.415387000	
H	-1.124844000	0.227392000	2.318178000	
H	-2.181929000	1.470599000	2.998681000	
H	-2.724110000	-0.228296000	2.953904000	
C	-5.736238000	2.064032000	-0.687428000	
H	-6.594457000	1.383022000	-0.733331000	
H	-6.026821000	2.929604000	-0.088222000	
H	-5.550308000	2.422472000	-1.708502000	
C	-3.774103000	3.021627000	1.730100000	
H	-2.801882000	3.526996000	1.713859000	
H	-4.519417000	3.718137000	1.341402000	
H	-4.022513000	2.821880000	2.780374000	
N	-0.939470000	-1.507270000	0.597988000	
N	-4.151591000	0.085101000	-0.532933000	
N	-2.733279000	0.797837000	1.101457000	
H	0.975149000	-0.737993000	0.928628000	
10^{Et}				DFT level: uB3LYP-D3/6-31G(d,p)
N	-0.976684000	-1.557317000	0.141555000	- Thermochemistry -
N	-3.794518000	0.633151000	-0.968858000	----------
N	-3.172004000	0.489016000	1.107407000	Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
C	0.017262000	-0.657624000	0.228518000	
C	-2.298601000	-1.343953000	-0.495007000	Zero-point correction= 0.853167
C	-3.035457000	-0.086502000	-0.107693000	(Hartree/Particle)
C	-3.096942000	-2.681680000	-0.256490000	Thermal correction to Energy= 0.896383
C	-1.944447000	-3.709927000	-0.218197000	Thermal correction to Enthalpy= 0.897327
H	-2.223891000	-4.602762000	0.345322000	Thermal correction to Gibbs Free Energy= 0.779072
H	-1.714309000	-4.033387000	-1.238243000	Sum of electronic and zero-point Energies= -1580.158116
C	-4.047638000	-2.952531000	-1.433315000	Sum of electronic and thermal Energies= -1580.114900
H	-4.507744000	-3.937088000	-1.317677000	Sum of electronic and thermal Enthalpies= -1580.113956
H	-3.525616000	-2.945141000	-2.395980000	Sum of electronic and thermal Free Energies= -1580.232211
H	-4.862267000	-2.222773000	-1.467537000	
C	-3.917748000	-2.675440000	1.045234000	Charge = 3 Multiplicity = 2
H	-4.705464000	-1.916599000	1.019004000	
H	-3.315704000	-2.516127000	1.939999000	
H	-4.410360000	-3.644031000	1.159541000	
C	0.573837000	-3.461230000	-0.364768000	
H	0.653658000	-4.550684000	-0.328513000	
H	1.487176000	-3.055193000	0.081811000	
H	0.526241000	-3.162145000	-1.416365000	
C	-0.521758000	-3.288387000	1.896602000	
H	-1.423372000	-3.065446000	2.467983000	
H	0.305845000	-2.699189000	2.305727000	
H	-0.284568000	-4.343198000	2.056440000	
C	-0.696164000	-3.035314000	0.391496000	
C	-4.428672000	1.672327000	-0.289016000	
C	-4.030212000	1.585328000	1.019950000	
C	-4.018956000	0.399067000	-2.404831000	
H	-3.373696000	-0.393025000	-2.773688000	
H	-3.812553000	1.319195000	-2.952793000	
H	-5.058054000	0.107986000	-2.567912000	
C	-2.564654000	0.085829000	2.381501000	
H	-3.350541000	-0.204016000	3.080717000	
H	-2.009320000	0.929370000	2.794977000	
H	-1.893960000	-0.750913000	2.227563000	
C	-5.361524000	2.619580000	-0.964312000	
H	-5.762110000	3.331982000	-0.242868000	
H	-6.209813000	2.092667000	-1.413401000	
H	-4.863024000	3.190751000	-1.754360000	
C	-4.384581000	2.417962000	2.204649000	
H	-5.078861000	3.207093000	1.915407000	
H	-3.502926000	2.896612000	2.643947000	
H	-4.869173000	1.821826000	2.984793000	
H	0.913276000	-1.032216000	0.706282000	
H	-2.104252000	-1.270204000	-1.571568000	
N	0.976730000	1.557338000	-0.141764000	
N	3.794364000	-0.633108000	0.969085000	
N	3.172142000	-0.489099000	-1.107279000	

