A Crystalline Monomeric Allenyl/Propargyl Radical

Max M. Hansmann, Mohand Melaimi and Guy Bertrand*

UCSD-CNRS Joint Research Laboratory (UMI 3555), Department of Chemistry and Biochemistry, University of California, San Diego, La Jolla, California 92093-0358, United States

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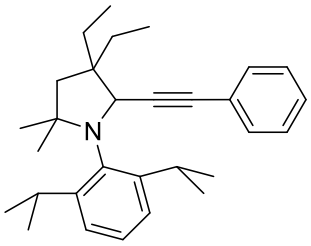
1. General procedures

Experiments were performed under an atmosphere of dry argon using standard Schlenk techniques. Solvents were dried by standard methods and distilled under argon. ^{1}H and ^{13}C NMR spectra were recorded on Varian Inova 500, and Bruker 300 MHz spectrometers. NMR multiplicities are abbreviated as follow: s=singlet, d=doublet, t=triplet, sept=septet, m=multiplet, br=broad signal. Melting points were measured with an Electrothermal MEL-TEMP apparatus. Electrochemical experiments were performed with an analyzer from CH Instruments (Model 620E) with platinum working and auxiliary electrodes.
The reference electrode was built from a silver wire inserted in a small glass tube fitted with a porous Vycor frit and filled with a $AgNO_3$ solution in acetonitrile (0.1 M). Ferrocene was used as a standard, and all reduction potentials are reported with respect to the $E_{1/2}$ of the Fc^{+}/Fc redox couple. EPR spectra were obtained using an X-band Bruker E500 spectrometer at either UCSD or UCR facilities. Field calibration was accomplished by using a standard of solid 2,2-diphenyl-1 picrylhydrazyl (DPPH), g = 2.0036. (Cyclic) (alkyl)aminocarbenes CAAC **1**$^{\mathbf{Et}}$ and **1**$^{\mathbf{Menth}}$, as well as their iminium precursor salts were prepared according to literature procedures.[i]

2. Characterization data

Synthesis of **2a**

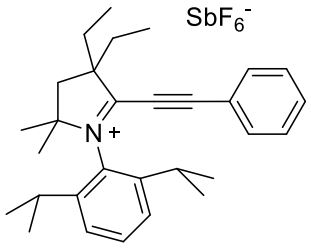


KHMDS (521 mg, 2.62 mmol, 1.05 eq.) was added at room temperature to a suspension of diethyl-CAAC iminium BF_4 (1.0 g, 2.49 mmol, 1.0 eq.) in Et_2O (25 mL). The mixture was stirred 15 min at room temperature after which phenylacetylene (330 µL, 2.99 mmol, 1.2 eq.) was added. The solution was then stirred for 16h at room temperature. Solvent and volatiles were removed under reduced pressure and the crude product purified by flash column chromatography (SiO_2, pure pentane) to give the desired product as colorless oil (940 mg, 2.26 mmol, 91%).

m.p. 106 ^{o}C; **^{1}H NMR** ($CDCl_3$, 298K, 500 MHz): δ = 7.21-7.18 (m, 2H), 7.17-7.09 (m, 4H), 7.06-7.04 (m, 2H), 4.74 (s, 1H), 3.89 (sept., J = 6.8 Hz, 1H), 3.33 (sept., J = 6.8 Hz, 1H), 2.13-2.04 (m, 1H), 2.02 (d, J =

12.9 Hz, 1H), 1.87-1.78 (m, 1H), 1.73-1.62 (m, 2H), 1.59-1.50 (m, 1H), 1.28-1.25 (m, 6H), 1.21 (d, *J* = 6.9 Hz, 3H), 1.16 (s, 3H), 1.11-1.08 (m, 6H), 1.03-0.95 (m, 6H); **^{13}C NMR** ($CDCl_3$, 298K, 125 MHz): δ = 153.23, 151.54, 137.41, 131.39, 128.07, 127.46, 126.62, 124.06, 123.89, 90.66, 85.93, 64.97, 61.54, 51.10, 47.06, 31.36, 30.18, 29.65, 27.91, 27.88, 26.68, 26.33, 25.78, 23.80, 23.75, 9.57, 8.85. **HR-ESI-TOF-MS** $[C30H41N]^+$ calc. $[M+H]^+$ 416.3312., found 416.3316.

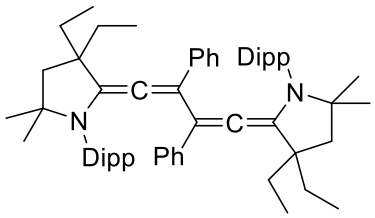
Synthesis of **3a**



DDQ (360 mg, 1.58 mm) was added at room temperature to a solution of **2a** (600 mg, 1.44 mmol) in diethyl ether (50 mL). The reaction mixture was stirred for 1 hour while a dark powder precipitated. The dark solid was recovered by filtration, and further washed with diethyl ether (3 x 30 mL). The remaining solid was then dissolved in mixture of methylene chloride (10 mL) and acetonitrile (10 mL). $NOSbF_6$ (420 mg, 1.58 mmol) was then added to the dark purple solution. A fast gas evolution was observed and the solution turned yellow. The solution was stirred for 1 h, the solvent removed under reduced pressure, redissolved in CH_2Cl_2 (8 mL) and filtered through a filter cannula. The solvent was concentrated (ca. 1-2 mL) and Et_2O (50 mL) added to precipitate the desired product. The solvent was removed by filtration and the solid wash with Et_2O (3 x 30 mL) to give the desired product **3a** as slightly yellow solid (660 mg, 1.01 mmol, 70%).

m.p. > 200 °C; **^{1}H NMR** (CD_3CN, 298K, 500 MHz): δ = 7.71-7.63 (m, 2H), 7.53 (d, *J* = 7.9 Hz, 2H), 7.48-7.44 (m, 2H), 7.33-7.29 (m, 2H), 2.72 (sept., *J* = 6.5 Hz, 2H), 2.50 (s, 2H), 2.16-2.02 (m, 4H), 1.58 (s, 6H), 1.35 (d, *J* = 6.7 Hz, 6H), 1.17-1.11 (12H); **^{13}C NMR** (CD_3CN, 298K, 125 MHz): δ = 179.78, 146.14, 135.45, 135.16, 132.89, 130.48, 126.91, 81.81, 81.71, 59.33, 42.87, 31.67, 30.48, 29.05, 26.16, 23.16, 9.24; **IR** (ATR) $\tilde{\nu}$ = 2972 cm^{-1}, 2199, 1716, 1567, 1456, 1373, 1140, 1052, 934, 815; **HR-ESI-TOF-MS** $[C_{35}H_{48}N]$ calc. $[M^+]$ 414.3155, found 414.3158.

Synthesis of **5a**



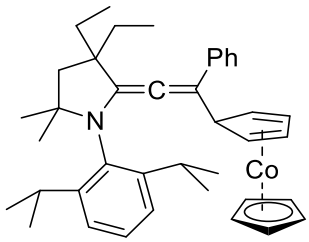
TDAE (56 mg, 0.15 mmol, 0.5 eq.) was added at room temperature to a solution of **3a** (200 mg, 0.31 mmol) in THF (25 mL). This solution was stirred for 1h at room temperature after which solvent and volatiles were removed under reduced pressure. The resulting solid extracted with pentane (2 x 15 mL). The solvent was removed under reduced pressure to give **5a** as brownish solid (100 mg, 0.16 mmol, 51%).

^{1}H and ^{13}C NMR of **5a** could not be recorded due to small amount of paramagnetic impurities that could not be separated.

m.p. 125 ºC;

HR-ESI-TOF-MS $[C_{36}H_{46}N_2]^+$ calc. $[M]^+$ 506.3661; found 506.3659.

Synthesis of **6a**

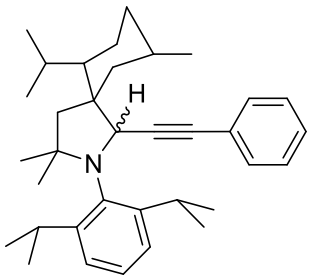


Cobaltocene (58.1 mg, 0.30 mmol, 2eq.) was added at room temperature to a solution of iminium **3a** (100 mg, 0.15 mmol). This reddish colored solution was stirred for 1h at room temperature after which solvent and volatiles were removed under reduced pressure. The remaining solid was extracted in pentane (10 mL), reduced to about 5 mL and stored at -40°C to yield deep red crystals suitable for x-ray diffraction (42 mg, 0.066 mmol, 44%).

m.p. 140°C; **^{1}H NMR** (C_6D_6, 298K, 500 MHz): δ = 7.18-7.16 (m, 2H), 7.11-7.07 (m, 2H), 7.05-7.02 (m, 1H), 7.02-6.98 (m, 3H), 5.99 (s, 1H), 4.76 (s, 1H), 4.58 (s, 2H), 3.78 (t, *J* = 2.3 Hz, 1H), 3.54 (sept., *J* = 6.7 Hz, 1H), 3.21 (sept., *J* = 6.7 Hz, 1H), 2.93 (s, 1H), 2.73 (s, 1H), 1.99-1.91 (m, 1H), 1.89-1.82 (m, 1H), 1.80 (d, *J* = 9.8 Hz, 2H), 1.78-1.66 (m, 2H), 1.50 (d, *J* = 6.7 Hz, 3H), 1.37 (d, *J* = 6.7 Hz, 3H), 1.21 (s, 3H), 1.16 (d, *J* = 6.7 Hz, 3H), 1.14-1.09 (m, 6H), 0.91 (t, *J* = 7.4 Hz, 3H), 0.64 (d, *J* = 6.7 Hz, 3H); **^{13}C NMR** (C_6D_6, 298K, 125 MHz): δ = 190.72, 151.26, 150.97, 139.95, 135.99, 132.08, 127.60, 125.98,

124.44, 124.08, 121.99, 79.19, 76.15, 75.07, 63.31, 55.94, 48.94, 48.28, 44.44, 33.50, 32.66, 30.27, 29.62, 28.69, 28.52, 27.38, 25.91, 24.70, 24.47, 10.20, 9.80; **IR** (ATR) $\tilde{\nu}$ = 2966 cm^{-1}, 2866, 1925, 1488, 1455, 1440, 1380, 1322, 1299, 1201, 1174, 1105, 1047, 933; **HR-ESI-TOF-MS** $[C_{40}H_{51}CoN]^+$ calc. $[M+H]^+$ 604.3348, found 604.3349.

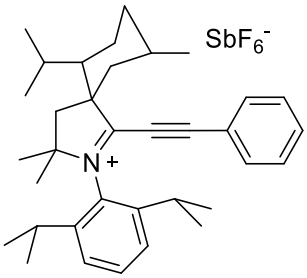
Synthesis of **2b**



Phenylacetylene (190 µL, 1.73 mmol, 1.1 eq.) was added at room temperature to a solution of menthyl-CAAC (600 mg, 1.57 mmol) in pentane (10 mL). the solution was stirred for 14h after which solvent and volatiles were removed under reduced pressure to afford white solid. This solid consist of a clean 1:1 mixture of epimers **2b** that was used in the next step without further purification (760mg, quant. yield, 1:1 mixture of diastereomers). Characterization data for the diasteromeric mixture.

m.p. 101 °C; **^{1}H NMR** ($CDCl_3$, 298K, 500 MHz): δ = 7.25-7.20 (m, 2H); 7.19-7.11 (m, 10H), 6.97-6.93 (m, 4H), 4.90 (s, 1H), 4.85 (s, 1H), 4.11 (sept., *J* = 6.3 Hz, 1H), 3.86 (sept., *J* = 6.3 Hz, 1H), 3.41 (sept., *J* = 6.8 Hz, 1H), 3.35 (sept., *J* = 6.8 Hz, 1H), 2.91 (d, *J* = 13.7 Hz, 1H), 2.61-2.48 (m, 2H), 2.42 (d, *J* = 12.7 Hz, 1H), 2.35-2.25 (m, 1H), 2.22 (d, *J* = 13.1 Hz, 1H), 2.17-2.06 (m, 2H), 1.85-1.78 (m, 2H), 1.77-1.71 (m, 1H), 1.70-1.52 (m, 6H), 1.32-1.21 (m, 27H), 1.14-1.10 (m, 9H), 1.08-1.03 (m, 9H), 1.01-0.98 (m, 2H), 0.95-0.92 (m, 4H), 0.89-0.85 (m, 4H); **^{13}C NMR** ($CDCl_3$, 298K, 125 MHz): δ = 153.40, 152.94, 151.66, 151.18, 137.41, 137.19, 131.05, 128.13, 127.49, 127.41, 126.61, 126.56, 124.14, 124.10, 124.00, 123.97, 123.86, 92.30, 91.98, 87.17, 86.92, 62.43, 61.61, 59.81, 57.82, 55.68, 55.49, 53.57, 50.60, 50.49, 48.94, 48.22, 48.08, 36.32, 35.70, 30.79, 30.11, 29.70, 29.51, 29.49, 29.34, 28.83, 28.79, 28.51, 27.89, 26.99, 26.87, 26.59, 26.57, 25.97, 25.63, 25.43, 25.40, 25.07, 23.97, 23.93, 23.80, 23.67, 23.56, 23.42, 23.21, 21.14, 19.26; **HR-ESI-TOF-MS** $[C_{35}H_{48}N]^+$ calc. $[M+H]^+$ 482.3781, found 482.3785.

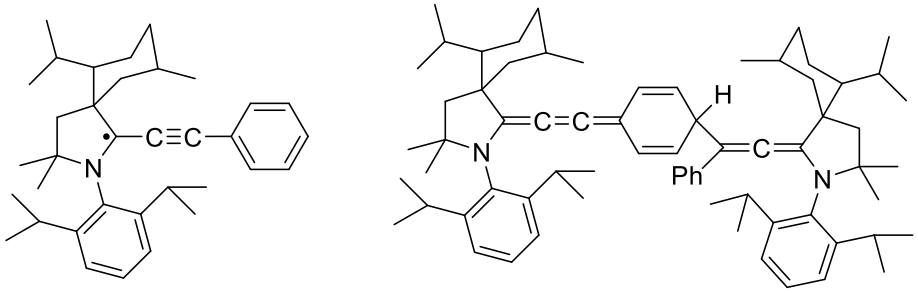
Synthesis of **3b**



DDQ (33 mg, 0. 145 mmol, 10 mol%) and $NOSbF_6$ (424 mg, 1.60 mmol, 1.1 eq.) were added at room temperature to a solution of **2b** (700 mg, 1.45 mmol) in CH_2Cl_2 (10 mL) and CH_3CN (10 mL). A fast gas formation was observed and the solution turns slightly yellow. The solution was stirred for 1 after which the solvent was removed under reduced pressure. The solid residue was extracted with CH_2Cl_2 (8 mL). The solution was then concentrated under reduced pressure to about ca. 1-2 mL, and Et_2O (25 mL) was added to precipitate the desired product. The solvent was removed by syringe and the solid wash with Et_2O (3x 10 mL) to give **3b** as a colorless solid (523 mg, 1.08 mmol, 75%).

m.p. > 200°C; **^{1}H NMR** (CD_3CN, 298K, 500 MHz): δ = 7.72-7.67 (m, 1H), 7.68-7.64 (m, 1H), 7.56-7.52 (m, 2H), 7.48-7.43 (m, 2H), 7.20-7.16 (m, 2H), 2.75 (d, *J* = 14.2 Hz, 1H), 2.73-2.66 (m, 2H), 2.44 (dt, *J* = 14.3 Hz, 2.2 Hz, 1H), 2.33 (d, *J* = 14.2 Hz, 1H), 2.18-2.11 (m, 2H), 2.09-2.03 (m, 1H), 1.88-1.83 (m, 1H), 1.80-1.74 (m, 1H), 1.68 (dd, *J* = 13.0 Hz, 3.8 Hz, 1H), 1.58 (d, *J* = 11.7 Hz, 6H), 1.37-1.34 (m, 6H), 1.12 (d, *J* = 6.7 Hz, 3H), 1.10-1.06 (m, 6H), 0.97 (d, *J* = 6.8 Hz, 6H); **^{13}C NMR** (CD_3CN, 298K, 125 MHz): δ = 177.68, 146.35, 146.22, 135.72, 134.55, 132.86, 130.57, 130.26, 127.07, 126.93, 124.59, 85.69, 79.74, 59.97, 52.42, 51.25, 48.83, 34.78, 30.60, 30.26, 29.74, 29.60, 29.29, 28.51, 26.90, 25.60, 24.71, 23.46, 23.33, 23.24, 22.14, 18.92; **IR** (ATR) $\tilde{\nu}$ = 2969 cm^{-1}, 2875, 2193, 1736, 1545, 1456, 1445, 1344, 1173, 1141, 1052, 997, 934, 802; **HR-ESI-TOF-MS** [$C_{35}H_{48}N$] calc. [M^+] 482.3781, found 482.3777.

