# Electronic Supplementary Information

## The curious case of a sterically crowded Stenhouse salt

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## General methods and materials

All manipulations were performed -unless otherwise noted- under an atmosphere of dry argon using standard Schlenk or dry box techniques. Solvents were dried by standard methods (Na for ethers and toluene, and $CaH_2$ for the rest) and distilled under argon. $^{1}H$, $^{13}C$ and $^{19}F$ NMR spectra were recorded on the NMR-ICMG platform of Grenoble with Bruker Avance 400 and 500 MHz spectrometers at 298 K. Chemical shifts are given in ppm and are referenced to $SiMe_4$ ($^{1}H$, $^{13}C$) and $CFCl_3$ ($^{19}F$). Coupling constants *J* are given in Hertz as positive values. NMR multiplicities are abbreviated as follows: s = singlet, d = doublet, t = triplet, q = quartet, sept = septet, m = multiplet, br = broad signal. Melting points were measured with a Büchi B-545 melting point apparatus system. Infrared (IR) data were recorded on Perkin-Elmer GS2000 IR spectrophotometer with a Golden-Gate ATR unit in the solid state unless otherwise noted. The intensities of the selected peaks are abbreviated as follows: s = strong, m = medium, w = weak, br = broad. Mass spectra were recorded on a Waters Gevo X2-S Qtof mass spectrometer or on a Thermo Scientific LTQ Orbitrap XL mass spectrometer. Single crystal X-ray diffraction data were collected at CEA-Grenoble with a Rigaku XCallibur S instrument.
For isolated products, UV-visible absorbance spectra were measured in a Varian Cary 300 Scan UV-vis spectrophotometer unless otherwise noted.

**CAAC**$HBF_4$ and **CAAC** were prepared according to reported procedures [1] and cinnamoyl chloride and methyl trifluoromethanesulfonate were distilled before use; all other starting materials were purchased from commercial sources and used without further purification.

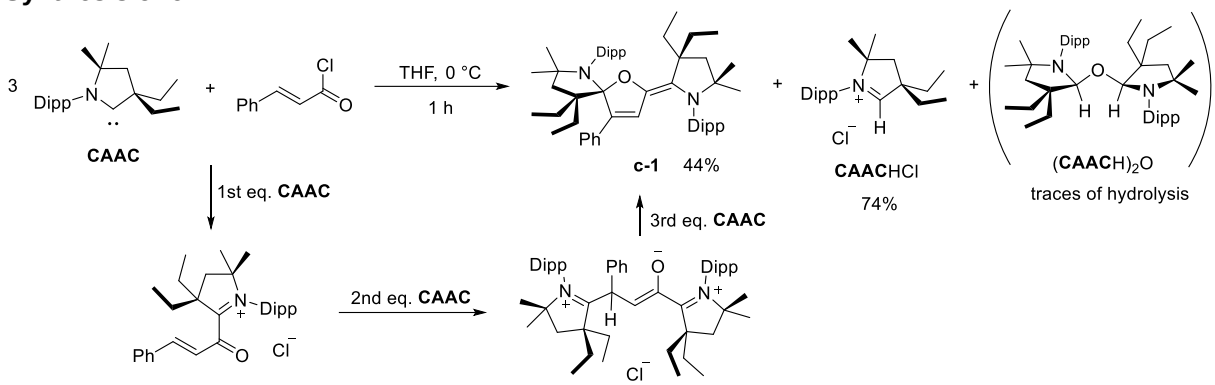
Electrochemical experiments run at 25 °C were carried out with a Biologic SP-300 potentiostat. Electrochemical experiments run at low temperatures were carried out with an Ivium technology potentiostat/galvanostat (compactStat). A silver reference electrode (0.01 M $AgNO_3$ in 0.1 M $[^nBu_4N]PF_6$ in $CH_3CN$) was used. Cyclic voltammetry experiments were performed in 0.1 M $[^nBu_4N]PF_6$ $CH_3CN$ solution. A vitreous carbon disk (3 mm in diameter) as working electrode and a platinum wire as auxiliary electrode were employed. Ferrocene was used as standard, and all reduction potentials are reported with respect to the $E_{1/2}$ of the $Fc/Fc^+$ redox couple. Electrochemical bulk reactions were performed using reticulated vitreous carbon electrode. Electrochemical reactions performed at 25 °C were monitored with a Zeiss MCS 501 UV-NIR spectrophotometer (1 mm cell). Electrochemical reactions performed at low temperatures were monitored with an Avantes Avalight-DH-S-BAL spectrophotometer (2 mm cell). EPR spectra were obtained using an X-band Bruker EMX Plus spectrometer and fitted with the EasySpin simulation package.[2]

The *in situ* electrochemical EPR experiments were performed with an Ivium Compacstat potentiostat. The electrochemistry cell was composed of a commercial Wilmad aqueous flat cell closed by silicon caps and metal wires: silver wire for the pseudo-reference electrode, platinum wires for the working electrode and the counter electrode. The cell was filled and tightly closed under argon atmosphere in glove box before measurement in the EPR cavity. The sample volume was 150 µl. The studied compounds were dissolved at a concentration of 1mM in an electrolytic solution of degassed acetonitrile (Fisher Chemical) with $TBAPF_6$ (Sigma Aldrich) at 0.2M. The potential from the pseudo-reference was controlled by a ferrocene solution at the end of the experiment. X-band EPR spectra were recorded at room temperature with an EMX Bruker spectrometer equipped with a standard ER4102ST Bruker cavity.

The reaction at low temperature in order to observe **o-1** was monitored with an Avantes Avalight-DH-S-BAL spectrophotometer (2 mm cell).

## Experimental procedures and characterization data

### Synthesis of c-1:

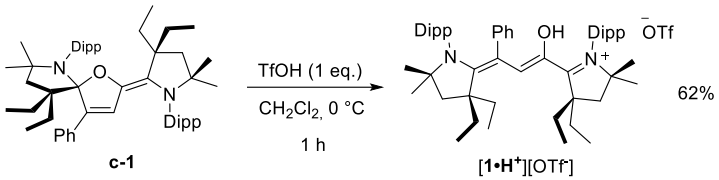



THF (10 mL) was added to a neat mixture of **CAAC** (0.752 g, 2.4 mmol, 3 eq.) and cinnamoyl chloride (0.131 g, 0.8 mmol) at 0 °C and the resulting mixture was stirred for 1 h at room temperature (until a green solution and abundant white to pale-yellow precipitate were obtained). The solution was concentrated to dryness under vacuum and the residue was extracted employing pentane (15 mL). The mother liquor was filtered by cannula into a new Schlenk flask (the solid that remained in the first flask is mainly **CAAC**H-Cl iminium salt (74%)). After evaporation of pentane under vacuum, a yellow to greenish residue remained. Acetonitrile (5 mL) was added and the sticky syrup was pulverized until a pale-yellow powder crashed out and the solution turned slightly green. The solid was filtered through canula and dried under vacuum. At this stage analysis of the solid by means of $^1$H NMR showed the presence of hydrolysis product (ca. 15-20%), namely (**CAAC**H)$_2$O, with a characteristic singlet at 4.63 ppm. *Note that since 3 equivalents of **CAAC** are employed with the accompanying traces of (**CAAC**H)$_2$O, the presence of such hydrolysis product may not be negligible at this point.* In order to remove the hydrolysis product, the pale-yellow solid was dissolved in the minimum amount of toluene and left in the freezer (-20 °C) until colorless crystals of (**CAAC**H)$_2$O appeared (a suitable single-crystal was measured by means of X-ray diffractometry for its unambiguous solid-state characterization). The mother liquor was filtered via canula in cold (sodium chloride-ice bath) and volatiles were removed under vacuum. The obtained solid residue was pulverized in minimum acetonitrile, filtered through canula and dried. Compound **c-1** was isolated as pale-yellow solid with a purity higher than 97% (0.266 g, 44% yield). *Note that compound **c-1** is a pale-yellow solid, however upon exposition to air and dissolving in polar solvents, it tends to ring-open generating the OH adduct **1•H**$^+$ with traces of water and/or radical **o-1**$^{\cdot+}$ in the air which are deep pink and red-brown solids, respectively.*

**Physical data:**
**m. p.:** 159 °C
**$^1$H NMR (500 MHz, $CDCl_3$):** $\delta$ (ppm) = 7.23 (dd, *J* = 7.6, 2.0 Hz, 1H), 7.19 (t, *J* = 7.6 Hz, 1H), 7.04-7.02 (m, 2H), 6.91-6.80 (m, 3H), 6.71 (t, *J* = 7.7 Hz, 2H), 5.89 (d, *J* = 7.1 Hz, 2H), 5.06 (s, 1H), 4.23 (sept, *J* = 6.6 Hz, 1H), 3.22-3.10 (m, 3H), 2.52 (sext, *J* = 7.4, 7.1 Hz, 1H), 2.22-2.12 (m, 3H), 2.07 (dd, *J* = 27.7, 12.6 Hz, 2H), 1.98 (dd, *J* = 13.4, 7.8 Hz, 1H), 1.92 (dd, *J* = 12.7, 3.7 Hz, 2H), 1.82 (sext, *J* = 7.7, 7.5 Hz, 1H), 1.52-1.44 (m, 2H), 1.46 (s, 3H), 1.43 (s, 3H), 1.32 (d, *J* = 6.6 Hz, 3H), 1.19 (d, *J* = 6.8 Hz, 3H), 1.16-1.06 (m, 18H), 0.95 (d, *J* = 6.6 Hz, 3H), 0.89 (td, *J* = 7.8, 3.9 Hz, 6H), 0.86 (s, 3H), 0.76 (d, *J* = 6.6 Hz, 3H), -0.27 (d, *J* = 6.7 Hz, 3H).
**$^{13}$C{$^1$H} NMR (126 MHz, $CDCl_3$):** $\delta$ (ppm) = 152.9, 152.4, 149.7, 149.6, 139.0, 138.5, 138.2, 134.6, 134.5, 132.3, 131.4, 131.2, 127.2, 126.7, 126.6, 125.8, 125.3, 125.0, 124.6, 124.4, 118.3, 64.0, 61.7, 57.6, 49.5, 45.6, 43.6, 33.2, 32.8, 31.5, 31.1, 30.4, 29.8, 29.6, 28.2, 27.8, 27.7, 27.4, 26.8, 26.3, 26.2, 26.1, 25.6, 24.2, 22.6, 12.0, 11.0, 10.8, 10.7.
**IR (neat):** 2950 (s), 2871 (m), 1597 (w), 1463 (w) cm$^{-1}$.
**HRMS (ESI):** m/z calculated for: $C_{53}H_{77}ON_2$ $[M+H]^+$ : 757.60304; found 757.60186.

**Physical data for (CAACH)$_2$O:**
**m. p.:** 153 °C
**$^1$H NMR (500 MHz, $CDCl_3$):** $\delta$ (ppm) = 7.22-7.17 (m, 4H), 7.11 (dd, *J* = 6.6, 2.8 Hz, 2H), 4.63 (s, 2H), 3.90 (sept, *J* = 6.7 Hz, 2H), 3.26 (sept, *J* = 6.7 Hz, 2H), 1.89 (d, *J* = 12.7 Hz, 2H), 1.86-1.81 (m, 2H), 1.55 (d, *J* = 12.7 Hz, 2H), 1.46-1.37 (m, 2H), 1.40 (d, *J* = 6.7 Hz, 6H), 1.28 (d, *J* = 6.7 Hz, 6H), 1.19 (d, *J* = 6.7 Hz, 6H), 1.19 (d, *J* = 6.8 Hz, 6H), 1.17 (s, 6H), 0.93 (s, 6H), 0.88 (t, *J* = 7.5 Hz, 6H), 0.86-0.79 (m, 2H), 0.71-0.64 (m, 2H), 0.27 (t, *J* = 7.5 Hz, 6H).
**$^{13}$C{$^1$H} NMR (126 MHz, $CDCl_3$):** $\delta$ (ppm) = 152.8, 149.8, 139.8, 126.8, 124.6, 124.4, 99.3, 62.2, 50.7, 49.4, 33.5, 32.2, 29.8, 28.0, 27.6, 26.6, 26.1, 26.1, 24.8, 10.6, 9.8.
**IR (neat):** 2971 (s), 2939 (s), 2871 (m), 1460 (m), 1437 (m), 1382 (w), 1361 (w), 1319 (w), 1186 (w), 1140 (w), 894 (m), 837 (m) cm$^{-1}$.
**HRMS (ESI):** *m/z* calculated for: $C_{22}H_{36}N$ $[(M-H_2O)/2+H]^+$: 314.28423 found 314.28386.

## Synthesis of [1•H$^+$][OTf$^-$]:




Compound **c-1** (0.035 g, 0.046 mmol) was dissolved in 2 mL of $CH_2Cl_2$ and at 0 °C, trifluoromethanesulfonic acid (0.004 mL, 0.046 mmol) was added. The resulting deep pink-reddish solution was stirred for 1 h at room temperature. The solution was concentrated to dryness under vacuum and diethyl ether (5 mL) was added. Deep pink-violet solid crashed out from the solution; upon standing the formed microcrystals tend to shine, similar to the golden rain, due to the formation of pink plates that are almost translucent-yellowish on one face. The solid was filtered through canula and dried under vacuum. Compound [**1•H$^+$**][OTf$^-$] was isolated as deep pink to violet powder (0.026 g, 62%). *Note that several attempts to obtain single-crystals of high quality for X-ray diffraction studies failed due to the formation of extremely thin plates. As shown below we decided to change the counter-anion to chloride in order to obtain better quality crystals.*

**Physical data:**
**m. p.:** 196 °C
**$^1$H NMR (500 MHz, $CDCl_3$, 25 °C):** *δ* (ppm) = 7.42 (br, 1H), 7.22 (br, 1H), 7.15 (t, *J* = 7.7 Hz, 1H), 6.95 (d, *J* = 7.7 Hz, 5H), 6.86 (br, 2H), 6.36 (br, 2H), 2.68 (br, 1H), 2.60 (br, 2H), 2.50 (br, 2H), 2.28-2.14 (br, 8H), 2.04 (br, 4H), 1.33 (s, 3H), 1.20 (br, 21H), 1.12 (br, 12H), 0.74 (br, 6H), 0.67 (d, *J* = 6.6 Hz, 6H).
**$^1$H NMR (500 MHz, $CDCl_3$, -38 °C):** *δ* (ppm) = 7.36 (s, 1H), 7.20 (t, *J* = 7.7 Hz, 1H), 7.14 (t, *J* = 7.7 Hz, 1H), 6.96-6.89 (m, 5H), 6.86 (t, *J* = 7.5 Hz, 2H), 6.30 (d, *J* = 7.3 Hz, 2H), 2.73 (s, 1H), 2.53 (sept, *J* = 6.4 Hz, 2H), 2.44 (sept, *J* = 6.4 Hz, 2H), 2.23 (s, 2H), 2.19 (s, 2H), 2.17-2.08 (m, 4H), 2.05-1.85 (m, 4H), 1.37-1.26 (m, 3H), 1.30 (s, 3H), 1.23-1.14 (m, 18H), 1.08 (t, *J* = 6.3 Hz, 10H), 0.85-0.78 (m, 2H), 0.67 (d, *J* = 6.3 Hz, 6H), 0.61 (d, *J* = 6.5 Hz, 6H).
**$^{13}$C{$^1$H} NMR (126 MHz, $CDCl_3$, -38 °C):** *δ* (ppm) = 175.2, 171.5, 146.6, 143.9, 137.0, 134.1, 132.8, 132.3, 130.4, 129.7, 129.2, 128.6, 128.1, 125.5, 123.6, 121.9, 119.4, 109.5, 73.0, 68.3, 54.4, 53.8, 46.4, 44.2, 33.8, 32.9, 29.5, 29.5, 29.3, 28.8, 26.5, 24.8, 24.0, 23.1, 10.0, 8.8.
**$^{19}$F{$^1$H} NMR (470 MHz, $CDCl_3$):** *δ* (ppm) = -78.0 (s).
**IR (neat):** 3497 (s), 2973 (s), 2873 (m), 1519 (w), 1390 (s), 1335 (s), 1267 (s), 1247 (s), 1128 (s), 1030 (s), 874 (m), 697 (m), 636 (s), 564 (m) cm$^{-1}$
**HRMS (ESI):** *m/z* calculated for: $C_{53}H_{77}ON_2$ [M-($CF_3SO_3$)]$^+$: 757.60304; found 757.60195.

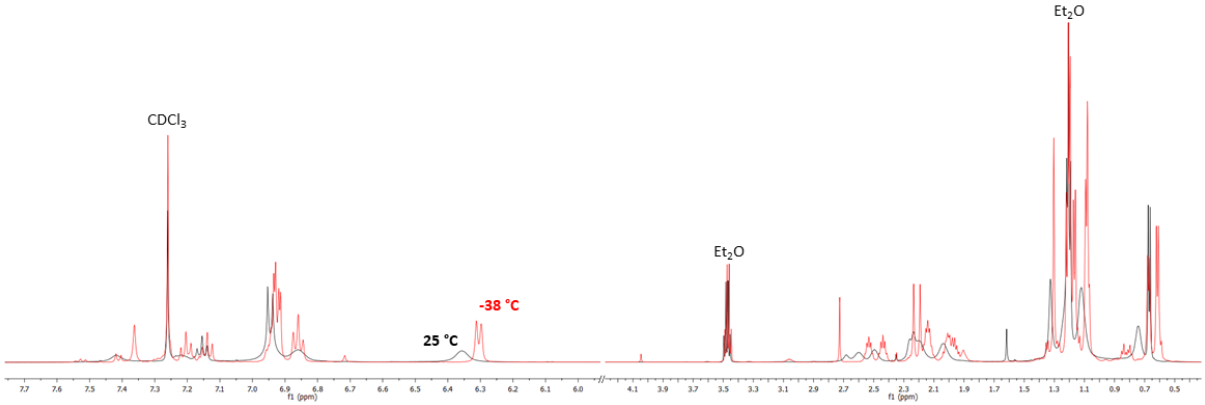
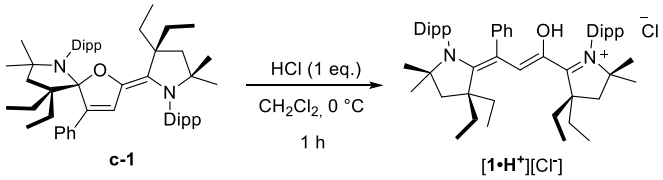



**Figure S1:** Superimposed $^1$H NMR spectra of compound [**1•H$^+$**][OTf$^-$] at 25 °C (in black) and -38 °C (in red) in $CDCl_3$.

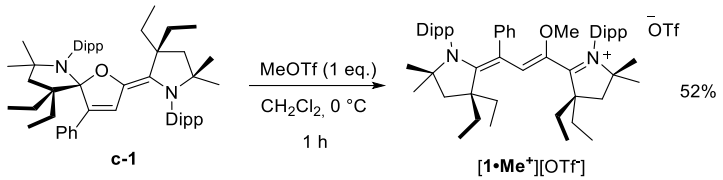
## Synthesis of [1•H$^+$][Cl$^-$] for single-crystal X-ray diffraction studies:




Compound **c-1** (0.047 g, 0.06 mmol) was dissolved in 2 mL of $CH_2Cl_2$ and at 0 °C, HCl 2 M ethereal solution (0.03 mL, 0.06 mmol) was added. The resulting deep pink-reddish solution was stirred for 1 h at room temperature. The solution was concentrated to dryness under vacuum and diethyl ether (5 mL) was added. Deep pink-violet solid crashed out from the solution. The solid was filtered through canula and dried under vacuum. In order to obtain single-crystals, a saturated solution of salt [**1•H$^+$**][Cl$^-$] in $CH_2Cl_2$ was layered with diethyl ether and stand at room temperature for slow diffusion.

**Physical data:**
**m. p.:** 124 °C

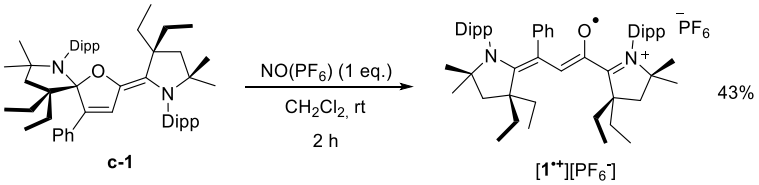
## Synthesis of [1•Me$^+$][OTf$^-$]:




Compound **c-1** (0.035 g, 0.046 mmol) was dissolved in 2 mL of $CH_2Cl_2$ and at 0 °C, methyl trifluoromethanesulfonate (0.005 mL, 0.046 mmol) was added. The resulting deep pink-reddish solution was stirred for 1 h at room temperature. The solution was concentrated to dryness under vacuum and diethyl ether (5 mL) was added. Deep pink-violet solid crashed out from the solution; upon standing the formed microcrystals tend to shine, similar to the golden rain, due to the formation of pink plates that are almost translucent-yellowish on one face. The solid was filtered through canula and dried under vacuum. Compound [**1•Me**$^+$][OTf$^-$] was isolated as deep pink to violet powder (0.022 g, 52%).

**Physical data:**
**m. p.:** 212 °C.
**$^1$H NMR (500 MHz, $CDCl_3$):** $\delta$ (ppm) = 7.66 (s, 1H), 7.25-7.16 (m, 2H), 7.09 (d, $J$ = 7.7 Hz, 2H), 6.95 (m, 3H), 6.84 (t, $J$ = 7.2 Hz, 1H), 6.76 (t, $J$ = 7.2 Hz, 1H), 6.43 (d, $J$ = 7.4 Hz, 2H), 2.71-2.64 (m, 2H), 2.60-2.52 (m, 2H), 2.25 (s, 4H), 2.15-2.01 (m, 4H), 1.98-1.94 (m, 3H), 1.67 (s, 3H), 1.38-1.28 (m, 5H), 1.37 (s, 3H), 1.30 (s, 3H), 1.24-1.07 (m, 25H), 0.94 (br s, 5H), 0.78 (br s, 6H), 0.66 (d, $J$ = 6.2 Hz, 2H).
**$^{13}$C{$^1$H} NMR (126 MHz, $CDCl_3$):** $\delta$ (ppm) = 178.1, 177.3, 146.8, 144.7, 137.8, 137.3, 137.0, 135.3, 131.2, 129.6, 129.3, 128.9, 127.7, 126.6, 125.6, 125.4, 123.8, 122.5, 113.2, 72.9, 69.4, 59.8, 55.6, 55.2, 46.6, 44.3, 33.9, 33.4, 33.0, 30.0, 29.7, 29.7, 29.5, 29.0, 26.9, 25.3, 24.9, 24.7, 23.3, 10.3, 10.2, 9.6.
**$^{19}$F{$^1$H} NMR (376 MHz, $CD_3CN$):** $\delta$ (ppm) = -79.3 (s).
**IR (neat):** 2970 (m), 2878 (w), 1466 (w), 1389 (m), 1331 (s), 1267 (s), 1248 (s), 1127 (s), 1031 (s), 864 (m), 701 (m), 637 (m) cm$^{-1}$.
**HRMS (ESI):** *m/z* calcd for $C_{54}H_{79}ON_2$ [M]$^+$: 771.61869; found: 771.61758.

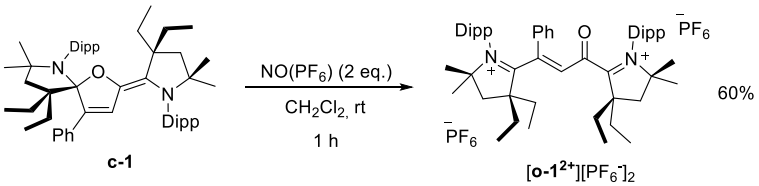
## Synthesis of [o-1$^{\bullet+}$][$PF_6^-$]:




Compound **c-1** (0.035 g, 0.046 mmol) was dissolved in 2 mL of $CH_2Cl_2$ and at room temperature, nitrosonium hexafluorophosphate (0.008 g, 0.046 mmol) was added. The resulting deep red solution was stirred for 2 h at room temperature. The solution was concentrated to ca. 0.5 mL under vacuum and diethyl ether (5 mL) was added. Dark red solid crashed out from the solution and it was filtered through canula and dried under vacuum. Compound [**o-1**$^{\bullet+}$][$PF_6^-$] was isolated as dark red powder (0.018 g, 43%).

**Physical data:**
**m. p.:** 142 °C
**IR (neat):** 2973 (s), 1473 (m), 1939 (m), 1334 (w), 1255 (w), 1027 (s), 836 (s), 556 (s) cm$^{-1}$
**HRMS (ESI):** *m/z* calculated for: $C_{53}H_{77}ON_2$ [M+H$^\bullet$]$^+$: 757.60304; found 757.60150.

## Synthesis of o-1$^{2+}$($PF_6$)$_2$:

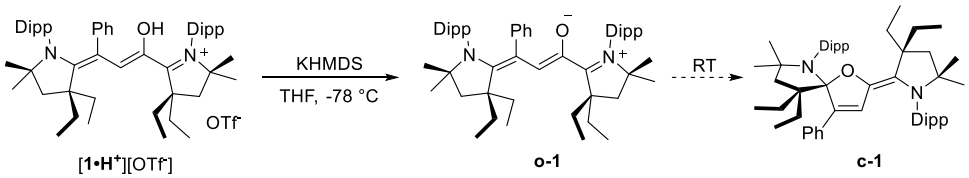



Compound **c-1** (0.035 g, 0.046 mmol) was dissolved in 2 mL of $CH_2Cl_2$ and at room temperature, nitrosonium hexafluorophosphate (0.016 g, 0.092 mmol) was added. The resulting yellow solution was stirred for 1 h at room temperature. The solution was concentrated to ca. 0.5 mL under vacuum and diethyl ether (5 mL) was added. Yellow solid crashed out from the solution and it was filtered through canula and dried under vacuum. Compound [**o-1**$^{2+}$][$PF_6^-$]$_2$ was isolated as yellow powder (0.029 g, 60%).

**Physical data:**
**m. p.:** 107 °C

**$^{1}$H NMR (500 MHz, $CD_3CN$):** $\delta$ (ppm) = 7.74 (t, *J* = 7.8 Hz, 2H), 7.58 (d, *J* = 7.8 Hz, 2H), 7.52 (d, *J* = 7.9 Hz, 2H), 7.38 (t, *J* = 7.6 Hz, 1H), 7.15 (t, *J* = 7.7 Hz, 2H), 6.49 (s, 1H), 6.28 (br s, 2H), 2.54 (sept, *J* = 6.5 Hz, 2H), 2.52 (s, 2H), 2.48 (sept, *J* = 6.5 Hz, 2H), 2.42 (s, 2H), 1.69-1.61 (m, 2H), 1.59 (s, 6H), 1.55-1.51 (m, 2H), 1.53 (s, 6H), 1.44-1.37 (m, 3H), 1.33 (d, *J* = 6.4 Hz, 6H), 1.27 (d, *J* = 6.4 Hz, 6H), 0.98-0.95 (m, 12H), 0.90 (t, *J* = 7.2 Hz, 6H), 0.84 (br s, 6H).
**$^{13}$C{$^{1}$H} NMR (126 MHz, $CD_3CN$):** $\delta$ (ppm) = 192.6, 192.1, 184.8, 150.5, 145.7, 144.8, 133.7, 133.7, 132.3, 132.0, 130.3, 130.1, 129.8, 129.0, 128.5, 128.3, 88.3, 88.1, 62.3, 59.7, 42.2, 40.2, 32.6, 31.2, 30.4, 30.3, 29.2, 29.0, 26.7, 25.4, 25.4, 25.1, 11.1, 9.2.
**$^{19}$F NMR (470 MHz, $CD_3CN$):** $\delta$ (ppm) = -72.9 (d, *J* = 706.4 Hz).
**IR (neat):** 2980 (m), 2951 (w), 1682 (w), 1622 (w), 1574 (w), 1469 (m), 1394 (w), 1337 (w), 1128 (w), 1045 (w), 834 (s), 556 (s) $cm^{-1}$.
**HRMS (ESI):** *m/z* calculated for: $C_{53}H_{76}ON_2$ $[M\text{-}2(PF_6)]^{2+}$: 378.29733; found 378.29683.

## Observation of o-1:




For the UV-visible spectroscopic observation and characterization of **o-1**, Stenhouse salt [**1•H$^+$**][OTf] (ca. 1 mg) was dissolved in 20 mL of dry THF under Argon atmosphere at -78 °C leading to a pink solution ($\lambda_{max}$ = 530 nm). The Schlenk flask was equipped with an UV-visible dip probe (2 mm path) for continuous monitorization of the reaction (see Figure S2). Upon addition of an excess of potassium bis(trimethylsilyl)amide in THF the reaction mixture instantaneously turned blue, attributed to **o-1** ($\lambda_{max}$ = 610 nm). The cold bath was then removed and the reaction mixture was allowed to reach room temperature. The blue colour slowly disappeared leading to a colourless solution with a band at 368 nm, which is characteristic of **c-1**.

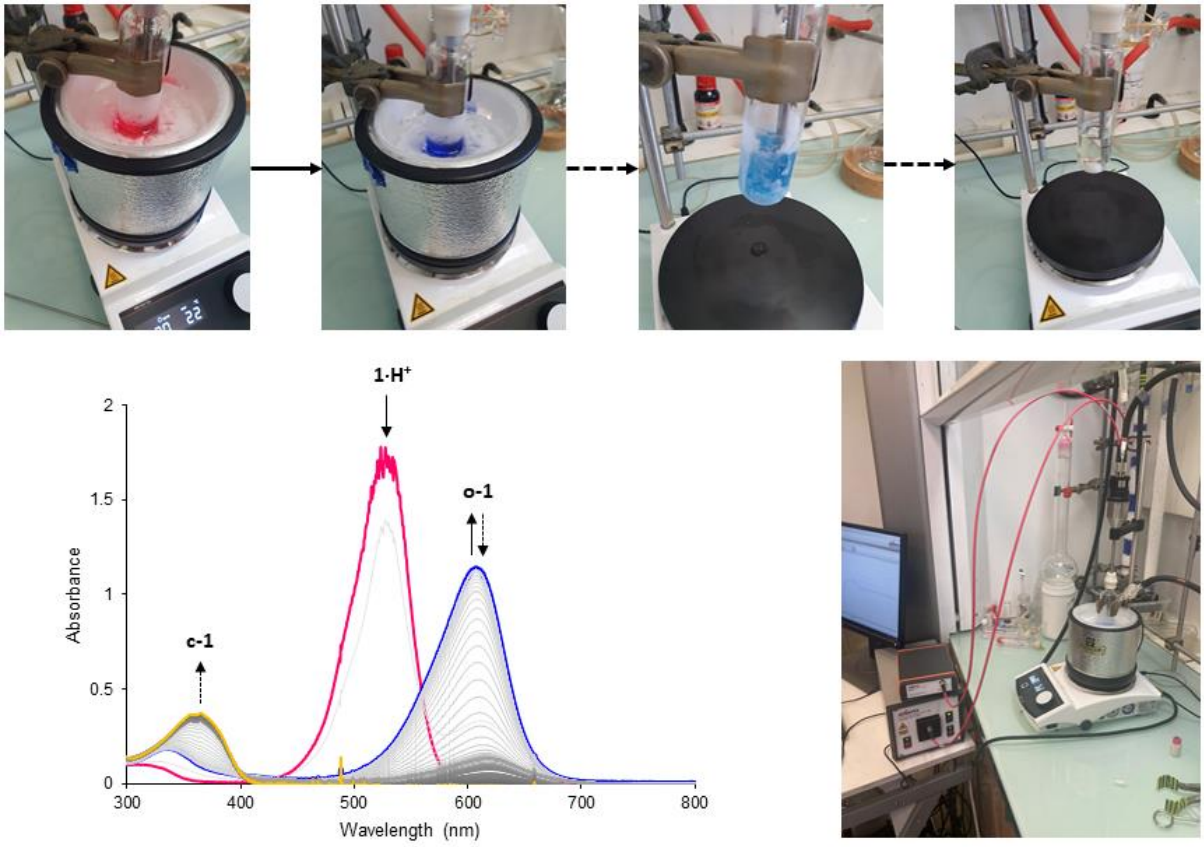



**Figure S2:** In situ monitorization of the reaction via UV-visible spectrometry.

## Electrochemical studies

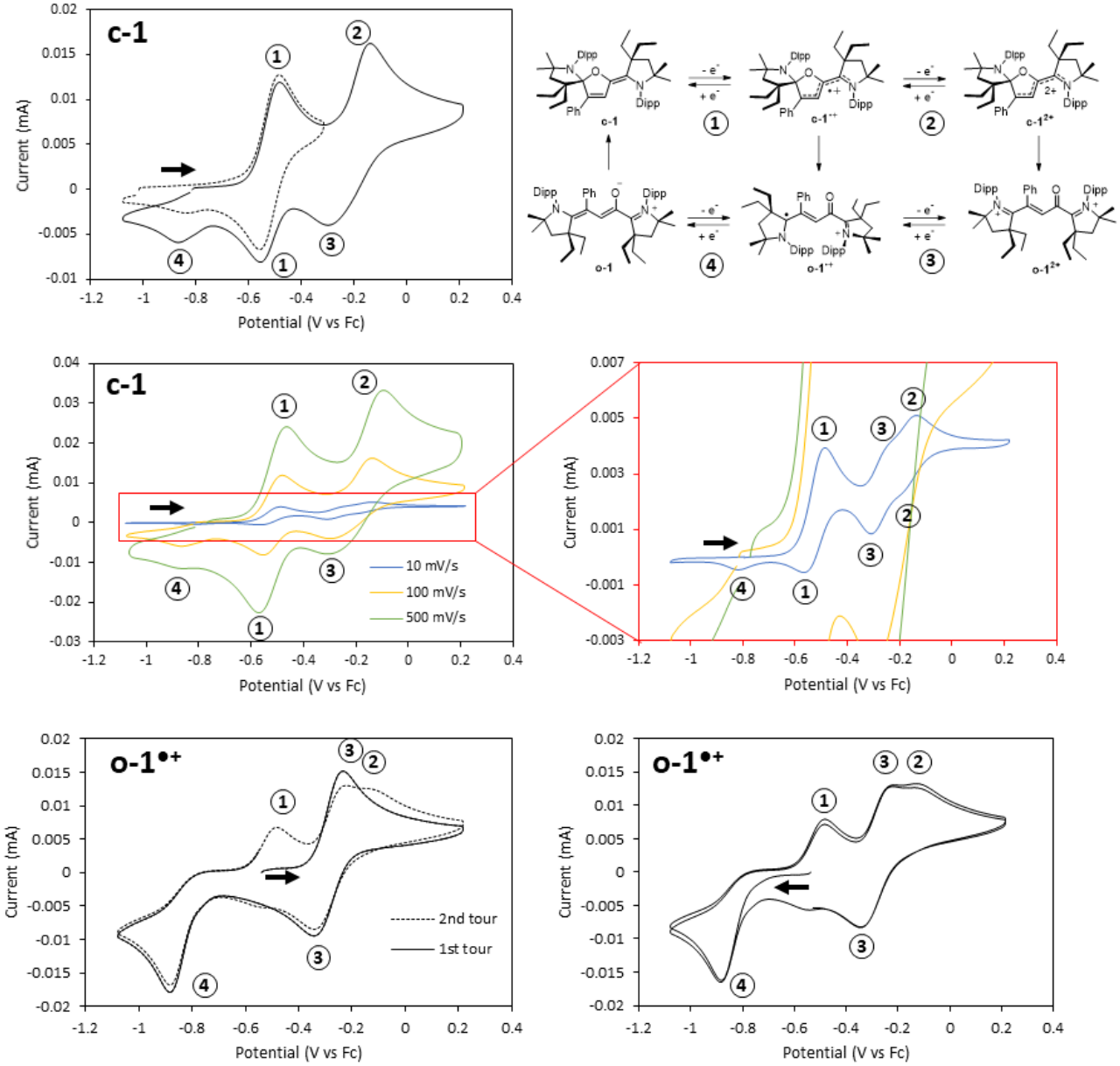



**Figure S3:** Up: Cyclic voltammogram of compound **c-1** (1 mM solution employing 0.1 M of $^{n}Bu_4NPF_6$ in acetonitrile electrolyte; 100 mV/s rate). Middle: Cyclic voltammograms of compound **c-1** at different rates (1 mM solution employing 0.1 M of $^{n}Bu_4NPF_6$ in acetonitrile electrolyte). Down: Cyclic voltammograms of compound **o-1$^{\bullet+}$** (1 mM solution employing 0.1 M of $^{n}Bu_4NPF_6$ in acetonitrile electrolyte; 100 mV/s rate). Radical cation **o-1$^{\bullet+}$** was generated by electrochemical reduction at $E$ = -0.47 V vs Fc of **c-1** on a reticulated vitreous carbon electrode, see Figure S4.