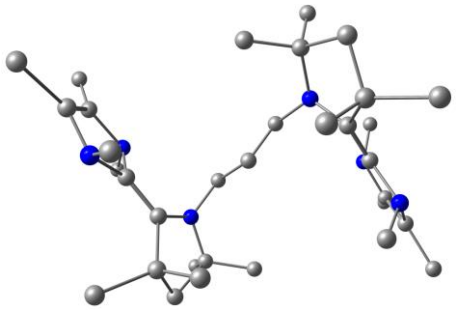


C	-0.017183000	0.657622000	-0.228751000	
C	2.298645000	1.344049000	0.494845000	
C	3.035497000	0.086548000	0.107746000	
C	3.096963000	2.681751000	0.256198000	
C	1.944449000	3.709973000	0.217931000	
H	2.223839000	4.602821000	-0.345592000	
H	1.714345000	4.033419000	1.237992000	
C	4.047713000	2.952631000	1.432979000	
H	4.507734000	3.937230000	1.317363000	
H	3.525766000	2.945120000	2.395681000	
H	4.862401000	2.222934000	1.467090000	
C	3.917720000	2.675451000	-1.045558000	
H	4.705397000	1.916569000	-1.019343000	
H	3.315648000	2.516161000	-1.940307000	
H	4.410380000	3.644016000	-1.159889000	
C	-0.573827000	3.461215000	0.364613000	
H	-0.653725000	4.550661000	0.328274000	
H	-1.487170000	3.055080000	-0.081870000	
H	-0.526138000	3.162221000	1.416229000	
C	0.521673000	3.288387000	-1.896804000	
H	1.423244000	3.065421000	-2.468239000	
H	-0.305968000	2.699207000	-2.305874000	
H	0.284502000	4.343204000	-2.056632000	
C	0.696159000	3.035325000	-0.391702000	
C	4.428470000	-1.672434000	0.289432000	
C	4.030182000	-1.585525000	-1.019595000	
C	4.018994000	-0.398539000	2.404947000	
H	3.372189000	0.392184000	2.774082000	
H	3.814624000	-1.319073000	2.952960000	
H	5.057564000	-0.105378000	2.567653000	
C	2.564998000	-0.085954000	-2.381482000	
H	3.351007000	0.203696000	-3.080641000	
H	2.009576000	-0.929453000	-2.794930000	
H	1.894420000	0.750910000	-2.227710000	
C	5.361195000	-2.619695000	0.964901000	
H	5.762320000	-3.331762000	0.243424000	
H	6.209117000	-2.092723000	1.414604000	
H	4.862426000	-3.191267000	1.754493000	
C	4.384558000	-2.418350000	-2.204157000	
H	5.078773000	-3.207485000	-1.914771000	
H	3.502892000	-2.897010000	-2.643424000	
H	4.869219000	-1.822356000	-2.984366000	
H	-0.913212000	1.032224000	-0.706486000	
H	2.104280000	1.270470000	1.571413000	
5^{Pr}				DFT level: B3LYP-D3/6-31G(d,p)
N	-2.098433000	1.441876000	0.036807000	- Thermochemistry -
N	-4.350425000	-1.228972000	0.648853000	----------
N	-4.423010000	-0.410365000	-1.372662000	Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
N	2.098341000	-1.441814000	0.036850000	
N	4.423117000	0.410245000	-1.372625000	Zero-point correction= 0.881479
N	4.350485000	1.228979000	0.648832000	(Hartree/Particle)
C	-3.311523000	1.065486000	0.329636000	Thermal correction to Energy= 0.926449
C	-3.917664000	-0.210181000	-0.129177000	Thermal correction to Enthalpy= 0.927393
C	3.311432000	-1.065409000	0.329675000	Thermal correction to Gibbs Free Energy= 0.804319
C	3.917595000	0.210225000	-0.129179000	Sum of electronic and zero-point Energies= -1618.979747
C	-1.082915000	0.652702000	-0.706267000	Sum of electronic and thermal Energies= -1618.934777
H	-0.627056000	1.341421000	-1.421342000	Sum of electronic and thermal Enthalpies= -1618.933833
H	-1.603137000	-0.119705000	-1.276735000	Sum of electronic and thermal Free Energies= -1619.056907
C	-0.000049000	0.000039000	0.191793000	
H	-0.469281000	-0.743756000	0.836311000	Charge = 4 Multiplicity = 1
H	0.469171000	0.743838000	0.836314000	
C	1.082824000	-0.652653000	-0.706243000	
H	0.626960000	-1.341385000	-1.421299000	
H	1.603049000	0.119735000	-1.276734000	
C	-4.128912000	2.139867000	1.023624000	
C	-3.052956000	3.217206000	1.308333000	
H	-3.441469000	4.225757000	1.156159000	
H	-2.731168000	3.145902000	2.350959000	
C	-1.857288000	2.936966000	0.375148000	
C	-4.820642000	1.661309000	2.317832000	