Synthesis of **4b**/**7b**



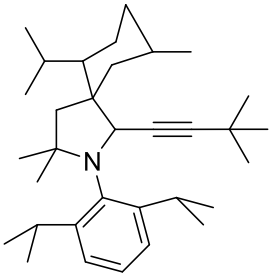
TDAE (56 mg, 0.28 mmol, 0.5 eq.) was added at room temperature to a solution of **3b** (400 mg, 0.56 mmol) in THF (25 mL). The solution stirred for 1 h at room temperature after which solvent and volatiles

were removed under reduced pressure. The resulting solid extracted with pentane (2x15 mL). The solvent was removed under reduced pressure to give **7b** as brownish solid (100 mg, 0.10 mmol, 37%).

^{1}H and ^{13}C NMR of **7b** could not be recorded due to the dynamic equilibrium between paramagnetic monomer **4b** and dimer **7b** in solution.

For **7b**: **m.p.** 160 °C; **IR** (ATR) $\tilde{\nu}$ = 2953 cm^{-1}, 2866, 2096, 1635, 1520, 1454, 1384, 1362, 1315, 1255, 1227, 1172, 1091, 993 **HR-ESI-TOF-MS** $[C_{70}H_{97}N_2]^+$ calc. $[M+H]^+$ 965.7646; found 965.7633.

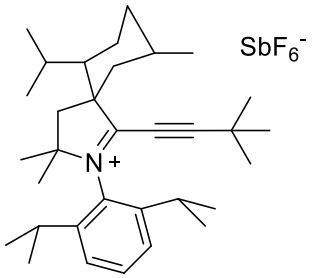
Synthesis of **2c**



KHMDS (425 mg, 2.1 mmol, 1.0 eq.) was added at room temperature to a suspension of menthyl-CAAC iminium BF_4 (1.0 g, 2.1 mmol, 1.0 eq.) in Et_2O (25 mL). The solution was stirred for 15 min after which 3,3-dimethylbut-1-yne (500 µL, 4.1 mmol, 2.0 eq.) was added. The solution was then stirred for another 36 h at 50°C. The solvent was removed under reduced pressure and the crude product purified by flash column chromatography (SiO_2, pure pentane) to give the desired product as ca. 1:1 diasteromeric mixture as colorless solid (340 mg, 0.73 mmol, 34%). Characterization data for the diasteromeric mixture.

m.p. 255 °C; **^{1}H NMR** ($CDCl_3$, 298K, 500 MHz): δ = 7.18-7.04 (m, 6H), 4.69 (s, 1H), 4.58 (s, 1H), 4.07 (sept., *J* = 6.8 Hz, 1H), 3.79 (sept., *J* = 6.8 Hz, 1H), 3.32 (sept., *J* = 6.8 Hz, 1H), 3.27 (sept., *J* = 6.8 Hz, 1H), 2.77 (*d*, = 14.7 Hz, 1H), 2.57-2.45 (m, 2H), 2.32-2.25 (m, 2H), 2.11-2.05 (m, 2H), 1.98-1.93 (m, 1H), 1.78-1.71 (m, 3H), 1.65-1.54 (m, 2H), 1.50-1.39 (m, 3H), 1.30-1.04 (m, 36H), 0.99 (d, *J* = 6.9 Hz, 3H), 0.93 (d, *J* = 6.9 Hz, 3H), 0.89-0.81 (m, 20H); **^{13}C NMR** ($CDCl_3$, 298K, 125 MHz): δ = 153.29, 152.74, 151.57, 150.99, 137.93, 137.62, 126.27, 126.16, 124.04, 123.88, 123.67, 123.56, 95.05, 94.77, 80.54, 80.37, 61.97, 61.13, 59.41, 57.01, 56.14, 55.44, 53.83, 50.56, 49.49, 48.32, 48.15, 48.03, 36.45, 35.77, 30.60, 30.49, 30.31, 29.96, 29.73, 29.20, 29.15, 29.02, 28.60, 28.57, 28.32, 27.77, 27.23, 26.55, 26.48, 26.18, 25.99, 25.21, 25.12, 25.09, 25.07, 24.38, 24.28, 23.76, 23.35, 23.25, 23.22, 21.36, 18.97; **IR** (ATR) $\tilde{\nu}$ = 2945 cm^{-1}, 2865, 2841, 1454, 1360, 1263, 1203, 1175, 1149, 1045, 927; **HR-ESI-TOF-MS** $[C_{33}H_{54}N]^+$ calc. $[M+H]^+$ 464.4251, found 464.4247.

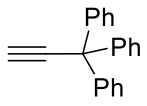
Synthesis of **3c**



$NOSbF_6$ (145 mg, 0.54 mmol) and DDQ (5.6 mg, 5 mol%) were added at room temperature to a solution of **2c** (230 mg, 0.50 mmol) in CH_2Cl_2 (5 mL) and CH_3CN (5 mL). A fast gas formation was observed and the solution turned slightly yellow. The solution was stirred for 30 min after which the solvent was removed under reduced pressure. The solid residue was extracted with CH_2Cl_2 (5 mL). The solution was then concentrated under reduced pressure to about ca. 1-2 mL, and Et_2O (25 mL) was added to precipitate the desired product. The solvent was removed by syringe and the solid wash with Et_2O (3 x 10 mL) to give **3c** as colorless solid (300 mg, 0.43 mmol, 86%).

^{1}H NMR ($CDCl_3$, 298K, 500 MHz): δ = 7.61 (t, *J* = 7.9 Hz, 1H), 7.50-7.46 (m, 2H), 2.68 (d, *J* = 14.3 Hz, 1H), 2.62 (sept., *J* = 6.4 Hz, 2H), 2.37-2.31 (m, 1H), 2.27 (d, *J* = 14.4 Hz, 1H), 2.17-2.10 (m, 2H), 2.10-2.05 (m, 1H), 2.04-1.99 (m, 1H), 1.98-1.95 (m, 1H), 1.79-1.74 (m, 1H), 1.73-1.70 (m, 1H), 1.63-1.58 (m, 1H), 1.55 (s, 3H), 1.53 (s, 3H), 1.36-1.32 (m, 6H), 1.21 (d, *J* = 6.7 Hz, 3H), 1.18 (d, *J* = 6.7 Hz, 3H), 1.06 (s, 9H), 0.95 (d, *J* = 6.7 Hz, 6H); **^{13}C NMR** ($CDCl_3$, 298K, 125 MHz): δ = 179.02, 145.86, 145.74, 136.23, 132.66, 127.13, 126.97, 79.74, 76.77, 60.09, 52.23, 51.17, 48.79, 34.66, 30.61, 30.36, 30.24, 29.61, 29.53, 29.20, 28.49, 28.43, 27.21, 25.94, 24.68, 23.50, 23.34, 22.94, 22.04, 19.07; **IR** (ATR) $\tilde{\nu}$ = 2968 cm^{-1}, 2932, 2871, 2210, 1589, 1566, 1456, 1328, 1260, 1200, 1151, 1123, 1052, 992, 933; **HR-ESI-TOF-MS** $[C_{33}H_{52}N]^+$ calc. $[M]^+$ 462.4094, found 462.4095.

Synthesis of prop-2-yne-1,1,1-triyltribenzene

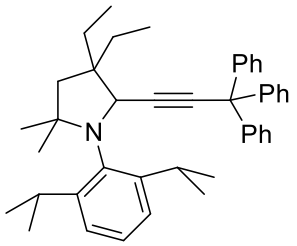


To a solution of trityl chloride (2.0 g, 7.17 mmol) in THF (80 mL) was added at room temperature ethynyl magnesium bromide (43 mL, 0.5 M, 21.5 mmol, 3.0 eq.). The solution was heated at reflux for 16 h, cooled down to 0 °C and a saturated aqueous solution of NH_4Cl added (100 mL). The phases were separated and the aqueous phases extracted with CH_2Cl_2 (3x50 mL). The combined organic phases were dried over $MgSO_4$, filtered and the solvent removed under reduced pressure. The crude product was

purified by flash column chromatography (SiO_2; pure pentane) to give the desired alkyne as colorless solid (1.5 g, 5.6 mmol, 78%). The characterization data is in agreement with previously published data.[ii]

^{1}H NMR ($CDCl_3$, 298K, 500 MHz): δ = 7.38-7.24 (m, 15H), 2.74 (s, 1H); **^{13}C NMR** ($CDCl_3$, 298K, 125 MHz): δ = 144.85, 129.21, 128.16, 127.06, 89.89, 73.54, 55.58.

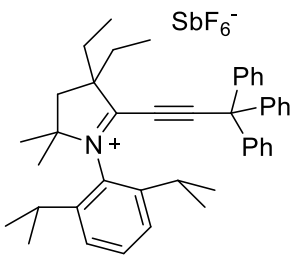
Synthesis of **2d**



KHMDS (550 mg, 2.75 mmol) was added at room temperature to a suspension of diethyl-CAAC iminium BF_4 (1.08 g, 2.69 mmol) in Et_2O (25 mL). The solution was stirred for 15 min after which prop-2-yne-1,1,1-triyltribenzene (600 mg, 2.23 mmol) was added. The solution was then stirred for another 48h at 45°C. The solution was cooled down and the solvent was removed under reduced pressure. The crude product purified by flash column chromatography (SiO_2; pure pentane) to give the **2d** product as colorless solid (850 mg, 1.46 mmol, 54%).

m.p. 163°C; **^{1}H NMR** ($CDCl_3$, 298K, 500 MHz): δ = 7.38-7.32 (m, 1H), 7.21-7.08 (m, 11H), 6.92-6.83 (m, 6H), 4.84 (s, 1H), 3.81-3.72 (m, 1H), 3.42-3.32 (m, 1H), 2.06-1.96 (m, 2H), 1.77-1.65 (m, 2H), 1.59-1.47 (m, 2H), 1.27-1.23 (m, 3H), 1.19-1.06 (m, 14H), 0.95-0.87 (m, 6H)0..59-0.52 (m, 3H); **^{13}C NMR** ($CDCl_3$, 298K, 125 MHz): δ = 153.12, 151.50, 145.28, 137.59, 129.23, 127.72, 126.58, 126.32, 124.39, 124.34, 91.27, 85.22, 64.43, 61.30, 55.75, 51.37, 47.24, 31.66, 29.63, 27.72, 27.14, 26.77, 25.59, 25.31, 24.14, 23.42, 9.52, 8.75. **HR-ESI-TOF-MS** $[C_{43}H_{52}N]^+$ calc. $[M+H]^+$ 582.4094, found 582.4086.

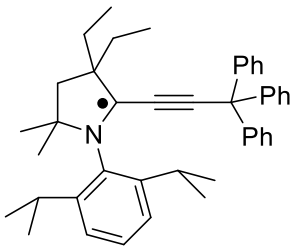
Synthesis of **3d**



$NOSbF_6$ (335 mg, 1.26 mmol) and DDQ (10 mg) were added at room temperature to a solution of **2d** (700 mg, 1.20 mmol) in CH_2Cl_2 (10 mL) and CH_3CN (10 mL). A fast gas formation was observed and the solution turns slightly yellow. The solution was stirred for 45 min after which the solvent was removed under reduced pressure. The solid residue was extracted with CH_2Cl_2 (10 mL). The solution was then concentrated under reduced pressure to about ca. 1-2 mL, and Et_2O (25 mL) was added to precipitate the desired product. The solvent was removed by syringe and the solid wash with Et_2O (3 x 10 mL) to give the desired product as colorless solid (850 mg, 1.04 mmol, 87%).

^{1}H NMR ($CDCl_3$, 298K, 500 MHz): δ = 7.87-7.81 (m, 1H), 7.58-7.52 (m, 2H), 7.40-7.24 (m, 9H), 6.84-6.75 (m, 6H), 2.69-2.60 (m, 2H), 2.51 (s, 2H), 2.07-1.92 (m, 12H), 1.56 (s, 6H), 1.36-1.28 (m, 6H), 0.81-0.70 (m, 6H); **^{13}C NMR** ($CDCl_3$, 298K, 125 MHz): δ = 180.88, 145.76, 141.89, 132.96, 129.68, 129.43, 129.03, 127.41, 82.54, 76.52, 66.17, 60.04, 41.98, 31.66, 30.32, 28.94, 25.63, 23.28, 9.29; **IR** (ATR) $\tilde{\nu}$ = 2972 cm^{-1}, 2209, 1596, 1581, 1490, 1447, 1388, 1351, 1268, 1144, 113, 1052; **HR-ESI-TOF-MS** $[C_{43}H_{50}N]^+$ calc. $[M]^+$ 580.3943, found 580.3937.

Synthesis of radical **4d**

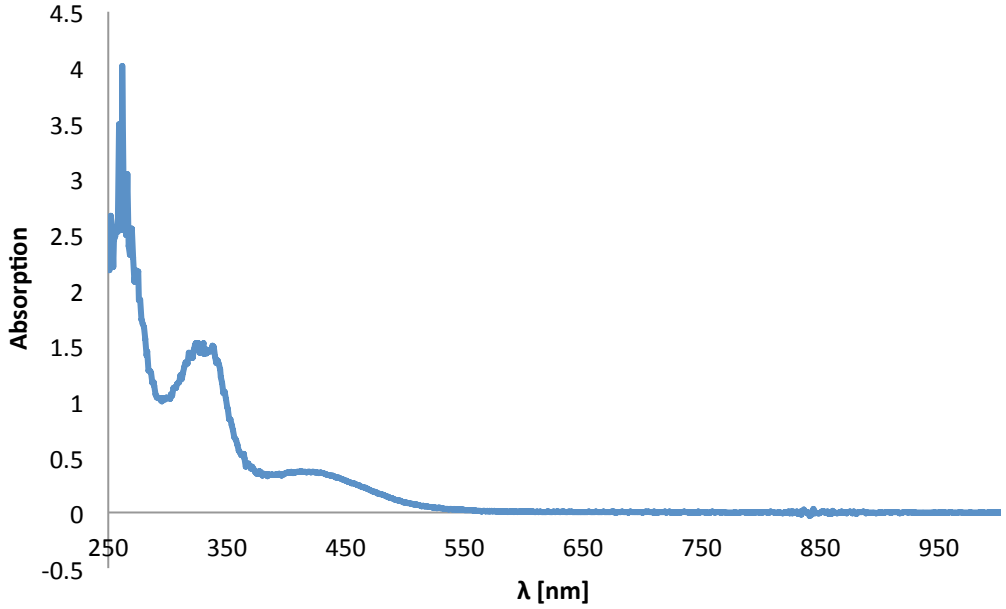


Option A: Cobaltocene (46 mg, 0.24 mmol) was added at room temperature to a solution of iminium **3d** (200 mg, 0.24 mmol) in THF (20 mL). The yellow/orange solution was stirred for 1 h after which the solvent was removed under reduced pressure. The solid residue was extracted with pentane (2 x 15 mL) and the solvent evaporated under reduced pressure to give **4d** as yellow/red solid (70 mg, 0.12 mmol, 50%). Single crystals suitable for x-ray diffraction were obtained from a saturated pentane solution at -40°C.

Option B: Sodium pieces (10 mg, 0.43 mmol) was added at room temperature to a solution of iminium **3d** (100 mg, 0.12 mmol) in THF (10 mL). The yellow/orange solution was stirred for 3h h after which the solvent was removed under reduced pressure. The solid residue was extracted with pentane (2 x 15 mL) and the solvent evaporated under reduced pressure to give **4d** as yellow/red solid (20 mg, 0.034 mmol, 28%).

m.p.143°C; UV-VIS absorption: λ_{max} = 330 nm and 414 nm (see below); Fitted EPR-parameters: a_N = 4.4 G.