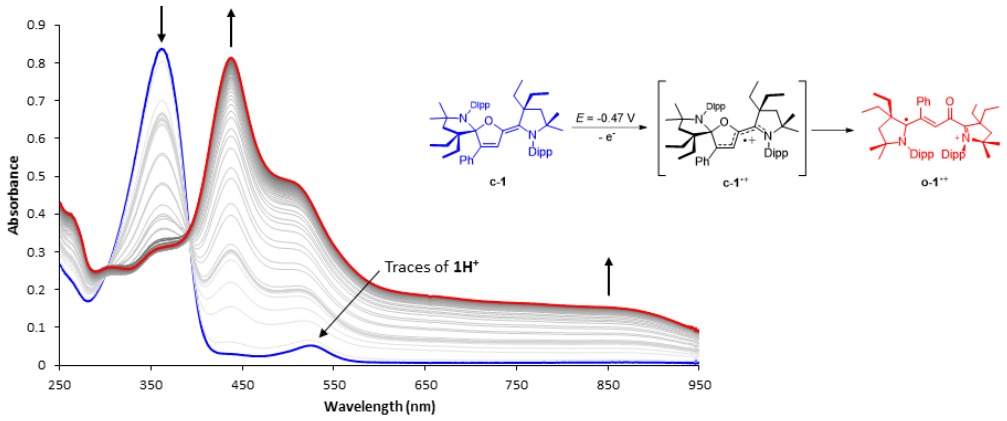



**Figure S4:** UV-vis monitoring of electrochemical reduction at $E$ = -0.47 V vs Fc of **c-1** on a reticulated vitreous carbon electrode (1 mM solution of **c-1** employing 0.1 M of $^{n}Bu_4NPF_6$ in acetonitrile electrolyte at room temperature).

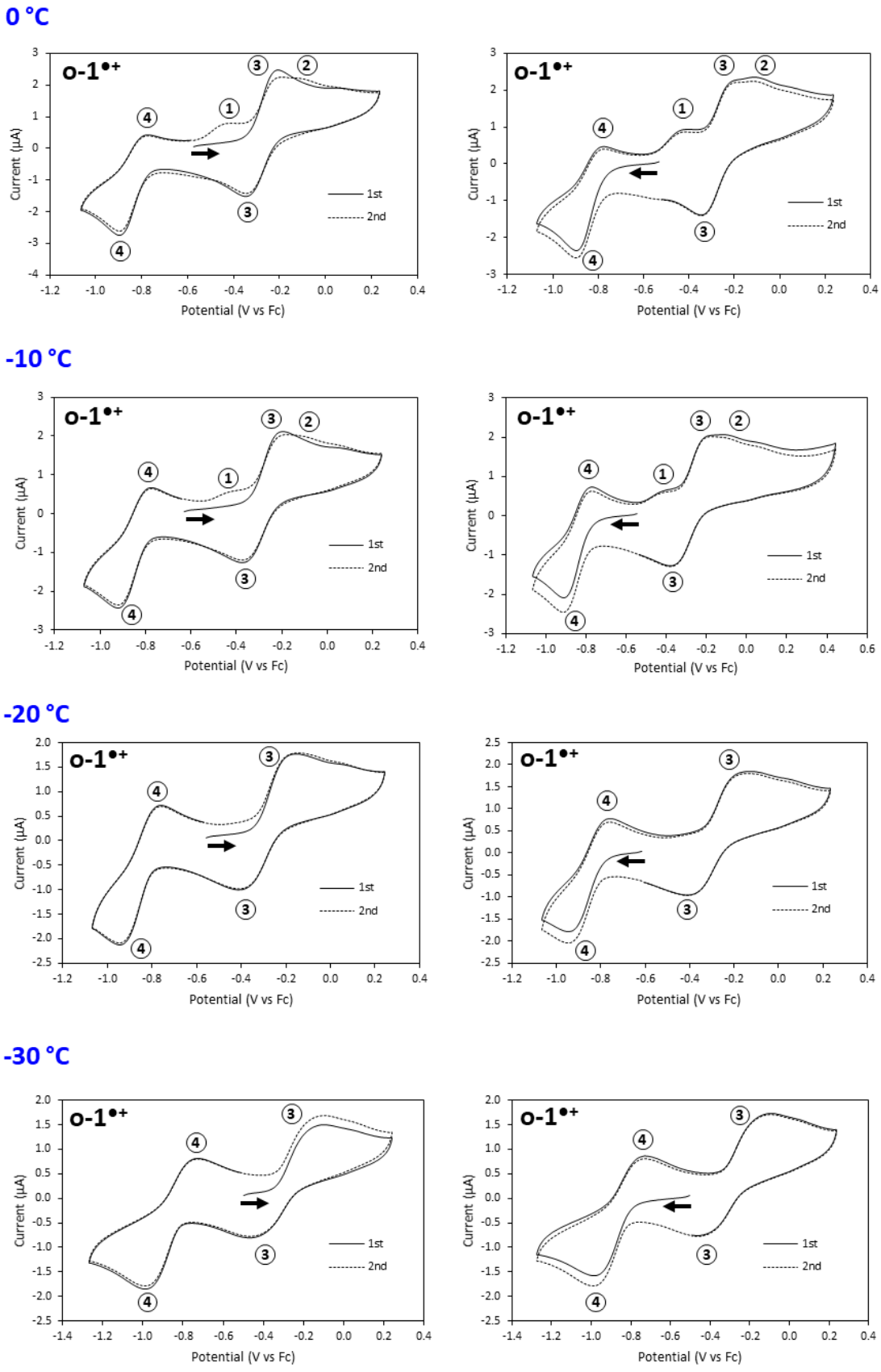



**Figure S5:** Cyclic voltammograms of compound **o-1**$^{\bullet+}$ at different temperatures (1 mM solution employing 0.1 M of $^{n}Bu_4NPF_6$ in acetonitrile electrolyte; 100 mV/s rate). Radical cation **o-1**$^{\bullet+}$ was generated by electrochemical reduction at $E$ = -0.47 V vs Fc of **c-1** on a reticulated vitreous carbon electrode (1 mM solution of **c-1** employing 0.1 M of $^{n}Bu_4NPF_6$ in acetonitrile electrolyte at room temperature).

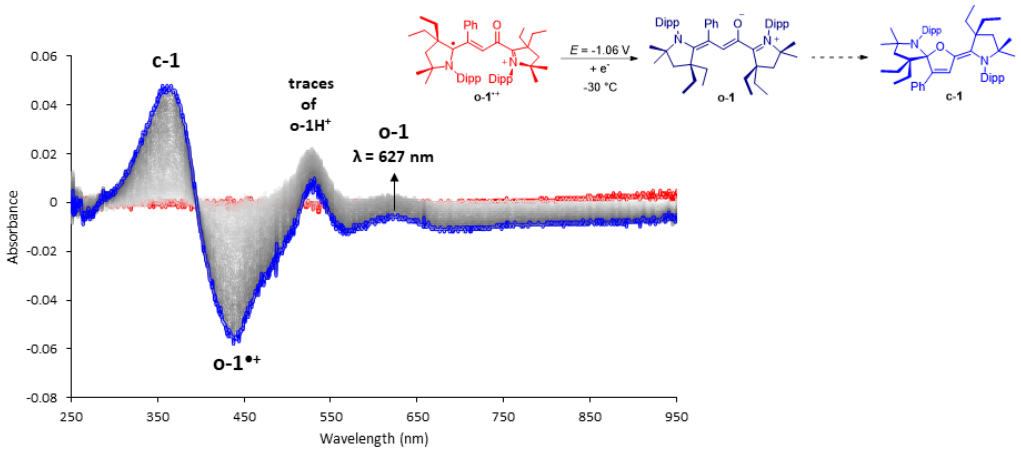



**Figure S6:** Early stages of the UV-vis monitoring of electrochemical reduction at *E* = -1.06 V vs Fc of **o-1**$^{\bullet+}$ on a reticulated vitreous carbon electrode (1 mM solution of **o-1**$^{\bullet+}$ employing 0.1 M of $^{n}Bu_4NPF_6$ in acetonitrile electrolyte at -30 °C). For more sensitive observation of transient species (attributed to **o-1** at 627 nm), the initial solution of substrate **o-1**$^{\bullet+}$ was set as the blank (red line). Positive absorbances correspond to forming species, whether negative absorbances correspond to consuming species (grey to blue lines).

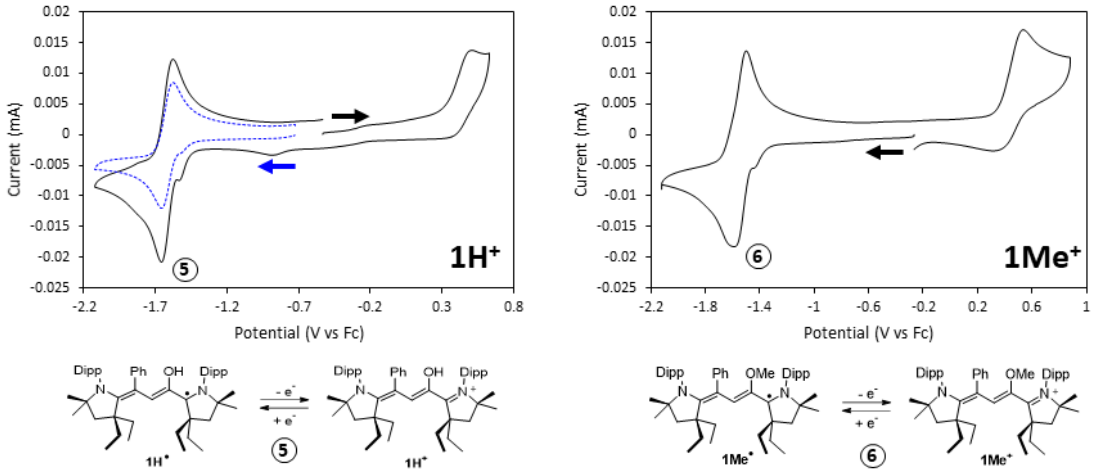



**Figure S7:** Cyclic voltammograms of salts [**1**•**H**$^{+}$][OTf$^{-}$] and [**1**•**Me**$^{+}$][OTf$^{-}$] (1 mM solution employing 0.1 M of $^{n}Bu_4NPF_6$ in acetonitrile electrolyte; 100 mV/s rate).

## UV-visible absorption spectra

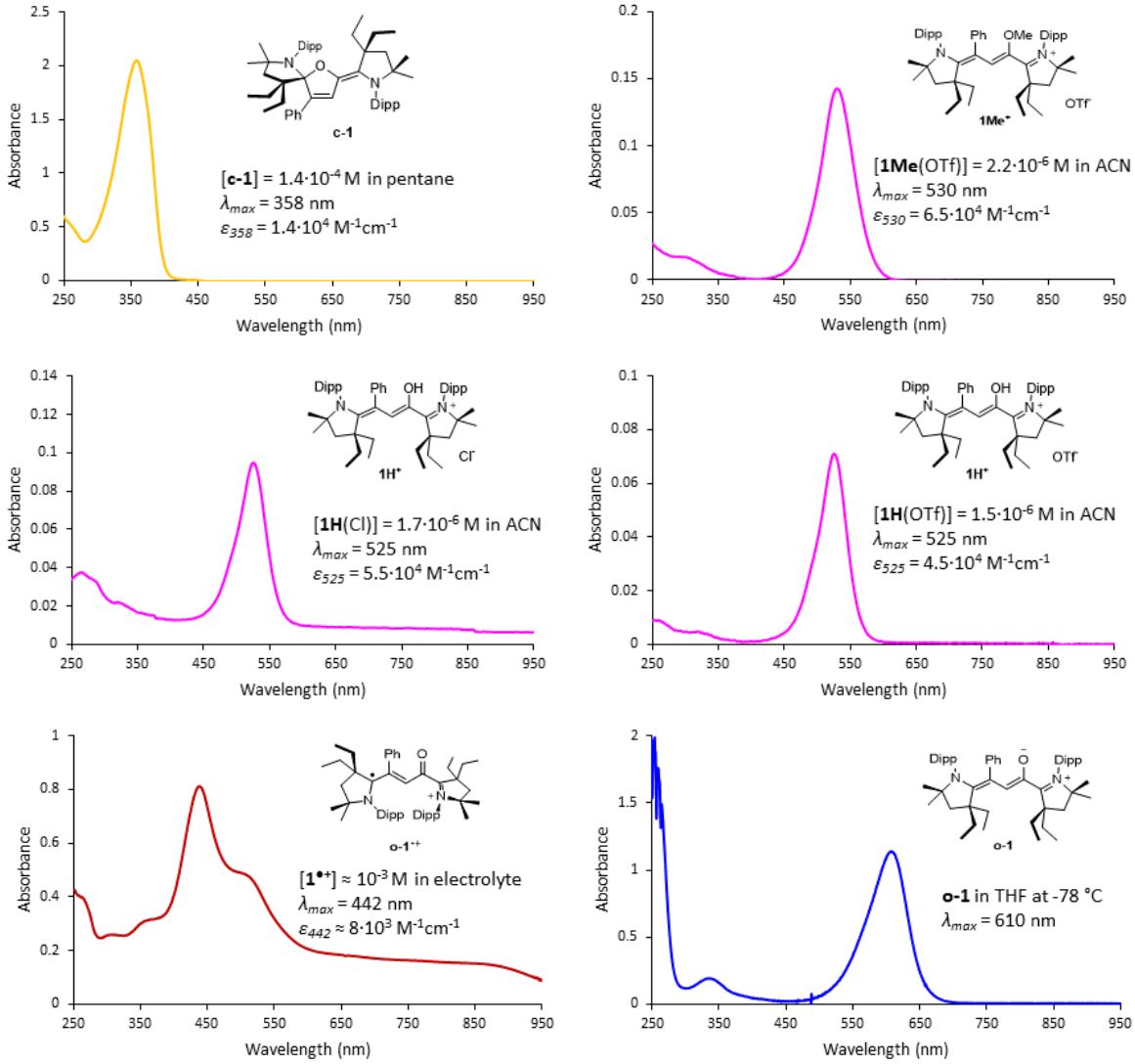



**Figure S8:** UV-visible absorption spectra of selected compounds (ACN = acetonitrile; electrolyte = a solution 0.1 M of $^{n}Bu_4NPF_6$ in acetonitrile).

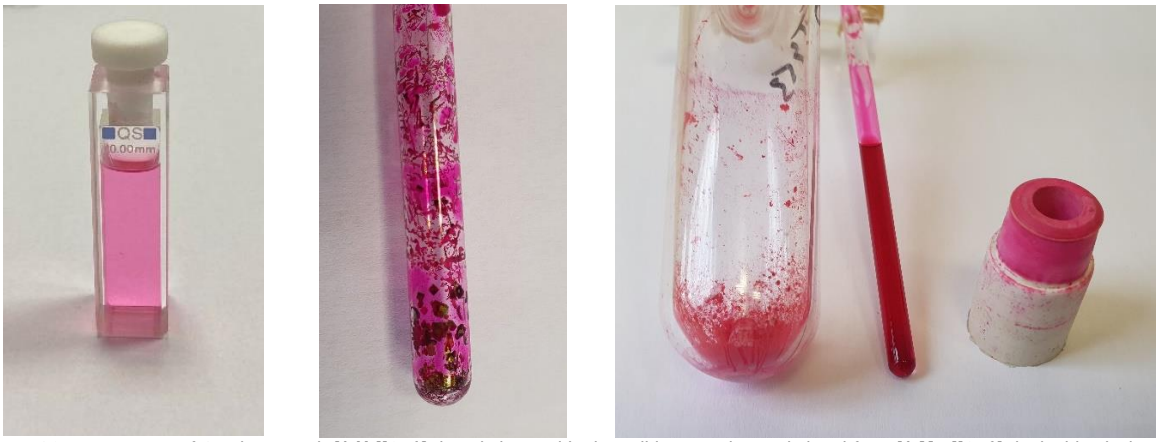


**Figure S9:** Appearance of Stenhouse salt [**1•H**$^+$][OTf] in solution and in the solid state. The methylated form [**1•Me**$^+$][OTf] looks identical. Note that upon exposure to air the septum employed during the synthesis of the closed form **c-1** turns pink; i. e. dye **1•H**$^+$ is formed with its characteristic color.

## X-ray diffraction studies

Single crystals of **c-1** grew by slow diffusion of acetonitrile into a saturated solution of the compound in chloroform at room temperature. Crystals of [**1•H**$^+$][Cl$^-$] grew by slow diffusion of $Et_2O$ into a saturated solution of the salt in $CH_2Cl_2$ at room temperature. Suitable single crystals of [**1•Me**$^+$][OTf$^-$] slowly grew from a saturated solution of the salt in $Et_2O$ kept at room temperature and obtained from the washing fractions during the work-up. Crystals of [**o-1**$^{2+}$][$PF_6^-$]$_2$ grew by slow diffusion of $Et_2O$ into a saturated solution of the salt in $CH_2Cl_2$ at 4 °C. During the purification of **c-1**, the crude mixture containing the former compound and (**CAAC**H)$_2$O was dissolved in the minimum amount of toluene and left in the freezer (-20 °C) until colorless crystals of (**CAAC**H)$_2$O appeared.

Diffraction data were collected using a Rigaku XCallibur S Kappa area detector four-circle diffractometer (Mo-$K_\alpha$ radiation λ = 0.71073 Å, graphite monochromator), controlled by the Rigaku CrysAlis CCD software.[3] Unique intensities with I > 10σ (I) detected on all frames using the Rigaku CrysAlis RED were used to refine the values of the cell parameters.

The substantial redundancy in data allows analytical absorption corrections to be applied using crystal shape determination for all compounds. The space group was determined from systematic absences, and it was confirmed by the successful resolution of the structure. The structures were solved by intrinsic phasing method using ShelXT software, in Olex1.2 environment.[4,5] All the atoms were found by difference Fourier syntheses. All non-hydrogen atoms were anisotropically refined on $F^2$ using ShelXL program.[6] Hydrogen atoms were fixed in ideal positions for compounds [**1•Me**$^+$][OTf$^-$], [**o-1**$^{2+}$][$PF_6^-$]$_2$ and [**1•H**$^+$][Cl$^-$] (except for hydroxide oxygen where hydrogen atom has been found by Fourier transform and refined isotropically) and found by Fourier transform and refined isotropically with a riding model for compound **c-1**.

CCDC 2163356-2163359 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Center via www.ccdc.cam.ac.uk/datarequest/cif.

**Table S1.** Crystal data for **c-1** and [**1•H**$^+$][Cl$^-$].

| | **c-1** | [**1•H**$^+$][Cl$^-$] |
|---|---|---|
| CCDC | 2163356 | 2163357 |
| Empirical formula | $C_{53}H_{76}N_2O$ | $C_{53}H_{79}ClN_2O_2$ |
| Formula weight | 757.15 | 811.63 |
| Temperature/K | 150.00(10) | 150.3(5) |
| Crystal system | triclinic | monoclinic |
| Space group | P-1 | P21/c |
| a/Å | 14.2247(5) | 13.0058(6) |
| b/Å | 18.7107(6) | 18.6532(8) |
| c/Å | 19.0753(10) | 20.2559(8) |
| α/° | 109.830(4) | 90 |
| β/° | 93.980(3) | 107.607(5) |
| γ/° | 103.160(3) | 90 |
| Volume/Å$^3$ | 4590.5(3) | 4683.9(4) |
| Z | 4 | 4 |
| $\rho_{calc}$g/cm$^3$ | 1.096 | 1.151 |
| μ/mm$^{-1}$ | 0.063 | 0.123 |
| F(000) | 1664.0 | 1776.0 |
| Crystal size/mm$^3$ | 0.31 × 0.19 × 0.16 | 0.27 × 0.08 × 0.05 |
| Radiation | Mo $K_\alpha$ (λ = 0.71073) | Mo $K_\alpha$ (λ = 0.71073) |
| 2Θ range for data collection/° | 3.884 to 52.744 | 3.944 to 52.744 |
| Index ranges | -17 ≤ h ≤ 17, -23 ≤ k ≤ 22, -23 ≤ l ≤ 23 | -16 ≤ h ≤ 12, -22 ≤ k ≤ 23, -25 ≤ l ≤ 25 |
| Reflections collected | 41469 | 22574 |
| Independent reflections | 18741 [$R_{int}$ = 0.0518, $R_{sigma}$ = 0.0957] | 9580 [$R_{int}$ = 0.1072, $R_{sigma}$ = 0.1931] |
| Data/restraints/parameters | 18741/0/1617 | 9580/0/546 |
| Goodness-of-fit on F$^2$ | 1.013 | 0.916 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0595, $wR_2$ = 0.0948 | $R_1$ = 0.0640, $wR_2$ = 0.0926 |
| Final R indexes [all data] | $R_1$ = 0.1188, $wR_2$ = 0.1136 | $R_1$ = 0.1626, $wR_2$ = 0.1241 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.21/-0.20 | 0.29/-0.27 |

[a] $R_1 = \Sigma(|F_o|-|F_c|)/\Sigma|F_o|$; $wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{½}$.

**Table S2.** Crystal data for [**1•Me**$^+$][OTf$^-$] and [**o-1**$^{2+}$][$PF_6^-$]$_2$.

| | [**1•Me**$^+$][OTf$^-$] | [**o-1**$^{2+}$][$PF_6^-$]$_2$ |
|---|---|---|
| CCDC | 2163358 | 2163359 |
| Empirical formula | $C_{57}H_{84}F_3N_2O_{4.5}S$ | $C_{54}H_{78}Cl_2F_{12}N_2OP_2$ |
| Formula weight | 958.32 | 1132.02 |
| Temperature/K | 150.00(14) | 150.00(14) |
| Crystal system | monoclinic | monoclinic |
| Space group | I2/a | $P2_1/n$ |
| a/Å | 17.3378(9) | 12.1520(8) |
| b/Å | 16.0403(10) | 31.9515(18) |
| c/Å | 38.924(2) | 14.2567(7) |
| α/° | 90 | 90 |
| β/° | 95.096(5) | 97.129(5) |
| γ/° | 90 | 90 |
| Volume/Å$^3$ | 10782.0(11) | 5492.7(6) |
| Z | 8 | 4 |
| $\rho_{calc}$g/cm$^3$ | 1.181 | 1.369 |
| μ/mm$^{-1}$ | 0.117 | 0.257 |
| F(000) | 4152.0 | 2384.0 |
| Crystal size/mm$^3$ | 0.539 × 0.245 × 0.015 | 0.87x0.14x0.01 |
| Radiation | Mo $K_\alpha$ (λ = 0.71073) | Mo $K_\alpha$ (λ = 0.71073) |
| 2Θ range for data collection/° | 4.048 to 52.744 | 2.1140 to 21.4940 |
| Index ranges | -13 ≤ h ≤ 21, -19 ≤ k ≤ 20, -48 ≤ l ≤ 43 | -15 ≤ h ≤ 15, -39 ≤ k ≤ 39, -17 ≤ l ≤ 17 |
| Reflections collected | 24739 | 47920 |
| Independent reflections | 11002 [$R_{int}$ = 0.0743, $R_{sigma}$ = 0.1286] | 11219 [$R_{int}$ = 0.1883, $R_{sigma}$ = 0.2034] |
| Data/restraints/parameters | 11002/55/681 | 11219/0/674 |
| Goodness-of-fit on F$^2$ | 1.014 | 1.002 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0859, $wR_2$ = 0.2195 | $R_1$ = 0.0942, $wR_2$ = 0.2009 |
| Final R indexes [all data] | $R_1$ = 0.1844, $wR_2$ = 0.2793 | $R_1$ = 0.2151, $wR_2$ = 0.2575 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.83/-0.56 | 0.55/-0.43 |

[a] $R_1 = \Sigma(|F_o|-|F_c|)/\Sigma|F_o|$; $wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{½}$.

**Table S3.** Crystal data for (**CAAC**H)$_2$O.

| | **(CAACH)$_2$O** | **(CAACH)$_2$O** |
|---|---|---|
| CCDC | *This work. Not deposited.* | *Previously deposited as 1967091.* |
| Space group | C2/c | C2/c |
| a/Å | 20.8603(6) | 20.8505(2) |
| b/Å | 10.6975(3) | 10.70890(10) |
| c/Å | 18.3341(7) | 18.3282(2) |
| α/° | 90 | 90 |
| β/° | 103.231(4) | 103.1900(10) |
| γ/° | 90 | 90 |

## DFT studies

**General considerations:** The DFT calculations were performed with the program package Gaussian09.[7] All optimized structures were submitted to vibrational analysis and minima were characterized by the absence of imaginary frequencies. E is the absolute electronic energy with zero point energy correction (in hartrees). When not otherwise stated, optimizations were performed at the D3-B3LYP/6-311g(d,p) level of theory, including the D3 version of Grimme's dispersion[8] and the Polarizing Continuum Model (PCM) for acetonitrile as solvent.
EPR hyperfine constants were calculated on previously optimized structures of the most stable conformer, with a single point calculation at the D3-B3LYP/EPRII level of theory. The NBO 3.1 program for natural bond orbital (NBO) analyses[9] was used as implemented in Gaussian 09.

As shown below in table S4, the elongated C1–O1 bond length in **c-1** was fairly reproduced at different level of theory. As expected for such bulky structure, results was very dependent on the model for dispersion forces, with D3-B3LYP/6-311g(d,p) with PCM model for acetonitrile affording the best fit with the experimental crystallographic data.

**Table S4:** Computed C–O bond lengths (pm) for optimized structures of **c-1**

| | | | C1 – O1 | C3–O1 |
|---|---|---|---|---|
| B3LYP | 6-31g(d) | | 151.4 | 140.0 |
| B3LYP | 6-311g(d,p) | | 151.7 | 139.8 |
| B3LYP | 6-311g(d,p) | PCM(ACN) | 151.5 | 139.9 |
| **D3-B3LYP** | **6-311g(d,p)** | **PCM(ACN)** | **150.6** | **139.5** |
| wb97xd | 6-311g(d,p) | PCM(ACN) | 147.8 | 138.6 |
| B97D3 | 6-311g(d,p) | PCM(ACN) | 153.3 | 139.6 |
| M06 | 6-311g(d,p) | PCM(ACN) | 148.1 | 138.6 |
| M06-2X | 6-311g(d,p) | PCM(ACN) | 147.6 | 139.2 |
| **Experimental XRD structure** | | | **150.7** | **139.1** |

**xyz coordinates of optimized structures of c-1**

(E = -2249.718306)

| | x | y | z | | x | y | z |
|---|---|---|---|---|---|---|---|
| O | -0.15023100 | -1.36519600 | 0.13927900 | C | -0.69605600 | -2.28018100 | 4.21809800 |
| N | -2.53697000 | -1.00434500 | -0.15021900 | H | -1.15706100 | -3.25983400 | 4.06093900 |
| N | 3.32547600 | -0.13584400 | -0.41029800 | H | -1.33353600 | -1.71588400 | 4.90289800 |
| C | -2.86431900 | -2.44971000 | 0.07443600 | H | 0.26171900 | -2.44252400 | 4.72102800 |
| C | -2.26346100 | -2.70013000 | 1.48935400 | C | -1.63055800 | 2.06117000 | 0.88613100 |
| H | -1.42941800 | -3.39996600 | 1.41045800 | C | -1.71314400 | 2.64094800 | 2.15885800 |
| H | -2.99728600 | -3.15370500 | 2.15405500 | H | -1.30688100 | 2.10914600 | 3.01005200 |
| C | -1.72469400 | -1.35175800 | 2.02144500 | C | -2.29670300 | 3.89391600 | 2.33935300 |
| C | -1.38113100 | -0.65607300 | 0.64013700 | H | -2.35133500 | 4.32309200 | 3.33376700 |
| C | -0.88949300 | 0.79105600 | 0.65905900 | C | -2.79653600 | 4.59812800 | 1.24437100 |
| C | 0.43627800 | 0.81112200 | 0.41678600 | H | -3.24905700 | 5.57360500 | 1.38312700 |
| H | 1.03851200 | 1.70374900 | 0.43701100 | C | -2.70323200 | 4.04116200 | -0.02998700 |
| C | 0.93808500 | -0.49302700 | 0.09549500 | H | -3.08307000 | 4.58138800 | -0.89006100 |
| C | 2.17392400 | -0.92647700 | -0.26989700 | C | -2.12609800 | 2.78569200 | -0.20759100 |
| C | 2.49661000 | -2.37790200 | -0.67393300 | H | -2.05923700 | 2.35902200 | -1.19982300 |
| C | 4.03295900 | -2.33782900 | -0.84421900 | C | 1.77215300 | -2.70990900 | -2.01123600 |
| H | 4.37865500 | -2.99382000 | -1.64339600 | H | 0.70617200 | -2.55990400 | -1.85241800 |
| H | 4.51772700 | -2.67064200 | 0.07437700 | H | 2.07220300 | -1.97851900 | -2.76194300 |
| C | 4.42987600 | -0.87314900 | -1.10334500 | C | 1.99145800 | -4.11568900 | -2.58248700 |
| C | -3.10286300 | -0.21561400 | -1.21535800 | H | 1.55399800 | -4.88952200 | -1.94794600 |
| C | -4.34245000 | 0.45730400 | -1.00274800 | H | 3.05133300 | -4.35056800 | -2.71514900 |
| C | -4.86569000 | 1.26833100 | -2.01337200 | H | 1.51498000 | -4.19185700 | -3.56410600 |
| H | -5.79930400 | 1.79076300 | -1.83951500 | C | 2.07703900 | -3.43270100 | 0.38561400 |
| C | -4.21370200 | 1.43772200 | -3.22547300 | H | 0.98615500 | -3.46906600 | 0.40882900 |
| H | -4.63264600 | 2.08133300 | -3.99145700 | H | 2.41868600 | -4.40843700 | 0.02710600 |
| C | -3.02202200 | 0.76605600 | -3.44389200 | C | 2.59913100 | -3.23214400 | 1.80901800 |
| H | -2.51403900 | 0.88498400 | -4.39402000 | H | 2.18196800 | -3.99494100 | 2.47250300 |
| C | -2.45665500 | -0.06616900 | -2.46922600 | H | 2.30974400 | -2.25923100 | 2.20036800 |
| C | -5.16549800 | 0.36399500 | 0.27880500 | H | 3.68778200 | -3.30902300 | 1.86985400 |
| H | -4.65912600 | -0.32900700 | 0.93940200 | C | 4.48482300 | -0.56803500 | -2.61362200 |
| C | -6.58410500 | -0.17833600 | 0.01239300 | H | 3.50775100 | -0.66195000 | -3.08574500 |
| H | -7.09370900 | -0.37314000 | 0.96104500 | H | 5.16930800 | -1.26560800 | -3.10415800 |
| H | -6.56928700 | -1.10570600 | -0.56143200 | H | 4.85350900 | 0.43937600 | -2.79386100 |
| H | -7.18607200 | 0.54718700 | -0.54171100 | C | 5.80349300 | -0.55349200 | -0.50547000 |
| C | -5.27005300 | 1.70752800 | 1.02314100 | H | 6.04441500 | 0.50733000 | -0.60437400 |
| H | -5.78059700 | 2.45992700 | 0.41547000 | H | 6.56655600 | -1.12464900 | -1.04005700 |
| H | -4.29206200 | 2.10271900 | 1.28826700 | H | 5.85471100 | -0.82466500 | 0.54776900 |
| H | -5.84683300 | 1.57424300 | 1.94370300 | C | 3.52492800 | 1.17017600 | 0.15855600 |
| C | -1.15051200 | -0.75411600 | -2.83322500 | C | 3.36243000 | 2.34471000 | -0.61618500 |
| H | -0.83817600 | -1.33829500 | -1.97628900 | C | 3.64435200 | 3.58573000 | -0.03184900 |
| C | -1.31241700 | -1.69937100 | -4.03761400 | H | 3.53428100 | 4.48628600 | -0.62460700 |
| H | -2.13101100 | -2.40751000 | -3.89306600 | C | 4.04427200 | 3.69231800 | 1.29150400 |
| H | -0.39218500 | -2.27129900 | -4.18911800 | H | 4.25314500 | 4.66453500 | 1.72422500 |
| H | -1.51264800 | -1.14230900 | -4.95773700 | C | 4.16193700 | 2.54197000 | 2.05964100 |
| C | -0.04339200 | 0.27312800 | -3.11323600 | H | 4.45654200 | 2.62503200 | 3.09926600 |
| H | -0.29671300 | 0.91779200 | -3.95969000 | C | 3.91326100 | 1.27822500 | 1.51797700 |
| H | 0.89702200 | -0.22937000 | -3.34669300 | C | 2.84593300 | 2.34957300 | -2.04886200 |
| H | 0.11988700 | 0.90103600 | -2.24157900 | H | 2.61141500 | 1.32171600 | -2.32178000 |
| C | -4.36624900 | -2.75344500 | 0.02592600 | C | 1.55340600 | 3.18206000 | -2.18038400 |
| H | -4.92084300 | -2.27400500 | 0.82837000 | H | 0.78176800 | 2.85702700 | -1.48210400 |
| H | -4.50999000 | -3.83206400 | 0.12330800 | H | 1.15019500 | 3.08947300 | -3.19213600 |
| H | -4.79599300 | -2.44407400 | -0.92911400 | H | 1.74707100 | 4.24173100 | -1.99392700 |
| C | -2.19400800 | -3.37695700 | -0.96028000 | C | 3.89587700 | 2.90141200 | -3.03363000 |
| H | -2.59513000 | -3.19458500 | -1.95883900 | H | 4.04958300 | 3.97253000 | -2.87376900 |
| H | -2.39850600 | -4.42055600 | -0.70179700 | H | 3.56041500 | 2.76278900 | -4.06545400 |
| H | -1.11710500 | -3.23183800 | -0.97701500 | H | 4.86491300 | 2.41298600 | -2.92035700 |
| C | -2.76599400 | -0.49167400 | 2.79959500 | C | 4.02446000 | 0.07284300 | 2.43826100 |
| H | -3.22727900 | 0.21829400 | 2.11946500 | H | 3.93486600 | -0.81999100 | 1.82347800 |
| H | -2.21577000 | 0.11763700 | 3.52173200 | C | 2.85868000 | 0.07135700 | 3.44273000 |
| C | -3.88274300 | -1.22437400 | 3.55146800 | H | 2.92215800 | 0.93372500 | 4.11324400 |
| H | -3.49889200 | -1.98864700 | 4.22995300 | H | 2.87486700 | -0.83453600 | 4.05560900 |
| H | -4.58415200 | -1.71327200 | 2.87215100 | H | 1.90286800 | 0.11546700 | 2.92143800 |
| H | -4.45628700 | -0.50787200 | 4.14677400 | C | 5.36990700 | -0.00000700 | 3.18125900 |
| C | -0.47358500 | -1.54668400 | 2.89189300 | H | 6.21717100 | 0.06051500 | 2.49473100 |
| H | -0.04566400 | -0.56090200 | 3.09676300 | H | 5.44128400 | -0.94420900 | 3.72887600 |
| H | 0.26399000 | -2.09192000 | 2.31034700 | H | 5.47240800 | 0.80980700 | 3.90876900 |