H	-5.572610000	0.893845000	2.119976000
H	-5.341246000	2.516614000	2.756984000
H	-4.106707000	1.297556000	3.060533000
C	-5.231236000	2.616098000	0.030842000
H	-4.828143000	2.991562000	-0.911295000
H	-5.777677000	3.434923000	0.506321000
H	-5.950241000	1.819708000	-0.178758000
C	-0.515918000	3.148773000	1.074467000
H	0.332286000	2.970484000	0.406362000
H	-0.423710000	2.537336000	1.976304000
H	-0.464598000	4.196583000	1.383223000
C	-1.914884000	3.723784000	-0.944105000
H	-1.828372000	4.788341000	-0.709865000
H	-2.858117000	3.581844000	-1.474486000
H	-1.089133000	3.476344000	-1.617052000
C	-5.132626000	-2.091389000	-0.104573000
C	-5.188889000	-1.566254000	-1.382255000
C	-3.987298000	-1.487517000	2.051920000
H	-3.266983000	-0.743612000	2.386376000
H	-3.547487000	-2.483212000	2.126839000
H	-4.877702000	-1.440114000	2.680287000
C	-5.741563000	-3.325506000	0.466966000
H	-6.397236000	-3.091667000	1.312127000
H	-4.978795000	-4.031201000	0.813842000
H	-6.342409000	-3.834620000	-0.286959000
C	-5.907682000	-2.040916000	-2.598618000
H	-6.456461000	-2.957123000	-2.379352000
H	-5.216441000	-2.255211000	-3.420534000
H	-6.632668000	-1.298200000	-2.948518000
C	-4.300215000	0.483621000	-2.536281000
H	-3.582734000	1.273667000	-2.323382000
H	-5.271451000	0.928723000	-2.760317000
H	-3.962204000	-0.094381000	-3.397283000
C	4.128823000	-2.139788000	1.023677000
C	3.052846000	-3.217085000	1.308446000
H	2.731054000	-3.145717000	2.351070000
H	3.441344000	-4.225651000	1.156333000
C	1.857194000	-2.936873000	0.375237000
C	4.820602000	-1.661208000	2.317856000
H	5.572625000	-0.893814000	2.119938000
H	5.341147000	-2.516531000	2.757042000
H	4.106699000	-1.297359000	3.060539000
C	5.231089000	-2.616050000	0.030863000
H	4.827962000	-2.991565000	-0.911239000
H	5.777561000	-3.434856000	0.506342000
H	5.950080000	-1.819670000	-0.178823000
C	0.515817000	-3.148667000	1.074568000
H	0.423584000	-2.537148000	1.976349000
H	0.464540000	-4.196449000	1.383423000
H	-0.332390000	-2.970470000	0.406439000
C	1.914791000	-3.723774000	-0.943973000
H	1.828242000	-4.788311000	-0.709666000
H	2.858041000	-3.581900000	-1.474337000
H	1.089060000	-3.476346000	-1.616947000
C	5.189107000	1.566054000	-1.382241000
C	5.132833000	2.091261000	-0.104587000
C	4.300040000	-0.483592000	-2.536319000
H	5.271461000	-0.927808000	-2.761302000
H	3.960782000	0.094292000	-3.396922000
H	3.583485000	-1.274337000	-2.322929000
C	5.907990000	2.040564000	-2.598608000
H	5.216810000	2.254750000	-3.420601000
H	6.632997000	1.297797000	-2.948362000
H	6.456765000	2.956792000	-2.379421000
C	5.741824000	3.325379000	0.466894000
H	6.343238000	3.834065000	-0.286870000
H	6.396959000	3.091637000	1.312494000
H	4.979058000	4.031410000	0.813101000
C	3.987397000	1.487588000	2.051900000
H	3.266801000	0.743922000	2.386287000