UV-VIS spectrum of **4d**



3. NMR spectra

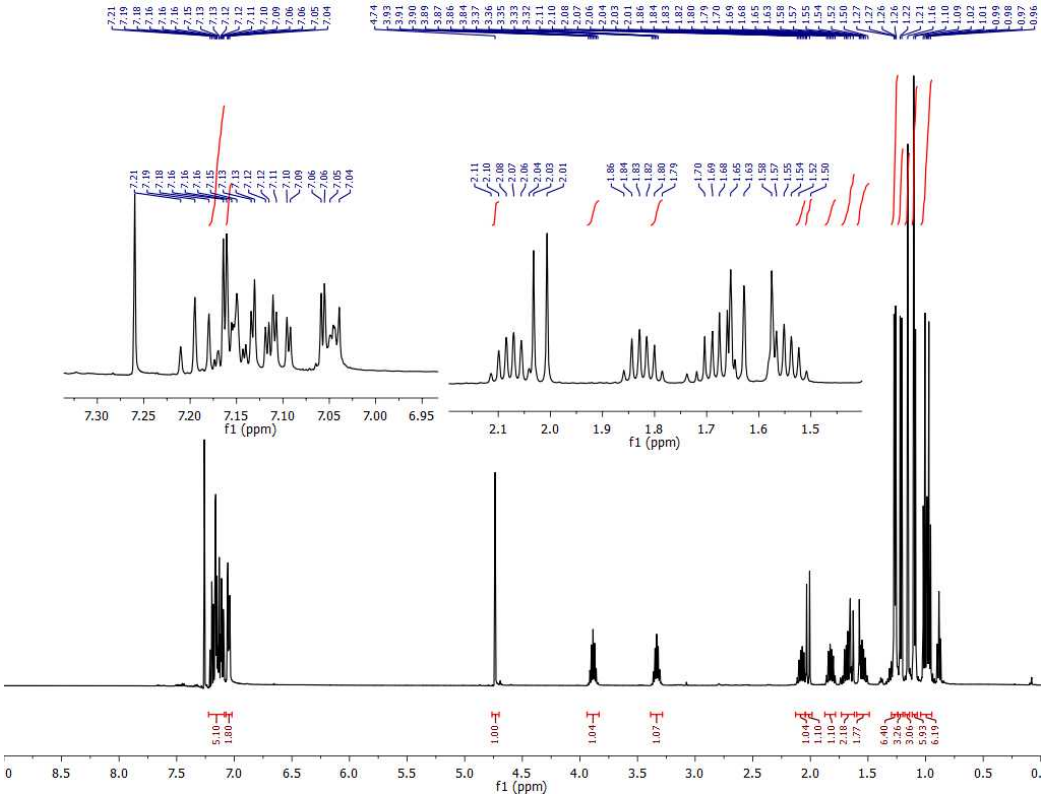


Figure S1. ^{1}H NMR ($CDCl_3$, 298K, 500 MHz) of **2a**

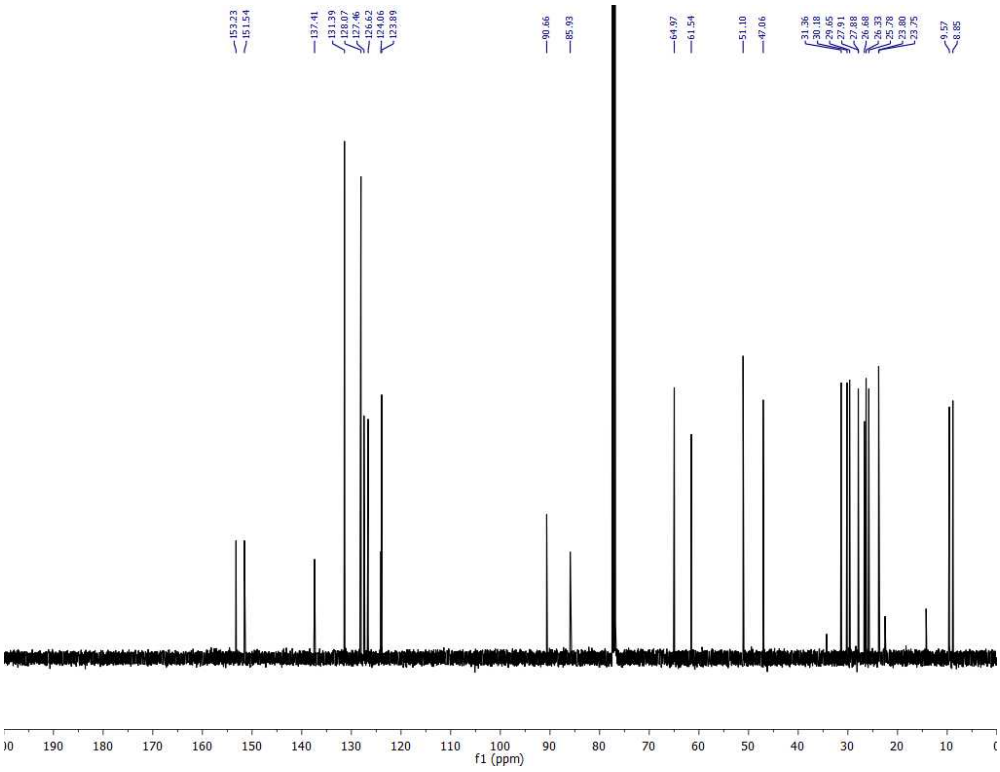


Figure S2. ^{13}C NMR ($CDCl_3$, 298K, 125 MHz) of **2a**

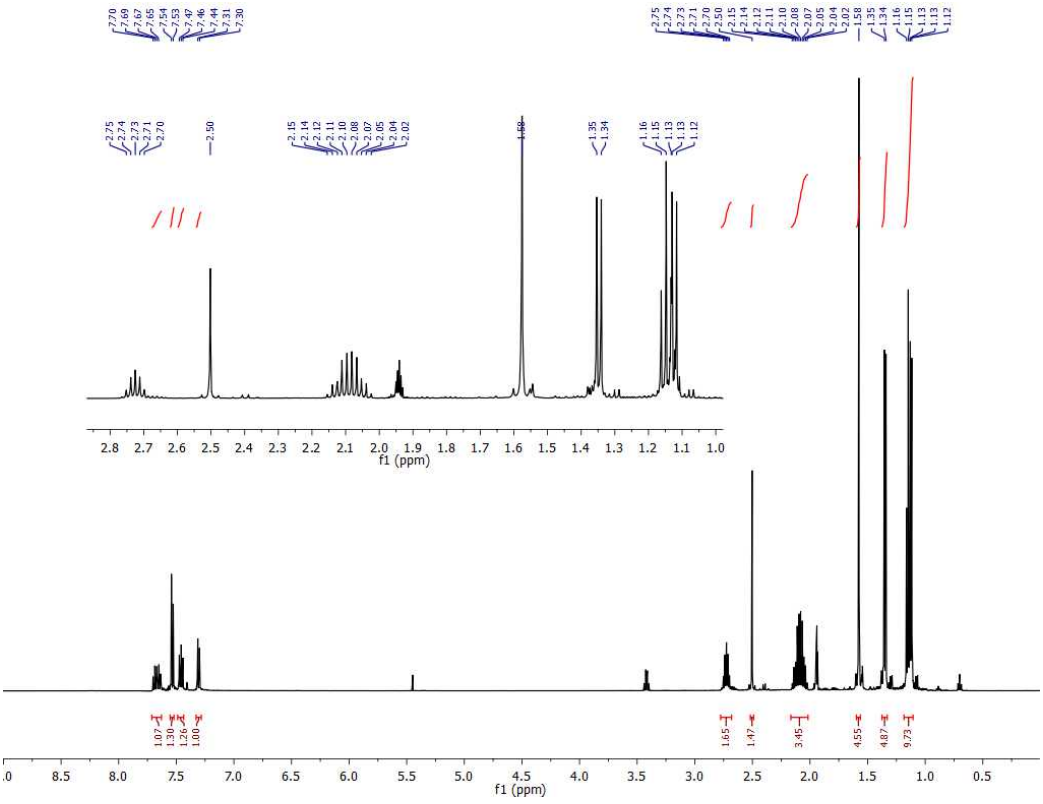


Figure S3. ^{1}H NMR (CD_3CN, 298K, 500 MHz) of **3a**

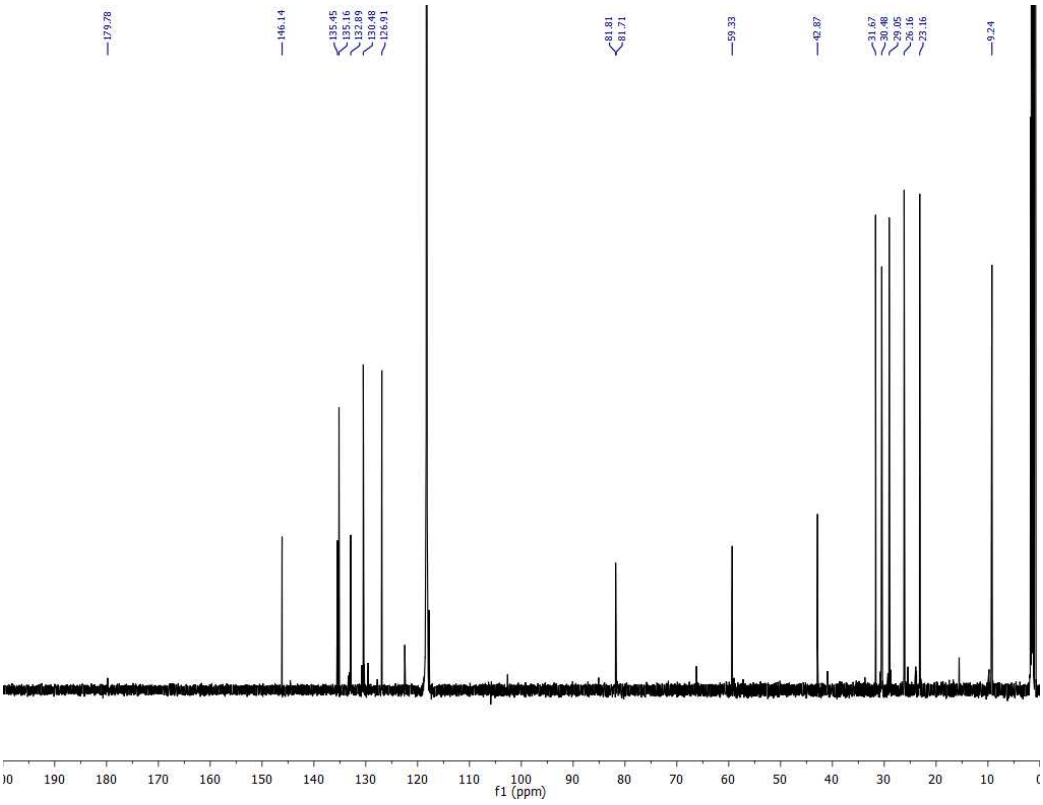


Figure S4. ^{13}C NMR (CD_3CN, 298K, 125 MHz) of **3a**

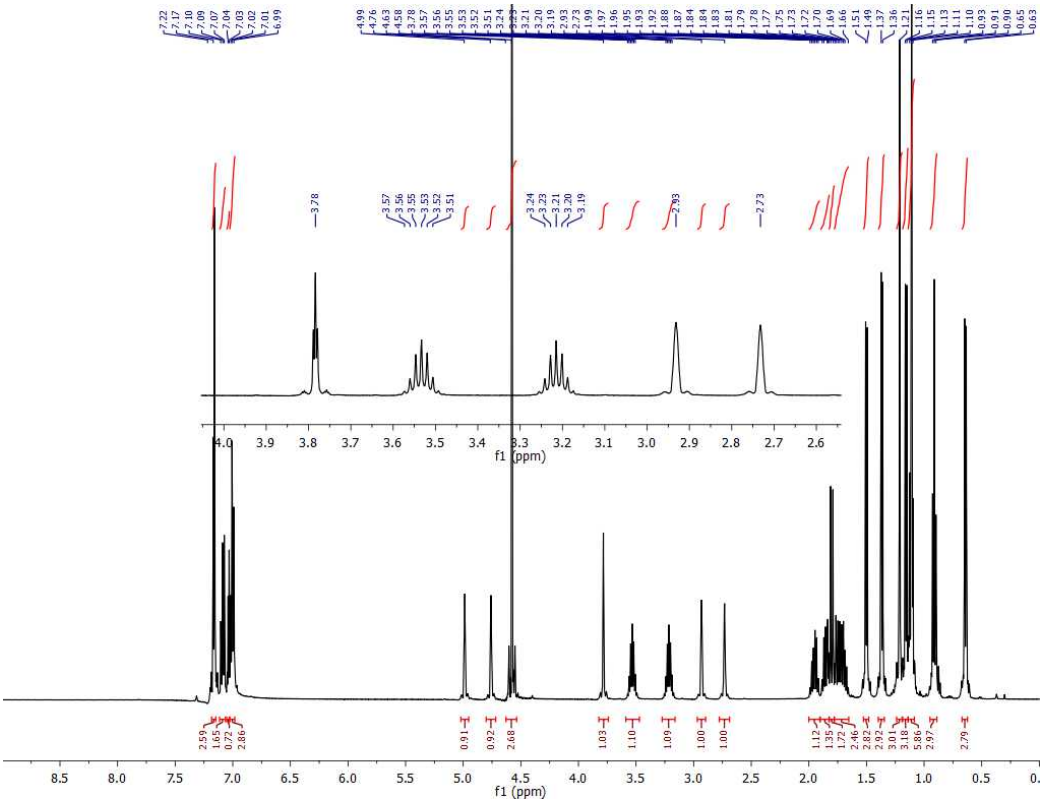


Figure S5. ^{1}H NMR (C_6D_6, 298K, 500 MHz) of **6a**

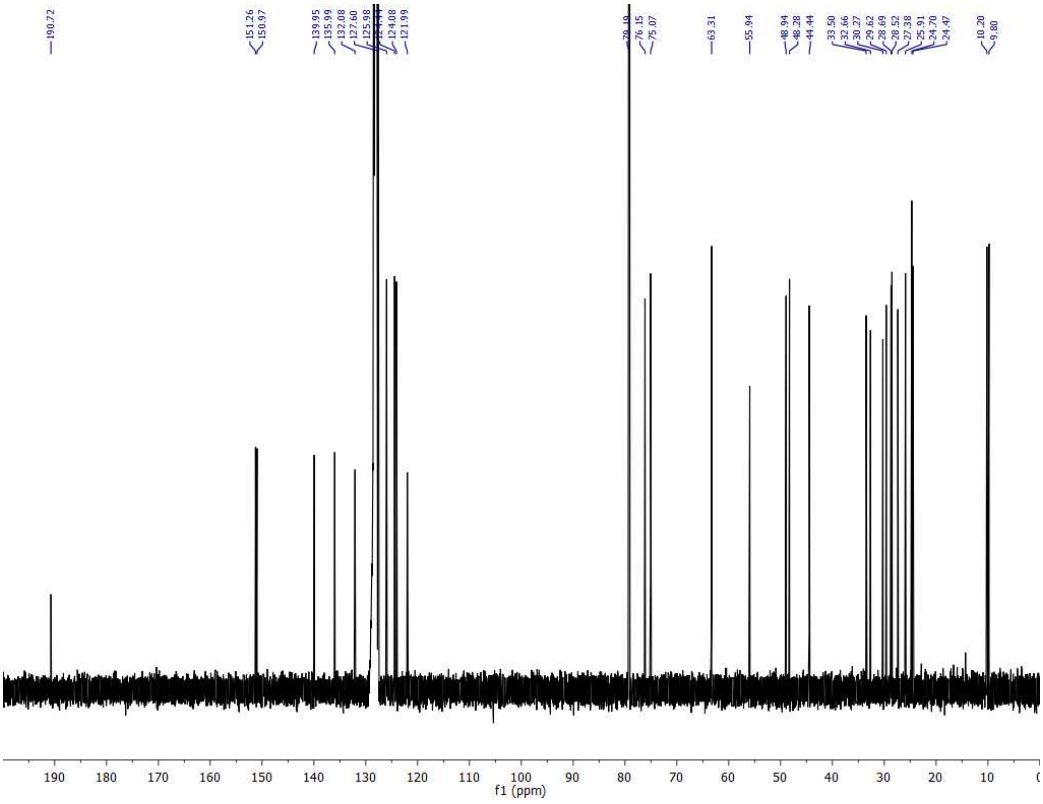