**xyz coordinates of optimized structures of c-1$^{\bullet+}$**

(E = -2249.570967)

| | x | y | z | | x | y | z |
|---|---|---|---|---|---|---|---|
| O | 0.22093400 | -1.84515800 | 0.03816600 | C | -0.84001600 | -2.40343900 | 4.17058300 |
| N | -2.69521600 | -1.03692600 | -0.12883200 | H | -1.37529300 | -3.35025600 | 4.05778000 |
| N | 3.36748300 | -0.08760500 | -0.34024500 | H | -1.38528200 | -1.78898500 | 4.88994500 |
| C | -3.21297500 | -2.45488500 | 0.16634600 | H | 0.13703900 | -2.62717400 | 4.60566700 |
| C | -2.61516500 | -2.72127300 | 1.56560900 | C | -1.49507400 | 1.95499500 | 0.76630300 |
| H | -1.84506700 | -3.48830400 | 1.48632800 | C | -1.51967900 | 2.56189100 | 2.02671400 |
| H | -3.37325700 | -3.09319500 | 2.24976700 | H | -1.20268900 | 2.00403400 | 2.89854300 |
| C | -1.94873700 | -1.41801700 | 2.05663500 | C | -1.92812300 | 3.88739100 | 2.16196400 |
| C | -1.79673200 | -0.64748400 | 0.74166200 | H | -1.94207600 | 4.34623600 | 3.14371100 |
| C | -0.94373600 | 0.57066700 | 0.59713000 | C | -2.30518600 | 4.62242500 | 1.03876200 |
| C | 0.37977300 | 0.45441400 | 0.34761600 | H | -2.62015900 | 5.65398700 | 1.14492000 |
| H | 0.96400400 | 1.36088900 | 0.32910600 | C | -2.27109200 | 4.02683500 | -0.22064800 |
| C | 0.99777100 | -0.83485500 | 0.05443500 | H | -2.55829500 | 4.59112800 | -1.10015000 |
| C | 2.38835900 | -1.01879900 | -0.25552000 | C | -1.87011700 | 2.70027800 | -0.35741400 |
| C | 2.92306500 | -2.41165000 | -0.60795300 | H | -1.84854900 | 2.24219800 | -1.33728500 |
| C | 4.44775400 | -2.16961700 | -0.65564700 | C | 2.34469500 | -2.84624000 | -1.98993600 |
| H | 4.93636700 | -2.76492300 | -1.42563400 | H | 1.25700300 | -2.82040100 | -1.91370800 |
| H | 4.89732500 | -2.44911100 | 0.29851200 | H | 2.62648700 | -2.10432500 | -2.73909700 |
| C | 4.66627900 | -0.66848600 | -0.89227600 | C | 2.78131200 | -4.22994400 | -2.48133900 |
| C | -3.14912600 | -0.24191200 | -1.27175500 | H | 2.39867400 | -5.02918900 | -1.84371000 |
| C | -4.29527400 | 0.57219200 | -1.08860500 | H | 3.86908700 | -4.32839500 | -2.52843200 |
| C | -4.70367000 | 1.37291900 | -2.15742300 | H | 2.39297400 | -4.39889100 | -3.48912800 |
| H | -5.56786000 | 2.01333500 | -2.03376900 | C | 2.58187200 | -3.50226300 | 0.44774400 |
| C | -4.02545900 | 1.37247900 | -3.36706800 | H | 1.54407900 | -3.80241900 | 0.30886000 |
| H | -4.36036400 | 2.00560300 | -4.18050300 | H | 3.20513400 | -4.36951700 | 0.20941800 |
| C | -2.91877800 | 0.55469200 | -3.52992300 | C | 2.80265800 | -3.12949800 | 1.91433700 |
| H | -2.39653300 | 0.55377000 | -4.47836400 | H | 2.53105200 | -3.97054800 | 2.55740000 |
| C | -2.45184900 | -0.26807900 | -2.49790700 | H | 2.18790400 | -2.27971200 | 2.21050100 |
| C | -5.12957400 | 0.64198300 | 0.18973600 | H | 3.84525000 | -2.88178800 | 2.13075500 |
| H | -4.72486900 | -0.06946000 | 0.90404300 | C | 4.81687200 | -0.34157300 | -2.38553700 |
| C | -6.59937500 | 0.25483800 | -0.07604400 | H | 3.92497200 | -0.59324200 | -2.95686500 |
| H | -7.13071400 | 0.14855000 | 0.87344300 | H | 5.65256900 | -0.92031700 | -2.78476900 |
| H | -6.68995400 | -0.68257400 | -0.62497500 | H | 5.04200200 | 0.71078400 | -2.53607700 |
| H | -7.10788300 | 1.03016600 | -0.65432700 | C | 5.89282500 | -0.14200700 | -0.14832700 |
| C | -5.08566700 | 2.02702700 | 0.85966900 | H | 5.98861000 | 0.94121800 | -0.24144800 |
| H | -5.47475300 | 2.80074500 | 0.19355700 | H | 6.78074000 | -0.59983200 | -0.58952200 |
| H | -4.07673600 | 2.31102200 | 1.14653800 | H | 5.87055100 | -0.40678900 | 0.90652800 |
| H | -5.70660900 | 2.01553300 | 1.75981600 | C | 3.33867000 | 1.27581600 | 0.16259600 |
| C | -1.21681900 | -1.11273600 | -2.78254600 | C | 3.09563500 | 2.37006100 | -0.69736100 |
| H | -0.95584900 | -1.66303500 | -1.88360000 | C | 3.17250400 | 3.65979500 | -0.15838300 |
| C | -1.46581300 | -2.12170600 | -3.92061800 | H | 2.99487200 | 4.51122300 | -0.80358500 |
| H | -2.36021500 | -2.72318500 | -3.75264200 | C | 3.45141600 | 3.87430400 | 1.18228300 |
| H | -0.61127900 | -2.79843900 | -4.00753000 | H | 3.49921500 | 4.88347000 | 1.57492400 |
| H | -1.58519300 | -1.61083900 | -4.87987500 | C | 3.65303200 | 2.78739400 | 2.02067400 |
| C | -0.01067700 | -0.22779600 | -3.13440700 | H | 3.84828700 | 2.95651400 | 3.07234600 |
| H | -0.19971900 | 0.37902600 | -4.02292500 | C | 3.60993900 | 1.47797700 | 1.53714200 |
| H | 0.86323500 | -0.84796800 | -3.33556300 | C | 2.67945500 | 2.24795000 | -2.15821900 |
| H | 0.23074700 | 0.44272300 | -2.31464300 | H | 2.60653400 | 1.18924700 | -2.40703200 |
| C | -4.73362300 | -2.56147500 | 0.12019800 | C | 1.29257900 | 2.88268700 | -2.38827300 |
| H | -5.22387700 | -2.00273500 | 0.91322000 | H | 0.54309900 | 2.48833700 | -1.70381600 |
| H | -4.99766000 | -3.61293600 | 0.24591500 | H | 0.95534900 | 2.68820300 | -3.40906100 |
| H | -5.12220800 | -2.23256700 | -0.84402900 | H | 1.32867500 | 3.96558000 | -2.24738400 |
| C | -2.61877300 | -3.41561800 | -0.86798700 | C | 3.69495700 | 2.91519100 | -3.10708000 |
| H | -3.01362100 | -3.21735000 | -1.86333600 | H | 3.66851600 | 4.00225400 | -2.99515000 |
| H | -2.90731100 | -4.43119100 | -0.58805000 | H | 3.44989800 | 2.68078600 | -4.14632200 |
| H | -1.53182800 | -3.35612800 | -0.88144400 | H | 4.71920200 | 2.59396000 | -2.91533000 |
| C | -2.87233600 | -0.47601200 | 2.93655600 | C | 3.79488000 | 0.34211000 | 2.53354200 |
| H | -3.30943300 | 0.31326600 | 2.32442100 | H | 3.88347800 | -0.59004200 | 1.97963800 |
| H | -2.21712400 | 0.04227100 | 3.63889300 | C | 2.55146900 | 0.23160900 | 3.43362100 |
| C | -4.00314700 | -1.15285600 | 3.71406900 | H | 2.44540900 | 1.12199100 | 4.05941000 |
| H | -3.64666800 | -1.98045800 | 4.32883500 | H | 2.62412300 | -0.64040100 | 4.08874100 |
| H | -4.78469000 | -1.53681700 | 3.05554600 | H | 1.64648600 | 0.13713800 | 2.83436300 |
| H | -4.46866000 | -0.41819500 | 4.37570400 | C | 5.06176300 | 0.49245100 | 3.39438600 |
| C | -0.64593800 | -1.70057800 | 2.82402200 | H | 5.95433400 | 0.64473800 | 2.78458800 |
| H | -0.12884600 | -0.75339700 | 2.98661300 | H | 5.20741700 | -0.40899700 | 3.99551400 |
| H | -0.00560900 | -2.31145100 | 2.19368200 | H | 4.98070100 | 1.33710500 | 4.08298700 |

Significant computed isotropic hyperfine coupling constants (B3LYP/EPR-II // PCM[ACN]):

$a(^{14}N)$: 13 MHz (exp: 15.0 MHz)

**xyz coordinates of optimized structures of o-1$^{\bullet+}$** (most stable conformer)
(E = -2249.571635)

| | x | y | z | | x | y | z |
|---|---|---|---|---|---|---|---|
| O | 1.36724600 | 0.45703200 | -1.71813500 | C | -4.44175800 | 4.48378400 | 0.06472600 |
| N | -3.33618300 | -0.03901300 | 0.12063500 | H | -5.45843800 | 4.11062200 | -0.07464800 |
| N | 3.21522200 | -0.82872300 | 0.13787700 | H | -4.31790500 | 5.33979900 | -0.60361300 |
| C | -4.79366500 | 0.37988500 | 0.27009400 | H | -4.35541200 | 4.85358300 | 1.08922900 |
| C | -4.62656500 | 1.64092200 | 1.11260900 | C | -0.47341500 | 2.27321700 | -0.62064000 |
| H | -4.64622500 | 1.36320800 | 2.16630200 | C | 0.47720400 | 2.92549400 | 0.17014600 |
| H | -5.44954300 | 2.33233900 | 0.95290500 | H | 0.75323400 | 2.50813900 | 1.13027400 |
| C | -3.24878200 | 2.24814500 | 0.74894100 | C | 1.08047100 | 4.10114200 | -0.26988700 |
| C | -2.49107100 | 1.01720600 | 0.18659900 | H | 1.81626100 | 4.59054400 | 0.35702300 |
| C | -1.10774100 | 0.99276900 | -0.15645600 | C | 0.75530700 | 4.62947600 | -1.51750000 |
| C | -0.25666700 | -0.12629400 | -0.06513800 | H | 1.23000100 | 5.54048300 | -1.86384000 |
| H | -0.54065600 | -0.98179500 | 0.52861500 | C | -0.16650200 | 3.96684100 | -2.32835300 |
| C | 0.99991800 | -0.19390600 | -0.72203200 | H | -0.41090000 | 4.35995000 | -3.30878500 |
| C | 2.07420700 | -1.19700300 | -0.35923800 | C | -0.77408600 | 2.79768700 | -1.88161700 |
| C | 2.05706400 | -2.62871600 | -0.83748300 | H | -1.48426400 | 2.28099600 | -2.51540700 |
| C | 3.50806000 | -3.10223500 | -0.55870400 | C | 0.97618400 | -3.46037400 | -0.10221200 |
| H | 3.52762200 | -4.01723900 | 0.03091200 | H | -0.00106400 | -3.03472600 | -0.33298000 |
| H | 4.01549700 | -3.31763200 | -1.49807300 | H | 0.98335900 | -4.45427100 | -0.55372200 |
| C | 4.25442700 | -1.96556700 | 0.17721200 | C | 1.13686400 | -3.61583700 | 1.40823800 |
| C | -2.98725500 | -1.38845800 | -0.26806600 | H | 0.33338600 | -4.24334700 | 1.79656300 |
| C | -2.77967200 | -1.71491700 | -1.62569600 | H | 1.08344700 | -2.66157700 | 1.93468100 |
| C | -2.49177200 | -3.04846100 | -1.93830000 | H | 2.07893700 | -4.09894700 | 1.67319300 |
| H | -2.32570300 | -3.32419800 | -2.97264600 | C | 1.73674800 | -2.60042900 | -2.36674100 |
| C | -2.41287200 | -4.02417500 | -0.95488700 | H | 0.75694700 | -2.14108300 | -2.50768100 |
| H | -2.18837000 | -5.04982500 | -1.22406700 | H | 2.46014500 | -1.94126000 | -2.85480000 |
| C | -2.59550900 | -3.67803900 | 0.37804000 | C | 1.75004200 | -3.97151200 | -3.04713500 |
| H | -2.50481700 | -4.44069600 | 1.14163000 | H | 1.63808800 | -3.83916700 | -4.12586800 |
| C | -2.87836600 | -2.36222600 | 0.75215800 | H | 0.92766200 | -4.60414300 | -2.70838600 |
| C | -2.84006400 | -0.70527900 | -2.76681700 | H | 2.68584600 | -4.51007700 | -2.87670300 |
| H | -3.10245700 | 0.26568000 | -2.35132900 | C | 5.52706400 | -1.55834100 | -0.55782800 |
| C | -3.91317500 | -1.08877800 | -3.80496100 | H | 5.32956800 | -1.31153400 | -1.59935400 |
| H | -4.04242600 | -0.27789800 | -4.52679100 | H | 6.21347600 | -2.40718800 | -0.53554400 |
| H | -4.88094700 | -1.29276500 | -3.34409200 | H | 6.01613800 | -0.71677900 | -0.06726600 |
| H | -3.61715100 | -1.98315600 | -4.35959200 | C | 4.60053100 | -2.30703200 | 1.62615200 |
| C | -1.48033100 | -0.54181600 | -3.47059800 | H | 5.05599600 | -1.45343800 | 2.12803400 |
| H | -1.15133100 | -1.48523100 | -3.91489100 | H | 5.32783100 | -3.12071400 | 1.61857700 |
| H | -0.70651800 | -0.19218900 | -2.79050300 | H | 3.73307700 | -2.63510300 | 2.19481000 |
| H | -1.57125000 | 0.18946500 | -4.27906300 | C | 3.51245000 | 0.51926100 | 0.63897500 |
| C | -3.02162100 | -2.03630800 | 2.23715800 | C | 3.22102400 | 0.80949700 | 1.98964300 |
| H | -3.36944200 | -1.00839600 | 2.32485700 | C | 3.57323100 | 2.07157600 | 2.47721700 |
| C | -1.67357800 | -2.10953800 | 2.97290500 | H | 3.35487600 | 2.31713200 | 3.50887800 |
| H | -1.28394700 | -3.12889100 | 2.97573800 | C | 4.18540500 | 3.01442400 | 1.66667300 |
| H | -1.79804600 | -1.79213600 | 4.01172200 | H | 4.45549100 | 3.98474500 | 2.06703600 |
| H | -0.92503400 | -1.46237700 | 2.51806700 | C | 4.42745400 | 2.71845700 | 0.33424100 |
| C | -4.03766500 | -2.95422400 | 2.94278200 | H | 4.87225100 | 3.47357100 | -0.30105500 |
| H | -4.98642800 | -3.00532700 | 2.40749600 | C | 4.09042700 | 1.48068600 | -0.22236500 |
| H | -4.23230700 | -2.58578300 | 3.95358200 | C | 2.48897200 | -0.13013400 | 2.94085600 |
| H | -3.65043200 | -3.97235000 | 3.03336300 | H | 2.34092700 | -1.08606500 | 2.44354700 |
| C | -5.39786500 | 0.67841200 | -1.11239300 | C | 1.09597100 | 0.43068500 | 3.27505100 |
| H | -4.81103500 | 1.40040900 | -1.67780300 | H | 0.56338600 | -0.25058900 | 3.94239400 |
| H | -6.39953700 | 1.09052700 | -0.97501000 | H | 0.50094200 | 0.55955900 | 2.37164000 |
| H | -5.48991000 | -0.23465000 | -1.69818800 | H | 1.16831600 | 1.40040200 | 3.77333800 |
| C | -5.67302400 | -0.66604100 | 0.95257700 | C | 3.27397800 | -0.39807600 | 4.23752600 |
| H | -5.62997700 | -1.62658700 | 0.43640300 | H | 4.28924400 | -0.74385000 | 4.04025600 |
| H | -6.70578200 | -0.31370400 | 0.91738000 | H | 2.76121800 | -1.16308100 | 4.82641600 |
| H | -5.41178900 | -0.80904100 | 1.99781400 | H | 3.34036500 | 0.50274200 | 4.85267400 |
| C | -2.53265100 | 2.77321500 | 2.02753600 | C | 4.32587100 | 1.30713900 | -1.72107800 |
| H | -1.59436200 | 3.24151000 | 1.72569000 | H | 3.96341700 | 0.32356600 | -2.01656500 |
| H | -3.15517600 | 3.57166300 | 2.44179400 | C | 3.51776900 | 2.34665400 | -2.52609300 |
| C | -2.24847600 | 1.74235000 | 3.12404400 | H | 3.91762100 | 3.35349900 | -2.37711100 |
| H | -3.16031900 | 1.35442700 | 3.58350500 | H | 2.47057100 | 2.34519700 | -2.23950500 |
| H | -1.65379400 | 2.19796400 | 3.91922700 | H | 3.58999500 | 2.11594500 | -3.59321700 |
| H | -1.68246800 | 0.89310300 | 2.74105100 | C | 5.81516500 | 1.43762200 | -2.10107400 |
| C | -3.37589400 | 3.43041900 | -0.26482400 | H | 5.94483800 | 1.21099000 | -3.16294500 |
| H | -2.41054700 | 3.93001200 | -0.31699700 | H | 6.46260500 | 0.77281700 | -1.53131400 |
| H | -3.56473300 | 3.04271800 | -1.26756900 | H | 6.16601900 | 2.45987500 | -1.93809100 |

Significant computed isotropic hyperfine coupling constants (B3LYP/EPR-II // PCM[ACN]):
*a*($^{14}$N): 10 MHz (exp: 11.4 MHz)
*a*($^{1}$H): 6 MHz (exp: 10.1 MHz)

**xyz coordinates of optimized structures of o-1$^{\bullet+}$** (conformer 2)
(E = -2249.568653)

| | x | y | z | | x | y | z |
|---|---|---|---|---|---|---|---|
| O | 1.54088200 | 1.18659000 | 0.08177200 | H | 5.24572300 | 2.97115800 | -3.40964600 |
| N | 3.77697200 | -0.33560000 | -0.34408000 | H | 6.33103000 | 2.26053700 | -2.20692400 |
| N | -3.53500700 | -0.46793500 | 0.42692000 | C | 5.95851100 | -0.46521400 | -1.62590600 |
| C | 4.11339400 | 0.66572100 | 1.88179200 | H | 5.53826100 | 0.03576800 | -2.49601400 |
| C | 4.11250200 | 0.81836500 | 0.48187400 | H | 6.70583400 | -1.17946000 | -1.97766000 |
| C | -3.74192100 | -0.02695900 | -1.98156900 | H | 6.46227900 | 0.26650500 | -0.99349300 |
| C | 2.62713100 | -2.13711300 | -1.32427700 | C | 1.69858100 | -0.88199200 | -3.41338700 |
| C | -1.11699300 | -0.08419500 | 0.22989400 | H | 1.06040400 | -1.01754800 | -4.28888100 |
| C | 4.89702800 | -1.24206400 | -0.84940800 | H | 2.70228100 | -0.64093400 | -3.77250100 |
| C | -1.14994100 | 2.16140200 | -0.93658200 | H | 1.32391400 | -0.01433600 | -2.86503200 |
| H | -1.26528800 | 1.65722900 | -1.88810800 | C | 4.44764000 | -1.15682100 | 3.64758500 |
| C | -1.17064000 | 1.41614600 | 0.24399600 | H | 5.40544900 | -1.44726100 | 3.21257700 |
| C | 1.37025400 | -0.02721500 | -0.16899500 | H | 3.98515900 | -2.04869600 | 4.07902700 |
| C | 2.56915700 | -0.81411300 | -0.56750300 | H | 4.64630400 | -0.46082500 | 4.46633200 |
| C | -3.93171300 | 0.42926500 | -0.65307600 | C | -1.87018300 | -1.29445100 | -3.11632100 |
| C | 4.58228100 | 1.73767500 | 2.64849400 | H | -1.47709500 | -2.29032300 | -3.33652300 |
| H | 4.59595600 | 1.64921000 | 3.72801600 | H | -1.12578100 | -0.74985400 | -2.53629700 |
| C | -4.51768800 | 1.68862000 | -0.39868600 | H | -1.99970000 | -0.77368100 | -4.06823100 |
| C | -3.20580100 | -1.40272900 | -2.36032600 | C | 2.27619700 | -4.69916800 | -1.00734600 |
| H | -3.02722900 | -1.97334500 | -1.45160700 | H | 1.46864900 | -4.78608800 | -1.73613300 |
| C | -1.03393900 | 2.07395800 | 1.46963200 | H | 2.11288800 | -5.46046400 | -0.24095500 |
| H | -1.04282400 | 1.49914800 | 2.38857500 | H | 3.21508000 | -4.93592600 | -1.51305400 |
| C | 0.09989400 | -0.69643500 | -0.04638400 | C | -2.21460000 | -2.09607500 | 1.53139600 |
| H | 0.10948400 | -1.76207300 | -0.16861100 | C | -4.82358600 | 2.24104600 | 0.98521500 |
| C | 1.68354600 | -2.15084300 | -2.55472300 | H | -4.33506100 | 1.60499100 | 1.72156500 |
| H | 1.97412900 | -3.00511400 | -3.17168600 | C | -5.06221300 | -0.68580400 | 2.46801200 |
| H | 0.66341500 | -2.35129400 | -2.22603600 | H | -4.25822800 | -0.26741000 | 3.07122100 |
| C | -0.94628400 | 3.53703700 | -0.89541200 | H | -5.55396900 | -1.46213000 | 3.05798400 |
| H | -0.92390300 | 4.10461200 | -1.81887200 | H | -5.79568000 | 0.08884400 | 2.27742000 |
| C | -2.26495500 | -0.85640800 | 0.62087100 | C | -4.22037000 | -2.20191200 | -3.20104300 |
| C | 4.11199400 | -2.19567100 | -1.76185000 | H | -4.36398000 | -1.74828600 | -4.18470900 |
| H | 4.20950800 | -1.86694500 | -2.79654400 | H | -5.19653500 | -2.25947100 | -2.71615500 |
| H | 4.51172100 | -3.20656600 | -1.70815000 | H | -3.85285800 | -3.22022500 | -3.35397800 |
| C | 2.30487300 | -3.31546700 | -0.35123100 | C | -1.72715000 | -1.55654300 | 2.92062400 |
| H | 3.04286300 | -3.31510600 | 0.45332800 | H | -0.69733300 | -1.21549300 | 2.78423100 |
| H | 1.34527700 | -3.14427600 | 0.13140300 | H | -2.30134100 | -0.66681900 | 3.18697900 |
| C | 3.50870800 | -0.53688000 | 2.59964600 | C | -6.34760100 | 2.24555100 | 1.23176200 |
| H | 3.28523800 | -1.31114300 | 1.86659100 | H | -6.56560400 | 2.50901100 | 2.27045100 |
| C | 5.57280800 | -1.94386500 | 0.33684700 | H | -6.81258200 | 1.28247800 | 1.01507200 |
| H | 6.05605600 | -1.21597000 | 0.98946700 | H | -6.82850200 | 2.98759300 | 0.58859900 |
| H | 6.34116300 | -2.61437200 | -0.05180800 | C | -3.68275400 | -2.56135900 | 1.50960900 |
| H | 4.87690400 | -2.53630300 | 0.92761300 | H | -3.81100900 | -3.31308200 | 0.73009400 |
| C | 4.45641600 | 2.03392200 | -0.13997600 | H | -3.98575300 | -3.02032600 | 2.44832500 |
| C | -4.86530700 | 2.48650500 | -1.49259700 | C | -5.72581900 | -1.69474500 | 0.27045500 |
| H | -5.31022900 | 3.45690100 | -1.31403600 | H | -6.28194000 | -0.80841000 | -0.03790900 |
| C | -4.09269100 | 0.82581500 | -3.03144200 | H | -6.40351400 | -2.34668900 | 0.82526400 |
| H | -3.94076700 | 0.49594600 | -4.05176000 | H | -5.39693500 | -2.22698400 | -0.62062200 |
| C | 4.91763400 | 3.06875400 | 0.67613400 | C | -1.30140100 | -3.28540500 | 1.13424400 |
| H | 5.18705400 | 4.01659900 | 0.22624100 | H | -0.26415000 | -3.03853400 | 1.36908200 |
| C | 5.00448800 | 2.91936300 | 2.05530400 | H | -1.56102500 | -4.09160200 | 1.82551900 |
| H | 5.36956700 | 3.73528200 | 2.66862000 | C | 3.01690800 | 3.27695100 | -1.78721200 |
| C | -4.54700000 | -1.33990900 | 1.17347800 | H | 2.12752500 | 2.88073700 | -1.30011900 |
| C | 4.21219300 | 2.31506300 | -1.61852500 | H | 2.80544200 | 3.42209300 | -2.85110000 |
| H | 3.93303800 | 1.37944500 | -2.10419300 | H | 3.24504400 | 4.25558300 | -1.35418100 |
| C | -0.80418100 | 3.44690600 | 1.51045200 | C | -4.28063100 | 3.66532700 | 1.19307900 |
| H | -0.66973900 | 3.94198700 | 2.46550700 | H | -4.82707200 | 4.39640600 | 0.59159100 |
| C | -0.74758300 | 4.18077600 | 0.32647100 | H | -3.22823900 | 3.72907400 | 0.93480700 |
| H | -0.56582700 | 5.24909000 | 0.35596000 | H | -4.39661900 | 3.95225200 | 2.24201500 |
| C | -4.64392900 | 2.07568900 | -2.79724500 | C | -1.41184000 | -3.83621300 | -0.28952400 |
| H | -4.90942600 | 2.72091000 | -3.62672000 | H | -1.14531300 | -3.10003600 | -1.04868600 |
| C | 2.16641200 | -0.13545700 | 3.24747400 | H | -2.42005100 | -4.18604400 | -0.51881800 |
| H | 2.32821700 | 0.57736300 | 4.06094400 | H | -0.74000300 | -4.68862900 | -0.40807100 |
| H | 1.67105700 | -1.01692300 | 3.66451200 | C | -1.78057400 | -2.54913100 | 4.08449100 |
| H | 1.49957300 | 0.32925700 | 2.52030000 | H | -2.79524700 | -2.90638600 | 4.27430200 |
| C | 5.44703400 | 2.88581600 | -2.33832300 | H | -1.43219400 | -2.05566900 | 4.99514700 |
| H | 5.68841500 | 3.88667100 | -1.97066700 | H | -1.13994600 | -3.41670800 | 3.91598100 |