H	3.547928000	2.483432000	2.126833000	
H	4.877752000	1.439852000	2.680310000	
4^{Pr}				DFT level: B3LYP-D3/6-31G(d,p)
N	-1.679272000	-1.860231000	-0.749600000	
N	-3.968708000	0.577222000	0.976837000	- Thermochemistry -
N	-3.720428000	0.140973000	-1.262557000	----------
N	1.678920000	1.859859000	-0.749364000	Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
N	3.720838000	-0.140510000	-1.262453000	
N	3.969328000	-0.576858000	0.976957000	Zero-point correction= 0.876095
C	-0.861327000	-0.945826000	-1.539711000	(Hartree/Particle)
H	-1.513070000	-0.339915000	-2.184883000	Thermal correction to Energy= 0.920843
H	-0.235177000	-1.543968000	-2.210305000	Thermal correction to Enthalpy= 0.921787
C	-0.000083000	-0.000263000	-0.700069000	Thermal correction to Gibbs Free Energy= 0.800320
H	-0.658804000	0.578951000	-0.048685000	Sum of electronic and zero-point Energies= -1620.198427
H	0.658529000	-0.579455000	-0.048538000	Sum of electronic and thermal Energies= -1620.153679
C	0.861273000	0.945303000	-1.539593000	Sum of electronic and thermal Enthalpies= -1620.152735
H	1.513238000	0.339422000	-2.184564000	Sum of electronic and thermal Free Energies= -1620.274202
H	0.235213000	1.543330000	-2.210381000	
C	-2.506248000	-1.341883000	0.288380000	Charge = 0 Multiplicity = 1
C	-2.399855000	-2.247012000	1.510675000	
C	-2.033698000	-3.586904000	0.803423000	
H	-1.491497000	-4.270702000	1.464333000	
H	-2.960949000	-4.087913000	0.504906000	
C	-1.217062000	-3.235266000	-0.462658000	
C	-3.723891000	-2.425719000	2.270825000	
H	-4.056320000	-1.506064000	2.756292000	
H	-3.616356000	-3.193714000	3.045434000	
H	-4.517798000	-2.734484000	1.584230000	
C	-1.275453000	-1.831922000	2.491565000	
H	-0.358267000	-1.571640000	1.960145000	
H	-1.049195000	-2.646249000	3.190648000	
H	-1.558936000	-0.959877000	3.083726000	
C	0.302301000	-3.355770000	-0.203345000	
H	0.891342000	-3.013665000	-1.059179000	
H	0.560159000	-4.405156000	-0.026084000	
H	0.618789000	-2.783401000	0.669125000	
C	-1.583948000	-4.157619000	-1.639998000	
H	-2.655069000	-4.090341000	-1.851777000	
H	-1.336384000	-5.203014000	-1.420929000	
H	-1.038027000	-3.867435000	-2.544794000	
C	-3.362440000	-0.309873000	0.039795000	
C	-4.547024000	1.286644000	-1.095178000	
C	-4.666293000	1.563242000	0.215131000	
C	-3.184743000	1.023978000	2.121825000	
H	-2.148716000	1.258899000	1.833946000	
H	-3.153453000	0.262813000	2.900633000	
H	-3.642155000	1.911936000	2.559775000	
C	-4.152142000	-0.879458000	-2.219016000	
H	-3.368994000	-1.632466000	-2.313847000	
H	-4.322092000	-0.418799000	-3.194513000	
H	-5.076115000	-1.380407000	-1.891518000	
C	-5.126293000	1.979667000	-2.281832000	
H	-5.866424000	1.363426000	-2.808357000	
H	-4.338937000	2.226316000	-3.004622000	
H	-5.618097000	2.909666000	-1.989637000	
C	-5.395329000	2.677642000	0.888331000	
H	-4.722362000	3.427162000	1.325156000	
H	-6.024081000	2.292183000	1.699657000	
H	-6.043108000	3.197286000	0.179238000	
C	2.506017000	1.341677000	0.288588000	
C	2.399082000	2.246563000	1.511018000	
C	2.032725000	3.586463000	0.803890000	
H	1.490218000	4.270023000	1.464795000	
H	2.959906000	4.087755000	0.505629000	
C	1.216413000	3.234788000	-0.462398000	
C	1.274473000	1.831014000	2.491473000	
H	0.357504000	1.570732000	1.959695000	
H	1.047877000	2.645116000	3.190704000	
H	1.557883000	0.958841000	3.083482000	
C	3.722846000	2.425512000	2.271573000	



H	4.055389000	1.505889000	2.757023000
H	3.614886000	3.193387000	3.046238000
H	4.516871000	2.734567000	1.585241000
C	-0.303032000	3.355021000	-0.203436000
H	-0.891805000	3.012817000	-1.059412000
H	-0.561107000	4.404364000	-0.026241000
H	-0.619652000	2.782607000	0.668955000
C	1.583412000	4.157308000	-1.639580000
H	2.654588000	4.090202000	-1.851138000
H	1.335656000	5.202648000	-1.420463000
H	1.037721000	3.867129000	-2.544516000
C	3.362609000	0.310025000	0.039947000
C	4.547974000	-1.285806000	-1.095167000
C	4.667370000	-1.562478000	0.215107000
C	4.152116000	0.880215000	-2.218789000
H	3.368593000	1.632824000	-2.313666000
H	4.322425000	0.419718000	-3.194295000
H	5.075784000	1.381640000	-1.891148000
C	3.185233000	-1.024520000	2.121528000
H	2.149920000	-1.261809000	1.832983000
H	3.151785000	-0.262912000	2.899769000
H	3.644170000	-1.911213000	2.560458000
C	5.127575000	-1.978449000	-2.281882000
H	5.619872000	-2.908210000	-1.989761000
H	5.867379000	-1.361789000	-2.808373000
H	4.340332000	-2.225451000	-3.004676000
C	5.396978000	-2.676565000	0.888203000
H	6.044835000	-3.195975000	0.179012000
H	4.724395000	-3.426337000	1.325185000
H	6.025722000	-2.290818000	1.699404000