Figure S6. ^{13}C NMR (C_6D_6, 298K, 125 MHz) of **6a**

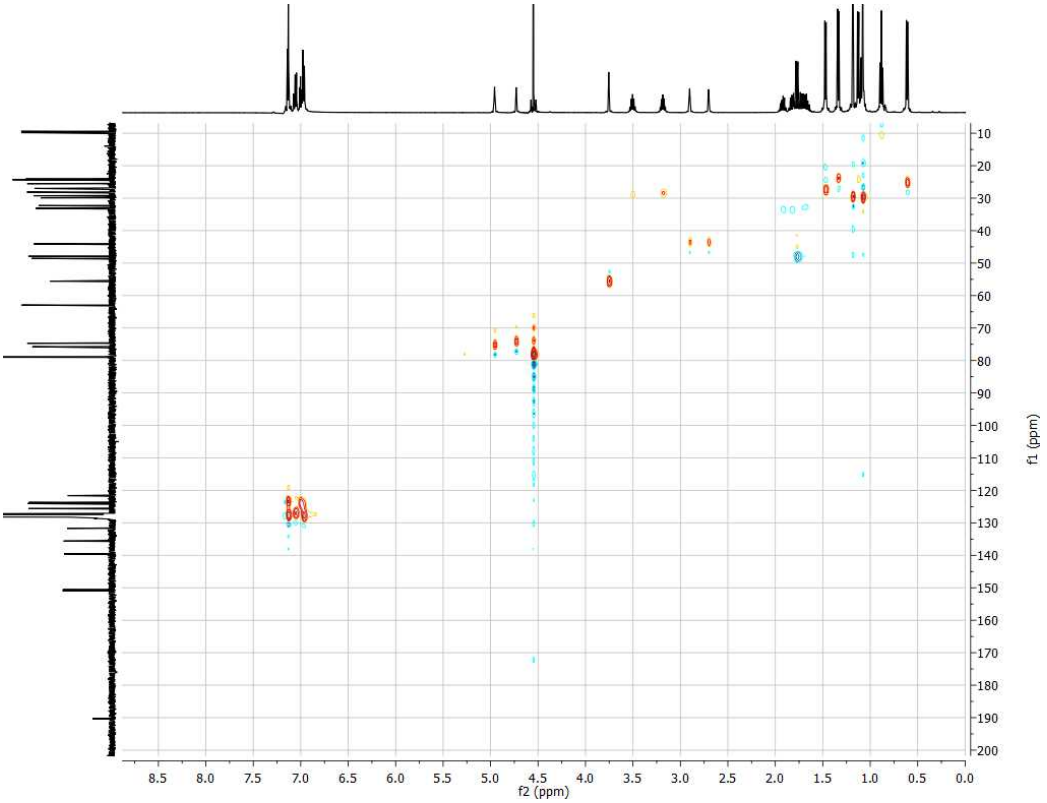


Figure S7. $^{1}H/^{13}C$ HSQC (C_6D_6, 298K, 500/125 MHz) of **6a**

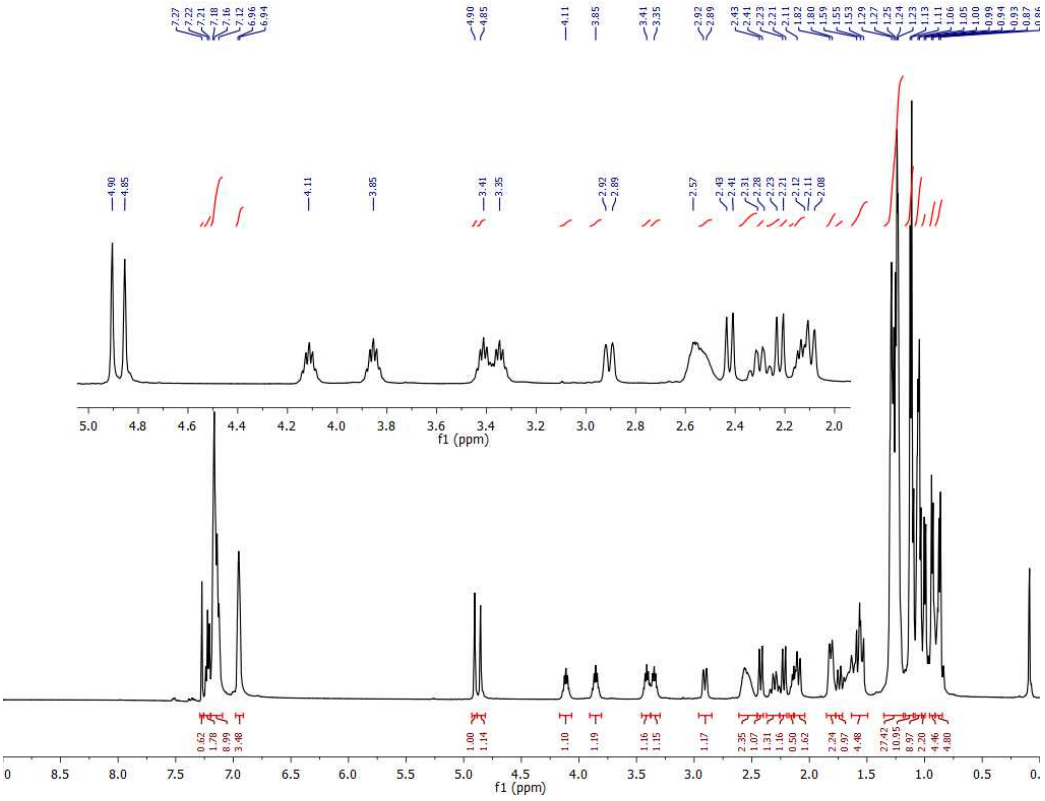


Figure S8. ^{1}H NMR ($CDCl_3$, 298K, 500 MHz) of **2b**

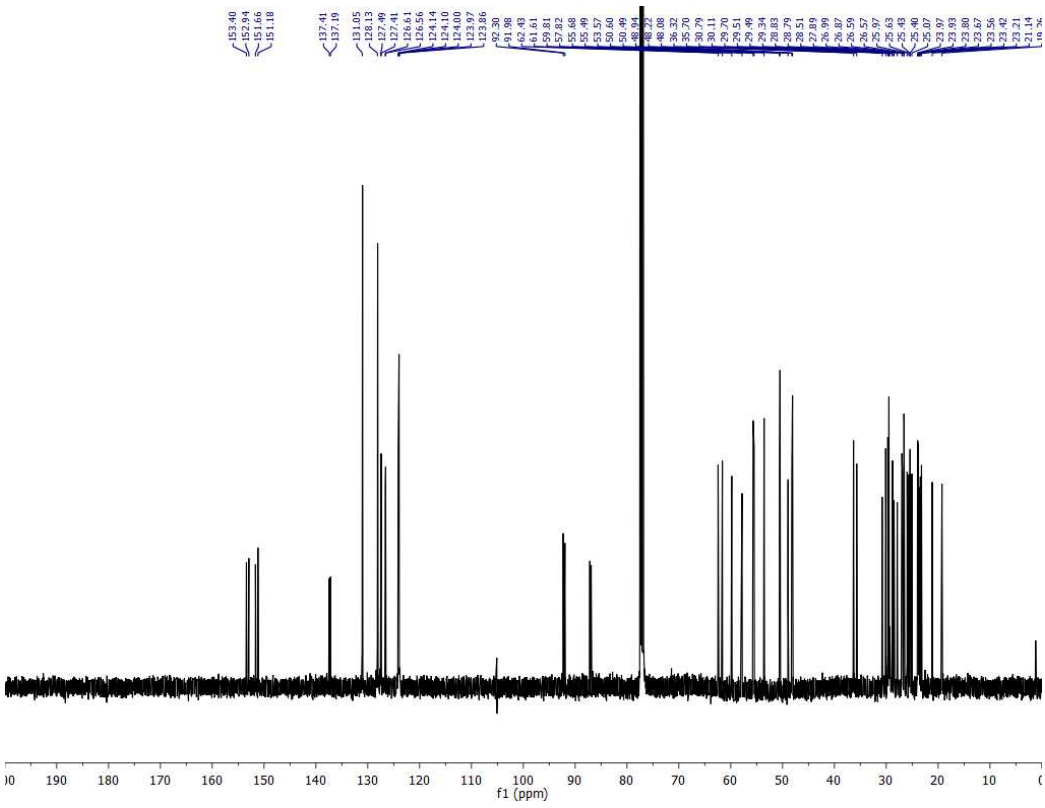


Figure S9. ^{13}C NMR ($CDCl_3$, 298K, 125 MHz) of **2b**

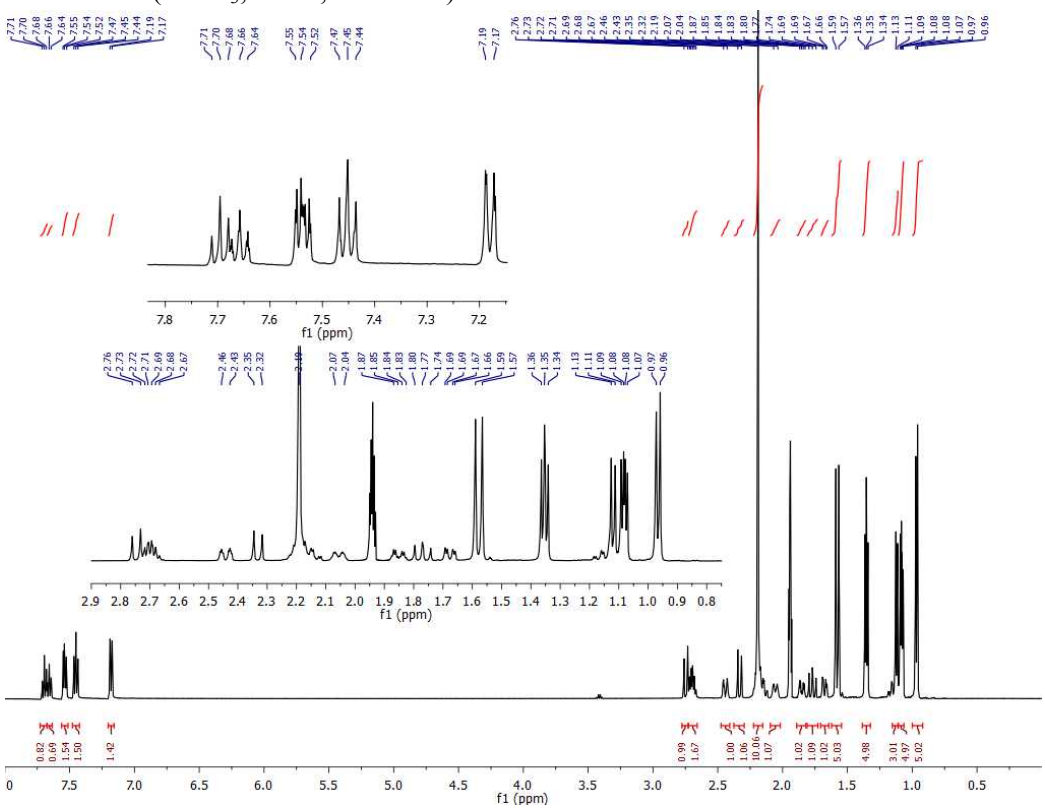


Figure S10. ^{1}H NMR (CD_3CN, 298K, 500 MHz) of **3b**

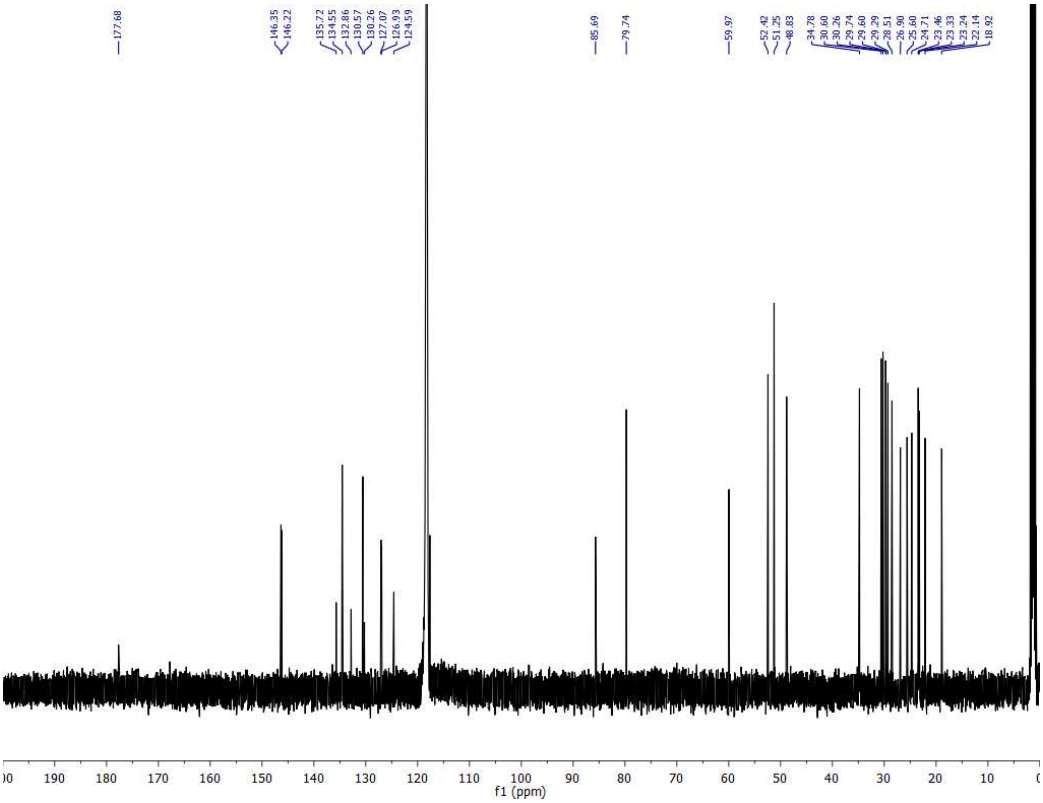


Figure S11. ^{13}C NMR (CD_3CN, 298K, 125 MHz) of **3b**

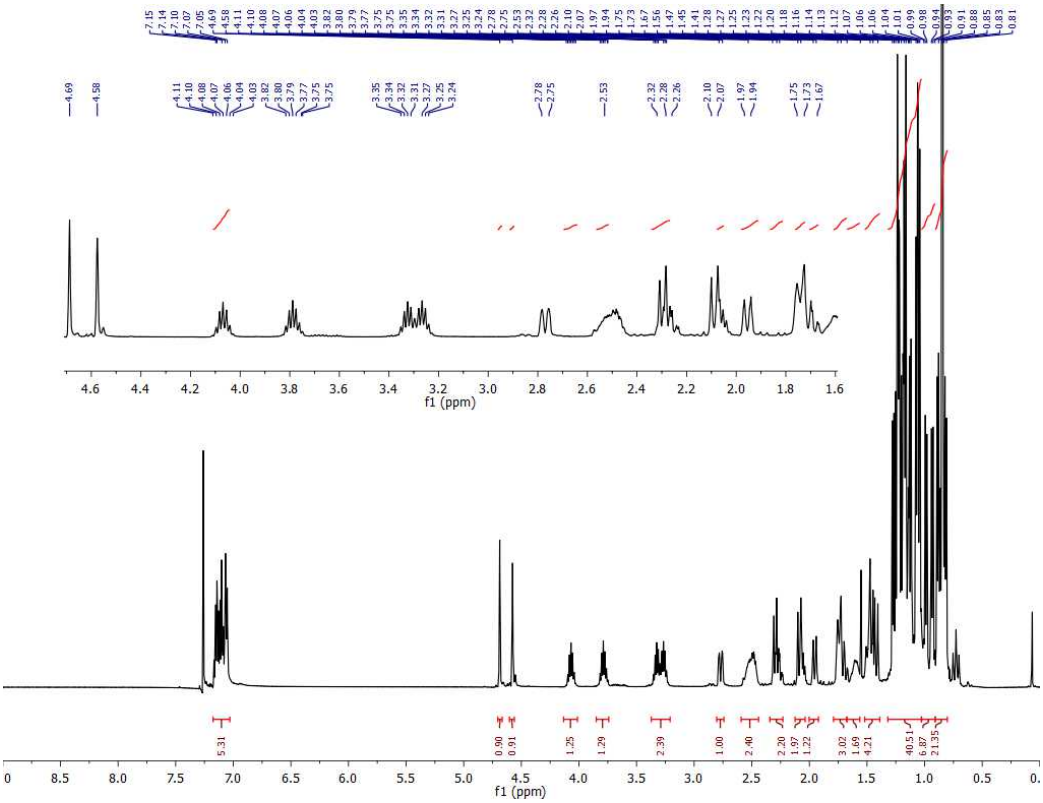