**xyz coordinates of optimized structures of o-1$^{\bullet+}$** (conformer 3)
(E = -2249.564979)

| | x | y | z | | x | y | z |
|---|---|---|---|---|---|---|---|
| O | 1.33085600 | 0.56512400 | -1.59769100 | C | -1.58067800 | -3.32365900 | 3.57640800 |
| N | -3.43915200 | -0.54453500 | 0.43430700 | H | -2.60322700 | -3.65971400 | 3.76374900 |
| N | 3.74106000 | -0.21841000 | -0.14640100 | H | -1.14794100 | -3.04131900 | 4.53947100 |
| C | -4.41849200 | -1.47957800 | 1.13005700 | H | -1.00943900 | -4.17311000 | 3.19633100 |
| C | -3.59355800 | -2.76568000 | 1.18234800 | C | -0.98079000 | 1.27361400 | -0.06198400 |
| H | -3.79841000 | -3.35300900 | 0.28506300 | C | -0.35544100 | 1.95389500 | 0.99365200 |
| H | -3.85952100 | -3.38604400 | 2.03636100 | H | -0.04544600 | 1.40055100 | 1.87082600 |
| C | -2.10507200 | -2.36417100 | 1.19106300 | C | -0.09663900 | 3.32053600 | 0.92134800 |
| C | -2.15048500 | -0.97800900 | 0.49115700 | H | 0.40771900 | 3.81310900 | 1.74383100 |
| C | -1.01908900 | -0.23103800 | 0.07862000 | C | -0.47484100 | 4.04010300 | -0.20881400 |
| C | 0.24652200 | -0.84986500 | -0.00655500 | H | -0.27165200 | 5.10279200 | -0.27507700 |
| H | 0.40151300 | -1.81609700 | 0.43911300 | C | -1.10903000 | 3.37785400 | -1.25864600 |
| C | 1.34832200 | -0.31977600 | -0.72308700 | H | -1.40122300 | 3.92369000 | -2.14863900 |
| C | 2.73581000 | -0.91460500 | -0.58221500 | C | -1.34955600 | 2.00895500 | -1.19083400 |
| C | 3.14471700 | -2.22745600 | -1.20830800 | H | -1.80386300 | 1.51619800 | -2.03534000 |
| C | 4.67196900 | -2.27184400 | -0.94767700 | C | 2.40776500 | -3.43703700 | -0.57703400 |
| H | 4.91869200 | -3.05291900 | -0.23059300 | H | 1.36299800 | -3.41172300 | -0.89222100 |
| H | 5.21762000 | -2.49952300 | -1.86180100 | H | 2.83725500 | -4.33332800 | -1.02971800 |
| C | 5.10244900 | -0.89517700 | -0.39783600 | C | 2.49955600 | -3.56556400 | 0.94631000 |
| C | -3.93142600 | 0.45893900 | -0.49176200 | H | 1.98278600 | -4.46910200 | 1.27567500 |
| C | -4.42436800 | 1.69489700 | -0.02687100 | H | 2.04182400 | -2.72132100 | 1.46662600 |
| C | -4.93272900 | 2.59917500 | -0.96438700 | H | 3.53267300 | -3.64133000 | 1.29248700 |
| H | -5.31043900 | 3.55554800 | -0.62396600 | C | 2.80410200 | -2.12355400 | -2.73020400 |
| C | -4.95076700 | 2.30669700 | -2.31947800 | H | 1.73881100 | -1.90325300 | -2.83603100 |
| H | -5.34056900 | 3.02784400 | -3.02883700 | H | 3.33916900 | -1.26234200 | -3.14095200 |
| C | -4.46950300 | 1.08214400 | -2.76156200 | C | 3.14387900 | -3.37402400 | -3.54524100 |
| H | -4.48665500 | 0.85648200 | -3.82091000 | H | 2.97963700 | -3.17015200 | -4.60572000 |
| C | -3.96428000 | 0.13315500 | -1.87014100 | H | 2.51359900 | -4.22188500 | -3.27122700 |
| C | -4.42626100 | 2.11264200 | 1.43552300 | H | 4.18768700 | -3.67404700 | -3.42458200 |
| H | -3.92673900 | 1.33296000 | 2.00832700 | C | 5.89433900 | -0.09160700 | -1.42766700 |
| C | -5.86730300 | 2.27953100 | 1.95822400 | H | 5.34657900 | 0.03502500 | -2.36121700 |
| H | -5.86435100 | 2.43276800 | 3.04093400 | H | 6.81484300 | -0.63633400 | -1.64546000 |
| H | -6.49351800 | 1.41323700 | 1.73558100 | H | 6.16777800 | 0.88389400 | -1.03239500 |
| H | -6.34202300 | 3.15042700 | 1.49796400 | C | 5.91115300 | -1.00208700 | 0.89248700 |
| C | -3.63904900 | 3.41313300 | 1.66926400 | H | 6.09932000 | -0.01940300 | 1.32730900 |
| H | -4.11793400 | 4.26473800 | 1.17868800 | H | 6.87427700 | -1.45390300 | 0.64871100 |
| H | -2.62353000 | 3.33102100 | 1.29207500 | H | 5.42388800 | -1.63585800 | 1.63105100 |
| H | -3.59458300 | 3.63054000 | 2.74058700 | C | 3.61404500 | 1.06464400 | 0.55594200 |
| C | -3.45900800 | -1.18460700 | -2.44515900 | C | 3.43273300 | 1.01461200 | 1.95639300 |
| H | -3.25477100 | -1.85821800 | -1.61748700 | C | 3.35153700 | 2.22535100 | 2.64885300 |
| C | -2.14461100 | -0.99367300 | -3.22664000 | H | 3.20234800 | 2.21140100 | 3.72121500 |
| H | -2.28893700 | -0.29849800 | -4.05833000 | C | 3.45012100 | 3.44032900 | 1.98833500 |
| H | -1.81170300 | -1.94846200 | -3.64179400 | H | 3.38909900 | 4.36898900 | 2.54383200 |
| H | -1.34588000 | -0.60502900 | -2.59301700 | C | 3.60527900 | 3.46265400 | 0.61108200 |
| C | -4.50573000 | -1.87318300 | -3.34097500 | H | 3.65067900 | 4.41684100 | 0.10173100 |
| H | -5.47379300 | -1.95994600 | -2.84311600 | C | 3.67865900 | 2.28864600 | -0.14676200 |
| H | -4.16381500 | -2.87837100 | -3.60200100 | C | 3.27245300 | -0.27319100 | 2.75766900 |
| H | -4.65857600 | -1.32492300 | -4.27394800 | H | 3.45205100 | -1.11999900 | 2.09889400 |
| C | -4.78604500 | -1.00049700 | 2.54733100 | C | 1.83285600 | -0.40823200 | 3.28245900 |
| H | -3.91396800 | -0.69511400 | 3.12260900 | H | 1.70639600 | -1.36034000 | 3.80478000 |
| H | -5.26438100 | -1.82927000 | 3.07394600 | H | 1.11634100 | -0.36728900 | 2.46263600 |
| H | -5.49326700 | -0.17701000 | 2.52654700 | H | 1.59097000 | 0.39667400 | 3.98111900 |
| C | -5.70162600 | -1.65915300 | 0.31880700 | C | 4.27483100 | -0.37329200 | 3.92170600 |
| H | -6.25703900 | -0.72463700 | 0.22617100 | H | 5.30340700 | -0.22886100 | 3.58818300 |
| H | -6.33620100 | -2.38197300 | 0.83621900 | H | 4.20063800 | -1.35905800 | 4.38833400 |
| H | -5.49609100 | -2.04319500 | -0.67899400 | H | 4.06411700 | 0.37281000 | 4.69160200 |
| C | -1.30364900 | -3.52629600 | 0.53026300 | C | 3.77383000 | 2.44401900 | -1.66213600 |
| H | -0.26080000 | -3.48825200 | 0.84601900 | H | 3.75004200 | 1.45347200 | -2.11237100 |
| H | -1.69328400 | -4.44234100 | 0.98428200 | C | 2.56432100 | 3.22132500 | -2.22148700 |
| C | -1.37299300 | -3.67548800 | -0.98851900 | H | 2.58931800 | 4.26759400 | -1.90474300 |
| H | -2.39581500 | -3.82288300 | -1.34102000 | H | 1.62413600 | 2.78395300 | -1.89899700 |
| H | -0.79897200 | -4.55199400 | -1.29922600 | H | 2.59877200 | 3.20698500 | -3.31505000 |
| H | -0.96055700 | -2.80644700 | -1.50173700 | C | 5.06611500 | 3.16947100 | -2.09004300 |
| C | -1.53172400 | -2.12503300 | 2.62464800 | H | 5.15171800 | 3.16107900 | -3.18003500 |
| H | -0.49382500 | -1.80921100 | 2.51459000 | H | 5.96743200 | 2.71808300 | -1.67662700 |
| H | -2.04438000 | -1.27973600 | 3.08642800 | H | 5.04505500 | 4.21400600 | -1.76810200 |

**xyz coordinates of optimized structures of o-1$^{\bullet+}$** (conformer 4)
(E = -2249.570309)

| | x | y | z | | x | y | z |
|---|---|---|---|---|---|---|---|
| O | -1.59196400 | 1.16023400 | 0.61451600 | C | 4.48013500 | 3.45216500 | 2.68308300 |
| N | 3.35565800 | -0.17961300 | 0.41236600 | H | 5.23426700 | 2.74491200 | 3.03343700 |
| N | -3.30710200 | -0.75518900 | -0.29341200 | H | 4.10194800 | 3.98561900 | 3.55871600 |
| C | 4.79239900 | 0.01747700 | 0.89815300 | H | 4.97449000 | 4.18380000 | 2.03929800 |
| C | 5.00805400 | 1.46775600 | 0.49053200 | C | 0.68235300 | 2.48232700 | -0.14752400 |
| H | 5.37914400 | 1.48689200 | -0.53427400 | C | 0.46722700 | 2.93976300 | -1.45011900 |
| H | 5.75514800 | 1.96076000 | 1.10673600 | H | 0.70034500 | 2.29658000 | -2.28957600 |
| C | 3.63053600 | 2.16029900 | 0.55390400 | C | -0.02518700 | 4.22271800 | -1.68494500 |
| C | 2.66622100 | 0.96921600 | 0.27685100 | H | -0.17064800 | 4.56371400 | -2.70342100 |
| C | 1.25233800 | 1.09802900 | 0.03528900 | C | -0.33933300 | 5.05419100 | -0.61423500 |
| C | 0.35410200 | 0.03642700 | -0.11919100 | H | -0.72237200 | 6.05256600 | -0.79184500 |
| H | 0.73451900 | -0.95463700 | -0.29330400 | C | -0.18285900 | 4.58405500 | 0.69120300 |
| C | -1.07849900 | 0.18232300 | 0.02656600 | H | -0.45890800 | 5.21092700 | 1.53153700 |
| C | -2.01049100 | -0.85627300 | -0.50396700 | C | 0.31517100 | 3.30616400 | 0.92012100 |
| C | -1.68344100 | -2.09716600 | -1.32994900 | H | 0.39843300 | 2.93318100 | 1.93188500 |
| C | -3.08096400 | -2.54390500 | -1.82201900 | C | -0.75934500 | -1.80139700 | -2.53932900 |
| H | -3.24205900 | -2.19293600 | -2.84134700 | H | 0.27480300 | -1.74305500 | -2.20115100 |
| H | -3.18467000 | -3.62605900 | -1.83838100 | H | -0.80679800 | -2.67424400 | -3.19628200 |
| C | -4.11975700 | -1.90466800 | -0.89668100 | C | -1.11627800 | -0.54758400 | -3.34345600 |
| C | 2.95563500 | -1.50396500 | -0.00965800 | H | -0.45628100 | -0.45407900 | -4.20758800 |
| C | 2.51594000 | -2.45203000 | 0.93634100 | H | -1.00909900 | 0.36205200 | -2.74742900 |
| C | 2.30308200 | -3.76118100 | 0.49262700 | H | -2.14172100 | -0.57844300 | -3.71929500 |
| H | 1.96758500 | -4.51113800 | 1.19835800 | C | -1.04130600 | -3.15462400 | -0.38092200 |
| C | 2.48974700 | -4.11373700 | -0.83613800 | H | -0.08555000 | -2.77288200 | -0.02648700 |
| H | 2.31562000 | -5.13388800 | -1.15571200 | H | -1.66594500 | -3.26686400 | 0.50860200 |
| C | 2.87597700 | -3.15255900 | -1.76095200 | C | -0.81207200 | -4.53194300 | -1.00779100 |
| H | 2.99513900 | -3.43431900 | -2.79953300 | H | -0.33041700 | -5.18526800 | -0.27744000 |
| C | 3.13216500 | -1.83522100 | -1.37403500 | H | -0.15732700 | -4.47694700 | -1.87825600 |
| C | 2.21448200 | -2.11583000 | 2.39206500 | H | -1.74590900 | -5.00975300 | -1.30977800 |
| H | 2.52282600 | -1.08841100 | 2.57599800 | C | -4.59340700 | -2.84327200 | 0.21968100 |
| C | 2.97773700 | -3.03619300 | 3.36336000 | H | -3.76876800 | -3.24856700 | 0.80348100 |
| H | 2.88360500 | -2.66200000 | 4.38585500 | H | -5.12636900 | -3.67814100 | -0.23870500 |
| H | 4.03935100 | -3.10346300 | 3.11794100 | H | -5.28233800 | -2.32874400 | 0.88870000 |
| H | 2.57091700 | -4.05052300 | 3.34327000 | C | -5.33809300 | -1.40634600 | -1.67336300 |
| C | 0.70533200 | -2.18741700 | 2.69173400 | H | -6.04271900 | -0.87699500 | -1.03128900 |
| H | 0.30718700 | -3.18502500 | 2.49053500 | H | -5.84619600 | -2.28019200 | -2.08657100 |
| H | 0.14119000 | -1.46729600 | 2.09956100 | H | -5.05289000 | -0.76298600 | -2.50299300 |
| H | 0.52992300 | -1.96054800 | 3.74610900 | C | -4.02024500 | 0.24158000 | 0.50014500 |
| C | 3.58592100 | -0.82833000 | -2.42807600 | C | -4.60042400 | 1.33768100 | -0.16540400 |
| H | 3.98239100 | 0.04605200 | -1.91441100 | C | -5.42553900 | 2.18393400 | 0.57913600 |
| C | 2.40756200 | -0.34983100 | -3.29336900 | H | -5.88125100 | 3.03867300 | 0.09478100 |
| H | 1.97336500 | -1.18416200 | -3.84983800 | C | -5.65509500 | 1.96258700 | 1.93131000 |
| H | 2.74899500 | 0.39703900 | -4.01468600 | H | -6.30778000 | 2.62527300 | 2.48803500 |
| H | 1.62121900 | 0.10017700 | -2.68757700 | C | -5.01473600 | 0.91273300 | 2.57571500 |
| C | 4.70621200 | -1.37514600 | -3.33168200 | H | -5.15258400 | 0.78089300 | 3.64206000 |
| H | 5.52974800 | -1.79749700 | -2.75276500 | C | -4.17001500 | 0.03856800 | 1.88457400 |
| H | 5.10244400 | -0.56754500 | -3.95236400 | C | -4.26135300 | 1.71309200 | -1.60336000 |
| H | 4.33648700 | -2.15369100 | -4.00334000 | H | -3.74383300 | 0.87510700 | -2.07095400 |
| C | 4.90693100 | -0.18435600 | 2.41777500 | C | -3.27971400 | 2.90110300 | -1.61124900 |
| H | 4.17041600 | 0.38879000 | 2.97719800 | H | -2.97044400 | 3.12904700 | -2.63531900 |
| H | 5.90056900 | 0.14492200 | 2.72911900 | H | -2.39055200 | 2.68239400 | -1.02285900 |
| H | 4.81221400 | -1.23388600 | 2.68476300 | H | -3.75384100 | 3.79491500 | -1.19467700 |
| C | 5.77605300 | -0.93041100 | 0.21221600 | C | -5.50039900 | 2.03673400 | -2.45542800 |
| H | 5.56218900 | -1.97515400 | 0.44266300 | H | -6.24090400 | 1.23552300 | -2.42388000 |
| H | 6.77599300 | -0.69972800 | 0.58569100 | H | -5.20481700 | 2.18928800 | -3.49689700 |
| H | 5.78701400 | -0.80010300 | -0.86704400 | H | -5.98538000 | 2.95528300 | -2.11568700 |
| C | 3.61084300 | 3.32003000 | -0.48173100 | C | -3.35385100 | -0.97145900 | 2.68371600 |
| H | 2.70820200 | 3.91265000 | -0.34875300 | H | -2.81577500 | -1.61780600 | 1.99017500 |
| H | 4.44549400 | 3.97374600 | -0.20819100 | C | -2.29584000 | -0.22715700 | 3.52539300 |
| C | 3.74994300 | 2.93259500 | -1.95615000 | H | -2.77994000 | 0.41194100 | 4.26906400 |
| H | 4.72566400 | 2.50100600 | -2.18899500 | H | -1.66358600 | 0.39902800 | 2.89549000 |
| H | 3.62969100 | 3.81865100 | -2.58375900 | H | -1.66500200 | -0.94463900 | 4.05532000 |
| H | 2.98680400 | 2.21505200 | -2.25798300 | C | -4.20849800 | -1.87140200 | 3.59270900 |
| C | 3.31404400 | 2.75947200 | 1.96994600 | H | -3.57267200 | -2.61691100 | 4.07767200 |
| H | 2.51767100 | 3.48787400 | 1.83627500 | H | -4.98584000 | -2.39857500 | 3.03793800 |
| H | 2.90124100 | 1.98758800 | 2.62375200 | H | -4.69365600 | -1.29076800 | 4.38128800 |

**xyz coordinates of optimized structures of $^{1}$o-1** (most stable conformer)
(E = -2249.715027)

| | x | y | z |
|---|---|---|---|
| O | -1.55190000 | 1.09637700 | 0.76399800 |
| N | 3.31023100 | -0.24481500 | 0.51214100 |
| N | -3.28612500 | -0.71102100 | -0.30605800 |
| C | 4.70041900 | -0.06555000 | 1.06365900 |
| C | 4.97216700 | 1.38288700 | 0.66375900 |
| H | 5.37835900 | 1.38433600 | -0.34879900 |
| H | 5.71384900 | 1.85990900 | 1.30177100 |
| C | 3.61323500 | 2.11338500 | 0.67153600 |
| C | 2.62167200 | 0.95704700 | 0.33604800 |
| C | 1.27697200 | 1.09945600 | 0.03540400 |
| C | 0.32616500 | 0.03826200 | -0.24008300 |
| H | 0.68292900 | -0.88544500 | -0.65904600 |
| C | -1.04722100 | 0.16960100 | 0.04314100 |
| C | -1.97674300 | -0.80593800 | -0.54925600 |
| C | -1.70068300 | -2.01290700 | -1.45610800 |
| C | -3.11898700 | -2.40272900 | -1.93614700 |
| H | -3.29874500 | -1.98249400 | -2.92659200 |
| H | -3.24404900 | -3.48042300 | -2.02301000 |
| C | -4.12258900 | -1.80332600 | -0.94824000 |
| C | 2.93654400 | -1.52249300 | -0.02541100 |
| C | 2.46227000 | -2.53972900 | 0.83173600 |
| C | 2.25097200 | -3.81694700 | 0.30317600 |
| H | 1.89041200 | -4.60679600 | 0.95182800 |
| C | 2.45935400 | -4.08443100 | -1.04237700 |
| H | 2.27907600 | -5.07838400 | -1.43463200 |
| C | 2.87288600 | -3.06407600 | -1.88891600 |
| H | 3.01095700 | -3.27232500 | -2.94340600 |
| C | 3.13317100 | -1.77935000 | -1.40433500 |
| C | 2.12298500 | -2.28934400 | 2.29435300 |
| H | 2.42491800 | -1.27084900 | 2.53064000 |
| C | 2.86549100 | -3.25470200 | 3.23615800 |
| H | 2.72642700 | -2.94998200 | 4.27724100 |
| H | 3.93759500 | -3.28534800 | 3.02893800 |
| H | 2.48199900 | -4.27414300 | 3.13612700 |
| C | 0.60623800 | -2.37548800 | 2.54306000 |
| H | 0.21900100 | -3.36812800 | 2.29600100 |
| H | 0.06474400 | -1.64020700 | 1.94681700 |
| H | 0.39323500 | -2.18487100 | 3.59833100 |
| C | 3.61413600 | -0.71211800 | -2.38030100 |
| H | 3.95637900 | 0.13868400 | -1.79524300 |
| C | 2.46522200 | -0.22005200 | -3.27734300 |
| H | 2.08019600 | -1.03477900 | -3.89718500 |
| H | 2.81565600 | 0.57374800 | -3.94336400 |
| H | 1.64204800 | 0.17170500 | -2.68113400 |
| C | 4.79318700 | -1.18374400 | -3.25030300 |
| H | 5.60409500 | -1.60039600 | -2.64894600 |
| H | 5.19104800 | -0.34085500 | -3.82237200 |
| H | 4.48352500 | -1.94946400 | -3.96666300 |
| C | 4.76862700 | -0.25791200 | 2.59225400 |
| H | 4.00132700 | 0.30900000 | 3.11644400 |
| H | 5.74502000 | 0.07876700 | 2.95109400 |
| H | 4.66534700 | -1.30716600 | 2.86206200 |
| C | 5.71560800 | -1.02018400 | 0.42682900 |
| H | 5.48497100 | -2.06361300 | 0.65098500 |
| H | 6.70482200 | -0.79646600 | 0.83382400 |
| H | 5.76170500 | -0.89943600 | -0.65362200 |
| C | 3.67712400 | 3.29939900 | -0.33179600 |
| H | 2.77412800 | 3.90087800 | -0.23614700 |
| H | 4.50372800 | 3.93809300 | 0.00022500 |
| C | 3.88656000 | 2.95698700 | -1.80809000 |
| H | 4.85387800 | 2.48600600 | -1.99889300 |
| H | 3.84488000 | 3.86828600 | -2.41096600 |
| H | 3.10855100 | 2.28635800 | -2.16954300 |
| C | 3.26232100 | 2.70440800 | 2.08086300 |
| H | 2.46532600 | 3.43079200 | 1.93127500 |
| H | 2.83068200 | 1.92391100 | 2.71081100 |
| C | 4.40227400 | 3.39125500 | 2.84247300 |
| H | 5.14404100 | 2.67826700 | 3.20885500 |
| H | 3.99932000 | 3.91725500 | 3.71250600 |
| H | 4.92192200 | 4.12849500 | 2.22473100 |
| C | 0.71138600 | 2.48110600 | -0.19139900 |
| C | 0.55585900 | 2.93281700 | -1.50612100 |
| H | 0.82261000 | 2.27585200 | -2.32459900 |
| C | 0.08738400 | 4.21704000 | -1.78264000 |
| H | -0.00310900 | 4.54768200 | -2.81184600 |
| C | -0.26843000 | 5.06756100 | -0.73948700 |
| H | -0.63204400 | 6.06813000 | -0.94690500 |
| C | -0.17807500 | 4.60927900 | 0.57640800 |
| H | -0.48707000 | 5.24911400 | 1.39637600 |
| C | 0.29266100 | 3.32677400 | 0.84141500 |
| H | 0.32837000 | 2.96494400 | 1.85950400 |
| C | -0.81306600 | -1.71271300 | -2.69356200 |
| H | 0.23706700 | -1.72568000 | -2.40415900 |
| H | -0.94236300 | -2.55091700 | -3.38619100 |
| C | -1.12792300 | -0.40638400 | -3.42681600 |
| H | -0.50251500 | -0.31296800 | -4.31782500 |
| H | -0.93631000 | 0.45694200 | -2.78739000 |
| H | -2.17125900 | -0.35941300 | -3.75117200 |
| C | -1.05999900 | -3.13041800 | -0.58116900 |
| H | -0.09524800 | -2.77290100 | -0.22787300 |
| H | -1.66908600 | -3.27528500 | 0.31512800 |
| C | -0.86271500 | -4.48020200 | -1.27539700 |
| H | -0.38320800 | -5.17819400 | -0.58522300 |
| H | -0.21530600 | -4.39424900 | -2.14950900 |
| H | -1.80818800 | -4.92706800 | -1.59119300 |
| C | -4.58974000 | -2.81308200 | 0.10945600 |
| H | -3.75740800 | -3.25814200 | 0.65247300 |
| H | -5.13778200 | -3.61440700 | -0.39053600 |
| H | -5.26157400 | -2.33840500 | 0.82419900 |
| C | -5.35391000 | -1.25589700 | -1.67519800 |
| H | -6.04271000 | -0.75557900 | -0.99343400 |
| H | -5.87854100 | -2.09898300 | -2.13089700 |
| H | -5.07623200 | -0.56617900 | -2.46998400 |
| C | -3.97423900 | 0.24990600 | 0.54411000 |
| C | -4.55392600 | 1.38192900 | -0.06057700 |
| C | -5.39556900 | 2.18298300 | 0.71507600 |
| H | -5.84460400 | 3.06460800 | 0.27321400 |
| C | -5.65124500 | 1.88221400 | 2.04796100 |
| H | -6.31737300 | 2.50865900 | 2.63095900 |
| C | -5.01833700 | 0.79562400 | 2.63895700 |
| H | -5.17316800 | 0.60081000 | 3.69380400 |
| C | -4.15862500 | -0.03296500 | 1.91126800 |
| C | -4.18067900 | 1.83537100 | -1.46594900 |
| H | -3.67790200 | 1.00849400 | -1.96862200 |
| C | -3.16047800 | 2.98614800 | -1.37814700 |
| H | -2.82039700 | 3.27266100 | -2.37760600 |
| H | -2.29658800 | 2.68906000 | -0.78436000 |
| H | -3.61606600 | 3.86629700 | -0.91269300 |
| C | -5.39089600 | 2.24645500 | -2.32034900 |
| H | -6.15504800 | 1.46691900 | -2.35080300 |
| H | -5.07029400 | 2.45254100 | -3.34554700 |
| H | -5.85783200 | 3.15756000 | -1.93655100 |
| C | -3.34287500 | -1.08031800 | 2.66045700 |
| H | -2.79730200 | -1.67984300 | 1.93132200 |
| C | -2.28944600 | -0.37112600 | 3.53688500 |
| H | -2.77789200 | 0.23869700 | 4.30339100 |
| H | -1.66486500 | 0.27279300 | 2.91714800 |
| H | -1.66054900 | -1.10851200 | 4.04233900 |
| C | -4.19215900 | -2.03077900 | 3.52099100 |
| H | -3.55216400 | -2.79481500 | 3.97156600 |
| H | -4.96460700 | -2.53682000 | 2.93974100 |
| H | -4.68431600 | -1.49441400 | 4.33675200 |

**xyz coordinates of optimized structures of $^{1}$o-1** (conformer 2)
(E = -2249.708697)

| | x | y | z | | x | y | z |
|---|---|---|---|---|---|---|---|
| O | 1.59135700 | 1.11341200 | 0.55259200 | H | 5.08827500 | 3.59052000 | -2.89290300 |
| N | 3.81488200 | -0.22121500 | -0.38010700 | H | 6.26275000 | 2.74177100 | -1.87652300 |
| N | -3.50667200 | -0.47198000 | 0.58562600 | C | 5.97789600 | -0.11139300 | -1.69797200 |
| C | 4.28964400 | 0.37335100 | 1.96699300 | H | 5.54926300 | 0.53877900 | -2.45836200 |
| C | 4.18433900 | 0.76800500 | 0.61905200 | H | 6.72067300 | -0.75033300 | -2.18094900 |
| C | -3.98008800 | 0.00345200 | -1.79346200 | H | 6.48924900 | 0.49921200 | -0.95260400 |
| C | 2.64246200 | -1.81525300 | -1.65673400 | C | 1.68613800 | -0.19638600 | -3.46592300 |
| C | -1.10872200 | -0.09266900 | 0.13777000 | H | 1.05394200 | -0.16816500 | -4.35711100 |
| C | 4.91867100 | -1.01226100 | -1.05939200 | H | 2.68462700 | 0.13709800 | -3.76163000 |
| C | -1.08249400 | 2.01481400 | -1.25759000 | H | 1.28956400 | 0.52622000 | -2.75048800 |
| H | -1.00181000 | 1.40335100 | -2.14707400 | C | 4.68799400 | -1.72524700 | 3.38279400 |
| C | -1.22125600 | 1.39438700 | -0.01181200 | H | 5.62544800 | -1.93895800 | 2.86579000 |
| C | 1.41144800 | 0.00696100 | -0.05787200 | H | 4.23699300 | -2.67781500 | 3.67518700 |
| C | 2.58440600 | -0.66087500 | -0.64797900 | H | 4.92636100 | -1.18085900 | 4.30040600 |
| C | -4.05607100 | 0.39814500 | -0.43183100 | C | -2.16243100 | -1.17669800 | -3.11192700 |
| C | 4.82246500 | 1.29336600 | 2.87591200 | H | -1.80177600 | -2.15169800 | -3.45189500 |
| H | 4.90915200 | 1.01693100 | 3.92020600 | H | -1.36701900 | -0.69906700 | -2.54128400 |
| C | -4.69507400 | 1.61888700 | -0.09679200 | H | -2.36035900 | -0.57024200 | -3.99999300 |
| C | -3.43111400 | -1.33962500 | -2.25782200 | C | 2.29734300 | -4.39540900 | -1.84984500 |
| H | -3.16563300 | -1.91550500 | -1.37636100 | H | 1.46646700 | -4.34537800 | -2.55619100 |
| C | -1.31790500 | 2.20267900 | 1.12429200 | H | 2.16204700 | -5.29613300 | -1.24572300 |
| H | -1.41211800 | 1.73126300 | 2.09589700 | H | 3.21999800 | -4.51794200 | -2.42257100 |
| C | 0.17931800 | -0.65382300 | -0.19479200 | C | -2.01897400 | -2.19683500 | 1.34988000 |
| H | 0.18796800 | -1.64750000 | -0.59893500 | C | -4.92743500 | 2.09864000 | 1.33011000 |
| C | 1.70205000 | -1.61015700 | -2.87700100 | H | -4.27985600 | 1.51361300 | 1.98315300 |
| H | 2.02047700 | -2.31708300 | -3.64969700 | C | -4.69821700 | -0.91677300 | 2.79604600 |
| H | 0.68491400 | -1.89252300 | -2.60490800 | H | -3.81211000 | -0.53049000 | 3.29697100 |
| C | -1.02575800 | 3.40238700 | -1.36585000 | H | -5.08437000 | -1.75094300 | 3.38791500 |
| H | -0.91706400 | 3.86303900 | -2.34213300 | H | -5.45619500 | -0.14024600 | 2.79877900 |
| C | -2.16429600 | -0.86873200 | 0.57151900 | C | -4.48714900 | -2.15144500 | -3.03292100 |
| C | 4.11992400 | -1.77596200 | -2.12292200 | H | -4.71875900 | -1.68985800 | -3.99659700 |
| H | 4.19471000 | -1.24673300 | -3.07361400 | H | -5.42148300 | -2.23958500 | -2.47432500 |
| H | 4.52645700 | -2.77434700 | -2.28033200 | H | -4.11061200 | -3.15961600 | -3.22943900 |
| C | 2.33826600 | -3.16556300 | -0.93737200 | C | -1.38029800 | -1.79788600 | 2.72276500 |
| H | 3.08903900 | -3.32034600 | -0.15904000 | H | -0.37220700 | -1.43982500 | 2.49929600 |
| H | 1.38697500 | -3.08975500 | -0.41676800 | H | -1.91218300 | -0.93601100 | 3.12868600 |
| C | 3.71118700 | -0.93408300 | 2.49782000 | C | -6.40316600 | 1.88832100 | 1.73554700 |
| H | 3.44607200 | -1.56714100 | 1.65154400 | H | -6.55178300 | 2.14070000 | 2.78991300 |
| C | 5.61622400 | -1.93551100 | -0.04904700 | H | -6.74569900 | 0.86584100 | 1.57900000 |
| H | 6.10890900 | -1.35102800 | 0.72853300 | H | -7.04763400 | 2.54134500 | 1.13973300 |
| H | 6.37721300 | -2.51739800 | -0.57294100 | C | -3.47918500 | -2.66874400 | 1.45387300 |
| H | 4.92588900 | -2.63062800 | 0.42506400 | H | -3.70629500 | -3.31556600 | 0.60421200 |
| C | 4.51256500 | 2.07162000 | 0.19972700 | H | -3.67055800 | -3.25037900 | 2.35540200 |
| C | -5.19109600 | 2.42726800 | -1.12581300 | C | -5.68000400 | -1.74102300 | 0.63801000 |
| H | -5.68065900 | 3.35963700 | -0.87250500 | H | -6.29472100 | -0.85313400 | 0.48906300 |
| C | -4.46787800 | 0.86306200 | -2.78079000 | H | -6.25517400 | -2.45802000 | 1.22898500 |
| H | -4.39424800 | 0.56801400 | -3.82116500 | H | -5.48180500 | -2.18467800 | -0.33756000 |
| C | 5.03582400 | 2.95161400 | 1.14951600 | C | -1.15659000 | -3.34841700 | 0.76622100 |
| H | 5.28711600 | 3.96341300 | 0.85380200 | H | -0.10246300 | -3.11173400 | 0.92267000 |
| C | 5.21363200 | 2.56385900 | 2.47303400 | H | -1.35388300 | -4.21944700 | 1.39956700 |
| H | 5.62838000 | 3.26008200 | 3.19363300 | C | 2.93025300 | 3.49203700 | -1.13084100 |
| C | -4.37542200 | -1.42212000 | 1.37343400 | H | 2.09967900 | 2.94462300 | -0.68583800 |
| C | 4.18068300 | 2.59219700 | -1.19391100 | H | 2.65142200 | 3.82020500 | -2.13752000 |
| H | 3.91989800 | 1.73853700 | -1.82022200 | H | 3.12924500 | 4.38453600 | -0.52862300 |
| C | -1.22760100 | 3.58808300 | 1.02631500 | C | -4.58594600 | 3.58570400 | 1.54236000 |
| H | -1.27067300 | 4.19565000 | 1.92395100 | H | -5.33133400 | 4.23840100 | 1.07956600 |
| C | -1.08346900 | 4.19655900 | -0.22115000 | H | -3.61220800 | 3.83528200 | 1.13045000 |
| H | -1.01655900 | 5.27619900 | -0.29892000 | H | -4.57723300 | 3.81234700 | 2.61263200 |
| C | -5.06568900 | 2.07269200 | -2.45996200 | C | -1.37763700 | -3.76779200 | -0.68712900 |
| H | -5.44344600 | 2.72432100 | -3.24011800 | H | -1.13894700 | -2.96772600 | -1.38600800 |
| C | 2.40144500 | -0.64516800 | 3.26087800 | H | -2.40821500 | -4.07573600 | -0.87804800 |
| H | 2.60498300 | -0.07045600 | 4.16986500 | H | -0.73574800 | -4.61900700 | -0.92877000 |
| H | 1.91963500 | -1.58253900 | 3.55490900 | C | -1.30667500 | -2.88774800 | 3.79626700 |
| H | 1.71824800 | -0.07131100 | 2.63392000 | H | -2.29536700 | -3.27058200 | 4.06303800 |
| C | 5.34833400 | 3.33789800 | -1.86093600 | H | -0.85982200 | -2.47760700 | 4.70632400 |
| H | 5.56924300 | 4.27490500 | -1.34240900 | H | -0.69082200 | -3.73405800 | 3.48418200 |