5^{Cy}			
N	4.162827000	-1.175064000	-1.097708000
N	4.170729000	-1.170670000	1.081827000
N	2.445347000	1.606685000	-0.041158000
C	3.860903000	-0.432480000	-0.008543000
C	4.664992000	-2.407166000	0.681295000
C	4.660371000	-2.409638000	-0.697664000
C	4.031559000	-0.773469000	-2.507135000
H	3.557324000	0.204230000	-2.568607000
H	3.421471000	-1.507878000	-3.035087000
H	5.019367000	-0.727881000	-2.968203000
C	4.018938000	-0.783019000	2.493284000
H	3.581727000	0.210501000	2.557368000
H	4.995322000	-0.779967000	2.980098000
H	3.370656000	-1.502783000	2.995600000
C	5.102203000	-3.445213000	1.657773000
H	5.442987000	-4.337844000	1.132587000
H	4.289085000	-3.742662000	2.328163000
H	5.934369000	-3.087135000	2.273311000
C	5.093378000	-3.449545000	-1.674053000
H	5.445175000	-4.337797000	-1.148695000
H	5.916537000	-3.089143000	-2.300171000
H	4.274681000	-3.754866000	-2.334097000
C	3.611268000	1.037118000	-0.031724000
C	4.774684000	2.018386000	-0.036779000
C	2.553891000	3.156385000	-0.055876000
C	5.833389000	1.673597000	-1.106626000
H	6.308627000	0.707071000	-0.917596000
H	6.617966000	2.433866000	-1.068341000
H	5.418451000	1.686686000	-2.116996000
C	5.460954000	2.005314000	1.358104000
H	5.947248000	1.048387000	1.560489000
H	4.773508000	2.244460000	2.172770000
H	6.242288000	2.769943000	1.350056000
C	1.690785000	3.734223000	-1.180464000
H	0.617387000	3.653379000	-0.988202000
H	1.925689000	3.280403000	-2.147328000
H	1.917149000	4.801620000	-1.256884000
C	2.113345000	3.665486000	1.322564000
H	2.735130000	3.265281000	2.126581000

DFT level: B3LYP-D3/6-31G(d,p)

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.947173 (Hartree/Particle)

Thermal correction to Energy= 0.994121

Thermal correction to Enthalpy= 0.995065

Thermal correction to Gibbs Free Energy= 0.868995

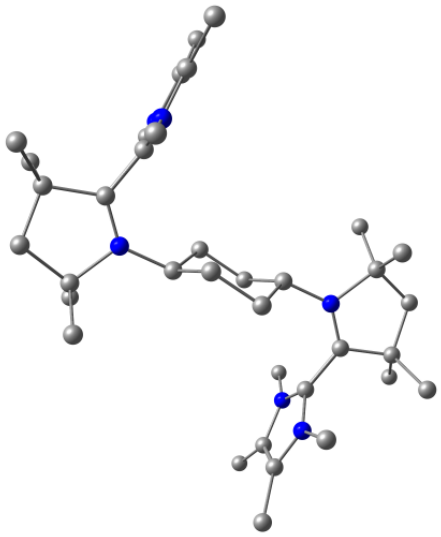
Sum of electronic and zero-point Energies= -1735.686114