Figure S12. ^{1}H NMR ($CDCl_3$, 298K, 500 MHz) of **2c**

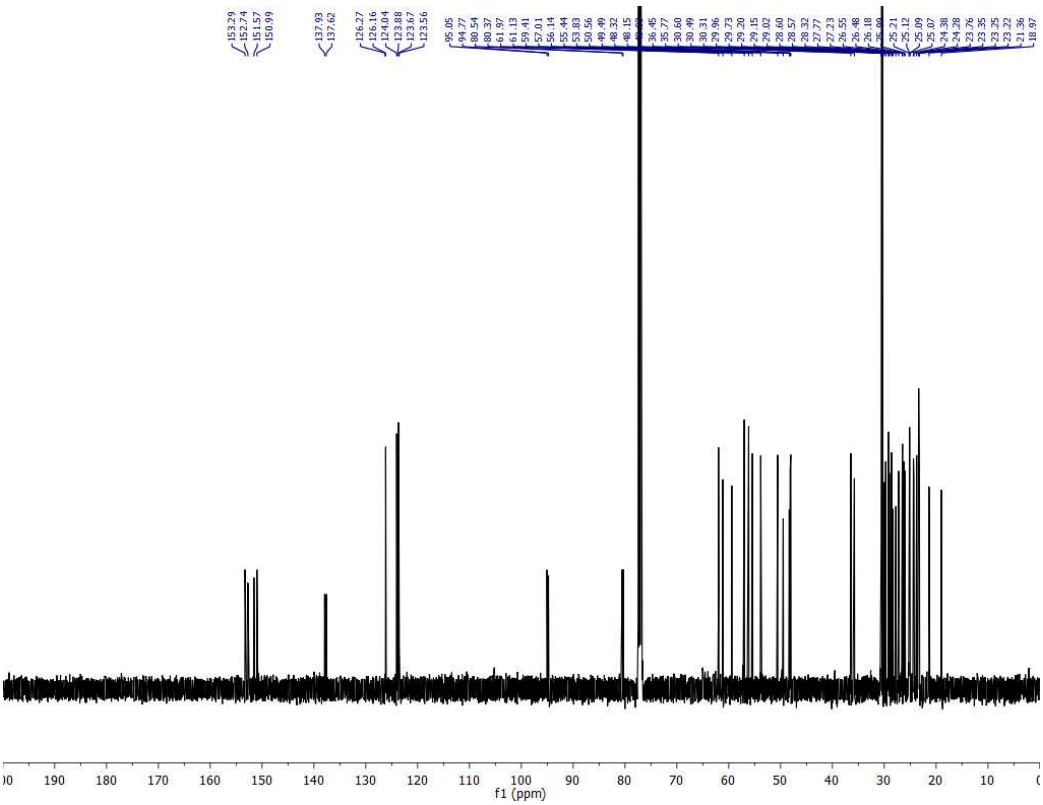


Figure S13. ^{13}C NMR ($CDCl_3$, 298K, 125 MHz) of **2c**

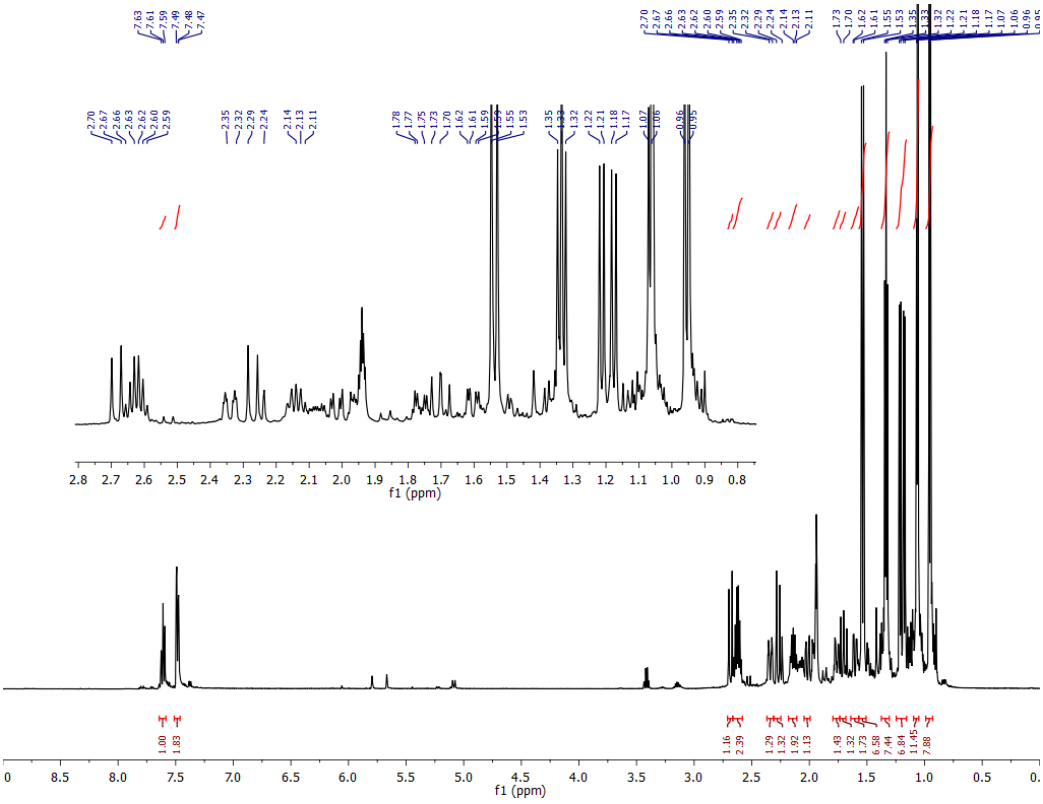


Figure S14. ^{1}H NMR (CD_3CN, 298K, 500 MHz) of **3c**

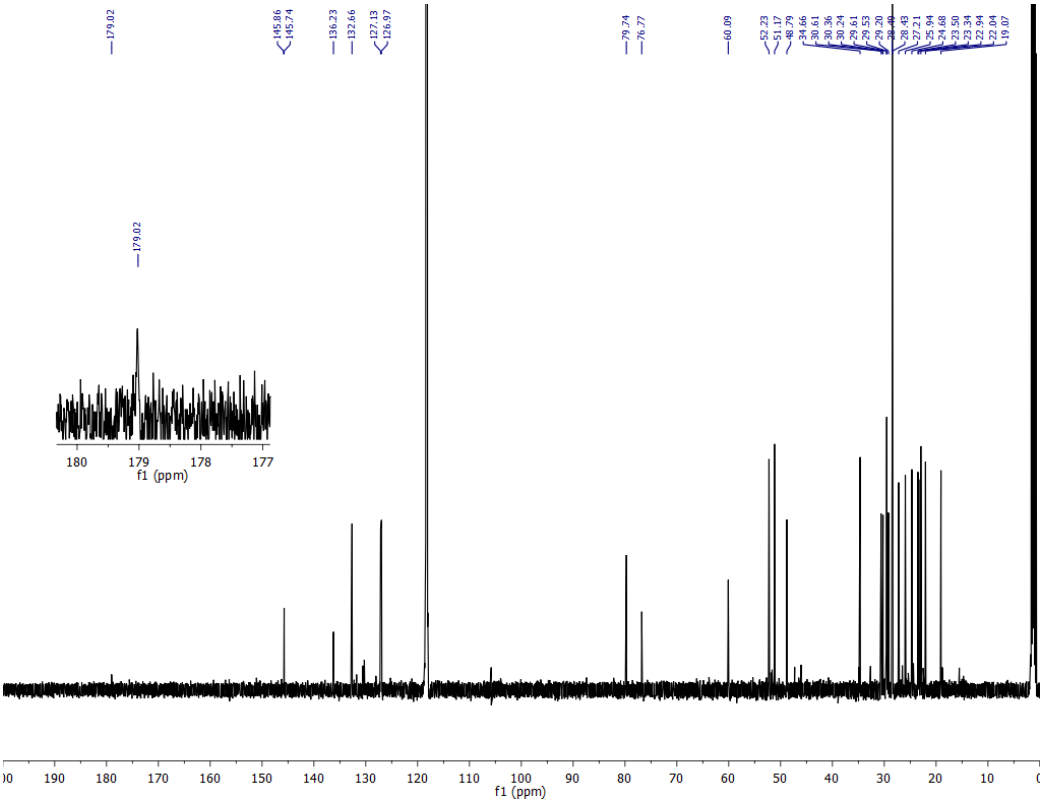


Figure S15. ^{13}C NMR (CD_3CN, 298K, 125 MHz) of **3c**

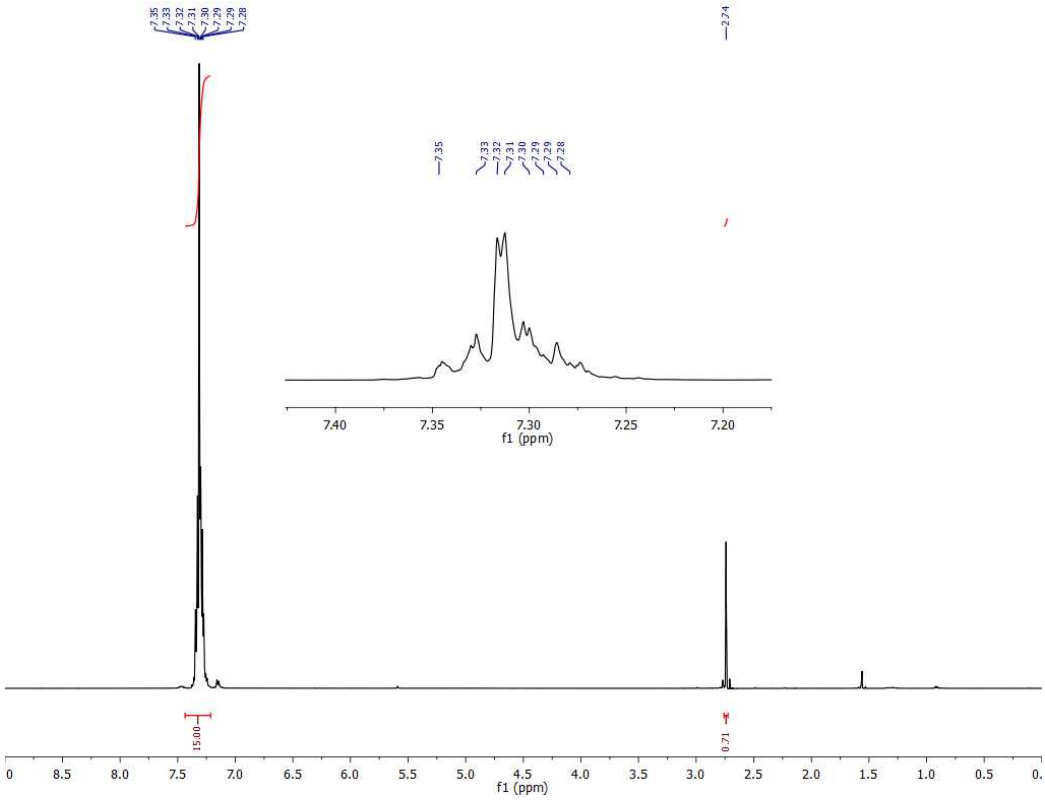


Figure S16. ^{1}H NMR ($CDCl_3$, 298K, 500 MHz) of prop-2-yne-1,1,1-triyltribenzene

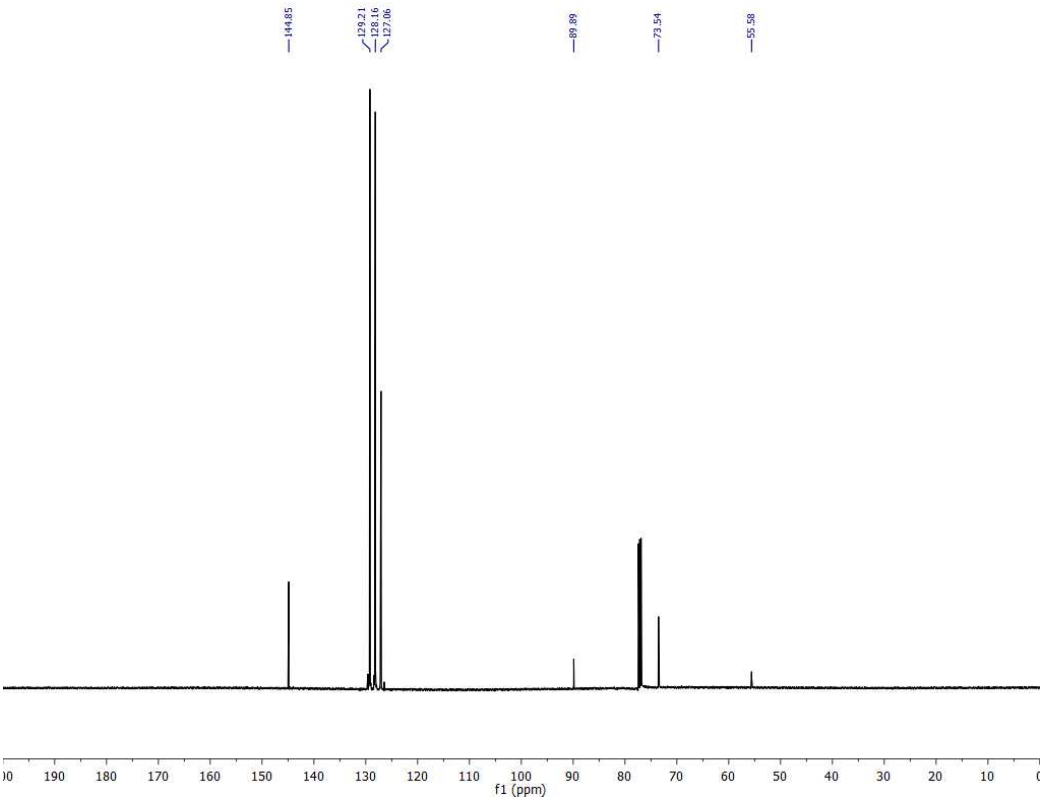


Figure S17. ^{13}C NMR ($CDCl_3$, 298K, 125 MHz) of prop-2-yne-1,1,1-triyltribenzene