**xyz coordinates of optimized structures of $^{1}$o-1** (conformer 3)
(E = -2249.706454)

| | x | y | z | | x | y | z |
|---|---|---|---|---|---|---|---|
| O | 1.31792400 | 0.52784600 | -1.78519000 | C | -5.10902800 | 3.81891500 | -0.75428700 |
| N | -3.25822600 | -0.14048800 | 0.39349400 | H | -5.99737300 | 3.18430800 | -0.71313400 |
| N | 3.19459800 | -0.79457700 | 0.00209400 | H | -5.19494200 | 4.43932300 | -1.65107400 |
| C | -4.70832000 | 0.17071300 | 0.63792300 | H | -5.13425100 | 4.48728900 | 0.11068800 |
| C | -4.59856200 | 1.58620700 | 1.19364100 | C | -0.46930200 | 2.37560700 | -0.39380100 |
| H | -4.40165700 | 1.51279800 | 2.26434600 | C | 0.47993300 | 2.91963300 | 0.48267600 |
| H | -5.52678600 | 2.14360300 | 1.07861900 | H | 0.73475100 | 2.38245200 | 1.38623800 |
| C | -3.39281500 | 2.25387300 | 0.49941200 | C | 1.10300400 | 4.13389700 | 0.21305800 |
| C | -2.48018100 | 1.03341800 | 0.20523300 | H | 1.83072800 | 4.52815900 | 0.91348200 |
| C | -1.14110500 | 1.06979000 | -0.07838300 | C | 0.80892300 | 4.82902100 | -0.96034900 |
| C | -0.20609900 | -0.06244700 | -0.00634800 | H | 1.29661600 | 5.77368300 | -1.17581100 |
| H | -0.37744300 | -0.84504500 | 0.71782500 | C | -0.08904300 | 4.27528400 | -1.87122900 |
| C | 0.93865000 | -0.13508900 | -0.75402800 | H | -0.29867200 | 4.78432700 | -2.80658800 |
| C | 2.04080400 | -1.12626300 | -0.51834800 | C | -0.70968100 | 3.05837000 | -1.59184900 |
| C | 2.05631800 | -2.51298100 | -1.12792100 | H | -1.37967700 | 2.61485600 | -2.31719400 |
| C | 3.53684800 | -2.94551000 | -0.97685300 | C | 1.03498900 | -3.43305300 | -0.40719800 |
| H | 3.63747500 | -3.94155100 | -0.54902600 | H | 0.06638500 | -2.93120000 | -0.42340200 |
| H | 4.01341900 | -2.97100200 | -1.95672000 | H | 0.91929100 | -4.32915800 | -1.01974700 |
| C | 4.25376000 | -1.89468000 | -0.09795800 | C | 1.36880400 | -3.87793200 | 1.01497700 |
| C | -2.90462400 | -1.44067100 | -0.11252800 | H | 0.57637200 | -4.53061700 | 1.38495900 |
| C | -2.80057000 | -1.68572100 | -1.50519400 | H | 1.44384500 | -3.03921100 | 1.70816400 |
| C | -2.52636300 | -2.98730100 | -1.93976400 | H | 2.30169900 | -4.44318900 | 1.06126600 |
| H | -2.43765100 | -3.18135900 | -3.00272200 | C | 1.64195700 | -2.38270400 | -2.62541500 |
| C | -2.37210500 | -4.03701700 | -1.04493600 | H | 0.62186200 | -1.99808300 | -2.66042100 |
| H | -2.16959700 | -5.03909800 | -1.40695200 | H | 2.27030500 | -1.61581500 | -3.08341200 |
| C | -2.44626300 | -3.78572900 | 0.31834000 | C | 1.73214200 | -3.67781900 | -3.43786500 |
| H | -2.28708300 | -4.59871500 | 1.01758900 | H | 1.51893900 | -3.46258400 | -4.48820300 |
| C | -2.69004100 | -2.49914900 | 0.80851000 | H | 1.00926700 | -4.42639600 | -3.10709300 |
| C | -2.96126400 | -0.60311400 | -2.56801500 | H | 2.72760600 | -4.12790600 | -3.39137800 |
| H | -3.23463400 | 0.31938500 | -2.06379700 | C | 5.52985400 | -1.39387000 | -0.76976300 |
| C | -4.06750600 | -0.94164100 | -3.58607100 | H | 5.33896600 | -1.04471600 | -1.78268600 |
| H | -4.24036000 | -0.08612200 | -4.24616500 | H | 6.23420600 | -2.22690100 | -0.82528300 |
| H | -5.01270000 | -1.19145800 | -3.10254400 | H | 5.99623200 | -0.59559700 | -0.19200100 |
| H | -3.78016100 | -1.78856800 | -4.21595000 | C | 4.60556500 | -2.40188500 | 1.30174600 |
| C | -1.64341200 | -0.33022000 | -3.31455700 | H | 5.07795600 | -1.61227800 | 1.88708000 |
| H | -1.31698400 | -1.21837800 | -3.86530500 | H | 5.31884700 | -3.22285000 | 1.20502600 |
| H | -0.84529900 | -0.02944300 | -2.63908100 | H | 3.73608300 | -2.76907100 | 1.84080800 |
| H | -1.79277400 | 0.47219300 | -4.04498000 | C | 3.48460200 | 0.48697900 | 0.64491200 |
| C | -2.64665200 | -2.29021000 | 2.32131600 | C | 3.19558000 | 0.64750000 | 2.01826000 |
| H | -2.91511300 | -1.25238500 | 2.51252800 | C | 3.59528900 | 1.83630000 | 2.63780700 |
| C | -1.22945100 | -2.50162800 | 2.87998800 | H | 3.38634500 | 1.97775600 | 3.69103100 |
| H | -0.91595600 | -3.54119200 | 2.76874300 | C | 4.23839300 | 2.84090200 | 1.93192200 |
| H | -1.20623100 | -2.25638600 | 3.94592800 | H | 4.54407600 | 3.75162100 | 2.43460800 |
| H | -0.49825700 | -1.87276000 | 2.37598000 | C | 4.45597700 | 2.68736100 | 0.57167800 |
| C | -3.61376100 | -3.21381800 | 3.08693300 | H | 4.91024600 | 3.49711200 | 0.01447600 |
| H | -4.63181900 | -3.16624000 | 2.70223900 | C | 4.07722000 | 1.52641300 | -0.10955300 |
| H | -3.63690700 | -2.93707900 | 4.14522300 | C | 2.41955800 | -0.35405700 | 2.86818500 |
| H | -3.28505200 | -4.25539800 | 3.02868500 | H | 2.18064200 | -1.21972100 | 2.25215000 |
| C | -5.56407500 | 0.10097100 | -0.64323400 | C | 1.08400200 | 0.25602500 | 3.33642100 |
| H | -5.21313000 | 0.76902600 | -1.42503500 | H | 0.54522700 | -0.45795500 | 3.96273400 |
| H | -6.59575100 | 0.37308100 | -0.40583300 | H | 0.45345300 | 0.50918500 | 2.48489500 |
| H | -5.56728800 | -0.91670700 | -1.03688200 | H | 1.25005700 | 1.15892200 | 3.92951700 |
| C | -5.37868500 | -0.75402400 | 1.65819600 | C | 3.21882500 | -0.84174900 | 4.09117000 |
| H | -5.40376500 | -1.78438200 | 1.30083500 | H | 4.19566500 | -1.24026300 | 3.81729700 |
| H | -6.41169400 | -0.42665900 | 1.80186500 | H | 2.66259000 | -1.62919200 | 4.60737600 |
| H | -4.88150800 | -0.72479700 | 2.62630200 | H | 3.37794600 | -0.02829200 | 4.80391000 |
| C | -2.77312600 | 3.30138700 | 1.46822000 | C | 4.26427000 | 1.51925000 | -1.62515300 |
| H | -2.01965800 | 3.87889700 | 0.93171900 | H | 3.90190000 | 0.56771200 | -2.01145800 |
| H | -3.56957300 | 4.00752200 | 1.73140700 | C | 3.39934500 | 2.61833200 | -2.27512200 |
| C | -2.14613500 | 2.75514600 | 2.75466100 | H | 3.75249200 | 3.61418600 | -1.99230300 |
| H | -2.88341100 | 2.29117700 | 3.41499200 | H | 2.35850900 | 2.51277800 | -1.98170800 |
| H | -1.67000000 | 3.56421700 | 3.31589100 | H | 3.46791600 | 2.53763800 | -3.36520100 |
| H | -1.38459000 | 2.00848000 | 2.52718000 | C | 5.73406300 | 1.72312200 | -2.04485300 |
| C | -3.81135700 | 3.00324900 | -0.81127400 | H | 5.82842400 | 1.60214500 | -3.12795400 |
| H | -2.99585000 | 3.67797100 | -1.06864700 | H | 6.41727600 | 1.02261300 | -1.56560900 |
| H | -3.87508700 | 2.29595300 | -1.64042700 | H | 6.07218900 | 2.73372700 | -1.79946800 |

**xyz coordinates of optimized structures of $^{3}$o-1** (most stable conformer )
(E = -2249.697218)

| | x | y | z | | x | y | z |
|---|---|---|---|---|---|---|---|
| O | -1.58042700 | 1.10881500 | 0.80635600 | C | 4.42469200 | 3.36247600 | 2.88933000 |
| N | 3.33513400 | -0.26186100 | 0.53637500 | H | 5.15424800 | 2.63897900 | 3.25925300 |
| N | -3.37566400 | -0.68442400 | -0.34933200 | H | 4.01852500 | 3.88825200 | 3.75801400 |
| C | 4.72249500 | -0.08030000 | 1.10170400 | H | 4.95930200 | 4.09717800 | 2.28139900 |
| C | 5.00118800 | 1.36775400 | 0.69933900 | C | 0.72510900 | 2.46972800 | -0.14338500 |
| H | 5.41078100 | 1.36673500 | -0.31190800 | C | 0.58521900 | 2.93483200 | -1.45387700 |
| H | 5.74254000 | 1.84211500 | 1.33961300 | H | 0.86852700 | 2.29361300 | -2.27825800 |
| C | 3.64446100 | 2.10295500 | 0.70096200 | C | 0.10375600 | 4.21705600 | -1.71764600 |
| C | 2.66237500 | 0.94929800 | 0.35564200 | H | 0.01694700 | 4.55837100 | -2.74340500 |
| C | 1.27558200 | 1.08452000 | 0.09315800 | C | -0.26909400 | 5.05105600 | -0.66725200 |
| C | 0.35890000 | 0.02808100 | -0.01483200 | H | -0.64342800 | 6.04912500 | -0.86633200 |
| H | 0.73173200 | -0.97938200 | -0.06800700 | C | -0.18069900 | 4.58099400 | 0.64412500 |
| C | -1.11209400 | 0.18539400 | 0.08562400 | H | -0.49864000 | 5.20958500 | 1.46896900 |
| C | -2.01508800 | -0.73263200 | -0.56321700 | C | 0.30138100 | 3.30060200 | 0.89871300 |
| C | -1.68743200 | -1.87379300 | -1.52171800 | H | 0.33715100 | 2.93002600 | 1.91382600 |
| C | -3.07938400 | -2.21629700 | -2.10609200 | C | -0.71566200 | -1.47443900 | -2.66151600 |
| H | -3.22372600 | -1.67454900 | -3.04188000 | H | 0.30369100 | -1.46332000 | -2.27399800 |
| H | -3.19097700 | -3.27573400 | -2.33274900 | H | -0.74425900 | -2.26998700 | -3.41327700 |
| C | -4.13469600 | -1.74590300 | -1.09528600 | C | -1.01431000 | -0.13313900 | -3.33689400 |
| C | 2.98205000 | -1.53022600 | -0.04599200 | H | -0.31587800 | 0.04228300 | -4.15891400 |
| C | 2.50381600 | -2.57770100 | 0.77353700 | H | -0.91706000 | 0.69431800 | -2.63173800 |
| C | 2.27335300 | -3.82954400 | 0.19490300 | H | -2.02532500 | -0.09689500 | -3.75179700 |
| H | 1.90607600 | -4.64001200 | 0.81363900 | C | -1.09460500 | -3.06795500 | -0.71417700 |
| C | 2.47261500 | -4.04612900 | -1.16103100 | H | -0.13649200 | -2.75610200 | -0.30063900 |
| H | 2.27364400 | -5.01995200 | -1.59255200 | H | -1.73711100 | -3.26724200 | 0.14689200 |
| C | 2.90629500 | -3.00087600 | -1.96485800 | C | -0.88205400 | -4.37087000 | -1.49055100 |
| H | 3.04466800 | -3.17011700 | -3.02626300 | H | -0.42350400 | -5.11792100 | -0.83771900 |
| C | 3.18473000 | -1.73960200 | -1.43104100 | H | -0.21166200 | -4.23129600 | -2.34047500 |
| C | 2.18188200 | -2.39140500 | 2.24995000 | H | -1.82077300 | -4.78974700 | -1.86086200 |
| H | 2.44579000 | -1.36987600 | 2.51842300 | C | -4.59799200 | -2.87241600 | -0.15545300 |
| C | 2.99047700 | -3.35945200 | 3.13378100 | H | -3.76902400 | -3.33476600 | 0.37759000 |
| H | 2.86095100 | -3.10838700 | 4.19030400 | H | -5.09784500 | -3.64623000 | -0.74300400 |
| H | 4.05746100 | -3.32861500 | 2.90199700 | H | -5.31113900 | -2.48966600 | 0.57572600 |
| H | 2.65424400 | -4.39072100 | 2.99362200 | C | -5.37287100 | -1.19203600 | -1.81100500 |
| C | 0.67738000 | -2.55594600 | 2.53636300 | H | -6.08536600 | -0.75882500 | -1.10657200 |
| H | 0.32375400 | -3.55341200 | 2.26076000 | H | -5.86986600 | -2.01249500 | -2.33442000 |
| H | 0.08205500 | -1.82268800 | 1.99238300 | H | -5.10503500 | -0.43739000 | -2.54849800 |
| H | 0.48781300 | -2.41633300 | 3.60422900 | C | -4.08125200 | 0.19614700 | 0.54653600 |
| C | 3.69128800 | -0.64933500 | -2.36659200 | C | -4.63597600 | 1.38707900 | 0.03270600 |
| H | 4.03845200 | 0.17894100 | -1.75352900 | C | -5.44317000 | 2.15982400 | 0.87159000 |
| C | 2.55504000 | -0.11747900 | -3.25505800 | H | -5.87561500 | 3.07982200 | 0.49522400 |
| H | 2.15609700 | -0.91064200 | -3.89363700 | C | -5.68303600 | 1.78294800 | 2.18822800 |
| H | 2.91716000 | 0.68710100 | -3.90129800 | H | -6.32022400 | 2.39024200 | 2.82200700 |
| H | 1.73841700 | 0.26768000 | -2.64599200 | C | -5.07198300 | 0.64430100 | 2.69829500 |
| C | 4.87390800 | -1.10932200 | -3.23769400 | H | -5.21601400 | 0.38569100 | 3.74121800 |
| H | 5.67535000 | -1.54874900 | -2.63960800 | C | -4.25031000 | -0.15870400 | 1.90034100 |
| H | 5.28472800 | -0.25512000 | -3.78316200 | C | -4.28312200 | 1.91573300 | -1.35195300 |
| H | 4.56445800 | -1.85298200 | -3.97680700 | H | -3.77223100 | 1.11970500 | -1.89415300 |
| C | 4.76386800 | -0.26421400 | 2.63214300 | C | -3.28508200 | 3.08334400 | -1.23048700 |
| H | 3.97789500 | 0.29355400 | 3.13761800 | H | -2.98668200 | 3.43333200 | -2.22319300 |
| H | 5.72795000 | 0.08870700 | 3.00775200 | H | -2.38979700 | 2.78056200 | -0.68915700 |
| H | 4.67089200 | -1.31287700 | 2.90674600 | H | -3.73933700 | 3.92634800 | -0.69970900 |
| C | 5.74310600 | -1.04050000 | 0.48375000 | C | -5.51321000 | 2.34337900 | -2.16988300 |
| H | 5.51150900 | -2.08180600 | 0.71662500 | H | -6.25897500 | 1.54815900 | -2.23056600 |
| H | 6.72790400 | -0.81147300 | 0.89825500 | H | -5.21230000 | 2.60887400 | -3.18756700 |
| H | 5.79969500 | -0.93173600 | -0.59748800 | H | -5.99637500 | 3.22197500 | -1.73324100 |
| C | 3.71426400 | 3.30032100 | -0.28965100 | C | -3.46448900 | -1.28652800 | 2.55832400 |
| H | 2.80686800 | 3.89591700 | -0.19482900 | H | -2.94546200 | -1.83846800 | 1.77551000 |
| H | 4.53310600 | 3.93962600 | 0.05956000 | C | -2.38338100 | -0.69310900 | 3.48462000 |
| C | 3.93887600 | 2.98189100 | -1.76818000 | H | -2.84225600 | -0.13926600 | 4.30957500 |
| H | 4.90236200 | 2.50207300 | -1.95577800 | H | -1.73554500 | -0.01333500 | 2.93063200 |
| H | 3.91638300 | 3.90462100 | -2.35447900 | H | -1.77262300 | -1.49231400 | 3.91274900 |
| H | 3.15740200 | 2.32874600 | -2.15214500 | C | -4.34528400 | -2.27594300 | 3.33906200 |
| C | 3.28543000 | 2.69277200 | 2.11163400 | H | -3.73352600 | -3.09589600 | 3.72647700 |
| H | 2.49933700 | 3.43022100 | 1.95652200 | H | -5.13010800 | -2.70566200 | 2.71431800 |
| H | 2.83699000 | 1.91515900 | 2.73335300 | H | -4.82512800 | -1.79231700 | 4.19443100 |

**xyz coordinates of optimized structures of $^{3}$o-1** (conformer 2)
(E = -2249.691776)

| | x | y | z | | x | y | z |
|---|---|---|---|---|---|---|---|
| O | 1.58679100 | 1.07722200 | 0.56535800 | H | 5.01607800 | 3.69211300 | -2.88051300 |
| N | 3.85842500 | -0.19089000 | -0.46698800 | H | 6.21433700 | 2.78918800 | -1.94277600 |
| N | -3.54900000 | -0.43890300 | 0.56294900 | C | 5.88553600 | -0.06228900 | -1.95969200 |
| C | 4.39240600 | 0.32233600 | 1.88993600 | H | 5.38150000 | 0.58992200 | -2.67199700 |
| C | 4.26159200 | 0.74694600 | 0.55033700 | H | 6.59272400 | -0.68533300 | -2.51277400 |
| C | -3.95973200 | -0.05450500 | -1.84418200 | H | 6.45381900 | 0.55154200 | -1.25821100 |
| C | 2.58689700 | -1.83215600 | -1.63178400 | C | 1.40373100 | -0.31743300 | -3.39320100 |
| C | -1.11145700 | -0.10081600 | 0.20081200 | H | 0.69753300 | -0.34429900 | -4.22716200 |
| C | 4.89359200 | -0.97203000 | -1.22546700 | H | 2.35862400 | 0.04996200 | -3.77941400 |
| C | -1.09138100 | 2.05543100 | -1.11598000 | H | 1.03780000 | 0.41189500 | -2.66818000 |
| H | -1.08464000 | 1.47700300 | -2.03135300 | C | 4.92459200 | -1.81994500 | 3.18544200 |
| C | -1.19671300 | 1.39346600 | 0.10947000 | H | 5.84623300 | -1.96711400 | 2.61937100 |
| C | 1.43843800 | -0.01593300 | -0.04133300 | H | 4.52619700 | -2.80439100 | 3.44791100 |
| C | 2.57658200 | -0.65506000 | -0.66288700 | H | 5.18035700 | -1.31030200 | 4.11842000 |
| C | -4.05017300 | 0.40170100 | -0.50371400 | C | -2.13891100 | -1.30339300 | -3.07291900 |
| C | 4.90550500 | 1.22780700 | 2.82470200 | H | -1.76226200 | -2.29349600 | -3.34429400 |
| H | 5.01510000 | 0.91938600 | 3.85822000 | H | -1.36086900 | -0.78357500 | -2.51529300 |
| C | -4.66271100 | 1.65137800 | -0.23334100 | H | -2.32156800 | -0.75333500 | -4.00003900 |
| C | -3.42455000 | -1.42398700 | -2.23866100 | C | 2.32283200 | -4.43792300 | -1.71990600 |
| H | -3.17987700 | -1.96428000 | -1.32912100 | H | 1.44746100 | -4.43848500 | -2.37276900 |
| C | -1.21857400 | 2.15099700 | 1.28375300 | H | 2.25637500 | -5.32186400 | -1.07983200 |
| H | -1.29537500 | 1.64121300 | 2.23748000 | H | 3.21034100 | -4.55237700 | -2.34791500 |
| C | 0.12821100 | -0.68952000 | -0.04591900 | C | -2.12506200 | -2.15752200 | 1.46819300 |
| H | 0.15693600 | -1.75785900 | -0.14630800 | C | -4.89181700 | 2.20883100 | 1.16463500 |
| C | 1.53498800 | -1.70766500 | -2.76513900 | H | -4.28415800 | 1.62669200 | 1.85667800 |
| H | 1.80076000 | -2.42985500 | -3.54367300 | C | -4.80262300 | -0.72650200 | 2.76393700 |
| H | 0.56040200 | -2.01797200 | -2.38681900 | H | -3.91793400 | -0.33011100 | 3.25960400 |
| C | -0.97661500 | 3.44312200 | -1.16708700 | H | -5.21761900 | -1.51709000 | 3.39450900 |
| H | -0.89249300 | 3.94213600 | -2.12646000 | H | -5.54468500 | 0.06306700 | 2.70613800 |
| C | -2.22297600 | -0.87159000 | 0.61920200 | C | -4.47450700 | -2.25733700 | -2.99768400 |
| C | 4.01886800 | -1.75447500 | -2.22071100 | H | -4.69337700 | -1.82868600 | -3.97936100 |
| H | 3.99708400 | -1.21983400 | -3.17161900 | H | -5.41546000 | -2.32387100 | -2.44717700 |
| H | 4.43666700 | -2.74133700 | -2.42086400 | H | -4.09938200 | -3.27289800 | -3.15486500 |
| C | 2.38541900 | -3.17247200 | -0.85728200 | C | -1.50878900 | -1.72357300 | 2.83962900 |
| H | 3.19188100 | -3.27681400 | -0.12801100 | H | -0.49232200 | -1.37801000 | 2.62971500 |
| H | 1.46727000 | -3.11118500 | -0.27251300 | H | -2.04577800 | -0.84928200 | 3.21066000 |
| C | 3.88115900 | -1.02775800 | 2.38066100 | C | -6.38129500 | 2.09427200 | 1.55548900 |
| H | 3.60717000 | -1.62284400 | 1.51162200 | H | -6.53021600 | 2.40190500 | 2.59499600 |
| C | 5.70126900 | -1.89242200 | -0.29323700 | H | -6.77288400 | 1.08367800 | 1.43944000 |
| H | 6.24501500 | -1.30235100 | 0.44654800 | H | -6.98385000 | 2.75098000 | 0.92117700 |
| H | 6.42973300 | -2.45251200 | -0.88413500 | C | -3.60330400 | -2.58307400 | 1.55188500 |
| H | 5.07156900 | -2.60843900 | 0.23158500 | H | -3.82131400 | -3.26806000 | 0.72965000 |
| C | 4.53520100 | 2.08114200 | 0.18249800 | H | -3.83620500 | -3.11195000 | 2.47597100 |
| C | -5.12425800 | 2.42292800 | -1.30529700 | C | -5.75977500 | -1.64079100 | 0.63137100 |
| H | -5.59254700 | 3.37829600 | -1.10276300 | H | -6.34560700 | -0.74417400 | 0.42676600 |
| C | -4.41468800 | 0.76941300 | -2.87705200 | H | -6.36733000 | -2.31224600 | 1.24291400 |
| H | -4.33299100 | 0.42524100 | -3.90151400 | H | -5.55280600 | -2.13648700 | -0.31693300 |
| C | 5.04897600 | 2.94613400 | 1.15207200 | C | -1.29311300 | -3.36910500 | 0.95467300 |
| H | 5.26578200 | 3.97456700 | 0.88646900 | H | -0.23495000 | -3.19003800 | 1.16066200 |
| C | 5.25538500 | 2.52197300 | 2.45969700 | H | -1.56811400 | -4.21456600 | 1.59401000 |
| H | 5.65853400 | 3.20653600 | 3.19811300 | C | 2.91982900 | 3.54944700 | -1.06476700 |
| C | -4.46420700 | -1.32108200 | 1.38058000 | H | 2.08690600 | 3.00814300 | -0.61775800 |
| C | 4.16000400 | 2.64074100 | -1.18465400 | H | 2.61772800 | 3.90566400 | -2.05504700 |
| H | 3.87478000 | 1.80064600 | -1.81752100 | H | 3.13814400 | 4.42575900 | -0.44585200 |
| C | -1.07022400 | 3.53389100 | 1.23944800 | C | -4.46968000 | 3.68313300 | 1.30574800 |
| H | -1.05771700 | 4.10492300 | 2.16143200 | H | -5.16340400 | 4.35048500 | 0.78704700 |
| C | -0.94356200 | 4.18606600 | 0.01222100 | H | -3.47187200 | 3.85175500 | 0.91074900 |
| H | -0.83012700 | 5.26389200 | -0.02398300 | H | -4.47368300 | 3.96817300 | 2.36201500 |
| C | -4.99085300 | 2.00423400 | -2.61994200 | C | -1.46153200 | -3.80392500 | -0.50134500 |
| H | -5.34431100 | 2.62717800 | -3.43410700 | H | -1.16894900 | -3.01891600 | -1.19712000 |
| C | 2.59579800 | -0.83303700 | 3.21161800 | H | -2.49164400 | -4.08475000 | -0.73294600 |
| H | 2.81319200 | -0.29628300 | 4.14015600 | H | -0.83369700 | -4.67584000 | -0.70306900 |
| H | 2.16276000 | -1.80293100 | 3.47529800 | C | -1.46356000 | -2.78429000 | 3.94361000 |
| H | 1.85532100 | -0.26120500 | 2.65204300 | H | -2.45797400 | -3.16988400 | 4.18388200 |
| C | 5.31075100 | 3.39699500 | -1.86914700 | H | -1.05388600 | -2.34679900 | 4.85837700 |
| H | 5.56543500 | 4.31037800 | -1.32399300 | H | -0.82950900 | -3.63227300 | 3.67610800 |

**xyz coordinates of optimized structures of $^{3}$o-1** (conformer 3)
(E = -2249.689167)

| | x | y | z | | x | y | z |
|---|---|---|---|---|---|---|---|
| O | -1.57602400 | 0.98202000 | -0.64785700 | C | 2.18648500 | -3.24304400 | -3.72956300 |
| N | 3.61767700 | -0.40737700 | -0.38196400 | H | 3.22260600 | -3.58882300 | -3.77670400 |
| N | -3.84068800 | -0.35476500 | 0.27542400 | H | 1.89951500 | -2.93542500 | -4.73900700 |
| C | 4.69637100 | -1.30176300 | -0.94940200 | H | 1.55998700 | -4.09523300 | -3.45733900 |
| C | 3.94249600 | -2.63131000 | -1.10458300 | C | 1.16385000 | 1.30352600 | -0.52854600 |
| H | 4.07563000 | -3.21369100 | -0.19100300 | C | 1.13899300 | 1.86230900 | -1.81079300 |
| H | 4.33840700 | -3.23047500 | -1.92409500 | H | 1.21656200 | 1.20755600 | -2.67183400 |
| C | 2.44676100 | -2.30845800 | -1.27637600 | C | 0.93833200 | 3.22802300 | -1.98795700 |
| C | 2.33966400 | -0.93931100 | -0.57534200 | H | 0.88909700 | 3.64164300 | -2.98949800 |
| C | 1.13806000 | -0.19452800 | -0.40109900 | C | 0.80330300 | 4.06363100 | -0.87831400 |
| C | -0.08994900 | -0.82060400 | -0.20136400 | H | 0.64754300 | 5.12846500 | -1.01248200 |
| H | -0.07230100 | -1.87932700 | -0.02671200 | C | 0.89545800 | 3.52298300 | 0.40309600 |
| C | -1.42670200 | -0.19114700 | -0.21607600 | H | 0.80978900 | 4.16601800 | 1.27215700 |
| C | -2.58738400 | -0.92900400 | 0.24288500 | C | 1.06669800 | 2.15129000 | 0.57471100 |
| C | -2.65157700 | -2.33614300 | 0.83498800 | H | 1.09846700 | 1.73134900 | 1.57181100 |
| C | -4.17577700 | -2.59781400 | 0.92124100 | C | -2.02321300 | -3.45698700 | -0.03877800 |
| H | -4.48620100 | -3.20753800 | 0.07094500 | H | -0.96269900 | -3.55268500 | 0.18401100 |
| H | -4.44385500 | -3.15100200 | 1.82172400 | H | -2.46558000 | -4.40491100 | 0.28416400 |
| C | -4.90123400 | -1.24626300 | 0.85694700 | C | -2.21839900 | -3.29570100 | -1.54774800 |
| C | 3.90795200 | 0.56212000 | 0.65141900 | H | -1.81877000 | -4.16285300 | -2.08040800 |
| C | 4.50646800 | 1.80698900 | 0.33716800 | H | -1.70782500 | -2.40515300 | -1.92115100 |
| C | 4.76238900 | 2.71353300 | 1.37074000 | H | -3.27548500 | -3.20378200 | -1.81239800 |
| H | 5.21864300 | 3.66704300 | 1.13391100 | C | -1.98431600 | -2.30644700 | 2.24205600 |
| C | 4.43263600 | 2.43261900 | 2.68764400 | H | -0.96765300 | -1.92302100 | 2.12792100 |
| H | 4.62550200 | 3.15852600 | 3.46979800 | H | -2.51312500 | -1.57270700 | 2.85753800 |
| C | 3.86661500 | 1.20345900 | 2.99252300 | C | -1.92764900 | -3.64472900 | 2.98639000 |
| H | 3.63041800 | 0.96944500 | 4.02418600 | H | -1.48782900 | -3.50254400 | 3.97732500 |
| C | 3.61679800 | 0.24782600 | 2.00441700 | H | -1.31363000 | -4.37672200 | 2.45702600 |
| C | 4.91287500 | 2.22383200 | -1.06856700 | H | -2.92100700 | -4.07957100 | 3.12717900 |
| H | 4.48029200 | 1.50577400 | -1.76275900 | C | -5.35307600 | -0.76934100 | 2.24671600 |
| C | 6.44906100 | 2.22218000 | -1.21559100 | H | -4.52676000 | -0.72211800 | 2.95535300 |
| H | 6.73579300 | 2.41545400 | -2.25375400 | H | -6.09478500 | -1.46974100 | 2.63828900 |
| H | 6.90074700 | 1.27791200 | -0.90838500 | H | -5.81879500 | 0.21424300 | 2.18496100 |
| H | 6.88691200 | 3.00960000 | -0.59502200 | C | -6.14157400 | -1.33002400 | -0.04281500 |
| C | 4.37907000 | 3.61137100 | -1.46255600 | H | -6.61992900 | -0.35561900 | -0.15925900 |
| H | 4.86351700 | 4.40745300 | -0.89027900 | H | -6.86309800 | -2.01081700 | 0.41540400 |
| H | 3.30682500 | 3.67891800 | -1.30493900 | H | -5.89232800 | -1.71830900 | -1.02924900 |
| H | 4.58451900 | 3.79866500 | -2.52105800 | C | -4.19689000 | 0.97152000 | -0.16488300 |
| C | 3.07179900 | -1.09726300 | 2.46360200 | C | -4.60442200 | 1.15921800 | -1.50227900 |
| H | 2.99281700 | -1.74040500 | 1.59275700 | C | -5.08305600 | 2.41585400 | -1.88204300 |
| C | 1.66651900 | -0.96082200 | 3.07626100 | H | -5.39881000 | 2.57818200 | -2.90620100 |
| H | 1.68526800 | -0.31879000 | 3.96150000 | C | -5.14280700 | 3.46763200 | -0.97485400 |
| H | 1.28789600 | -1.93906300 | 3.38586100 | H | -5.52500000 | 4.43424300 | -1.28475800 |
| H | 0.96445900 | -0.53616700 | 2.35816500 | C | -4.67845200 | 3.28318100 | 0.32155200 |
| C | 4.01908400 | -1.79212500 | 3.46009900 | H | -4.67607600 | 4.12128400 | 1.00905500 |
| H | 5.03448500 | -1.87070100 | 3.06549100 | C | -4.18420900 | 2.04620100 | 0.74792600 |
| H | 3.65788500 | -2.80237800 | 3.67411400 | C | -4.42740500 | 0.07888100 | -2.56152600 |
| H | 4.07198900 | -1.25050800 | 4.40846500 | H | -4.18718300 | -0.85339200 | -2.05109500 |
| C | 5.22133600 | -0.83262100 | -2.32305400 | C | -3.22497500 | 0.41675900 | -3.46600900 |
| H | 4.40997800 | -0.53872300 | -2.98746100 | H | -3.04200100 | -0.39798000 | -4.17379200 |
| H | 5.76078100 | -1.65892400 | -2.79314900 | H | -2.32788200 | 0.57508300 | -2.86694800 |
| H | 5.91425900 | -0.00113700 | -2.23995300 | H | -3.41968400 | 1.32723600 | -4.04187700 |
| C | 5.87267800 | -1.45292200 | 0.01805700 | C | -5.68930100 | -0.15316300 | -3.40929500 |
| H | 6.37563500 | -0.50318000 | 0.20303900 | H | -6.56469600 | -0.35017700 | -2.78685800 |
| H | 6.59983000 | -2.14492000 | -0.41372300 | H | -5.54280600 | -1.00955900 | -4.07394800 |
| H | 5.54410000 | -1.85701400 | 0.97555700 | H | -5.91360800 | 0.71335300 | -4.03762400 |
| C | 1.62602700 | -3.52031200 | -0.75283200 | C | -3.51974500 | 1.95167600 | 2.11643700 |
| H | 0.60087500 | -3.43719000 | -1.11629200 | H | -3.29219800 | 0.90383000 | 2.30682000 |
| H | 2.03574400 | -4.39974100 | -1.26019400 | C | -2.17521700 | 2.70340400 | 2.09048800 |
| C | 1.61845900 | -3.80666400 | 0.74950400 | H | -2.33371700 | 3.77859500 | 1.95836200 |
| H | 2.62465400 | -3.95079200 | 1.14954100 | H | -1.55155700 | 2.34927700 | 1.27210500 |
| H | 1.06014600 | -4.72543100 | 0.94863500 | H | -1.63833700 | 2.55611400 | 3.03335100 |
| H | 1.14776200 | -3.00496900 | 1.31822300 | C | -4.39753900 | 2.47065400 | 3.26729800 |
| C | 2.01712300 | -2.06728800 | -2.76188100 | H | -3.89666600 | 2.30087200 | 4.22487400 |
| H | 0.96450100 | -1.76823000 | -2.73704500 | H | -5.36898000 | 1.97395500 | 3.30160400 |
| H | 2.56020100 | -1.20507000 | -3.15219500 | H | -4.57488500 | 3.54601900 | 3.17762300 |