Sum of electronic and thermal Energies= -1735.639167

Sum of electronic and thermal Enthalpies= -1735.638222

Sum of electronic and thermal Free Energies= -1735.764293

Charge = 4 Multiplicity = 1

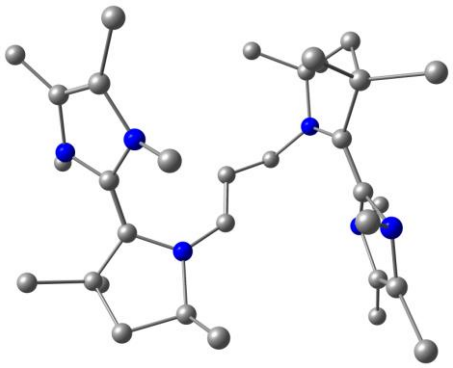


H	1.065116000	3.436077000	1.536363000	
H	2.213595000	4.754079000	1.335394000	
C	1.072499000	1.004142000	0.007486000	
H	0.422964000	1.877541000	0.077678000	
C	0.797139000	0.140338000	1.250407000	
H	1.045132000	0.692150000	2.161452000	
H	1.413893000	-0.764516000	1.229338000	
C	0.696282000	0.259116000	-1.286833000	
H	1.316346000	-0.638569000	-1.393121000	
H	0.878662000	0.892396000	-2.159217000	
C	4.057742000	3.358144000	-0.334689000	
H	4.461311000	4.173078000	0.268810000	
H	4.205954000	3.628621000	-1.383260000	
N	-4.162723000	1.175093000	1.097673000	
N	-4.170639000	1.170690000	-1.081859000	
N	-2.445431000	-1.606767000	0.041148000	
C	-3.860841000	0.432488000	0.008512000	
C	-4.664772000	2.407239000	-0.681330000	
C	-4.660138000	2.409718000	0.697630000	
C	-4.031484000	0.773481000	2.507098000	
H	-3.557346000	-0.204267000	2.568559000	
H	-3.421314000	1.507827000	3.035044000	
H	-5.019291000	0.727991000	2.968177000	
C	-4.018929000	0.783000000	-2.493313000	
H	-3.581792000	-0.210552000	-2.557393000	
H	-4.995329000	0.780012000	-2.980097000	
H	-3.370611000	1.502708000	-2.995663000	
C	-5.101894000	3.445323000	-1.657808000	
H	-5.442572000	4.337994000	-1.132622000	
H	-4.288759000	3.742683000	-2.328216000	
H	-5.934110000	3.087326000	-2.273326000	
C	-5.093027000	3.449675000	1.674018000	
H	-5.444751000	4.337956000	1.148658000	
H	-5.916206000	3.089356000	2.300156000	
H	-4.274286000	3.754927000	2.334041000	
C	-3.611314000	-1.037125000	0.031706000	
C	-4.774797000	-2.018312000	0.036801000	
C	-2.554068000	-3.156463000	0.055917000	
C	-5.833448000	-1.673440000	1.106673000	
H	-6.308648000	-0.706899000	0.917629000	
H	-6.618064000	-2.433673000	1.068446000	
H	-5.418470000	-1.686511000	2.117028000	
C	-5.461105000	-2.005183000	-1.358064000	
H	-5.947368000	-1.048232000	-1.560411000	
H	-4.773693000	-2.244333000	-2.172756000	
H	-6.242470000	-2.769780000	-1.350011000	
C	-1.691048000	-3.734331000	1.180555000	
H	-0.617636000	-3.653585000	0.988328000	
H	-1.925947000	-3.280456000	2.147394000	
H	-1.917502000	-4.801706000	1.257008000	
C	-2.113502000	-3.665643000	-1.322488000	
H	-2.735223000	-3.265427000	-2.126548000	
H	-1.065248000	-3.436309000	-1.536249000	
H	-2.213822000	-4.754230000	-1.335282000	
C	-1.072557000	-1.004284000	-0.007501000	
H	-0.423043000	-1.877697000	-0.077692000	
C	-0.797192000	-0.140481000	-1.250422000	
H	-1.045186000	-0.692292000	-2.161468000	
H	-1.413946000	0.764373000	-1.229353000	
C	-0.696336000	-0.259259000	1.286817000	
H	-1.316399000	0.638427000	1.393108000	
H	-0.878717000	-0.892538000	2.159201000	
C	-4.057940000	-3.358120000	0.334696000	
H	-4.461556000	-4.173029000	-0.268807000	
H	-4.206178000	-3.628590000	1.383265000	
8^{Pr}				DFT level: B3LYP-D3/6-31G(d,p)
N	-1.303067000	1.563301000	0.160270000	- Thermochemistry -
N	-2.264608000	-1.040640000	-0.997586000	----------
N	-4.158952000	-0.861254000	0.210598000	Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
N	1.997106000	-1.589210000	1.252189000	