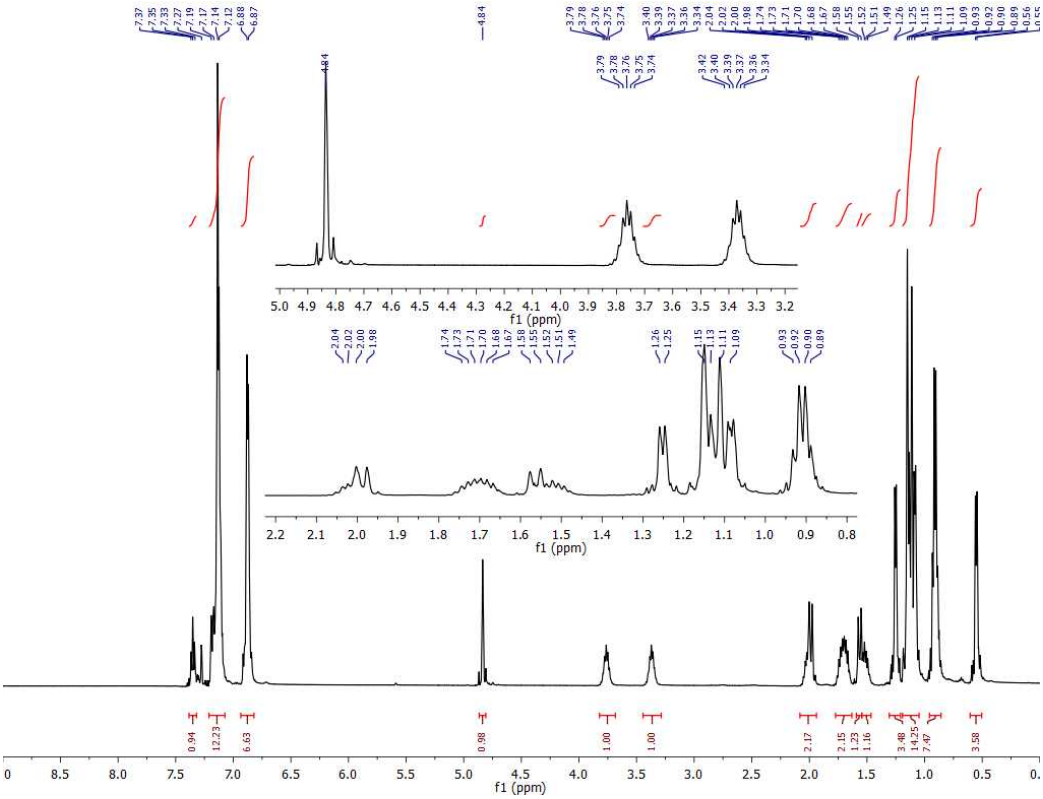


Figure S18. ^{1}H NMR ($CDCl_3$, 298K, 500 MHz) of **2d**

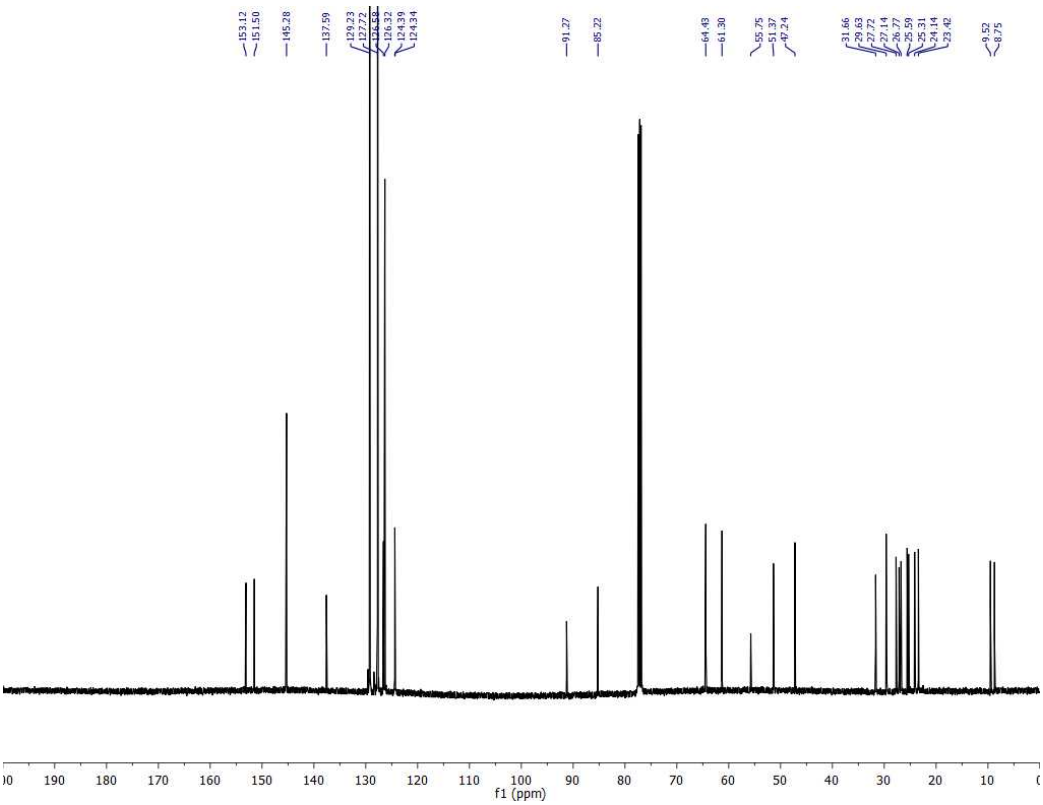


Figure S19. ^{13}C NMR ($CDCl_3$, 298K, 125 MHz) of **2d**

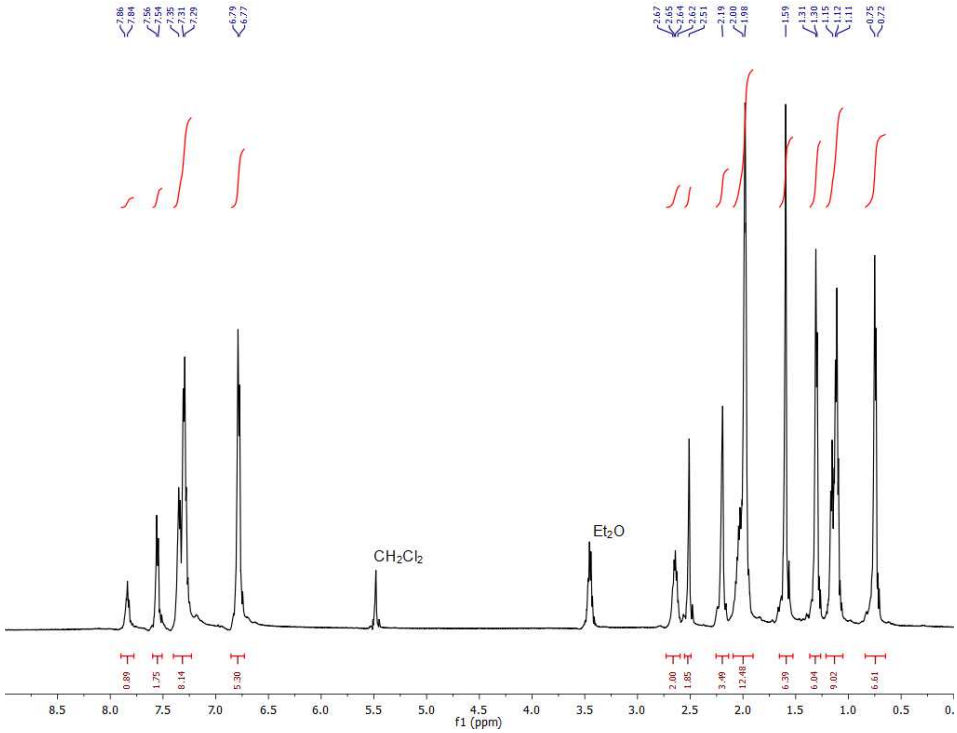


Figure S20. ^{1}H NMR (CD_3CN, 298K, 500 MHz) of **3d**

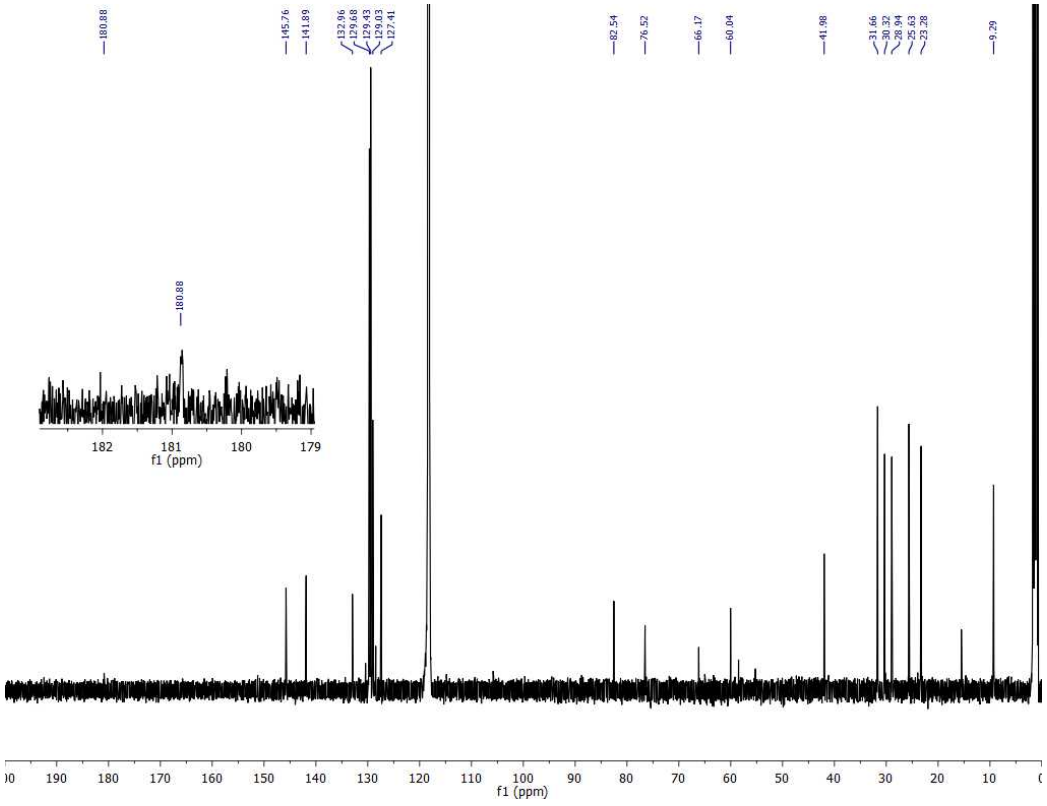


Figure S21. ^{13}C NMR (CD_3CN, 298K, 125 MHz) of **3d**

4. EPR spectroscopy

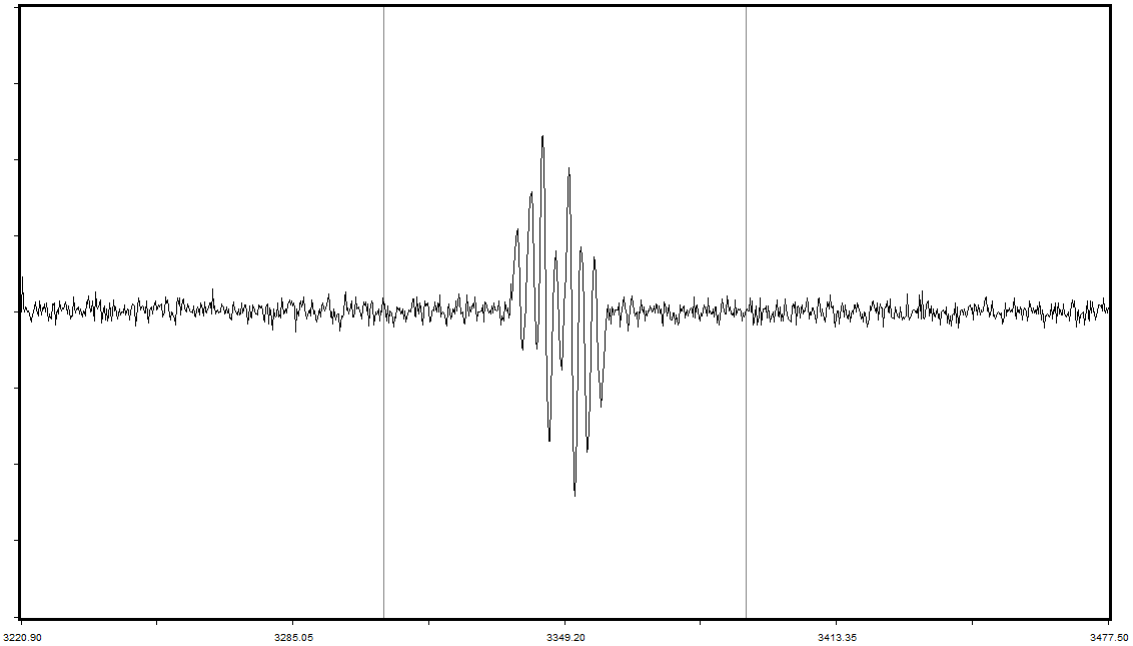
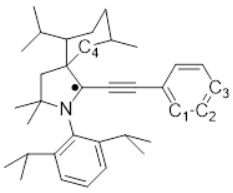


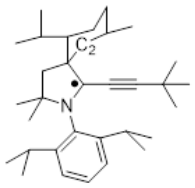
Figure S22. Epr spectrum of **4a** in THF.

In order to fit the experimental EPR parameters a benchmark of three different basis-sets were used in combination with the B3LYP functional.



	Fitted [G]	B3LYP/TZVP [G]	EPR-II (from TZVP)	EPR-III (from TZVP)
N (1)	4.3	2.8 (7.8)	3.1 (8.8)	3.3 (9.1)
$H_{[C1]}$ (2)	2.9	-3.0 (-8.3)	-3.1 (-8.7)	-3.0 (-8.5)
$H_{[C2]}$ (2)	0.5	1.2 (3.5)	1.2 (3.6)	1.3 (3.6)
$H_{[C3]}$ (1)	2.8	-3.5 (-9.8)	-3.7 (-10.3)	-3.7 (-10.2)
$H_{[C4]}$ (1)	2.3	2.4 (6.9)	2.6 (7.4)	2.7 (7.5)

Table S1. Simulated EPR parameters for **4b** together with benchmark of different methods. Values in Gauss (MHz).



	Fitted [G]	B3LYP/TZVP [G]
N (1)	4.4	3.0
$H_{[C2]}$ (1)	3.7	3.2

Table S2. Experimental and fitted EPR parameters for **4c**.

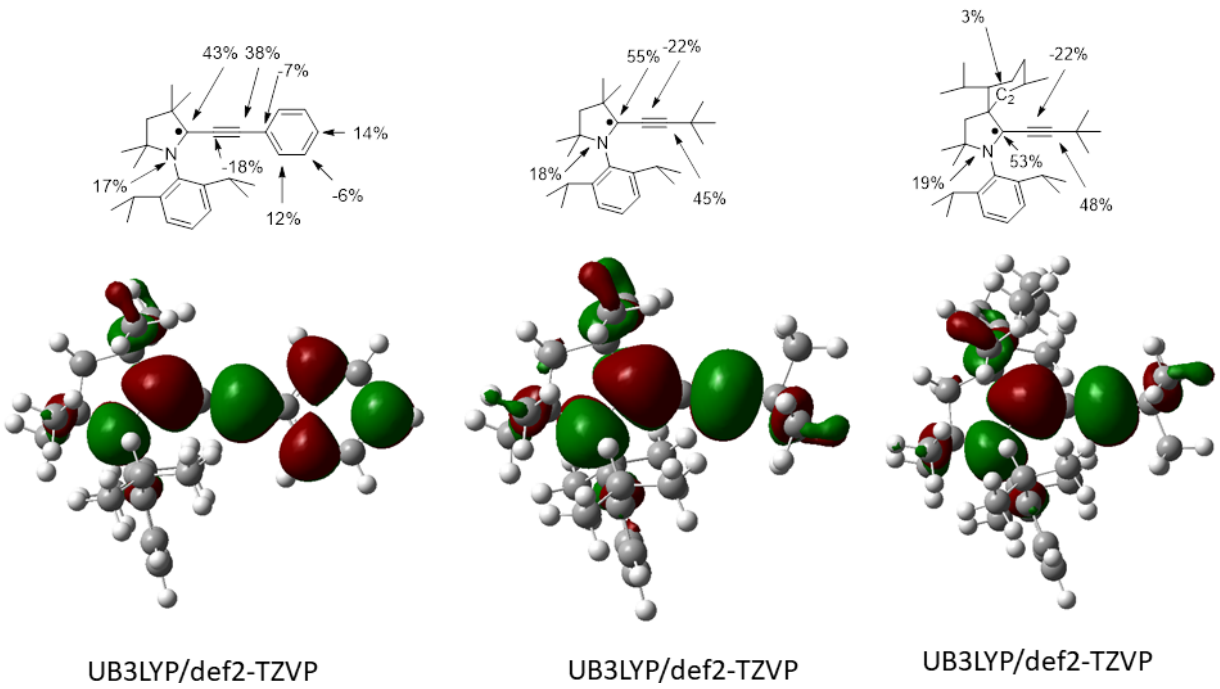


Figure S23. Calculated SOMOs and Mulliken spin densities at the UB3LYP/def2-TZVP level of theory.

5. X-ray crystallography

X-ray analysis of compounds **3a** (CCDC: 1573244), **5a** (CCDC: 1573246), **6a** (CCDC: 1573249), **7b** (CCDC: 1573247), **3d** (CCDC: 1573248)and **4d** (CCDC: 1573245) were performed at the UCSD crystallography facility using Bruker single-crystal diffractometers with CCD detectors, low-temperature cryostats and with either hi-flux Cu (λ = 1.54178 Å) and Mo (λ = 0.71073 Å) radiation sources. Suitable single crystals were covered with perfluoropolyalkyl ether oil and then mounted on the edge of a loop. Subsequently, they were placed in the cold nitrogen stream of a low-temperature for the duration of the data collection. All calculations were performed with Olex2 software[3] or SHELXTL (v6.12) and SHELXL-97.[4] The structures were solved by direct methods and successive interpretation of the difference Fourier maps, followed by full matrix least-squares refinement (against F2). All non-hydrogen atoms were refined anisotropically. The contribution of the hydrogen atoms, in their calculated positions, was included in the refinement using a riding model. Upon convergence, the final Fourier difference map of the X-ray structures showed no significant peaks.

5.1 Cyclic iminium 3a

Single crystals suitable for X-ray crystallography were obtained by vapor diffusion of pentane into a THF solution of **3a**.

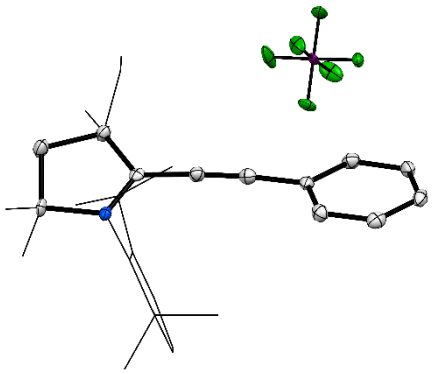


Table S3. Crystal data and structure refinement for **3a**.