**xyz coordinates of optimized structures of 1•H⁺** (most stable conformer )
(E = -2250.184796)

| | x | y | z | | x | y | z |
|---|---|---|---|---|---|---|---|
| O | -1.69804400 | 1.27832500 | 0.39968900 | H | 5.41594900 | 2.80789800 | 2.76903800 |
| N | 3.36133700 | -0.16235500 | 0.37171300 | H | 4.36256300 | 4.11726800 | 3.29144000 |
| N | -3.29322600 | -0.78875100 | -0.22674300 | H | 5.16905200 | 4.21452500 | 1.72698800 |
| C | 4.80668700 | 0.04418600 | 0.79871000 | C | 0.71652300 | 2.53265400 | -0.15749300 |
| C | 5.02550900 | 1.46444400 | 0.29662100 | C | 0.36913100 | 2.99049700 | -1.43680500 |
| H | 5.33753400 | 1.41545200 | -0.74708200 | H | 0.54075900 | 2.35056300 | -2.29320300 |
| H | 5.81525800 | 1.97872600 | 0.83795700 | C | -0.18639900 | 4.25262500 | -1.61852000 |
| C | 3.66410900 | 2.18396700 | 0.39568900 | H | -0.43789100 | 4.58986000 | -2.61719800 |
| C | 2.66417300 | 0.99475200 | 0.21395800 | C | -0.43481500 | 5.07470800 | -0.51903700 |
| C | 1.27559700 | 1.13979800 | -0.00670200 | H | -0.87269300 | 6.05575400 | -0.66019500 |
| C | 0.33012300 | 0.07973000 | -0.18886700 | C | -0.13968000 | 4.61723000 | 0.76292600 |
| H | 0.71476000 | -0.89714700 | -0.42319400 | H | -0.35328100 | 5.23579800 | 1.62659500 |
| C | -1.05887400 | 0.16854400 | -0.08729700 | C | 0.42751400 | 3.35457100 | 0.94242700 |
| C | -1.97484200 | -0.86704700 | -0.45454800 | H | 0.63109000 | 2.99504500 | 1.94306200 |
| C | -1.64204200 | -2.18670500 | -1.16549700 | C | -0.75972400 | -2.01760500 | -2.43031200 |
| C | -3.04078800 | -2.69313300 | -1.58576500 | H | 0.28459800 | -1.91619700 | -2.13833300 |
| H | -3.24042800 | -2.40105700 | -2.61658700 | H | -0.81875500 | -2.96020900 | -2.98214000 |
| H | -3.11578500 | -3.77683700 | -1.54409000 | C | -1.15215700 | -0.86738800 | -3.36221400 |
| C | -4.06549400 | -2.02570400 | -0.67168200 | H | -0.52383300 | -0.87485400 | -4.25477900 |
| C | 2.94805400 | -1.49476700 | 0.01011300 | H | -1.02974100 | 0.10343400 | -2.87761800 |
| C | 2.54093200 | -2.40478600 | 1.00758800 | H | -2.19032400 | -0.94343500 | -3.69507200 |
| C | 2.34150800 | -3.73777900 | 0.63387700 | C | -0.96433300 | -3.14314400 | -0.14126000 |
| H | 2.03579900 | -4.45867400 | 1.38245200 | H | 0.02063000 | -2.74794000 | 0.09540700 |
| C | 2.49736500 | -4.14915300 | -0.68233800 | H | -1.52307400 | -3.12334100 | 0.79693200 |
| H | 2.32911700 | -5.18542900 | -0.94957900 | C | -0.81044500 | -4.59641600 | -0.59606000 |
| C | 2.84154000 | -3.22645800 | -1.66169900 | H | -0.25043100 | -5.15336200 | 0.15786300 |
| H | 2.93638600 | -3.55513900 | -2.68913700 | H | -0.25886200 | -4.67362800 | -1.53437000 |
| C | 3.09230300 | -1.88994400 | -1.34152700 | H | -1.77354300 | -5.09491300 | -0.72153500 |
| C | 2.26148400 | -1.99145600 | 2.44770600 | C | -4.44227900 | -2.88558100 | 0.54313900 |
| H | 2.57849800 | -0.95701800 | 2.56838700 | H | -3.57609400 | -3.19276700 | 1.12619100 |
| C | 3.02967200 | -2.85867800 | 3.46183600 | H | -4.94554000 | -3.78613800 | 0.18646600 |
| H | 2.93582300 | -2.43400400 | 4.46467500 | H | -5.13247800 | -2.34847700 | 1.19306100 |
| H | 4.09155600 | -2.93218500 | 3.21881600 | C | -5.34806600 | -1.67887400 | -1.43020400 |
| H | 2.62785100 | -3.87479900 | 3.49479500 | H | -6.04577800 | -1.11272600 | -0.81221300 |
| C | 0.75471200 | -2.03494900 | 2.76475700 | H | -5.83175100 | -2.61570200 | -1.71468900 |
| H | 0.35407100 | -3.04420600 | 2.64016600 | H | -5.14282900 | -1.12170500 | -2.34166600 |
| H | 0.18669100 | -1.36132000 | 2.12279600 | C | -4.03327200 | 0.25064500 | 0.47493800 |
| H | 0.58823500 | -1.73130600 | 3.80147300 | C | -4.66405400 | 1.25422500 | -0.28604000 |
| C | 3.52015100 | -0.92805800 | -2.44745200 | C | -5.47255300 | 2.17180900 | 0.38876200 |
| H | 3.92577600 | -0.03460800 | -1.97586800 | H | -5.96487000 | 2.95760900 | -0.17125700 |
| C | 2.32685600 | -0.48292100 | -3.30982200 | C | -5.63738200 | 2.11013400 | 1.76726200 |
| H | 1.88331000 | -1.33799000 | -3.82562900 | H | -6.27529100 | 2.82735400 | 2.27134600 |
| H | 2.65737700 | 0.23339300 | -4.06647800 | C | -4.95358500 | 1.15025600 | 2.50105400 |
| H | 1.55159400 | -0.00516100 | -2.71088100 | H | -5.04285500 | 1.14345500 | 3.58070800 |
| C | 4.61961800 | -1.51269400 | -3.35357300 | C | -4.12459700 | 0.21102600 | 1.87865500 |
| H | 5.45499800 | -1.91577800 | -2.77788600 | C | -4.40757000 | 1.45085200 | -1.77634500 |
| H | 5.00435800 | -0.73157600 | -4.01433600 | H | -3.88115500 | 0.57307100 | -2.15152100 |
| H | 4.23243200 | -2.31569200 | -3.98564900 | C | -3.47593000 | 2.65728300 | -2.00350400 |
| C | 4.97658800 | -0.07202400 | 2.32383000 | H | -3.25671900 | 2.76803300 | -3.06962700 |
| H | 4.25378700 | 0.52484600 | 2.87624700 | H | -2.53698700 | 2.53264300 | -1.46774800 |
| H | 5.97821600 | 0.27476400 | 2.58786500 | H | -3.94704000 | 3.58205500 | -1.65720700 |
| H | 4.89281200 | -1.10665300 | 2.64849200 | C | -5.69961200 | 1.61728400 | -2.59489200 |
| C | 5.76634700 | -0.94979600 | 0.14177500 | H | -6.40850800 | 0.80789600 | -2.41214100 |
| H | 5.54776800 | -1.97835800 | 0.43355800 | H | -5.46340200 | 1.63158400 | -3.66236300 |
| H | 6.77817100 | -0.71156400 | 0.47697400 | H | -6.20044800 | 2.55976900 | -2.35847100 |
| H | 5.75059900 | -0.88014800 | -0.94286700 | C | -3.27055800 | -0.70100400 | 2.75345600 |
| C | 3.60841800 | 3.29301400 | -0.69206700 | H | -2.75353600 | -1.41450800 | 2.11287100 |
| H | 2.72793100 | 3.91359700 | -0.53585800 | C | -2.18559700 | 0.12471300 | 3.47533400 |
| H | 4.46937600 | 3.94204700 | -0.50010500 | H | -2.64135600 | 0.85960000 | 4.14450700 |
| C | 3.64826500 | 2.83883300 | -2.15317200 | H | -1.55856900 | 0.65661600 | 2.76050300 |
| H | 4.59432600 | 2.36361200 | -2.42100000 | H | -1.55111300 | -0.53249300 | 4.07479000 |
| H | 3.52113200 | 3.70106200 | -2.81219800 | C | -4.09008100 | -1.49953900 | 3.78200400 |
| H | 2.84700600 | 2.13440400 | -2.37687100 | H | -3.43920500 | -2.20113600 | 4.31056700 |
| C | 3.44780400 | 2.86399300 | 1.79379400 | H | -4.89416900 | -2.06998600 | 3.31471300 |
| H | 2.68774900 | 3.63151100 | 1.66457100 | H | -4.53798300 | -0.83966200 | 4.52972800 |
| H | 3.02629600 | 2.14511700 | 2.49999100 | H | -1.06884000 | 1.98673600 | 0.59128400 |
| C | 4.67566000 | 3.53147400 | 2.42332800 | | | | |

**xyz coordinates of optimized structures of 1•H$^+$** (conformer 2)
(E = -2250.182058)

| | x | y | z |
|---|---|---|---|
| O | 1.59841300 | 1.16994500 | 0.32105400 |
| N | 3.79038300 | -0.28749300 | -0.35770400 |
| N | -3.54161900 | -0.48133100 | 0.46446700 |
| C | 4.21940800 | 0.59092000 | 1.90698200 |
| C | 4.16072200 | 0.81391700 | 0.51705000 |
| C | -3.81562500 | 0.12161600 | -1.90459400 |
| C | 2.61388900 | -2.06866900 | -1.37399900 |
| C | -1.13681000 | -0.13087900 | 0.19211500 |
| C | 4.89068600 | -1.15936200 | -0.94212200 |
| C | -1.11810600 | 2.08360300 | -1.04113500 |
| H | -1.16706200 | 1.55110000 | -1.98153200 |
| C | -1.21170200 | 1.36940900 | 0.15925800 |
| C | 1.38137400 | -0.11575000 | -0.10099800 |
| C | 2.55773300 | -0.77638800 | -0.55050100 |
| C | -3.96647000 | 0.48131600 | -0.54095500 |
| C | 4.67982700 | 1.63526800 | 2.71520800 |
| H | 4.73466200 | 1.49098500 | 3.78751100 |
| C | -4.53334200 | 1.72834500 | -0.18962700 |
| C | -3.32494400 | -1.23825700 | -2.38848500 |
| H | -3.15406500 | -1.87204500 | -1.52214700 |
| C | -1.15318400 | 2.07470600 | 1.37042700 |
| H | -1.22770000 | 1.52992800 | 2.30480800 |
| C | 0.12654600 | -0.71925400 | -0.07138600 |
| H | 0.13135100 | -1.76999400 | -0.28646400 |
| C | 1.65442800 | -2.05624000 | -2.59455200 |
| H | 1.95833200 | -2.88215600 | -3.24342700 |
| H | 0.64011500 | -2.29135900 | -2.27169100 |
| C | -0.93665000 | 3.46287100 | -1.03216900 |
| H | -0.85704300 | 3.99956000 | -1.97033200 |
| C | -2.25234900 | -0.90663200 | 0.55950700 |
| C | 4.08364200 | -2.08171500 | -1.86317100 |
| H | 4.13776600 | -1.70632300 | -2.88485600 |
| H | 4.49766900 | -3.08847200 | -1.87046000 |
| C | 2.34244700 | -3.29503900 | -0.44902800 |
| H | 3.10137700 | -3.31145400 | 0.33601700 |
| H | 1.39363900 | -3.16239300 | 0.06686200 |
| C | 3.69895400 | -0.67661100 | 2.57880900 |
| H | 3.48478800 | -1.41594900 | 1.80951000 |
| C | 5.63129200 | -1.91827900 | 0.16998300 |
| H | 6.13074900 | -1.22368500 | 0.84631100 |
| H | 6.39388600 | -2.54922300 | -0.29038200 |
| H | 4.97193400 | -2.55982200 | 0.75115400 |
| C | 4.45110200 | 2.07192300 | -0.04743200 |
| C | -4.88108600 | 2.61200100 | -1.21601900 |
| H | -5.30910000 | 3.57299500 | -0.96050900 |
| C | -4.16531400 | 1.05413800 | -2.88408200 |
| H | -4.03846000 | 0.79541500 | -3.92830000 |
| C | 4.90904000 | 3.07787300 | 0.80724000 |
| H | 5.13789600 | 4.05534000 | 0.39994700 |
| C | 5.04329900 | 2.86074600 | 2.17299400 |
| H | 5.40208200 | 3.65544100 | 2.81734900 |
| C | -4.52267100 | -1.40124000 | 1.17633400 |
| C | 4.16455400 | 2.42396200 | -1.50415200 |
| H | 3.88721900 | 1.50997100 | -2.02999400 |
| C | -0.93772900 | 3.45412700 | 1.37894600 |
| H | -0.86290800 | 3.97976200 | 2.32355100 |
| C | -0.82194700 | 4.14942000 | 0.17703700 |
| H | -0.64969500 | 5.21917700 | 0.18205600 |
| C | -4.68482400 | 2.29544100 | -2.55097200 |
| H | -4.94836500 | 3.00536900 | -3.32662200 |
| C | 2.36719900 | -0.39062200 | 3.30295300 |
| H | 2.51662400 | 0.30879700 | 4.13025100 |
| H | 1.95518800 | -1.31716900 | 3.71277700 |
| H | 1.63202700 | 0.04086200 | 2.62378900 |
| C | 5.37634700 | 3.04667900 | -2.22080700 |
| H | 5.61699200 | 4.02882600 | -1.80532700 |
| H | 5.15014900 | 3.18630400 | -3.28150800 |
| H | 6.26833800 | 2.42374800 | -2.14213600 |
| C | 5.91449900 | -0.33985400 | -1.72731800 |
| H | 5.45350300 | 0.19231600 | -2.55719600 |
| H | 6.65882000 | -1.02537100 | -2.13789500 |
| H | 6.43076200 | 0.37372400 | -1.08426400 |
| C | 1.63507200 | -0.76056900 | -3.41152600 |
| H | 0.98385500 | -0.87830600 | -4.28026800 |
| H | 2.62865400 | -0.49222900 | -3.77926100 |
| H | 1.25891500 | 0.08067400 | -2.82587700 |
| C | 4.71024300 | -1.30369700 | 3.55323500 |
| H | 5.66537200 | -1.51195700 | 3.06822400 |
| H | 4.31482400 | -2.24521900 | 3.94409700 |
| H | 4.90155200 | -0.64827200 | 4.40657500 |
| C | -1.99788200 | -1.12604300 | -3.15929500 |
| H | -1.66002000 | -2.11426200 | -3.48237600 |
| H | -1.21523500 | -0.68284100 | -2.54455100 |
| H | -2.11447600 | -0.50936200 | -4.05397200 |
| C | 2.32334400 | -4.65230500 | -1.15878600 |
| H | 1.49967700 | -4.72605400 | -1.87092300 |
| H | 2.19427300 | -5.44784300 | -0.42109200 |
| H | 3.25304600 | -4.84982100 | -1.69759700 |
| C | -2.19589700 | -2.23348800 | 1.34630000 |
| C | -4.83567600 | 2.16659700 | 1.23608900 |
| H | -4.30115400 | 1.50171700 | 1.91382300 |
| C | -4.94515200 | -0.87928800 | 2.56312800 |
| H | -4.09506000 | -0.53289000 | 3.14856300 |
| H | -5.41469300 | -1.70186900 | 3.10717300 |
| H | -5.67228400 | -0.07726400 | 2.50192400 |
| C | -4.37979600 | -1.94565200 | -3.26167700 |
| H | -4.51875100 | -1.42904000 | -4.21473500 |
| H | -5.35105300 | -1.99481900 | -2.76546200 |
| H | -4.05463400 | -2.96652100 | -3.48047600 |
| C | -1.65202400 | -1.83976900 | 2.76307100 |
| H | -0.60747100 | -1.54351100 | 2.62898700 |
| H | -2.16763300 | -0.94333500 | 3.11194600 |
| C | -6.35369500 | 2.07283900 | 1.50653500 |
| H | -6.56901700 | 2.27710000 | 2.55924200 |
| H | -6.76915800 | 1.09672500 | 1.25493700 |
| H | -6.88367900 | 2.81525400 | 0.90347500 |
| C | -3.67268300 | -2.66863000 | 1.32869700 |
| H | -3.84438700 | -3.31286800 | 0.46543300 |
| H | -3.94898800 | -3.24098500 | 2.21240700 |
| C | -5.76287300 | -1.65170800 | 0.31905000 |
| H | -6.31725800 | -0.73273700 | 0.12647500 |
| H | -6.42192800 | -2.34184900 | 0.85004500 |
| H | -5.49953800 | -2.10160200 | -0.63744300 |
| C | -1.32538600 | -3.40298100 | 0.81670700 |
| H | -0.27859200 | -3.21242200 | 1.06004900 |
| H | -1.59880600 | -4.26897300 | 1.42600100 |
| C | 2.95451400 | 3.37671200 | -1.60031200 |
| H | 2.07187400 | 2.93784700 | -1.13810600 |
| H | 2.73133200 | 3.58911500 | -2.65027200 |
| H | 3.16792700 | 4.32793300 | -1.10373900 |
| C | -4.37721900 | 3.60309700 | 1.54795900 |
| H | -5.00428700 | 4.34364800 | 1.04482900 |
| H | -3.34754100 | 3.77019900 | 1.24570900 |
| H | -4.45606600 | 3.78700700 | 2.62307200 |
| C | -1.46209500 | -3.80113000 | -0.65339900 |
| H | -1.19116400 | -2.99297100 | -1.33199700 |
| H | -2.47925800 | -4.10785500 | -0.90473300 |
| H | -0.80641200 | -4.64728300 | -0.86906800 |
| C | -1.73835900 | -2.91603600 | 3.84775000 |
| H | -2.76934600 | -3.21799700 | 4.04627900 |
| H | -1.32837100 | -2.52303600 | 4.78160100 |
| H | -1.16646400 | -3.80953300 | 3.59004400 |
| H | 0.80926400 | 1.52765600 | 0.74922500 |

**xyz coordinates of optimized structures of c-1 at other levels of theory**

*B3LYP/6-31g(d)* (E = -2248.912418)

| | x | y | z | | x | y | z |
|---|---|---|---|---|---|---|---|
| O | -0.18219400 | -1.33458300 | 0.27563700 | C | -0.62138200 | -1.71022700 | 4.47524500 |
| N | -2.58765800 | -0.99116400 | 0.00208000 | H | -1.10287400 | -2.69562700 | 4.47945500 |
| N | 3.34305400 | -0.22065100 | -0.40283600 | H | -1.21889200 | -1.04277300 | 5.10485900 |
| C | -2.93809800 | -2.38497900 | 0.44859900 | H | 0.35570900 | -1.82283600 | 4.95991000 |
| C | -2.30621500 | -2.44328300 | 1.87241100 | C | -1.57466800 | 2.21016000 | 0.63093800 |
| H | -1.50045300 | -3.18433000 | 1.88367300 | C | -1.54195400 | 2.95370000 | 1.82244100 |
| H | -3.04032300 | -2.76842400 | 2.61352800 | H | -1.10106200 | 2.51278100 | 2.71101600 |
| C | -1.71254000 | -1.05081100 | 2.19387700 | C | -2.04384900 | 4.25496800 | 1.87541400 |
| C | -1.40064100 | -0.54915300 | 0.71086300 | H | -2.00635700 | 4.80782200 | 2.81071000 |
| C | -0.88792600 | 0.88604800 | 0.52576800 | C | -2.57407100 | 4.84968800 | 0.72940100 |
| C | 0.43656400 | 0.85095700 | 0.25361600 | H | -2.95965600 | 5.86520100 | 0.76752000 |
| H | 1.04715400 | 1.73512600 | 0.14665300 | C | -2.59436800 | 4.13262500 | -0.46735400 |
| C | 0.92497200 | -0.49444000 | 0.10682900 | H | -2.99379300 | 4.58744800 | -1.37014500 |
| C | 2.17199000 | -0.98607500 | -0.16796700 | C | -2.10075500 | 2.82804400 | -0.51661800 |
| C | 2.50034300 | -2.48558800 | -0.36544100 | H | -2.11632800 | 2.28233800 | -1.45396700 |
| C | 4.03825500 | -2.46826000 | -0.54037700 | C | 1.77670800 | -3.01174200 | -1.64628300 |
| H | 4.38534100 | -3.23041000 | -1.24340700 | H | 0.70258700 | -2.88468500 | -1.49376100 |
| H | 4.52397700 | -2.67666900 | 0.41733200 | H | 2.03781000 | -2.36355900 | -2.48803500 |
| C | 4.44136500 | -1.05283900 | -0.99692800 | C | 2.04396500 | -4.46831200 | -2.05424100 |
| C | -3.19784500 | -0.35650300 | -1.15147000 | H | 1.64802500 | -5.18534300 | -1.32821200 |
| C | -4.43072500 | 0.35756500 | -0.99726000 | H | 3.11142900 | -4.68098500 | -2.18472300 |
| C | -4.99686200 | 0.99931700 | -2.10619100 | H | 1.55422000 | -4.67702200 | -3.01277000 |
| H | -5.92411200 | 1.54992800 | -1.97576300 | C | 2.08705000 | -3.39922700 | 0.82604200 |
| C | -4.40746100 | 0.95958500 | -3.36154500 | H | 0.99464600 | -3.39982500 | 0.88664000 |
| H | -4.86465400 | 1.47124800 | -4.20488700 | H | 2.38252900 | -4.42376700 | 0.56725800 |
| C | -3.23171500 | 0.24323900 | -3.52188600 | C | 2.66168500 | -3.08620700 | 2.21173000 |
| H | -2.77502700 | 0.18867600 | -4.50599600 | H | 2.23998300 | -3.77770900 | 2.95087900 |
| C | -2.61861700 | -0.42580300 | -2.45175900 | H | 2.42011300 | -2.07111700 | 2.53562100 |
| C | -5.22601100 | 0.48566100 | 0.30570300 | H | 3.75054900 | -3.20287800 | 2.25307400 |
| H | -4.71474900 | -0.09802700 | 1.06663100 | C | 4.50639400 | -0.97077600 | -2.53985200 |
| C | -6.65850900 | -0.07470800 | 0.16089700 | H | 3.53023500 | -1.12132600 | -3.00567900 |
| H | -7.15156500 | -0.10148200 | 1.14050500 | H | 5.18340900 | -1.74575200 | -2.91922000 |
| H | -6.67068500 | -1.08628100 | -0.25361800 | H | 4.89710700 | -0.00770100 | -2.87235600 |
| H | -7.27062700 | 0.55762000 | -0.49236100 | C | 5.82729800 | -0.67343700 | -0.45826800 |
| C | -5.30956400 | 1.93610800 | 0.82163600 | H | 6.08866000 | 0.36206900 | -0.69875600 |
| H | -5.80045400 | 2.59241500 | 0.09364200 | H | 6.57990100 | -1.32276000 | -0.91988600 |
| H | -4.32443200 | 2.35454400 | 1.03284600 | H | 5.89187500 | -0.80444100 | 0.62345100 |
| H | -5.90094800 | 1.96738400 | 1.74545600 | C | 3.55363800 | 1.15759800 | -0.02393500 |
| C | -1.35272600 | -1.20571700 | -2.79163600 | C | 3.41131200 | 2.21507200 | -0.96648200 |
| H | -0.98141000 | -1.65600000 | -1.87373700 | C | 3.69012600 | 3.52861100 | -0.56235100 |
| C | -1.63587200 | -2.32721000 | -3.81375900 | H | 3.58594000 | 4.33499300 | -1.28263400 |
| H | -2.45872500 | -2.97634400 | -3.49863600 | C | 4.08278600 | 3.82781400 | 0.73473700 |
| H | -0.74428800 | -2.95199400 | -3.94806200 | H | 4.28914600 | 4.85489000 | 1.02450800 |
| H | -1.89997800 | -1.91681800 | -4.79578500 | C | 4.20014600 | 2.79803000 | 1.65878800 |
| C | -0.24520200 | -0.28327900 | -3.33377800 | H | 4.49824400 | 3.02991000 | 2.67749600 |
| H | -0.55748800 | 0.22833300 | -4.25208900 | C | 3.95042800 | 1.46568400 | 1.30900700 |
| H | 0.65216100 | -0.86547700 | -3.57116800 | C | 2.93944100 | 2.02574100 | -2.40695100 |
| H | 0.02701800 | 0.47536200 | -2.59742400 | H | 2.71734300 | 0.96629600 | -2.55097500 |
| C | -4.44816500 | -2.66661500 | 0.48402600 | C | 1.64785600 | 2.81850800 | -2.70079900 |
| H | -4.97816800 | -2.07122500 | 1.22800200 | H | 0.84059000 | 2.56591600 | -2.00863400 |
| H | -4.60302100 | -3.72115900 | 0.73815200 | H | 1.29930400 | 2.60379500 | -3.71776000 |
| H | -4.90769900 | -2.49368000 | -0.49382800 | H | 1.81806400 | 3.89914100 | -2.63256700 |
| C | -2.31805400 | -3.48287000 | -0.44384800 | C | 4.02168000 | 2.44943500 | -3.42358200 |
| H | -2.75242700 | -3.46923400 | -1.44787700 | H | 4.16836200 | 3.53592100 | -3.40884000 |
| H | -2.52737500 | -4.46819100 | -0.00860800 | H | 3.72179000 | 2.17184700 | -4.44113900 |
| H | -1.23694300 | -3.36855200 | -0.52237800 | H | 4.99328000 | 1.99045000 | -3.21710200 |
| C | -2.70530800 | -0.06762500 | 2.89325600 | C | 4.09194700 | 0.41967200 | 2.41015100 |
| H | -3.19774700 | 0.55178100 | 2.14396600 | H | 3.95772800 | -0.56295400 | 1.95512000 |
| H | -2.11051200 | 0.62975500 | 3.49544400 | C | 2.99222300 | 0.59896900 | 3.47473700 |
| C | -3.79416600 | -0.65736000 | 3.80271200 | H | 3.10496400 | 1.55436300 | 4.00122600 |
| H | -3.39162700 | -1.32122800 | 4.57410300 | H | 3.04354900 | -0.20159500 | 4.22273200 |
| H | -4.54322100 | -1.22488900 | 3.24067800 | H | 1.99904800 | 0.58103800 | 3.01989200 |
| H | -4.32396700 | 0.15607500 | 4.31287400 | C | 5.47716800 | 0.44428200 | 3.08848000 |
| C | -0.43673400 | -1.16751700 | 3.05124200 | H | 6.29465800 | 0.36805600 | 2.36479500 |
| H | 0.02478400 | -0.17430700 | 3.11619800 | H | 5.56551900 | -0.39258900 | 3.79168600 |
| H | 0.27258100 | -1.80685400 | 2.52678800 | H | 5.63003100 | 1.36656000 | 3.66074500 |

*B3LYP/6-311g(d,p)*
(E = -2249.480290)

| | x | y | z | | x | y | z |
|---|---|---|---|---|---|---|---|
| O | -0.18378600 | -1.32645500 | 0.29245200 | C | -0.60953700 | -1.60796300 | 4.50125500 |
| N | -2.58828900 | -0.98512200 | 0.02289000 | H | -1.08650100 | -2.59225100 | 4.52757000 |
| N | 3.34284600 | -0.23358300 | -0.39029500 | H | -1.20535400 | -0.93040000 | 5.11692400 |
| C | -2.93988600 | -2.36921500 | 0.50192300 | H | 0.36674500 | -1.70740700 | 4.98434000 |
| C | -2.29669600 | -2.39869800 | 1.91935100 | C | -1.56710200 | 2.22657300 | 0.58733400 |
| H | -1.48698200 | -3.13117900 | 1.93415400 | C | -1.52635500 | 2.99459600 | 1.75961800 |
| H | -3.02167700 | -2.71401000 | 2.66950600 | H | -1.08178000 | 2.57468800 | 2.65343800 |
| C | -1.70778700 | -1.00021600 | 2.21130200 | C | -2.02417500 | 4.29543300 | 1.78652500 |
| C | -1.40205000 | -0.52890800 | 0.71825600 | H | -1.97896800 | 4.86827700 | 2.70639500 |
| C | -0.88290600 | 0.89979300 | 0.50622300 | C | -2.55963700 | 4.86448200 | 0.63321300 |
| C | 0.43746400 | 0.85572600 | 0.23261300 | H | -2.94087900 | 5.87945400 | 0.65052900 |
| H | 1.04903200 | 1.73412400 | 0.10871200 | C | -2.59108900 | 4.12134600 | -0.54387200 |
| C | 0.92356800 | -0.49135000 | 0.11369000 | H | -2.99572100 | 4.55509200 | -1.45165000 |
| C | 2.16884500 | -0.98733200 | -0.14696700 | C | -2.10245200 | 2.81686500 | -0.56648900 |
| C | 2.49223500 | -2.49089600 | -0.31232100 | H | -2.12905500 | 2.25052700 | -1.48843300 |
| C | 4.02945300 | -2.48432800 | -0.47728100 | C | 1.77086000 | -3.03654300 | -1.58468100 |
| H | 4.37669500 | -3.26037300 | -1.16031500 | H | 0.69885200 | -2.92016600 | -1.42558300 |
| H | 4.50546300 | -2.67334500 | 0.48611000 | H | 2.01871800 | -2.39251000 | -2.43007600 |
| C | 4.44287300 | -1.08280400 | -0.95938000 | C | 2.05575800 | -4.49192700 | -1.98019300 |
| C | -3.20151500 | -0.37796800 | -1.14359000 | H | 1.68834400 | -5.20557000 | -1.23981500 |
| C | -4.43192700 | 0.33813200 | -1.00332400 | H | 3.12132300 | -4.68637000 | -2.13064900 |
| C | -4.99937800 | 0.95407000 | -2.12273800 | H | 1.55197400 | -4.72104600 | -2.92365900 |
| H | -5.92420400 | 1.50653400 | -2.00399200 | C | 2.06786500 | -3.37627900 | 0.89465600 |
| C | -4.41360300 | 0.88483900 | -3.37562000 | H | 0.97832000 | -3.35912700 | 0.95319500 |
| H | -4.87127100 | 1.37644300 | -4.22743700 | H | 2.34767700 | -4.40679100 | 0.65367200 |
| C | -3.24197200 | 0.16466200 | -3.52286400 | C | 2.64876400 | -3.04446300 | 2.27219300 |
| H | -2.79035600 | 0.08752900 | -4.50505600 | H | 2.21352500 | -3.70849200 | 3.02472800 |
| C | -2.62762200 | -0.47901100 | -2.44111700 | H | 2.42916600 | -2.02007700 | 2.57323300 |
| C | -5.22215700 | 0.49449900 | 0.29844400 | H | 3.73207800 | -3.18435700 | 2.31620100 |
| H | -4.70753500 | -0.07380000 | 1.06525800 | C | 4.51850800 | -1.03432100 | -2.50188100 |
| C | -6.65489700 | -0.06642400 | 0.17085100 | H | 3.54838100 | -1.19935000 | -2.96920900 |
| H | -7.14139300 | -0.07775800 | 1.15124300 | H | 5.19943600 | -1.81418000 | -2.85601800 |
| H | -6.66966100 | -1.08148500 | -0.22747800 | H | 4.90767200 | -0.07984600 | -2.85152000 |
| H | -7.26752300 | 0.55577900 | -0.48732900 | C | 5.82447600 | -0.69865600 | -0.41713300 |
| C | -5.29957300 | 1.95432000 | 0.78456100 | H | 6.09107900 | 0.32860400 | -0.67558200 |
| H | -5.80798100 | 2.59088800 | 0.05491000 | H | 6.57592800 | -1.35900100 | -0.85850700 |
| H | -4.31380700 | 2.37958600 | 0.96295800 | H | 5.87708400 | -0.80843100 | 0.66478900 |
| H | -5.86835100 | 2.00385400 | 1.71856400 | C | 3.55247900 | 1.15471900 | -0.04953700 |
| C | -1.36556900 | -1.26965400 | -2.76639400 | C | 3.41399900 | 2.18417600 | -1.01888000 |
| H | -0.99596800 | -1.69968500 | -1.84095900 | C | 3.68852700 | 3.50633000 | -0.64986000 |
| C | -1.65533400 | -2.41159300 | -3.76216300 | H | 3.58899500 | 4.29171200 | -1.39004300 |
| H | -2.48095200 | -3.04564800 | -3.43333000 | C | 4.07138400 | 3.84002000 | 0.63859000 |
| H | -0.77024200 | -3.04397500 | -3.88041400 | H | 4.27426700 | 4.87251800 | 0.90112900 |
| H | -1.91505300 | -2.02191300 | -4.75088700 | C | 4.18492800 | 2.83801900 | 1.58923100 |
| C | -0.25747900 | -0.36270600 | -3.32917500 | H | 4.47728500 | 3.09806700 | 2.60011800 |
| H | -0.57487300 | 0.13727600 | -4.24893100 | C | 3.93977800 | 1.49875200 | 1.27446400 |
| H | 0.63160900 | -0.95244800 | -3.56591800 | C | 2.95153300 | 1.95434800 | -2.45542400 |
| H | 0.02631300 | 0.40141700 | -2.60718700 | H | 2.73321700 | 0.89315500 | -2.56750900 |
| C | -4.44906600 | -2.64405300 | 0.55665300 | C | 1.66072800 | 2.73449100 | -2.77751100 |
| H | -4.96935000 | -2.02764500 | 1.28611100 | H | 0.85190100 | 2.49456500 | -2.08719400 |
| H | -4.60300400 | -3.68865400 | 0.83991100 | H | 1.32111800 | 2.49521600 | -3.78918900 |
| H | -4.91367600 | -2.49781700 | -0.42033200 | H | 1.82688200 | 3.81428900 | -2.73255100 |
| C | -2.33034800 | -3.48473700 | -0.37340000 | C | 4.03920800 | 2.34872600 | -3.47659600 |
| H | -2.77876300 | -3.49349700 | -1.36830800 | H | 4.17468800 | 3.43381800 | -3.50136600 |
| H | -2.53241700 | -4.45711100 | 0.08712100 | H | 3.75284000 | 2.02998500 | -4.48324700 |
| H | -1.25329000 | -3.36889100 | -0.46804700 | H | 5.00998800 | 1.90799900 | -3.24310700 |
| C | -2.70239500 | -0.00564600 | 2.88803600 | C | 4.08485400 | 0.48248700 | 2.40152600 |
| H | -3.20145500 | 0.58687700 | 2.12529800 | H | 3.94850400 | -0.50829900 | 1.97132800 |
| H | -2.10783300 | 0.71033500 | 3.46269800 | C | 2.99214600 | 0.68737500 | 3.46723000 |
| C | -3.78156200 | -0.57556800 | 3.81964100 | H | 3.11007200 | 1.65248400 | 3.96889500 |
| H | -3.37166700 | -1.20656700 | 4.61057400 | H | 3.04833000 | -0.09364500 | 4.23145300 |
| H | -4.52403000 | -1.16835600 | 3.28072200 | H | 1.99808400 | 0.65989800 | 3.02162100 |
| H | -4.31742800 | 0.24733900 | 4.30211300 | C | 5.47323400 | 0.52532100 | 3.07094000 |
| C | -0.43017200 | -1.09451400 | 3.06660200 | H | 6.28499300 | 0.44379300 | 2.34564900 |
| H | 0.02612000 | -0.10079200 | 3.10846900 | H | 5.57085400 | -0.29812900 | 3.78480700 |
| H | 0.27694600 | -1.74073100 | 2.55316800 | H | 5.62153000 | 1.45563200 | 3.62627100 |