N	3.210563000	1.022888000	0.977935000
N	3.221920000	0.900915000	-1.315621000
C	-0.253050000	0.916829000	0.779618000
C	-2.652610000	1.110628000	0.169952000
C	-3.548538000	2.320969000	0.394323000
C	-2.696354000	3.399036000	-0.343537000
H	-2.973102000	3.395757000	-1.403234000
H	-2.885416000	4.407036000	0.039490000
C	-1.204025000	3.001702000	-0.203264000
C	-4.926161000	2.227969000	-0.277840000
H	-4.821248000	1.944846000	-1.329598000
H	-5.434903000	3.197462000	-0.228871000
H	-5.575383000	1.490325000	0.197539000
C	-3.707110000	2.688523000	1.887282000
H	-4.142225000	3.688784000	2.004207000
H	-2.741902000	2.672179000	2.399253000
H	-4.361586000	1.979110000	2.399810000
C	-0.491863000	3.841743000	0.875559000
H	-0.943872000	3.698809000	1.859270000
H	-0.562231000	4.902441000	0.614422000
H	0.571008000	3.593677000	0.946297000
C	-0.447528000	3.159704000	-1.533293000
H	0.597390000	2.856176000	-1.414184000
H	-0.463778000	4.202353000	-1.871495000
H	-0.903925000	2.537901000	-2.308961000
C	-3.005370000	-0.161396000	-0.196273000
C	-3.000075000	-2.240778000	-1.139481000
C	-4.120061000	-2.148469000	-0.392539000
C	-1.400927000	-0.504355000	-2.032640000
H	-1.917447000	0.287356000	-2.594878000
H	-1.107474000	-1.299112000	-2.716997000
H	-0.500328000	-0.085751000	-1.584249000
C	-2.507327000	-3.358487000	-1.994330000
H	-3.156549000	-4.230524000	-1.895606000
H	-1.494301000	-3.659616000	-1.703384000
H	-2.472879000	-3.090896000	-3.058279000
C	-5.211643000	-3.140626000	-0.172636000
H	-5.113985000	-3.979636000	-0.864882000
H	-6.193208000	-2.680440000	-0.336509000
H	-5.213932000	-3.557460000	0.843196000
C	-4.648771000	-0.688831000	1.573290000
H	-5.089170000	-1.619510000	1.934706000
H	-5.414260000	0.088654000	1.641876000
H	-3.814071000	-0.405728000	2.227812000
C	-0.209742000	-0.321656000	1.318860000
C	1.041477000	-0.773473000	2.024180000
H	1.568794000	0.115013000	2.388760000
H	0.786125000	-1.358926000	2.913479000
C	2.517563000	-1.130917000	0.010613000
C	2.684320000	-2.320951000	-0.935829000
C	2.758138000	-3.480821000	0.099001000
H	2.425656000	-4.434914000	-0.322124000
H	3.800874000	-3.607922000	0.409586000
C	1.920064000	-3.060093000	1.324449000
C	1.479276000	-2.544618000	-1.878717000
H	0.540373000	-2.450226000	-1.333587000
H	1.522008000	-3.543694000	-2.329934000
H	1.454935000	-1.817745000	-2.691583000
C	3.994312000	-2.287503000	-1.741211000
H	4.027166000	-1.467210000	-2.460583000
H	4.123180000	-3.224689000	-2.295219000
H	4.848926000	-2.161702000	-1.069786000
C	2.567691000	-3.564881000	2.627440000
H	3.593530000	-3.193677000	2.708973000
H	2.588975000	-4.660766000	2.656992000
H	2.009670000	-3.220589000	3.504798000
C	0.471541000	-3.599140000	1.256583000
H	-0.094345000	-3.318565000	2.150082000
H	0.478145000	-4.693196000	1.201018000
H	-0.069392000	-3.207994000	0.394494000

Zero-point correction= 0.852557
(Hartree/Particle)
Thermal correction to Energy= 0.896773
Thermal correction to Enthalpy= 0.897717
Thermal correction to Gibbs Free Energy= 0.780048
Sum of electronic and zero-point Energies= -1619.004322
Sum of electronic and thermal Energies= -1618.960106
Sum of electronic and thermal Enthalpies= -1618.959161
Sum of electronic and thermal Free Energies= -1619.076831