Identification code	**3a** (CCDC 1573244)	
Empirical formula	C30 H40 F6 N Sb	
Molecular formula	F6 Sb, C30 H40 N	
Formula weight	650.38	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 11.1422(3) Å	α= 90°.
	b = 15.1771(4) Å	β= 96.155(2)°.
	c = 17.5455(5) Å	γ = 90°.
Volume	2949.95(14) $Å^3$	
Z	4	
Density (calculated)	1.464 Mg/m^3	
Absorption coefficient	0.992 mm^{-1}	
F(000)	1328	
Crystal size	0.25 x 0.2 x 0.19 mm^3	
Crystal color, habit	colourless block	
Theta range for data collection	2.276 to 25.687°.	
Index ranges	-13<=h<=13, -18<=k<=15, -21<=l<=21	
Reflections collected	18652	
Independent reflections	5601 [R(int) = 0.0256, R(sigma) = 0.0271]	
Completeness to theta = 25.000°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.4903 and 0.4438	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5601 / 0 / 351	
Goodness-of-fit on F^2	1.021	
Final R indices [I>2sigma(I)]	R1 = 0.0237, wR2 = 0.0522	
R indices (all data)	R1 = 0.0308, wR2 = 0.0552	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.474 and -0.752 $e.Å^{-3}$	

5.2 neutral β-β dimer 5a

Single crystals suitable for X-ray crystallography were obtained by slow evaporation of a saturated solution of **5a** in benzene.

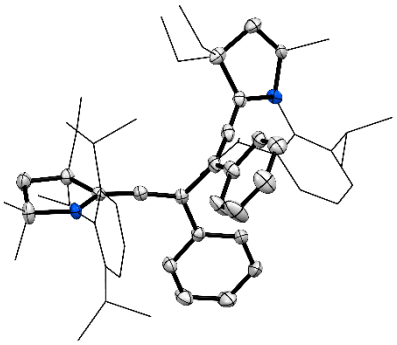


Table S4. Crystal data and structure refinement for **5a**.

Identification code	**5a** (CCDC: 1573246)	
Empirical formula	C60 H80 N2	
Molecular formula	C60 H80 N2	
Formula weight	829.26	
Temperature	100.0 K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 11.340(3) Å	α= 78.37(2)°.
	b = 12.577(4) Å	β= 81.016(19)°.
	c = 18.802(5) Å	γ = 75.52(2)°.
Volume	2527.2(12) $Å^3$	
Z	2	
Density (calculated)	1.090 Mg/m^3	
Absorption coefficient	0.458 mm^{-1}	
F(000)	908	
Crystal size	0.35 x 0.25 x 0.115 mm^3	
Crystal color, habit	red plate	
Theta range for data collection	2.414 to 68.958°.	
Index ranges	-13<=h<=13, -14<=k<=14, -22<=l<=22	
Reflections collected	15019	
Independent reflections	8997 [R(int) = 0.0386, R(sigma) = 0.0483]	
Completeness to theta = 67.500°	97.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.521 and 0.407	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8997 / 474 / 857	
Goodness-of-fit on F^2	1.183	
Final R indices [I>2sigma(I)]	R1 = 0.0687, wR2 = 0.1543	
R indices (all data)	R1 = 0.0793, wR2 = 0.1583	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.400 and -0.300 $e.Å^{-3}$	

5.3 Cobaltocene adduct 6a

Single crystals suitable for X-ray crystallography were obtained by storing a saturated solution of **6a** at -40 °C.

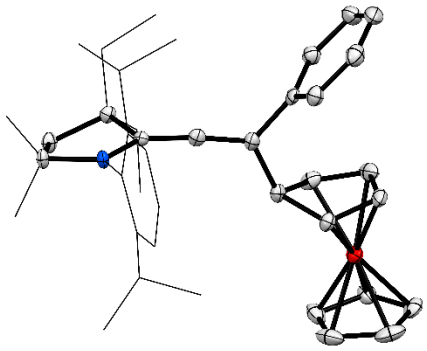


Table S5. Crystal data and structure refinement for **6a**

Identification code	**6a** (CCDC: 1573249))	
Empirical formula	C40 H50 Co N	
Molecular formula	C40 H50 Co N	
Formula weight	603.74	
Temperature	100.0 K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.3348(5) Å	α= 86.599(2)°.
	b = 10.9124(5) Å	β= 75.345(2)°.
	c = 17.2615(8) Å	γ = 75.325(2)°.
Volume	1645.62(14) $Å^3$	
Z	2	
Density (calculated)	1.218 Mg/m^3	
Absorption coefficient	4.278 mm^{-1}	
F(000)	648	
Crystal size	0.175 x 0.05 x 0.05 mm^3	
Crystal color, habit	dark red needle	
Theta range for data collection	2.646 to 70.067°.	
Index ranges	-11<=h<=11, -13<=k<=13, -21<=l<=21	
Reflections collected	49417	
Independent reflections	6159 [R(int) = 0.0422, R(sigma) = 0.0207]	
Completeness to theta = 67.500°	98.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.5231 and 0.3937	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6159 / 30 / 439	
Goodness-of-fit on F^2	1.055	
Final R indices [I>2sigma(I)]	R1 = 0.0297, wR2 = 0.0817	
R indices (all data)	R1 = 0.0302, wR2 = 0.0821	

Extinction coefficient	n/a
Largest diff. peak and hole	0.335 and -0.379 e.Å^{-3}

5.4 β-para dimer 7b

Single crystals suitable for X-ray crystallography were obtained by storing a saturated solution of **7b** at -40 °C.

During refinement, 1 Voids per cell was treated with the squeeze function. Each Void equates to 49 electrons which is assign to one molecule of disordered Diethyl Ether.

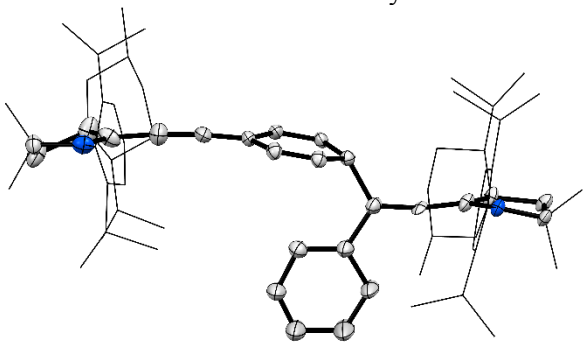


Table S6. Crystal data and structure refinement for **7b**.

Identification code	**7b** (CCDC: 1573247)	
Empirical formula	C70 H96 N2	
Molecular formula	1(C70 H96 N2)	
Formula weight	965.48	
Temperature	100.0 K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P1	
Unit cell dimensions	a = 12.5961(12) Å	α= 78.446(3)°.
	b = 15.6929(16) Å	β= 84.586(3)°.
	c = 16.3566(17) Å	γ = 88.562(3)°.
Volume	3153.5(5) Å^3	
Z	2	
Density (calculated)	1.017 Mg/m^3	
Absorption coefficient	0.057 mm^{-1}	
F(000)	1060	
Crystal size	0.2 x 0.2 x 0.2 mm^3	
Crystal color, habit	colourless block	
Theta range for data collection	1.276 to 21.725°.	
Index ranges	-12<=h<=13, -16<=k<=16, -17<=l<=16	
Reflections collected	49730	
Independent reflections	13473 [R(int) = 0.0419, R(sigma) = 0.0421]	
Completeness to theta = 21.725°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.4889 and 0.4653	
Refinement method	Full-matrix least-squares on F^2	

Data / restraints / parameters	13473 / 2031 / 1777
Goodness-of-fit on F^2	1.299
Final R indices [I>2sigma(I)]	R1 = 0.1063, wR2 = 0.2914
R indices (all data)	R1 = 0.1402, wR2 = 0.3244
Absolute structure parameter	0.5(10)
Extinction coefficient	n/a
Largest diff. peak and hole	0.581 and -0.238 e.$Å^{-3}$

5.5 Cyclic iminium 3d

Single crystals suitable for X-ray crystallography were obtained by slow diffusion of Et_2O into a saturated solution of **2d** at room temperature.

During refinement, 4 Voids per cell were treated with the squeeze function. Each Void equates to 42 electrons which correspond to one molecule of disordered methylene chloride.

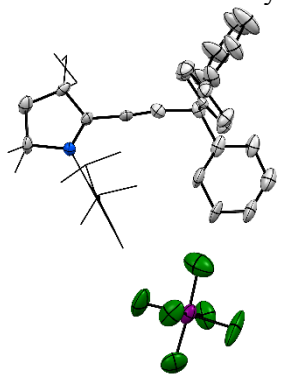


Table S7. Crystal data and structure refinement for **3d**.

Identification code	**3d** (CCDC: 1573248)	
Empirical formula	C43 H50 F6 N Sb	
Molecular formula	F6 Sb, C43 H50 N	
Formula weight	816.59	
Temperature	100.0 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 1 21/n 1	
Unit cell dimensions	a = 13.4623(5) Å	α= 90°.
	b = 23.1356(7) Å	β= 94.923(2)°.
	c = 14.0612(5) Å	γ = 90°.
Volume	4363.3(3) $Å^3$	
Z	4	
Density (calculated)	1.243 Mg/m^3	
Absorption coefficient	0.685 mm^{-1}	

F(000)	1680
Crystal size	0.25 x 0.25 x 0.2 mm^3
Crystal color, habit	colourless block
Theta range for data collection	1.699 to 25.357°.
Index ranges	-11<=h<=16, -27<=k<=21, -16<=l<=16
Reflections collected	27487
Independent reflections	7947 [R(int) = 0.0760, R(sigma) = 0.1008]
Completeness to theta = 25.242°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.4868 and 0.4352
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7947 / 304 / 544
Goodness-of-fit on F^2	1.168
Final R indices [I>2sigma(I)]	R1 = 0.0914, wR2 = 0.1839
R indices (all data)	R1 = 0.1268, wR2 = 0.1962
Extinction coefficient	n/a
Largest diff. peak and hole	1.017 and -1.937 e.$Å^{-3}$

5.6 Neutral Radical monomer 4d

Single crystals of **4d** suitable for x-ray diffraction were obtained from a saturated pentane solution at -40°C.

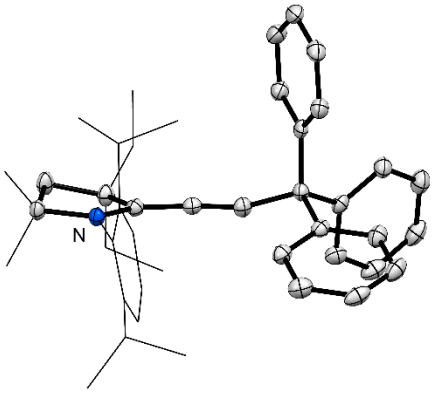


Table S8. Crystal data and structure refinement for **4d**.

Identification code	**4d** (CCDC: 1573245)
Empirical formula	C43 H50 N
Molecular formula	C43 H50 N

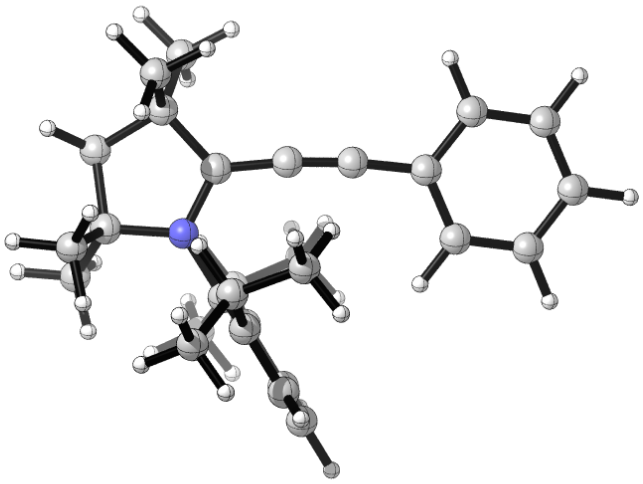
Formula weight	580.84	
Temperature	100 K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.2489(4) Å	α= 72.6260(10)°.
	b = 11.6580(6) Å	β= 83.8110(10)°.
	c = 17.0457(8) Å	γ = 77.388(2)°.
Volume	1709.96(14) $Å^3$	
Z	2	
Density (calculated)	1.128 Mg/m^3	
Absorption coefficient	0.476 mm^{-1}	
F(000)	630	
Crystal size	0.31 x 0.29 x 0.28 mm^3	
Crystal color, habit	orange block	
Theta range for data collection	2.719 to 68.331°.	
Index ranges	-10<=h<=11, -14<=k<=14, -20<=l<=20	
Reflections collected	20730	
Independent reflections	6129 [R(int) = 0.0415, R(sigma) = 0.0321]	
Completeness to theta = 67.679°	98.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.5849 and 0.5075	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6129 / 0 / 405	
Goodness-of-fit on F^2	1.033	
Final R indices [I>2sigma(I)]	R1 = 0.0399, wR2 = 0.1023	
R indices (all data)	R1 = 0.0421, wR2 = 0.1046	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.266 and -0.188 $e.Å^{-3}$	

6. Computational part

General part

All calculations were performed with the Gaussian09 program package[5] (version g09, rev.d01). The theoretical approach is based on the framework of density functional theory (DFT).[6] All calculations were performed with the B3LYP functional and employing Ahlrich's def2-TZVP basis set[7] or Dunning's cc-pVDZ basis set. Ground states were fully optimized without constraints at the corresponding level of theory. Gibbs free reaction energies and enthalpies were calculated for standard conditions (p = 1 atm, T = 298 K) and are unscaled. Grimme's D3 dispersion correction with Becke-Johnson damping was used in order to take dispersion effects into account.[8] For the visualization of optimized structures CYLview,[9] and for the visualization of frontier molecular orbitals GaussView 5.0.9[10] was used.

Optimized x,y,z-coordinates



Zero-point correction=	0.566186 (Hartree/Particle)
Thermal correction to Energy=	0.595536
Thermal correction to Enthalpy=	0.596480
Thermal correction to Gibbs Free Energy=	0.507119
Sum of electronic and zero-point Energies=	-1142.984620
Sum of electronic and thermal Energies=	-1142.955270
Sum of electronic and thermal Enthalpies=	-1142.954326
Sum of electronic and thermal Free Energies=	-1143.043687

65

scf done: -1143.550806

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C	-0.041261	-2.971903	-1.090542
C	0.257475	-3.552945	0.139826
C	0.003458	-2.851555	1.315627
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C	-0.810029	1.408480	-0.093358
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C	-3.080405	1.999966	-0.478433
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H	2.798560	-1.214960	0.089936
H	0.286276	-3.289665	2.274438
H	0.714934	-4.543963	0.180953
H	0.208315	-3.503271	-2.010568
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H	-1.366155	-0.118106	-2.382184
H	0.592111	0.188351	4.033369
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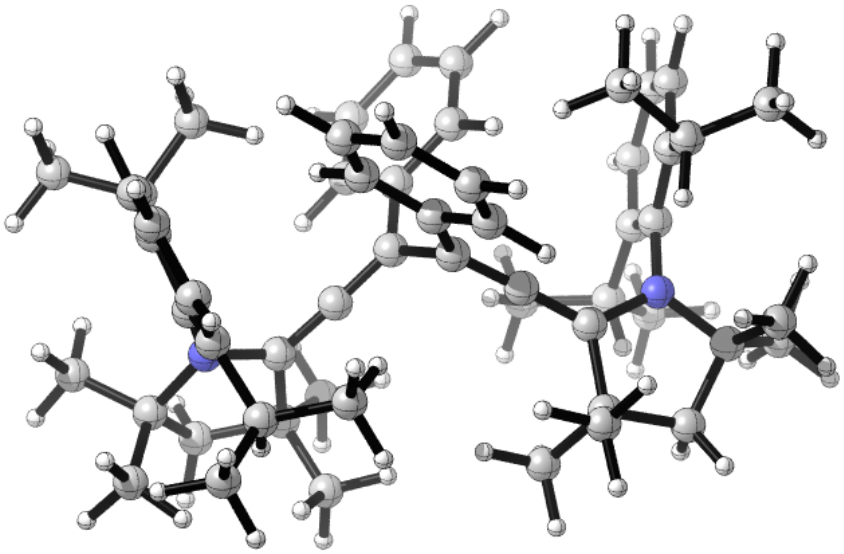

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Thermal correction to Energy=	1.198437
Thermal correction to Enthalpy=	1.199381
Thermal correction to Gibbs Free Energy=	1.049257
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Sum of electronic and thermal Enthalpies=	-2286.001917
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130

scf done: -2287.201299

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C	4.510755	-0.053514	-1.400764
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C	4.453225	-3.293735	2.283163
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C	0.315555	3.886144	-2.288283
C	-0.766099	3.684753	-3.155534
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C	-1.092975	1.480853	-2.201001
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C	2.097402	-2.772533	1.523360
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H	-1.670141	0.560303	-2.152629
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H	-5.134730	0.532180	-3.404005
H	0.868498	4.828237	-2.311902
H	-3.597781	-1.247838	-3.805935
H	-3.290958	-2.853782	-3.098074
H	-2.384450	-1.445980	-2.516804
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H	-2.317618	2.308096	-3.763859