*B3LYP/6-311g(d,p) with PCM model for acetonitrile*
(E = -2249.488451)

| | x | y | z | | x | y | z |
|---|---|---|---|---|---|---|---|
| O | -0.18774600 | -1.32073900 | 0.29707400 | C | -0.60198100 | -1.56820800 | 4.50995200 |
| N | -2.59237800 | -0.98174100 | 0.03172500 | H | -1.07925700 | -2.55210500 | 4.54406000 |
| N | 3.34210900 | -0.23867000 | -0.38899100 | H | -1.19689300 | -0.88567900 | 5.12103100 |
| C | -2.94210700 | -2.36283200 | 0.52366600 | H | 0.37589200 | -1.66349700 | 4.99102700 |
| C | -2.29344700 | -2.38073400 | 1.93857000 | C | -1.56510500 | 2.23590700 | 0.56760800 |
| H | -1.48249800 | -3.11168300 | 1.95563600 | C | -1.53311500 | 3.00887300 | 1.73772900 |
| H | -3.01515100 | -2.69138200 | 2.69355600 | H | -1.10120400 | 2.59137300 | 2.63880700 |
| C | -1.70551500 | -0.97948200 | 2.21787400 | C | -2.02540200 | 4.31309000 | 1.75476100 |
| C | -1.40257700 | -0.52027400 | 0.72065700 | H | -1.98623900 | 4.88912900 | 2.67287000 |
| C | -0.88385900 | 0.90687100 | 0.49504400 | C | -2.54707300 | 4.88102300 | 0.59343100 |
| C | 0.43612000 | 0.85869100 | 0.21686300 | H | -2.92256600 | 5.89817400 | 0.60275200 |
| H | 1.04886800 | 1.73434200 | 0.07979600 | C | -2.57107700 | 4.13248600 | -0.58165500 |
| C | 0.92189400 | -0.48857600 | 0.11068100 | H | -2.96414500 | 4.56594600 | -1.49481000 |
| C | 2.16823200 | -0.98830800 | -0.14347800 | C | -2.08821400 | 2.82484700 | -0.59320300 |
| C | 2.48931100 | -2.49388900 | -0.29937600 | H | -2.10936500 | 2.25337700 | -1.51238500 |
| C | 4.02671400 | -2.49125700 | -0.46026400 | C | 1.76855100 | -3.04392800 | -1.57054200 |
| H | 4.37510200 | -3.27186900 | -1.13687000 | H | 0.69598000 | -2.93454200 | -1.40881900 |
| H | 4.50010500 | -2.67360900 | 0.50551600 | H | 2.01056600 | -2.39966400 | -2.41735000 |
| C | 4.44370200 | -1.09459800 | -0.95212100 | C | 2.06245700 | -4.49741900 | -1.96689000 |
| C | -3.20780200 | -0.38719800 | -1.13931000 | H | 1.71165900 | -5.21338200 | -1.22040500 |
| C | -4.44137800 | 0.32587600 | -1.00431600 | H | 3.12807200 | -4.68015700 | -2.12971200 |
| C | -5.01615200 | 0.92658500 | -2.12921300 | H | 1.54918100 | -4.73122900 | -2.90424400 |
| H | -5.94340300 | 1.47608600 | -2.01469200 | C | 2.05924200 | -3.37174400 | 0.91121500 |
| C | -4.43360700 | 0.84587400 | -3.38399400 | H | 0.96983700 | -3.34686900 | 0.97075800 |
| H | -4.89584400 | 1.32601400 | -4.23986900 | H | 2.33224100 | -4.40449900 | 0.67278800 |
| C | -3.25787500 | 0.12972700 | -3.52610100 | C | 2.64416700 | -3.04102300 | 2.28753600 |
| H | -2.80845200 | 0.04508200 | -4.50873600 | H | 2.20502900 | -3.70150900 | 3.04115000 |
| C | -2.63701300 | -0.49909500 | -2.43812600 | H | 2.43163300 | -2.01478700 | 2.58784100 |
| C | -5.22709700 | 0.49395700 | 0.29867100 | H | 3.72653300 | -3.18677400 | 2.32952700 |
| H | -4.70886600 | -0.06507100 | 1.06959900 | C | 4.52110000 | -1.05706100 | -2.49446200 |
| C | -6.66041400 | -0.06798600 | 0.18422000 | H | 3.55140000 | -1.22132000 | -2.96312300 |
| H | -7.14152700 | -0.06523000 | 1.16718800 | H | 5.19898900 | -1.84352300 | -2.83875300 |
| H | -6.67543200 | -1.08962900 | -0.19746900 | H | 4.91684400 | -0.10752400 | -2.85033800 |
| H | -7.27496800 | 0.54494900 | -0.48095600 | C | 5.82488000 | -0.70987900 | -0.41064800 |
| C | -5.30337800 | 1.95934400 | 0.76870700 | H | 6.09681100 | 0.31311000 | -0.68091600 |
| H | -5.82687500 | 2.58414400 | 0.03922600 | H | 6.57302700 | -1.37804800 | -0.84528300 |
| H | -4.31470700 | 2.38749500 | 0.92595900 | H | 5.87556200 | -0.81053800 | 0.67212600 |
| H | -5.85753500 | 2.01660500 | 1.71095800 | C | 3.55163200 | 1.15100200 | -0.05360200 |
| C | -1.37056800 | -1.28482700 | -2.75864000 | C | 3.41812900 | 2.17611300 | -1.02886600 |
| H | -0.99349100 | -1.70013400 | -1.82948600 | C | 3.68621500 | 3.50171600 | -0.66442000 |
| C | -1.65454800 | -2.44074600 | -3.74009200 | H | 3.59230700 | 4.28354200 | -1.40919000 |
| H | -2.46983900 | -3.08151100 | -3.39782200 | C | 4.05908400 | 3.84265500 | 0.62614800 |
| H | -0.76253300 | -3.06348700 | -3.85699500 | H | 4.25796100 | 4.87679700 | 0.88539300 |
| H | -1.92467900 | -2.06355100 | -4.73096300 | C | 4.17097100 | 2.84415400 | 1.58214500 |
| C | -0.27283200 | -0.37619500 | -3.33902500 | H | 4.45820400 | 3.10990000 | 2.59302200 |
| H | -0.59604900 | 0.10198900 | -4.26833400 | C | 3.93248200 | 1.50175300 | 1.27121800 |
| H | 0.62302300 | -0.96004900 | -3.56386800 | C | 2.97205700 | 1.93781600 | -2.46918800 |
| H | 0.00239900 | 0.40461600 | -2.63140700 | H | 2.75767100 | 0.87577700 | -2.57910200 |
| C | -4.45052800 | -2.63927900 | 0.58829800 | C | 1.68405300 | 2.71461200 | -2.81037800 |
| H | -4.96839400 | -2.01662900 | 1.31407900 | H | 0.86779700 | 2.47383300 | -2.12839800 |
| H | -4.59977100 | -3.68098400 | 0.88409700 | H | 1.35792600 | 2.46969300 | -3.82514700 |
| H | -4.92112500 | -2.50551800 | -0.38781400 | H | 1.84907400 | 3.79472300 | -2.76855700 |
| C | -2.33550400 | -3.48459300 | -0.34553100 | C | 4.07100700 | 2.32899500 | -3.47955500 |
| H | -2.79070300 | -3.50279600 | -1.33744400 | H | 4.20647600 | 3.41407500 | -3.50550900 |
| H | -2.53357400 | -4.45243600 | 0.12595600 | H | 3.79421800 | 2.00640600 | -4.48757200 |
| H | -1.25928100 | -3.36643900 | -0.44787800 | H | 5.03794100 | 1.88633100 | -3.23389600 |
| C | -2.69937900 | 0.01926700 | 2.88975900 | C | 4.08343100 | 0.49105100 | 2.40287500 |
| H | -3.20122900 | 0.60457200 | 2.12289000 | H | 3.94441900 | -0.50223000 | 1.97960300 |
| H | -2.10367800 | 0.73922300 | 3.45800500 | C | 3.00065400 | 0.70340200 | 3.47756300 |
| C | -3.77560900 | -0.54502500 | 3.82847100 | H | 3.12943100 | 1.66804100 | 3.97748200 |
| H | -3.36146300 | -1.16996900 | 4.62190600 | H | 3.06062000 | -0.07760400 | 4.24135200 |
| H | -4.51904400 | -1.14244500 | 3.29615400 | H | 2.00159800 | 0.67960500 | 3.04239100 |
| H | -4.30998100 | 0.28123100 | 4.30716000 | C | 5.47654000 | 0.53831500 | 3.06283700 |
| C | -0.42575700 | -1.06540600 | 3.07094200 | H | 6.28336500 | 0.44824400 | 2.33301200 |
| H | 0.02840100 | -0.07042900 | 3.10497200 | H | 5.57668700 | -0.28042600 | 3.78152500 |
| H | 0.28101600 | -1.71485800 | 2.56104500 | H | 5.62749700 | 1.47332400 | 3.60950700 |

*wb97xd/6-311g(d,p) with PCM model for acetonitrile*
(E = -2248.888173)

| | x | y | z | | x | y | z |
|---|---|---|---|---|---|---|---|
| O | -0.14639100 | -1.34366400 | 0.13570000 | C | -0.67641100 | -2.29924400 | 4.18363800 |
| N | -2.51154700 | -1.00776300 | -0.15216800 | H | -1.14320800 | -3.27518500 | 4.01846600 |
| N | 3.30569400 | -0.11507500 | -0.42895500 | H | -1.31273000 | -1.73427100 | 4.86982000 |
| C | -2.82023200 | -2.44770700 | 0.05427400 | H | 0.27952400 | -2.46932800 | 4.68664800 |
| C | -2.23310000 | -2.70198200 | 1.46841200 | C | -1.63554300 | 2.05445400 | 0.89176400 |
| H | -1.40141500 | -3.40752500 | 1.39673400 | C | -1.73836400 | 2.62742300 | 2.16061600 |
| H | -2.97555500 | -3.15242900 | 2.12737700 | H | -1.33895500 | 2.09696700 | 3.01699100 |
| C | -1.69798700 | -1.35929300 | 2.00417100 | C | -2.33269000 | 3.87204000 | 2.33446500 |
| C | -1.35795300 | -0.66052600 | 0.63502400 | H | -2.40501400 | 4.29991400 | 3.32815200 |
| C | -0.88500700 | 0.79061600 | 0.66728300 | C | -2.82252200 | 4.57161300 | 1.23677800 |
| C | 0.43254700 | 0.82576600 | 0.42790100 | H | -3.28526900 | 5.54277400 | 1.37149300 |
| H | 1.02934600 | 1.72380000 | 0.45169400 | C | -2.70638500 | 4.02084900 | -0.03418100 |
| C | 0.93578600 | -0.47946900 | 0.09216200 | H | -3.07667400 | 4.56065600 | -0.89866400 |
| C | 2.15903600 | -0.90591600 | -0.29233400 | C | -2.11729900 | 2.77432600 | -0.20506100 |
| C | 2.47917100 | -2.34623400 | -0.71950200 | H | -2.02849200 | 2.35009100 | -1.19845400 |
| C | 4.00767300 | -2.29508100 | -0.90520100 | C | 1.74584400 | -2.66478400 | -2.04728700 |
| H | 4.34957600 | -2.94070100 | -1.71569400 | H | 0.68124900 | -2.50952700 | -1.88020200 |
| H | 4.50538500 | -2.63305100 | 0.00616400 | H | 2.04302200 | -1.93387900 | -2.80058900 |
| C | 4.38875600 | -0.82846000 | -1.15163800 | C | 1.94951100 | -4.06577100 | -2.62131600 |
| C | -3.08802800 | -0.21936900 | -1.20390200 | H | 1.50518700 | -4.83674900 | -1.98779700 |
| C | -4.33144400 | 0.42963200 | -0.98117500 | H | 3.00709300 | -4.30976000 | -2.75743500 |
| C | -4.87298900 | 1.23536400 | -1.98033200 | H | 1.46977000 | -4.13406700 | -3.60144900 |
| H | -5.81648400 | 1.73901000 | -1.79883500 | C | 2.07449100 | -3.41310200 | 0.32444600 |
| C | -4.23188700 | 1.42169200 | -3.19217400 | H | 0.98243400 | -3.45833400 | 0.35477600 |
| H | -4.66540700 | 2.06248700 | -3.95220800 | H | 2.42053000 | -4.38155700 | -0.05047200 |
| C | -3.03231100 | 0.77439100 | -3.41954700 | C | 2.60215400 | -3.23112700 | 1.74246900 |
| H | -2.52868600 | 0.90913500 | -4.37093400 | H | 2.18691100 | -4.00204700 | 2.39756200 |
| C | -2.45144400 | -0.05024500 | -2.45385800 | H | 2.31451300 | -2.26273200 | 2.14837100 |
| C | -5.13625900 | 0.31718600 | 0.30511600 | H | 3.69128100 | -3.31062900 | 1.79940000 |
| H | -4.61001200 | -0.37321900 | 0.95445800 | C | 4.40986100 | -0.50094900 | -2.65392000 |
| C | -6.54478600 | -0.23961200 | 0.05409500 | H | 3.41893000 | -0.56580500 | -3.10348500 |
| H | -7.03935500 | -0.44499100 | 1.00841800 | H | 5.06823100 | -1.20152800 | -3.17510800 |
| H | -6.52517500 | -1.16445300 | -0.52451000 | H | 4.79309000 | 0.50363800 | -2.82689600 |
| H | -7.16338200 | 0.48130400 | -0.48863700 | C | 5.77132700 | -0.51366400 | -0.58419900 |
| C | -5.24681800 | 1.65024000 | 1.05391500 | H | 6.00754400 | 0.54959500 | -0.67738500 |
| H | -5.78862700 | 2.39445500 | 0.46207800 | H | 6.52169600 | -1.07594900 | -1.14583200 |
| H | -4.26817500 | 2.06272000 | 1.29447800 | H | 5.85093800 | -0.79868900 | 0.46480900 |
| H | -5.79546800 | 1.50252000 | 1.98939800 | C | 3.50561300 | 1.16596200 | 0.17821800 |
| C | -1.12850600 | -0.69799300 | -2.81177500 | C | 3.31825700 | 2.36035400 | -0.54913500 |
| H | -0.81602100 | -1.28619100 | -1.95620200 | C | 3.57386600 | 3.58142300 | 0.07676100 |
| C | -1.24383400 | -1.62458300 | -4.02714200 | H | 3.43918500 | 4.50221400 | -0.48027200 |
| H | -2.03201000 | -2.37026800 | -3.90011900 | C | 3.97857200 | 3.64643400 | 1.39792900 |
| H | -0.29829300 | -2.15332800 | -4.18207700 | H | 4.16472600 | 4.60597000 | 1.86732800 |
| H | -1.46128600 | -1.06144700 | -4.94020400 | C | 4.13146700 | 2.47356500 | 2.11747700 |
| C | -0.05132700 | 0.36102300 | -3.05629100 | H | 4.43289300 | 2.52361300 | 3.15822400 |
| H | -0.29352200 | 0.98914800 | -3.91959400 | C | 3.90718400 | 1.23032600 | 1.53065000 |
| H | 0.91540600 | -0.11187600 | -3.24467000 | C | 2.80796600 | 2.40059400 | -1.97890400 |
| H | 0.05542700 | 1.00320400 | -2.18433700 | H | 2.57262800 | 1.37773400 | -2.27416700 |
| C | -4.31264500 | -2.77301100 | -0.01028500 | C | 1.52472800 | 3.23695200 | -2.10054200 |
| H | -4.88335200 | -2.31091000 | 0.79241100 | H | 0.75249400 | 2.91301800 | -1.40066300 |
| H | -4.43853900 | -3.85486200 | 0.07679000 | H | 1.11712800 | 3.15064100 | -3.11136700 |
| H | -4.74061300 | -2.46426300 | -0.96742100 | H | 1.72404200 | 4.29564600 | -1.91176900 |
| C | -2.13190000 | -3.35722800 | -0.97792200 | C | 3.86583100 | 2.96836200 | -2.93637500 |
| H | -2.52383600 | -3.16842900 | -1.98018200 | H | 4.00261600 | 4.04056900 | -2.76525700 |
| H | -2.33160200 | -4.40497900 | -0.73305000 | H | 3.55415200 | 2.83262600 | -3.97587800 |
| H | -1.05462500 | -3.20332800 | -0.97959200 | H | 4.83921100 | 2.49224500 | -2.80471700 |
| C | -2.73398800 | -0.50861700 | 2.78727400 | C | 4.05632600 | -0.00411200 | 2.39886400 |
| H | -3.18337200 | 0.22208600 | 2.11845600 | H | 3.97746900 | -0.87472500 | 1.74919400 |
| H | -2.18415300 | 0.07945300 | 3.52856100 | C | 2.90917700 | -0.06750000 | 3.41254900 |
| C | -3.85947100 | -1.24516800 | 3.51055600 | H | 2.96348900 | 0.76964800 | 4.11561300 |
| H | -3.48568000 | -2.02652700 | 4.17648200 | H | 2.95040300 | -0.99614500 | 3.98963100 |
| H | -4.55831100 | -1.71448300 | 2.81377300 | H | 1.94644900 | -0.02325600 | 2.90173000 |
| H | -4.43308300 | -0.53784000 | 4.11582100 | C | 5.40938800 | -0.07355800 | 3.11569700 |
| C | -0.44995500 | -1.55955300 | 2.86794200 | H | 6.24371100 | 0.04524500 | 2.42028300 |
| H | -0.02307000 | -0.57407300 | 3.08220400 | H | 5.51618800 | -1.04083100 | 3.61490400 |
| H | 0.28741500 | -2.10189500 | 2.27997500 | H | 5.49958200 | 0.70273200 | 3.88105000 |

*B97D3/6-311g(d,p) with PCM model for acetonitrile*
(E = -2248.167231)

| | x | y | z | | x | y | z |
|---|---|---|---|---|---|---|---|
| O | -0.13456600 | -1.39086600 | 0.14081700 | C | -0.67967500 | -2.24906300 | 4.23004300 |
| N | -2.54050600 | -1.02343000 | -0.14279200 | H | -1.13553900 | -3.23769900 | 4.08913000 |
| N | 3.33618100 | -0.13143700 | -0.40147300 | H | -1.32081600 | -1.67739500 | 4.91148300 |
| C | -2.87878600 | -2.46398300 | 0.10422900 | H | 0.28479700 | -2.39768200 | 4.73301100 |
| C | -2.28254000 | -2.69348000 | 1.52598100 | C | -1.63674500 | 2.05207400 | 0.83883300 |
| H | -1.45922200 | -3.41280900 | 1.46432700 | C | -1.68865800 | 2.66942000 | 2.10168300 |
| H | -3.03024700 | -3.11765000 | 2.20013600 | H | -1.26078800 | 2.15566800 | 2.95864300 |
| C | -1.72388400 | -1.34258000 | 2.02976200 | C | -2.26984500 | 3.93159300 | 2.26235100 |
| C | -1.38908900 | -0.66349100 | 0.63677500 | H | -2.30142700 | 4.38978000 | 3.24928800 |
| C | -0.89680600 | 0.77939000 | 0.63278600 | C | -2.79775400 | 4.60799000 | 1.15633600 |
| C | 0.44162600 | 0.79733600 | 0.39719700 | H | -3.24971300 | 5.59028600 | 1.27963900 |
| H | 1.04539000 | 1.69383500 | 0.41006100 | C | -2.73245400 | 4.01489400 | -0.10907200 |
| C | 0.94497400 | -0.50685400 | 0.09262000 | H | -3.13255100 | 4.53421100 | -0.97801100 |
| C | 2.19604500 | -0.93725800 | -0.26343000 | C | -2.15708500 | 2.75081100 | -0.26678000 |
| C | 2.53892700 | -2.38510400 | -0.65847700 | H | -2.10520400 | 2.29790700 | -1.25167700 |
| C | 4.07726500 | -2.32922400 | -0.81863800 | C | 1.82522200 | -2.73246600 | -1.99899200 |
| H | 4.43426900 | -2.98359000 | -1.61865300 | H | 0.75260000 | -2.59607900 | -1.84301900 |
| H | 4.56031300 | -2.65501800 | 0.10759700 | H | 2.11938500 | -1.99405300 | -2.75100400 |
| C | 4.46055100 | -0.85938900 | -1.08017100 | C | 2.07031900 | -4.13800800 | -2.56281800 |
| C | -3.10964900 | -0.24172100 | -1.20731300 | H | 1.64224300 | -4.91793600 | -1.92274200 |
| C | -4.34713400 | 0.44130700 | -0.98910700 | H | 3.13856000 | -4.35582400 | -2.68971400 |
| C | -4.87435200 | 1.25173100 | -2.00455500 | H | 1.59833500 | -4.22840600 | -3.54961500 |
| H | -5.80732000 | 1.78157600 | -1.82496800 | C | 2.12402300 | -3.43935500 | 0.40458800 |
| C | -4.22340600 | 1.41394700 | -3.22439100 | H | 1.02984500 | -3.48573200 | 0.41998900 |
| H | -4.64342600 | 2.05955100 | -3.99391200 | H | 2.47924300 | -4.41620600 | 0.05062400 |
| C | -3.03042100 | 0.73368700 | -3.44574100 | C | 2.63494900 | -3.22034200 | 1.82991000 |
| H | -2.52175900 | 0.84609900 | -4.40089900 | H | 2.21926800 | -3.98254600 | 2.50129400 |
| C | -2.46468300 | -0.10173900 | -2.46718400 | H | 2.33326200 | -2.24213000 | 2.20922600 |
| C | -5.15524100 | 0.35953500 | 0.30150300 | H | 3.72781800 | -3.28657500 | 1.89896100 |
| H | -4.64020400 | -0.33732900 | 0.95872400 | C | 4.52667000 | -0.56048900 | -2.59190300 |
| C | -6.58222900 | -0.17291400 | 0.05249400 | H | 3.55170100 | -0.66736700 | -3.07379700 |
| H | -7.08227400 | -0.36623400 | 1.01078200 | H | 5.22479100 | -1.25787300 | -3.07143000 |
| H | -6.58036400 | -1.10184500 | -0.52610900 | H | 4.88956300 | 0.45267400 | -2.77393000 |
| H | -7.18619300 | 0.56204500 | -0.49433100 | C | 5.81944600 | -0.51377100 | -0.46268800 |
| C | -5.23971200 | 1.70833300 | 1.04163900 | H | 6.03519700 | 0.55722300 | -0.54914200 |
| H | -5.75223400 | 2.46393500 | 0.43305600 | H | 6.60388000 | -1.06347700 | -0.99601800 |
| H | -4.25111500 | 2.09572700 | 1.29196700 | H | 5.86069400 | -0.79663200 | 0.59160900 |
| H | -5.80879200 | 1.58268200 | 1.97240500 | C | 3.50759300 | 1.18278200 | 0.15523500 |
| C | -1.16831900 | -0.80661900 | -2.83228900 | C | 3.33915500 | 2.35005500 | -0.63682600 |
| H | -0.85851900 | -1.39139600 | -1.96868600 | C | 3.59385500 | 3.60558000 | -0.05962800 |
| C | -1.35323400 | -1.75538200 | -4.03281400 | H | 3.47739400 | 4.49992200 | -0.66766000 |
| H | -2.19108500 | -2.44524900 | -3.88032200 | C | 3.97393000 | 3.73256500 | 1.27337500 |
| H | -0.44322100 | -2.34978600 | -4.18442600 | H | 4.16308700 | 4.71580700 | 1.70034700 |
| H | -1.54486800 | -1.19530700 | -4.95745500 | C | 4.09811800 | 2.58729600 | 2.05768200 |
| C | -0.05163000 | 0.20865600 | -3.12248300 | H | 4.38026100 | 2.68249800 | 3.10394100 |
| H | -0.31424700 | 0.86550700 | -3.96141200 | C | 3.87444400 | 1.31057500 | 1.52339800 |
| H | 0.88063400 | -0.30610200 | -3.37805400 | C | 2.84535300 | 2.33080100 | -2.07647300 |
| H | 0.13387000 | 0.82675600 | -2.24373200 | H | 2.63497800 | 1.29147700 | -2.34056100 |
| C | -4.38311600 | -2.75798500 | 0.05120700 | C | 1.53946000 | 3.14035400 | -2.23258600 |
| H | -4.93921500 | -2.26978800 | 0.85221900 | H | 0.76244400 | 2.80117700 | -1.54155300 |
| H | -4.53156800 | -3.83925700 | 0.15279600 | H | 1.15372600 | 3.03795500 | -3.25400200 |
| H | -4.80770900 | -2.45028200 | -0.91080400 | H | 1.71472200 | 4.20690400 | -2.04524200 |
| C | -2.20788500 | -3.40792200 | -0.91685900 | C | 3.90346100 | 2.89301700 | -3.04921700 |
| H | -2.61212600 | -3.24111400 | -1.92084400 | H | 4.02694800 | 3.97341800 | -2.90093300 |
| H | -2.41516300 | -4.44992000 | -0.63880300 | H | 3.59277300 | 2.72984100 | -4.08907500 |
| H | -1.12766200 | -3.26092000 | -0.93562400 | H | 4.88459900 | 2.42856400 | -2.90490000 |
| C | -2.75051000 | -0.45458000 | 2.79588800 | C | 3.98970300 | 0.11548900 | 2.45474100 |
| H | -3.20025100 | 0.25243400 | 2.09921100 | H | 3.89863500 | -0.78387900 | 1.84310200 |
| H | -2.18628500 | 0.16089500 | 3.50786600 | C | 2.82385900 | 0.12254500 | 3.46155100 |
| C | -3.87883200 | -1.15611200 | 3.56088500 | H | 2.89957600 | 0.98319800 | 4.13901500 |
| H | -3.50598400 | -1.91168300 | 4.26118400 | H | 2.82950800 | -0.79020300 | 4.07083900 |
| H | -4.58703800 | -1.65284800 | 2.88788300 | H | 1.86633600 | 0.18305700 | 2.93813600 |
| H | -4.44723400 | -0.41573400 | 4.13881800 | C | 5.33779100 | 0.05597000 | 3.19745600 |
| C | -0.46737500 | -1.53178600 | 2.89208600 | H | 6.18638300 | 0.11869900 | 2.50710800 |
| H | -0.03796100 | -0.53996000 | 3.08218300 | H | 5.41602900 | -0.88693000 | 3.75381900 |
| H | 0.26579300 | -2.08420300 | 2.30464300 | H | 5.43315700 | 0.87565600 | 3.92051900 |

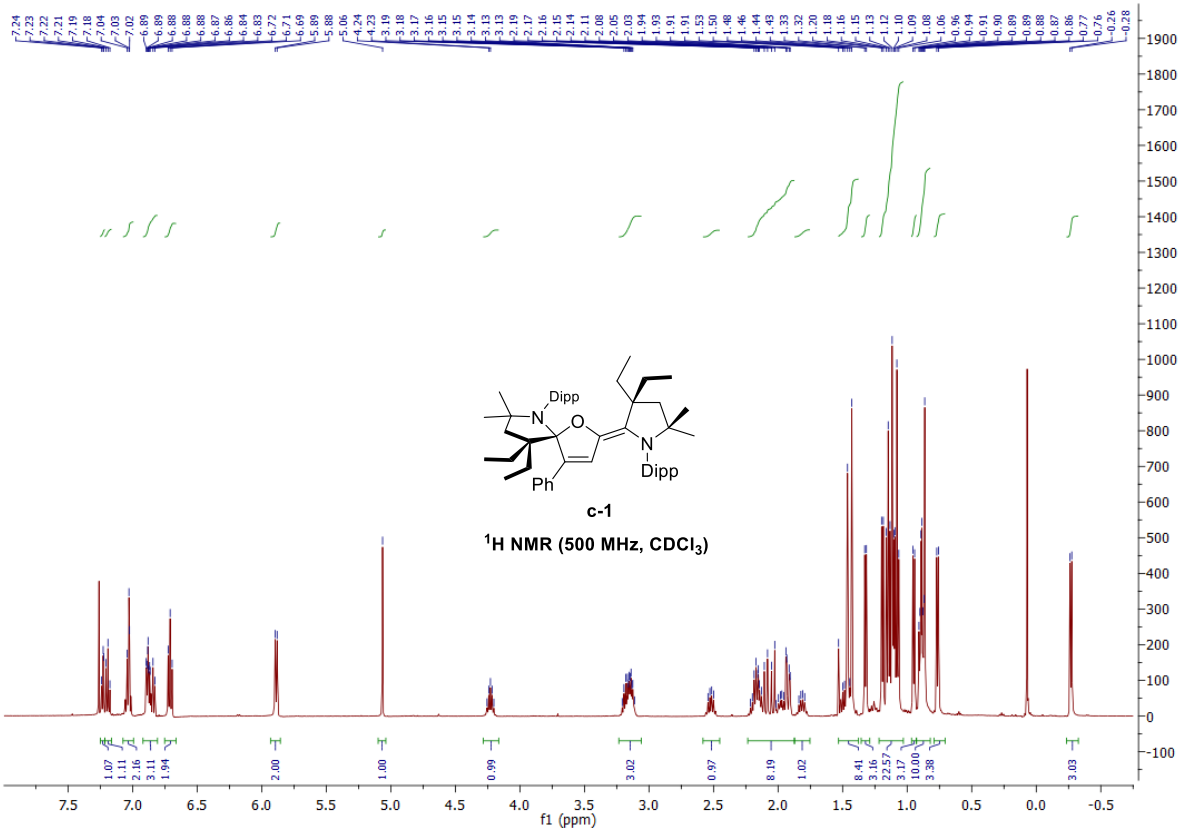
*M06/6-311g(d,p) with PCM model for acetonitrile*
(E = -2247.815622)