Charge = 0 Multiplicity = 1



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C	3.505742000	2.306578000	0.440410000	
C	3.478992000	2.242384000	-0.903115000	
C	4.095861000	0.515406000	2.030582000	
H	3.717029000	-0.447564000	2.376187000	
H	4.104031000	1.213439000	2.871104000	
H	5.125285000	0.377196000	1.666624000	
C	3.776623000	3.457571000	1.349359000	
H	3.857161000	4.391027000	0.788505000	
H	4.705413000	3.331974000	1.920618000	
H	2.963204000	3.568789000	2.077232000	
C	3.692260000	3.328923000	-1.904154000	
H	4.073820000	4.228257000	-1.416644000	
H	2.771581000	3.608800000	-2.432516000	
H	4.422970000	3.019902000	-2.660891000	
C	2.369172000	0.696684000	-2.476381000	
H	1.311640000	0.629926000	-2.188182000	
H	2.636993000	-0.215426000	-3.007937000	
H	2.494432000	1.522283000	-3.177656000	
H	0.655138000	1.510154000	0.818904000	
H	-1.050152000	-1.001083000	1.259700000	
7^{cy}				DFT level: uB3LYP-D3/6-31G(d,p)
N	2.416888000	1.610291000	0.058159000	- Thermochemistry -
N	4.043281000	-1.168123000	1.134996000	----------
N	4.054660000	-1.301359000	-1.032877000	Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
N	-2.416822000	-1.610281000	0.058031000	
N	-4.043367000	1.168112000	1.134963000	Zero-point correction= 0.945531
N	-4.054672000	1.301328000	-1.032910000	(Hartree/Particle)
C	1.063846000	1.022170000	0.058167000	Thermal correction to Energy= 0.992659
H	0.395042000	1.886008000	0.056644000	Thermal correction to Enthalpy= 0.993604
C	0.740615000	0.212940000	1.328143000	Thermal correction to Gibbs Free Energy= 0.866116
H	0.957815000	0.809100000	2.219491000	Sum of electronic and zero-point Energies= -1736.133514
H	1.374669000	-0.680041000	1.367798000	Sum of electronic and thermal Energies= -1736.086385
C	-0.740564000	-0.212996000	1.328134000	Sum of electronic and thermal Enthalpies= -1736.085441
H	-0.957752000	-0.809226000	2.219440000	Sum of electronic and thermal Free Energies= -1736.212929
H	-1.374622000	0.679981000	1.367864000	
C	-1.063777000	-1.022139000	0.058102000	Charge = 3 Multiplicity = 2
H	-0.394975000	-1.885975000	0.056543000	
C	-0.741510000	-0.209125000	-1.208563000	
H	-1.370477000	0.687615000	-1.243556000	
H	-0.964176000	-0.800547000	-2.101924000	
C	0.741587000	0.209237000	-1.208550000	
H	1.370566000	-0.687494000	-1.243630000	
H	0.964233000	0.800730000	-2.101870000	
C	3.601442000	0.990337000	-0.067614000	
C	4.766554000	1.965063000	-0.198694000	
C	4.090868000	3.296372000	0.219280000	
H	4.457923000	4.140970000	-0.366843000	
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C	4.426625000	-2.465862000	0.818463000	
C	4.433681000	-2.550635000	-0.553559000	
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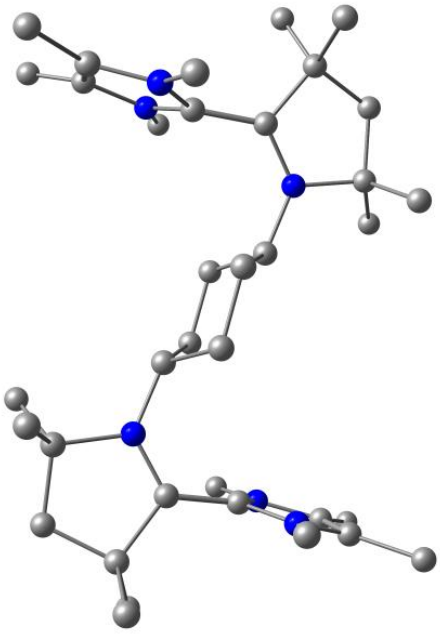

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N	4.795094000	-0.974938000	0.919951000	----------
N	2.438239000	1.470157000	-0.692282000	Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
C	4.062334000	-0.258813000	-0.049675000	
C	5.172104000	-2.224334000	0.362338000	Zero-point correction= 0.940219
C	4.693882000	-2.289716000	-0.897118000	(Hartree/Particle)
C	3.964209000	-0.520831000	-2.500803000	Thermal correction to Energy= 0.987252
H	3.199728000	0.254096000	-2.536544000	Thermal correction to Enthalpy= 0.988196
H	3.734193000	-1.288972000	-3.242066000	Thermal correction to Gibbs Free Energy= 0.862187
H	4.934824000	-0.063161000	-2.745843000	Sum of electronic and zero-point Energies= -1736.873522
C	4.481013000	-0.837755000	2.332563000	Sum of electronic and thermal Energies= -1736.826489
H	3.529354000	-0.302921000	2.421690000	Sum of electronic and thermal Enthalpies= -1736.825545

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H	0.681909000	1.921518000	1.412541000
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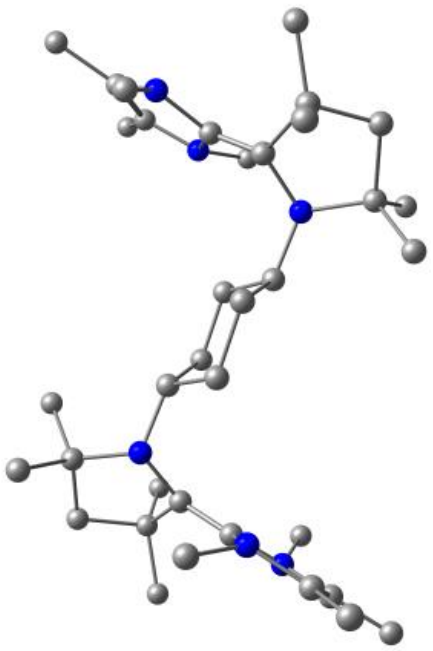

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H	-4.775016000	-3.138723000	1.074947000	

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