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H	-5.037455	2.964431	-2.937884	H	5.549061	-0.709743	2.714364
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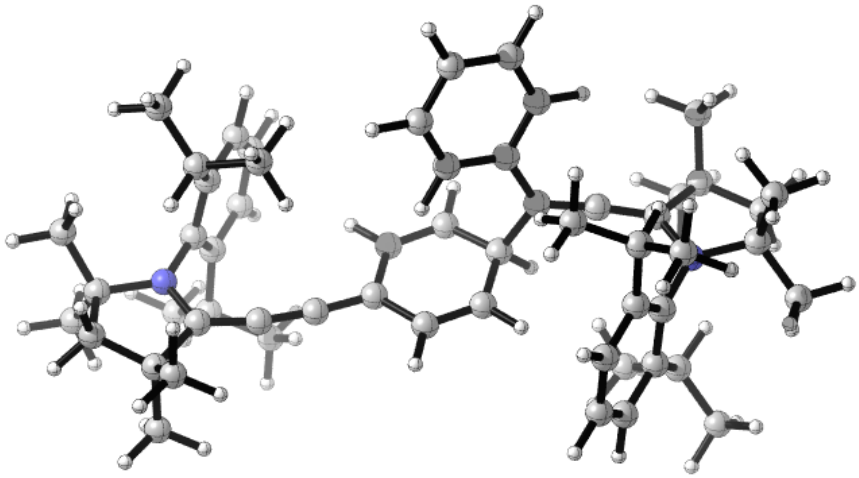
H	3.513178	-1.365942	2.281782	H	4.116320	-3.505842	3.310889
H	1.420650	-1.989272	1.159111	H	5.498628	-2.950780	2.326736
H	1.741055	-3.110523	2.510770	H	-6.581140	-1.077635	0.508813
H	2.029078	-3.623639	0.826647	H	-6.727447	-2.155772	1.916759
H	-6.624431	-1.864279	-1.605763	H	-5.651600	-2.600267	0.568836
H	-5.762106	-3.131527	-2.516404	H	-1.930661	-3.565167	1.852144
H	-6.089346	-1.558390	-3.272004	H	-0.594253	-2.536454	2.413251
H	4.294641	-3.823113	-0.431511	H	6.647437	1.697058	-1.539666
H	3.750952	1.025238	-3.896155	H	5.871916	2.942851	-2.555299
H	3.407682	2.658431	-3.275854	H	6.214100	1.329639	-3.221230
H	2.466159	1.275484	-2.686941	H	-4.369590	-1.999363	3.781778
H	1.114886	3.268258	1.844357	H	-4.177848	-3.021087	2.343320
H	2.829431	3.675716	1.619138	H	-4.776548	0.604434	3.365085

H	-6.296194	-0.313211	3.358172	H	-5.965944	0.862021	2.065392



Zero-point correction=	1.137002 (Hartree/Particle)
Thermal correction to Energy=	1.195262
Thermal correction to Enthalpy=	1.196206
Thermal correction to Gibbs Free Energy=	1.047867
Sum of electronic and zero-point Energies=	-2286.000629
Sum of electronic and thermal Energies=	-2285.942369
Sum of electronic and thermal Enthalpies=	-2285.941425
Sum of electronic and thermal Free Energies=	-2286.089764

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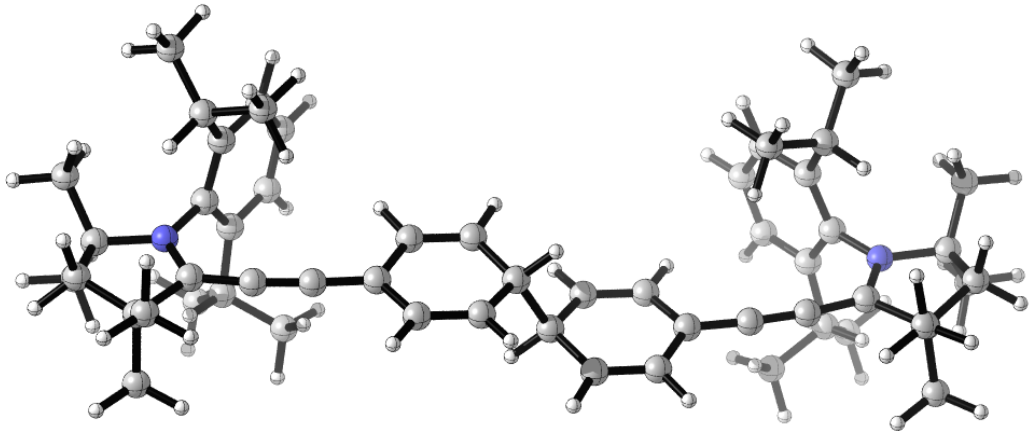
scf done: -2287.137631

C	7.096979	0.009580	-0.424985	C	5.079464	-1.032957	0.868863
C	7.088137	0.185368	-1.962606	C	4.810979	-2.397781	0.594761
C	5.690079	0.737372	-2.353753	C	4.193773	-3.175782	1.581578
C	4.849967	0.417946	-1.106635	C	3.836799	-2.626185	2.811419
N	5.657240	-0.233096	-0.165538	C	4.082539	-1.279551	3.062498
C	3.574324	0.713423	-0.943893	C	4.692354	-0.460477	2.101385
C	2.279338	0.895095	-0.754889	C	4.894190	1.013208	2.412361
C	5.117998	-0.005013	-3.571549	C	5.126673	-3.030590	-0.752949
C	5.712510	2.245171	-2.647079	C	5.944636	-4.322938	-0.614503
				C	3.841897	-3.278539	-1.558362
				C	3.580077	1.698888	2.814972

C	5.956938	1.204057	3.507197
C	7.965327	-1.163074	0.029077
C	7.598074	1.292789	0.265624
C	1.310052	-0.283569	-1.024339
C	0.029832	0.122239	-1.706903
C	-1.190697	-0.148963	-1.208485
C	-1.364312	-0.855058	0.061365
C	-0.158513	-1.321855	0.734936
C	1.070460	-1.065137	0.246430
C	-2.608297	-1.009218	0.561815
C	-3.807927	-1.065316	0.940798
C	-5.123737	-0.963537	1.189396
C	-5.883547	-1.535867	2.375949
C	-7.247941	-0.810032	2.261336
C	-7.408429	-0.338402	0.794781
N	-5.990240	-0.308164	0.341964
C	-5.504892	0.319226	-0.852895
C	-6.016000	-3.063270	2.221861
C	-5.171075	-1.214272	3.695496
C	-8.054996	1.047917	0.714482
C	-8.255002	-1.312310	-0.040427
C	-5.387040	-0.432241	-2.043943
C	-4.917535	0.213862	-3.195499
C	-4.534062	1.552158	-3.165147
C	-4.577163	2.256416	-1.964264
C	-5.042835	1.654605	-0.788352
C	-4.937338	2.421463	0.522087
C	-5.642486	-1.931282	-2.095376
C	-6.677509	-2.317385	-3.161923
C	-4.321390	-2.689344	-2.319621
C	-3.459964	2.605765	0.912832
C	-5.659776	3.775878	0.471168
C	1.767614	2.182381	-0.205608
C	2.510020	3.363458	-0.393522
C	2.094440	4.573620	0.157485
C	0.918161	4.635611	0.912669
C	0.168767	3.473016	1.103174
C	0.581797	2.259854	0.547056
H	7.900411	0.843185	-2.303881
H	7.240114	-0.798377	-2.431857
H	5.756724	0.149962	-4.457427
H	5.050093	-1.086542	-3.379686
H	4.106211	0.360925	-3.805782
H	4.697049	2.607314	-2.869269
H	6.096137	2.823162	-1.793989
H	6.350489	2.457736	-3.520753
H	3.979256	-4.227008	1.380630
H	3.354792	-3.246947	3.570001
H	3.781989	-0.847409	4.018543
H	5.247568	1.494461	1.491928
H	5.727199	-2.308763	-1.319366
H	6.249441	-4.691824	-1.607421
H	6.852068	-4.163743	-0.011703
H	5.361321	-5.123808	-0.132322

H	4.078751	-3.723611	-2.539080
H	3.303675	-2.336345	-1.730786
H	3.161724	-3.964884	-1.028154
H	3.726992	2.787373	2.900889
H	2.794601	1.525415	2.069626
H	3.214806	1.334942	3.789623
H	6.170312	2.274550	3.661271
H	6.901100	0.696781	3.255633
H	5.608586	0.789543	4.467729
H	7.844663	-1.346476	1.107615
H	7.718780	-2.088673	-0.506253
H	9.024819	-0.931694	-0.159616
H	8.616005	1.537496	-0.078516
H	6.946088	2.149152	0.042928
H	7.631801	1.167359	1.355724
H	1.875655	-0.932523	-1.718346
H	0.125941	0.668404	-2.649100
H	-2.093231	0.171270	-1.733629
H	-0.276059	-1.879661	1.666952
H	1.960962	-1.411494	0.775191
H	-7.241825	0.072200	2.918771
H	-8.084955	-1.450394	2.573439
H	-5.021801	-3.534829	2.229533
H	-6.608154	-3.481747	3.052429
H	-6.508110	-3.338201	1.277693
H	-5.755407	-1.589830	4.551396
H	-4.176071	-1.683929	3.722347
H	-5.034968	-0.128500	3.815437
H	-8.049474	1.427474	-0.318441
H	-9.102171	0.984200	1.048180
H	-7.537346	1.773439	1.354415
H	-8.286162	-0.993397	-1.091852
H	-7.865088	-2.337820	-0.002707
H	-9.288477	-1.326121	0.339863
H	-4.829117	-0.350195	-4.125609
H	-4.169615	2.038731	-4.072468
H	-4.219637	3.287007	-1.932810
H	-5.407365	1.810639	1.303775
H	-6.026932	-2.237295	-1.115723
H	-6.891272	-3.397587	-3.116898
H	-7.626070	-1.775301	-3.028868
H	-6.308527	-2.097092	-4.176735
H	-4.496221	-3.777549	-2.290108
H	-3.582132	-2.435530	-1.547208
H	-3.884968	-2.445894	-3.302291
H	-3.385306	3.113542	1.889016
H	-2.942588	1.638871	0.982794
H	-2.923966	3.220842	0.172299
H	-5.628172	4.264244	1.458702
H	-6.713971	3.666091	0.175008
H	-5.180910	4.459985	-0.247660
H	3.428780	3.313456	-0.978836
H	2.689352	5.475332	-0.006185
H	0.589625	5.582459	1.346834

H	-0.747241	3.502366	1.696324
H	-0.009973	1.367383	0.729737



Zero-point correction=	1.136147 (Hartree/Particle)
Thermal correction to Energy=	1.192866
Thermal correction to Enthalpy=	1.193810
Thermal correction to Gibbs Free Energy=	1.050542
Sum of electronic and zero-point Energies=	-2285.947173
Sum of electronic and thermal Energies=	-2285.890454
Sum of electronic and thermal Enthalpies=	-2285.889510
Sum of electronic and thermal Free Energies=	-2286.032779

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scf done: -2287.083320

C	9.205568	-0.235277	-0.444606
C	9.523390	1.186003	-0.970048
C	8.400135	2.132195	-0.476997
C	7.259678	1.157053	-0.226179
N	7.739691	-0.134226	-0.199237
C	5.967184	1.465893	-0.034368
C	4.730338	1.613455	0.151789
C	8.021118	3.173270	-1.536843
C	8.770122	2.847479	0.836896
C	6.869326	-1.237067	0.086870
C	6.201841	-1.881962	-0.979741
C	5.375666	-2.974405	-0.685854
C	5.181282	-3.397243	0.626897
C	5.779239	-2.699641	1.673399
C	6.612787	-1.600038	1.428928
C	7.114581	-0.781127	2.609163
C	6.261567	-1.365895	-2.410246
C	6.677839	-2.450030	-3.414738
C	4.908848	-0.744202	-2.802669
C	5.936698	-0.067024	3.296581
C	7.905363	-1.622723	3.621009
C	9.529374	-1.307371	-1.490460
C	9.979309	-0.572291	0.840271
C	3.396062	1.669378	0.347151

C	2.639543	0.442016	0.584582
C	1.298569	0.450986	0.718919
C	0.458782	1.687522	0.548465
C	1.302752	2.932573	0.519236
C	2.643866	2.916741	0.381713
C	-0.445246	1.584515	-0.772666
C	-1.291521	2.817433	-0.936544
C	-2.633729	2.818948	-0.809631
C	-3.384970	1.589642	-0.591993
C	-2.624199	0.342820	-0.629308
C	-1.282152	0.334631	-0.753172
C	-4.721635	1.561601	-0.406641
C	-5.961362	1.442364	-0.219481
C	-7.261314	1.175148	-0.015781
N	-7.756896	-0.102876	0.124080
C	-9.225721	-0.153669	0.364401
C	-9.642970	1.289872	-0.009142
C	-8.387703	2.189932	0.116335
C	-6.882152	-1.236785	0.062762
C	-8.299648	2.888984	1.486771
C	-8.321600	3.240915	-0.998246
C	-9.907588	-1.191194	-0.533397
C	-9.555337	-0.495569	1.826475
C	-6.216380	-1.678277	1.228999
C	-5.379135	-2.798001	1.133343
C	-5.172756	-3.441680	-0.083973
C	-5.773772	-2.946667	-1.238962
C	-6.619330	-1.830925	-1.193408
C	-6.290633	-0.926938	2.550028
C	-6.738082	-1.823262	3.713924
C	-4.937378	-0.263492	2.862275
C	-7.134940	-1.241379	-2.498404
C	-5.975931	-0.606090	-3.287430
C	-7.881682	-2.271644	-3.358234
H	10.519622	1.522731	-0.649849
H	9.517251	1.166725	-2.070058
H	8.873871	3.839922	-1.745694
H	7.720061	2.686796	-2.477260
H	7.176956	3.789080	-1.191047
H	7.922322	3.451551	1.193415
H	9.029366	2.134176	1.632489
H	9.633740	3.514468	0.679219
H	4.858835	-3.487817	-1.498430
H	4.536444	-4.253399	0.836996
H	5.578837	-2.999631	2.703483
H	7.778349	-0.002322	2.216677
H	7.009104	-0.562869	-2.443032
H	6.780168	-2.018481	-4.423685
H	7.637489	-2.913634	-3.140422
H	5.925233	-3.252584	-3.477174
H	4.965289	-0.312922	-3.815795
H	4.618662	0.051207	-2.101798
H	4.109788	-1.503943	-2.804124
H	6.304586	0.584141	4.106669

H	5.376103	0.551789	2.582050
H	5.237211	-0.793958	3.741306
H	8.312179	-0.980838	4.419194
H	8.745367	-2.152241	3.146453
H	7.264125	-2.378649	4.102265
H	9.182359	-2.298339	-1.161187
H	9.066036	-1.080849	-2.459185
H	10.619236	-1.360086	-1.637542
H	11.056875	-0.627709	0.620230
H	9.830800	0.180355	1.625100
H	9.664229	-1.548943	1.234490
H	3.205298	-0.488755	0.674699
H	0.775903	-0.484128	0.931736
H	-0.277041	1.754952	1.371799
H	0.782512	3.890799	0.582451
H	3.206100	3.851860	0.323170
H	0.291661	1.526833	-1.595933
H	-0.772719	3.756906	-1.139214
H	-3.197442	3.750822	-0.898234
H	-3.187313	-0.592410	-0.579327
H	-0.756068	-0.620509	-0.815481
H	-9.988407	1.300200	-1.053678
H	-10.472700	1.646025	0.617712
H	-7.360112	3.456491	1.564540
H	-9.142599	3.588039	1.614747
H	-8.323475	2.168164	2.316795
H	-9.169188	3.941435	-0.919895
H	-7.387279	3.818561	-0.929741
H	-8.352340	2.765909	-1.990792
H	-9.501529	-2.197698	-0.351747
H	-10.986367	-1.214737	-0.314812
H	-9.781125	-0.952954	-1.597059
H	-9.177555	-1.495059	2.084242
H	-9.121853	0.227724	2.528839
H	-10.647254	-0.498287	1.969580
H	-4.863104	-3.157270	2.025388
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H	-5.565203	-3.421427	-2.199186
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H	-6.856295	-1.227401	4.633445
H	-7.696586	-2.321771	3.503389
H	-5.994076	-2.608390	3.924701
H	-5.009087	0.333498	3.786431
H	-4.623263	0.399401	2.044348
H	-4.148569	-1.019177	3.010938
H	-7.835286	-0.435075	-2.245503
H	-6.354697	-0.129460	-4.206690
H	-5.458495	0.156552	-2.688589
H	-5.235340	-1.367366	-3.583084
H	-8.307991	-1.787710	-4.251986
H	-8.702243	-2.749904	-2.802028
H	-7.207202	-3.069435	-3.709291

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