| | x | y | z | | x | y | z |
|---|---|---|---|---|---|---|---|
| O | -0.14786000 | -1.32611400 | 0.23596200 | C | -0.65708200 | -1.92870000 | 4.34649200 |
| N | -2.51793100 | -1.00610000 | -0.05862700 | H | -1.11329800 | -2.92236100 | 4.26113100 |
| N | 3.33075200 | -0.18532800 | -0.39140800 | H | -1.29611200 | -1.32399500 | 4.99894700 |
| C | -2.85371400 | -2.41210400 | 0.30533000 | H | 0.30247300 | -2.05519400 | 4.86087400 |
| C | -2.24720700 | -2.53153600 | 1.72290400 | C | -1.58830500 | 2.14112100 | 0.70763000 |
| H | -1.42331500 | -3.25569700 | 1.71069700 | C | -1.61382800 | 2.84524800 | 1.91275200 |
| H | -2.98416200 | -2.91316300 | 2.43544900 | H | -1.18642700 | 2.38818000 | 2.80201400 |
| C | -1.68824100 | -1.15554300 | 2.11625800 | C | -2.16025200 | 4.11981300 | 1.98358200 |
| C | -1.35349200 | -0.59294200 | 0.68449600 | H | -2.16866600 | 4.65000400 | 2.93139000 |
| C | -0.87179900 | 0.84850700 | 0.57989300 | C | -2.68084700 | 4.71996500 | 0.84414500 |
| C | 0.44711700 | 0.85147900 | 0.32254700 | H | -3.10602200 | 5.71764400 | 0.89814900 |
| H | 1.04602600 | 1.75241300 | 0.26429300 | C | -2.63911500 | 4.04133800 | -0.36619700 |
| C | 0.94009400 | -0.47653300 | 0.11073800 | H | -3.02939000 | 4.50617400 | -1.26745600 |
| C | 2.17318500 | -0.94878000 | -0.20254700 | C | -2.09511200 | 2.76631400 | -0.43348400 |
| C | 2.48988000 | -2.42127500 | -0.47184100 | H | -2.05174200 | 2.24325800 | -1.38577900 |
| C | 4.01473800 | -2.40847400 | -0.66017500 | C | 1.77042400 | -2.87053200 | -1.76297600 |
| H | 4.33955600 | -3.11872500 | -1.42799200 | H | 0.70637100 | -2.64132400 | -1.65387900 |
| H | 4.51263600 | -2.69925300 | 0.27100600 | H | 2.12522600 | -2.24735400 | -2.59284000 |
| C | 4.42792300 | -0.97831100 | -1.01205900 | C | 1.92246800 | -4.33457800 | -2.14374800 |
| C | -3.11157300 | -0.31438800 | -1.16794200 | H | 1.38321800 | -4.99626300 | -1.45835700 |
| C | -4.33307700 | 0.38737600 | -0.98427900 | H | 2.97013200 | -4.65695600 | -2.16186500 |
| C | -4.88624400 | 1.09130400 | -2.05091000 | H | 1.51321400 | -4.50631300 | -3.14475400 |
| H | -5.81385500 | 1.63742800 | -1.89760000 | C | 2.09523100 | -3.37004000 | 0.67696800 |
| C | -4.28198500 | 1.12215200 | -3.29362200 | H | 1.00102800 | -3.43890400 | 0.70823900 |
| H | -4.72781500 | 1.68266600 | -4.11025400 | H | 2.45810500 | -4.37165800 | 0.40851500 |
| C | -3.11003800 | 0.41747200 | -3.48371000 | C | 2.61706800 | -3.03198700 | 2.06300200 |
| H | -2.64090600 | 0.42015900 | -4.46441200 | H | 2.20030500 | -3.72495600 | 2.80250900 |
| C | -2.51680600 | -0.30828000 | -2.45023200 | H | 2.33446200 | -2.02035800 | 2.36690600 |
| C | -5.11365000 | 0.42090100 | 0.31542700 | H | 3.70843700 | -3.10663100 | 2.13380900 |
| H | -4.58752000 | -0.21506300 | 1.02506900 | C | 4.51938200 | -0.78812600 | -2.52716700 |
| C | -6.53015900 | -0.12819800 | 0.14457800 | H | 3.55703700 | -0.93065900 | -3.02571500 |
| H | -7.00029100 | -0.26361000 | 1.12652200 | H | 5.22606400 | -1.51565100 | -2.94272600 |
| H | -6.54523100 | -1.09170500 | -0.37288600 | H | 4.89028000 | 0.20782100 | -2.77921500 |
| H | -7.15904800 | 0.56519400 | -0.42607000 | C | 5.78547600 | -0.63943200 | -0.41921300 |
| C | -5.19196200 | 1.81415900 | 0.93295000 | H | 6.05229300 | 0.41032300 | -0.58828900 |
| H | -5.70399800 | 2.52034000 | 0.26762100 | H | 6.54858300 | -1.25906200 | -0.90262800 |
| H | -4.20214400 | 2.22144800 | 1.15208000 | H | 5.81955300 | -0.84313800 | 0.65406100 |
| H | -5.76019400 | 1.77153400 | 1.87069500 | C | 3.50914200 | 1.16882400 | 0.03795900 |
| C | -1.25027000 | -1.06105400 | -2.78669600 | C | 3.34068500 | 2.25158300 | -0.85077300 |
| H | -0.92047000 | -1.56535500 | -1.87868300 | C | 3.57268300 | 3.54763700 | -0.39047400 |
| C | -1.48349300 | -2.11274900 | -3.86874000 | H | 3.45205000 | 4.38248400 | -1.07578400 |
| H | -2.34141100 | -2.75441000 | -3.64291800 | C | 3.93352200 | 3.79589500 | 0.91998500 |
| H | -0.59785000 | -2.75314300 | -3.96806500 | H | 4.10408200 | 4.81343200 | 1.25887000 |
| H | -1.66545000 | -1.64887700 | -4.84594300 | C | 4.06402900 | 2.73520000 | 1.79784000 |
| C | -0.13386200 | -0.11544800 | -3.21431600 | H | 4.33369500 | 2.92974400 | 2.83281600 |
| H | -0.41626000 | 0.47335900 | -4.09596500 | C | 3.86270700 | 1.42227200 | 1.38196600 |
| H | 0.77069800 | -0.68016400 | -3.47086200 | C | 2.86446000 | 2.09989800 | -2.27860700 |
| H | 0.11920300 | 0.57645300 | -2.40726800 | H | 2.67361800 | 1.03557200 | -2.45382500 |
| C | -4.34750900 | -2.71132200 | 0.29589500 | C | 1.55910000 | 2.85844400 | -2.52297500 |
| H | -4.90897800 | -2.15305500 | 1.04617300 | H | 0.77200000 | 2.57145100 | -1.81761600 |
| H | -4.48959800 | -3.77661000 | 0.50660000 | H | 1.19154300 | 2.65620900 | -3.53544500 |
| H | -4.78398300 | -2.51098500 | -0.68915500 | H | 1.70624400 | 3.94099200 | -2.43687600 |
| C | -2.21597000 | -3.44632100 | -0.62884300 | C | 3.91454700 | 2.58625400 | -3.27725600 |
| H | -2.64307700 | -3.38321400 | -1.63574600 | H | 4.00316700 | 3.67855400 | -3.24556400 |
| H | -2.42528700 | -4.45264400 | -0.24599400 | H | 3.63348000 | 2.30804500 | -4.29922700 |
| H | -1.13347500 | -3.32504900 | -0.69088600 | H | 4.90806200 | 2.17525500 | -3.07184500 |
| C | -2.69767900 | -0.21692100 | 2.82222600 | C | 3.98869000 | 0.33026200 | 2.41808000 |
| H | -3.12837300 | 0.47052200 | 2.09168900 | H | 3.86274000 | -0.62613100 | 1.90322800 |
| H | -2.12850900 | 0.42390900 | 3.50926200 | C | 2.87880700 | 0.45514000 | 3.45951700 |
| C | -3.83878600 | -0.84407800 | 3.60786300 | H | 3.01092000 | 1.35928300 | 4.06565300 |
| H | -3.49365800 | -1.55308700 | 4.36780600 | H | 2.88606100 | -0.40529200 | 4.14011300 |
| H | -4.54619500 | -1.37941600 | 2.96468200 | H | 1.89354400 | 0.50980400 | 2.98566400 |
| H | -4.40603900 | -0.06120400 | 4.12324900 | C | 5.34798600 | 0.31832200 | 3.11241500 |
| C | -0.44223200 | -1.28880600 | 2.98545400 | H | 6.17795500 | 0.29620100 | 2.39903600 |
| H | -0.01164900 | -0.28721800 | 3.12630300 | H | 5.43078300 | -0.56401300 | 3.75765200 |
| H | 0.29646500 | -1.87220600 | 2.43467000 | H | 5.48191400 | 1.20058900 | 3.74880700 |

*M06-2X/6-311g(d,p) with PCM model for acetonitrile*
(E = -2248.550152)

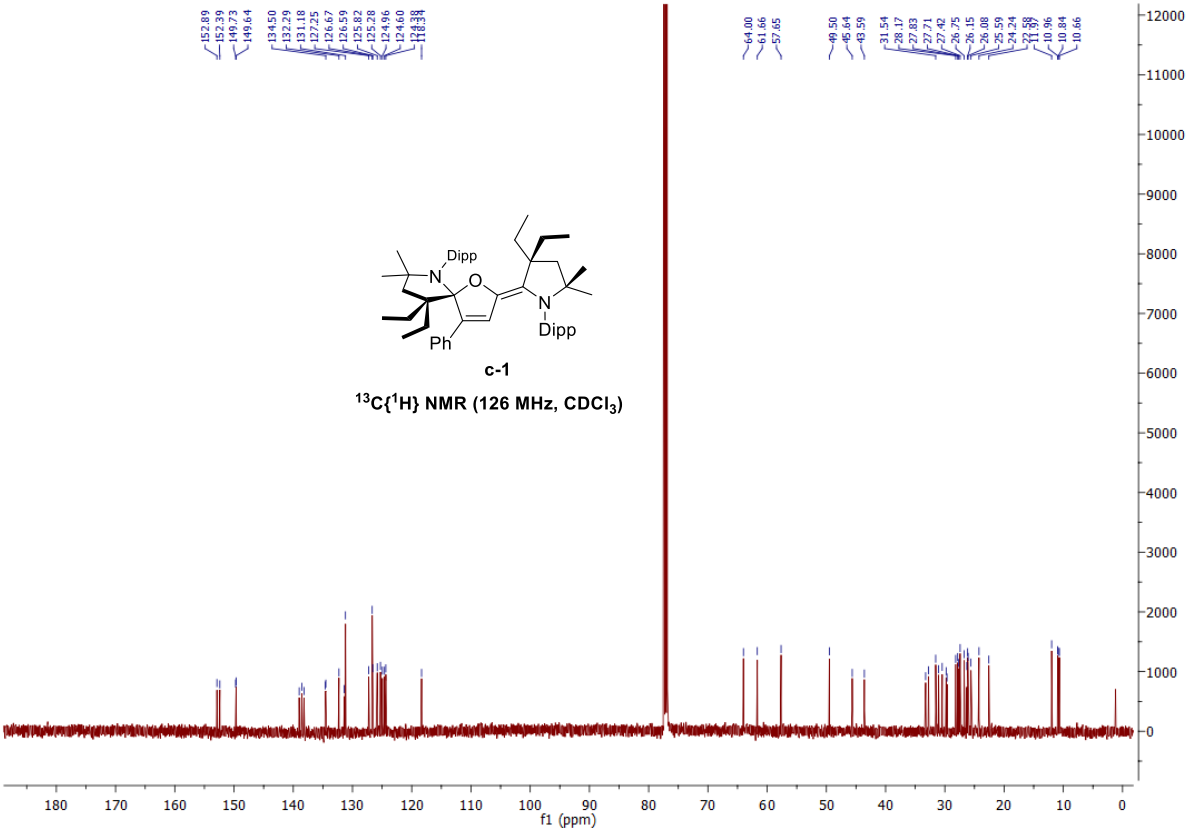
| | x | y | z | | x | y | z |
|---|---|---|---|---|---|---|---|
| O | -0.14743200 | -1.34867100 | 0.12072400 | C | -0.68174000 | -2.31536400 | 4.16951700 |
| N | -2.52026900 | -1.00209300 | -0.14961300 | H | -1.17419500 | -3.27876100 | 4.00778900 |
| N | 3.32166300 | -0.13038100 | -0.42580500 | H | -1.30342400 | -1.72848000 | 4.84962800 |
| C | -2.83684600 | -2.44307500 | 0.05056900 | H | 0.26827400 | -2.50793700 | 4.67408400 |
| C | -2.24787400 | -2.70721200 | 1.46369200 | C | -1.64686400 | 2.04666800 | 0.90460500 |
| H | -1.42231200 | -3.42036600 | 1.38470100 | C | -1.72600000 | 2.61719500 | 2.17861300 |
| H | -2.99356200 | -3.14905600 | 2.12552000 | H | -1.29222700 | 2.09188800 | 3.02161400 |
| C | -1.69120000 | -1.36934400 | 1.99746200 | C | -2.34107200 | 3.85032000 | 2.37180900 |
| C | -1.35380200 | -0.66688900 | 0.62932500 | H | -2.39470500 | 4.27435600 | 3.36777800 |
| C | -0.88438300 | 0.78839800 | 0.66890700 | C | -2.87409400 | 4.54226100 | 1.28787500 |
| C | 0.43730500 | 0.82677500 | 0.43272900 | H | -3.35159600 | 5.50375300 | 1.43666800 |
| H | 1.03482300 | 1.72577900 | 0.46561600 | C | -2.77698200 | 3.99808700 | 0.01120500 |
| C | 0.94044600 | -0.48106500 | 0.08726000 | H | -3.17666700 | 4.53456100 | -0.84192900 |
| C | 2.16707600 | -0.90956700 | -0.29687600 | C | -2.16642700 | 2.76228500 | -0.18017100 |
| C | 2.47844000 | -2.35484000 | -0.71541700 | H | -2.08909400 | 2.34655200 | -1.17944400 |
| C | 4.00651300 | -2.31875700 | -0.92145700 | C | 1.73856700 | -2.69004000 | -2.03425800 |
| H | 4.32200800 | -2.94956300 | -1.75481600 | H | 0.68439100 | -2.45236800 | -1.89611300 |
| H | 4.51536600 | -2.68100300 | -0.02558100 | H | 2.10452200 | -2.02942300 | -2.82228400 |
| C | 4.40332100 | -0.85126900 | -1.14900600 | C | 1.85889900 | -4.13901000 | -2.51076600 |
| C | -3.09876500 | -0.20507200 | -1.19468900 | H | 1.30925000 | -4.82441300 | -1.86280600 |
| C | -4.33766900 | 0.44945400 | -0.95829800 | H | 2.89838300 | -4.47603100 | -2.55218300 |
| C | -4.87640900 | 1.27383000 | -1.94593300 | H | 1.44216000 | -4.23414500 | -3.51604400 |
| H | -5.81472400 | 1.78299400 | -1.75339300 | C | 2.08293600 | -3.40015500 | 0.35270200 |
| C | -4.23460600 | 1.47151900 | -3.15877600 | H | 0.99023800 | -3.45533400 | 0.38425900 |
| H | -4.66425700 | 2.12678500 | -3.90791400 | H | 2.44064800 | -4.37344300 | 0.00303700 |
| C | -3.04234300 | 0.81145000 | -3.40217900 | C | 2.61702000 | -3.16545900 | 1.76327900 |
| H | -2.54170600 | 0.94924600 | -4.35474000 | H | 2.19527200 | -3.90317400 | 2.45096100 |
| C | -2.46763400 | -0.03303700 | -2.44768500 | H | 2.34098500 | -2.17638000 | 2.12638200 |
| C | -5.13786900 | 0.31990700 | 0.32940200 | H | 3.70489400 | -3.25609400 | 1.81792400 |
| H | -4.61314100 | -0.38017400 | 0.96985400 | C | 4.43307300 | -0.49974700 | -2.64391100 |
| C | -6.55020200 | -0.22380900 | 0.06634600 | H | 3.44540500 | -0.56668300 | -3.10051100 |
| H | -7.04356300 | -0.45032300 | 1.01592100 | H | 5.10490200 | -1.18364600 | -3.16910400 |
| H | -6.53772300 | -1.13135000 | -0.53833700 | H | 4.80631500 | 0.51268600 | -2.79105900 |
| H | -7.16156300 | 0.51839000 | -0.45373300 | C | 5.78440300 | -0.55359000 | -0.56840900 |
| C | -5.25087000 | 1.64599500 | 1.09305000 | H | 6.02948800 | 0.50844100 | -0.65098700 |
| H | -5.77309600 | 2.39989400 | 0.49675600 | H | 6.53202000 | -1.11805500 | -1.13074000 |
| H | -4.27458800 | 2.04892300 | 1.36092600 | H | 5.85151500 | -0.85063900 | 0.47838900 |
| H | -5.82384200 | 1.48943900 | 2.01197400 | C | 3.52887200 | 1.16480500 | 0.15238900 |
| C | -1.16341400 | -0.71020700 | -2.81768700 | C | 3.32877700 | 2.34735800 | -0.59308400 |
| H | -0.86479200 | -1.31230800 | -1.96642900 | C | 3.61138500 | 3.57940300 | 0.00327200 |
| C | -1.31382500 | -1.61791200 | -4.04504400 | H | 3.46958300 | 4.48955500 | -0.56895800 |
| H | -2.14211800 | -2.32084400 | -3.93936300 | C | 4.05595900 | 3.66584500 | 1.31224200 |
| H | -0.39394300 | -2.19122100 | -4.19651000 | H | 4.26516100 | 4.63213300 | 1.75647300 |
| H | -1.48981600 | -1.02845900 | -4.94960400 | C | 4.21989600 | 2.50421400 | 2.05122900 |
| C | -0.06150400 | 0.32274300 | -3.07277100 | H | 4.55299300 | 2.56934400 | 3.08112700 |
| H | -0.31430900 | 0.96604700 | -3.92130100 | C | 3.96767900 | 1.25103400 | 1.49329900 |
| H | 0.88476000 | -0.17662100 | -3.29799400 | C | 2.78184300 | 2.36860600 | -2.00993200 |
| H | 0.08641500 | 0.95025500 | -2.19490700 | H | 2.54527600 | 1.34130100 | -2.29207800 |
| C | -4.33248900 | -2.75577000 | -0.02454000 | C | 1.49433700 | 3.20414200 | -2.10531800 |
| H | -4.90594600 | -2.31222900 | 0.78674100 | H | 0.72990300 | 2.87386500 | -1.40000500 |
| H | -4.46248500 | -3.83871200 | 0.03255700 | H | 1.07757100 | 3.12914000 | -3.11303200 |
| H | -4.75081000 | -2.41909300 | -0.97687400 | H | 1.70185000 | 4.25866500 | -1.90730900 |
| C | -2.15265100 | -3.34965300 | -0.98727400 | C | 3.80796400 | 2.95016200 | -2.99628700 |
| H | -2.53388100 | -3.13964700 | -1.98969500 | H | 3.90635400 | 4.02882400 | -2.84496100 |
| H | -2.37541600 | -4.39510100 | -0.75484200 | H | 3.48127400 | 2.78642300 | -4.02640000 |
| H | -1.07183800 | -3.21661200 | -0.97624900 | H | 4.79955700 | 2.51365900 | -2.87272700 |
| C | -2.70870500 | -0.50751700 | 2.79207100 | C | 4.12689800 | 0.03112700 | 2.38036800 |
| H | -3.15197600 | 0.23528100 | 2.13038500 | H | 4.04975900 | -0.85269400 | 1.74710000 |
| H | -2.14576000 | 0.06497500 | 3.53619200 | C | 2.98267800 | -0.01142600 | 3.40031200 |
| C | -3.83846400 | -1.24120200 | 3.51624900 | H | 3.04080400 | 0.84670300 | 4.07633500 |
| H | -3.46708900 | -2.04343200 | 4.15731800 | H | 3.03009100 | -0.92361200 | 4.00225400 |
| H | -4.55327000 | -1.68328800 | 2.81820400 | H | 2.01811800 | 0.01848700 | 2.89024500 |
| H | -4.39059700 | -0.53831700 | 4.14477000 | C | 5.47997600 | -0.01184200 | 3.10027900 |
| C | -0.43745800 | -1.58994400 | 2.84701200 | H | 6.31316400 | 0.12189200 | 2.40726000 |
| H | 0.01401200 | -0.61254400 | 3.05085800 | H | 5.60100800 | -0.97516600 | 3.60239400 |
| H | 0.27797700 | -2.15874800 | 2.25563300 | H | 5.55063000 | 0.76709000 | 3.86364400 |

## NMR spectra



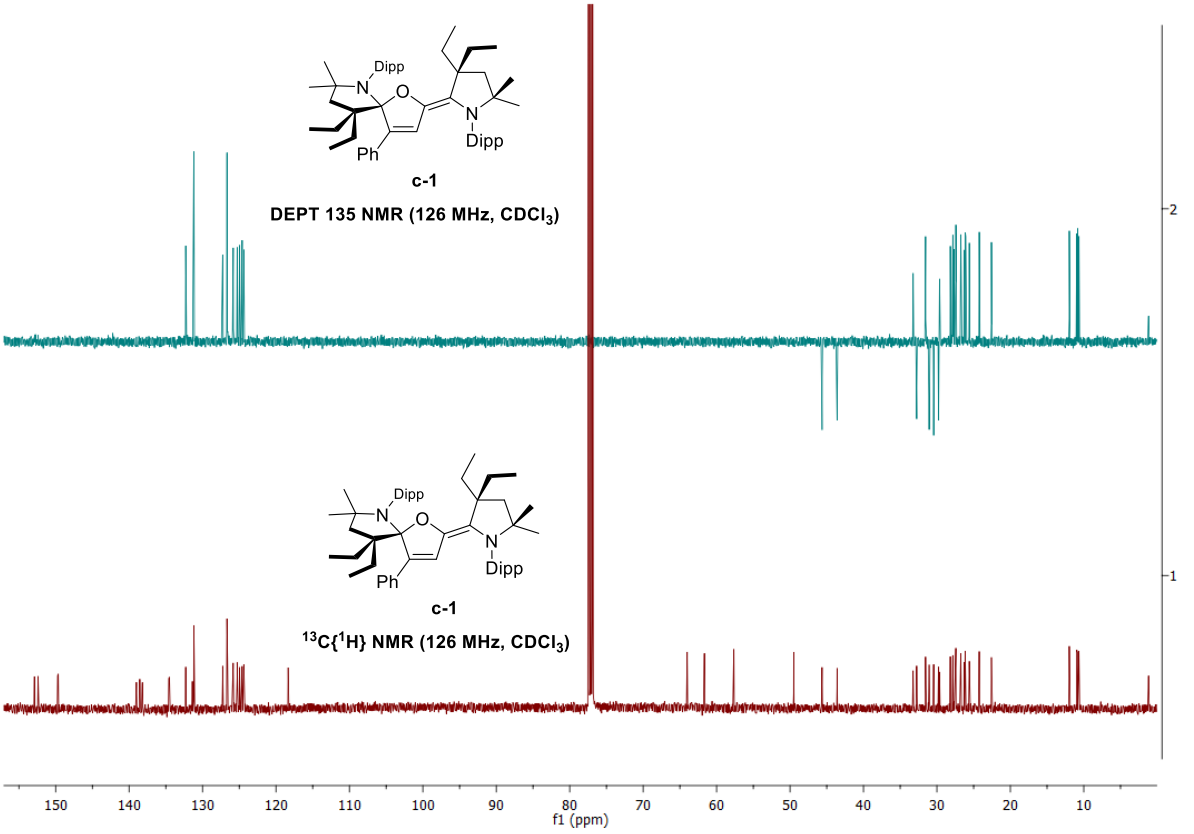

**c-1**

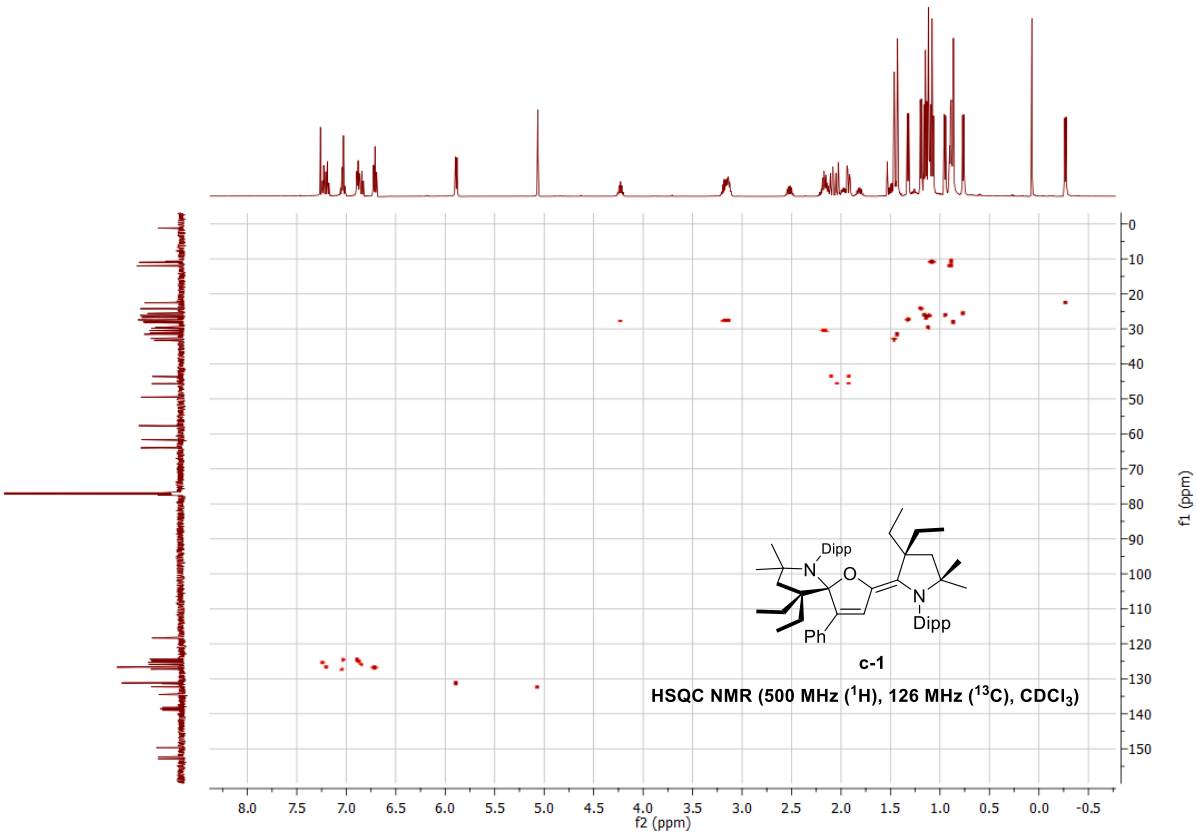
**$^{1}$H NMR (500 MHz, $CDCl_3$)**

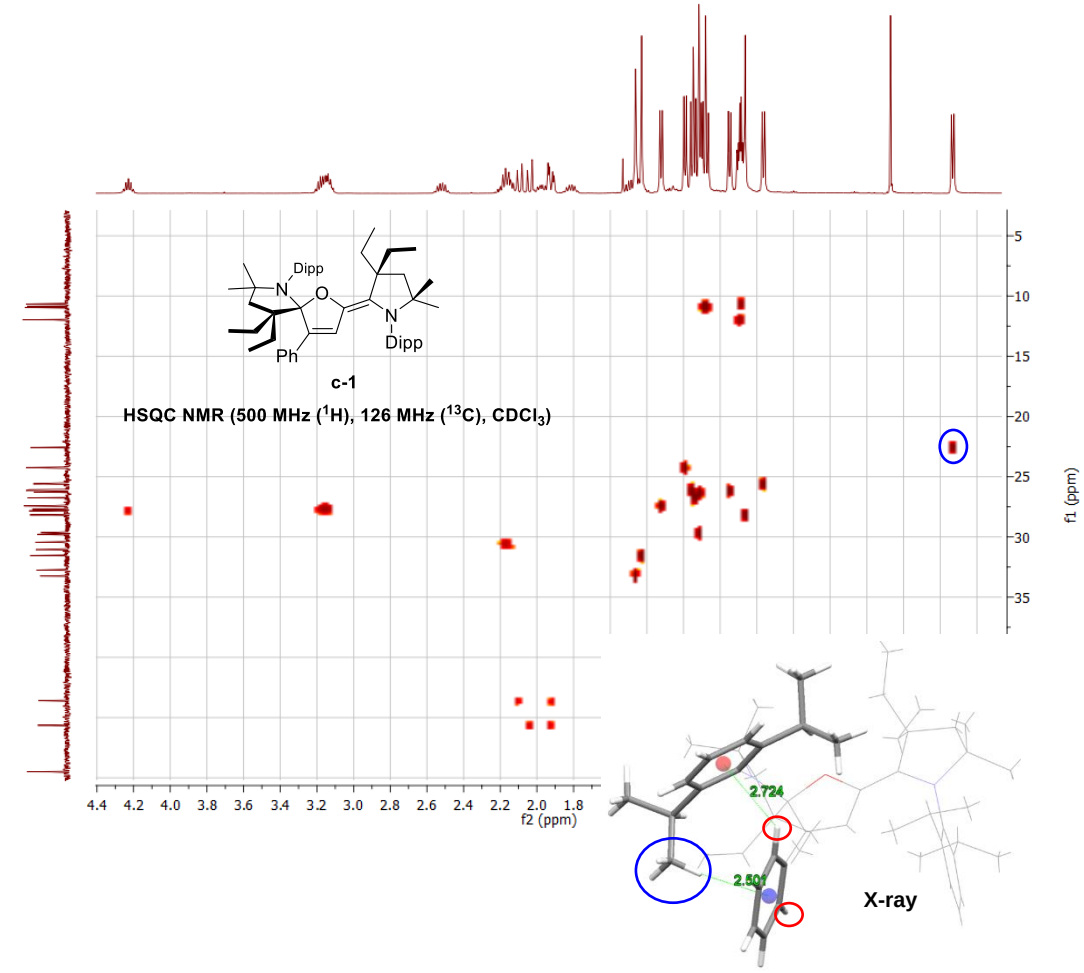


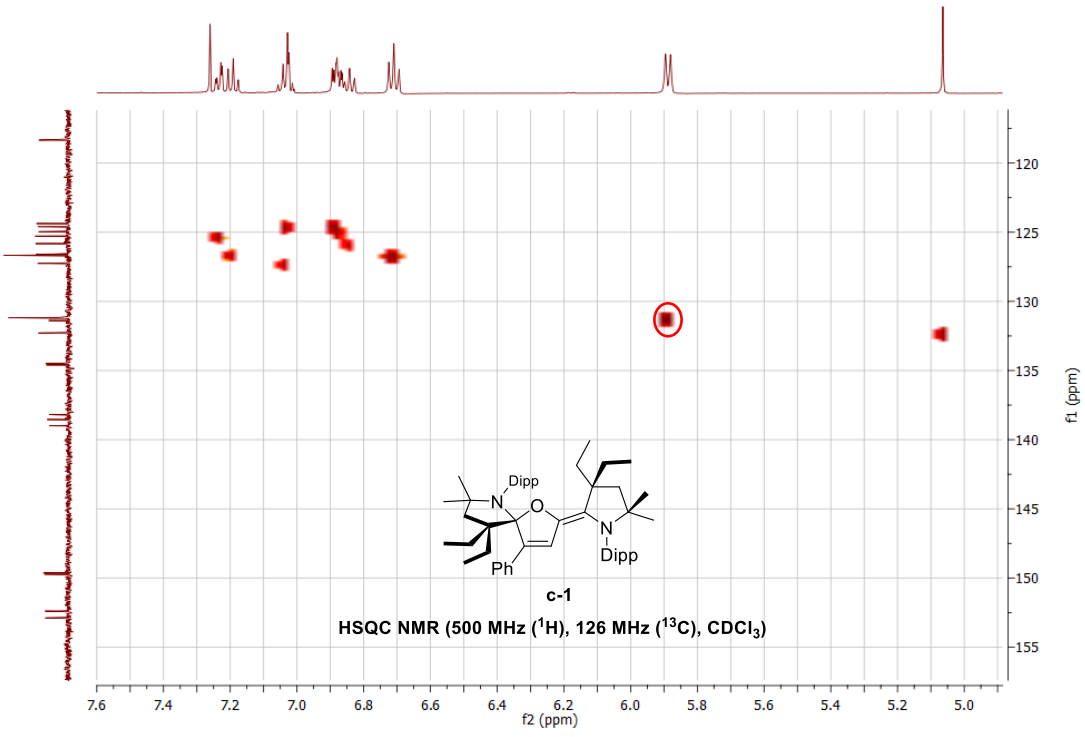

**c-1**

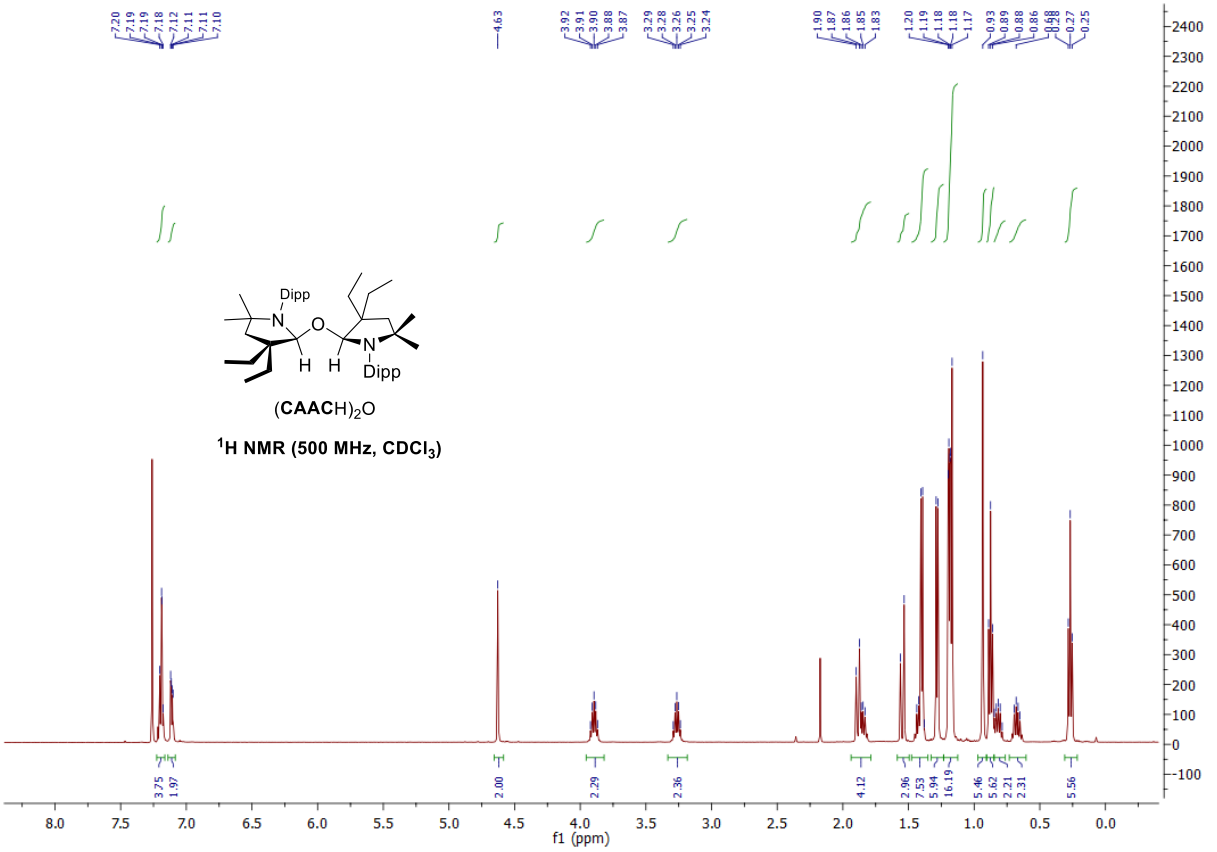
**$^{13}$C{$^{1}$H} NMR (126 MHz, $CDCl_3$)**


Dipp
N
O
N
Dipp
Ph
c-1
DEPT 135 NMR (126 MHz, CDCl3)
2
1
Dipp
N
O
N
Dipp
Ph
c-1
13C{1H} NMR (126 MHz, CDCl3)
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150
f1 (ppm)
Dipp
N
O
N
Dipp
Ph
c-1
HSQC NMR (500 MHz (1H), 126 MHz (13C), CDCl3)
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f2 (ppm)

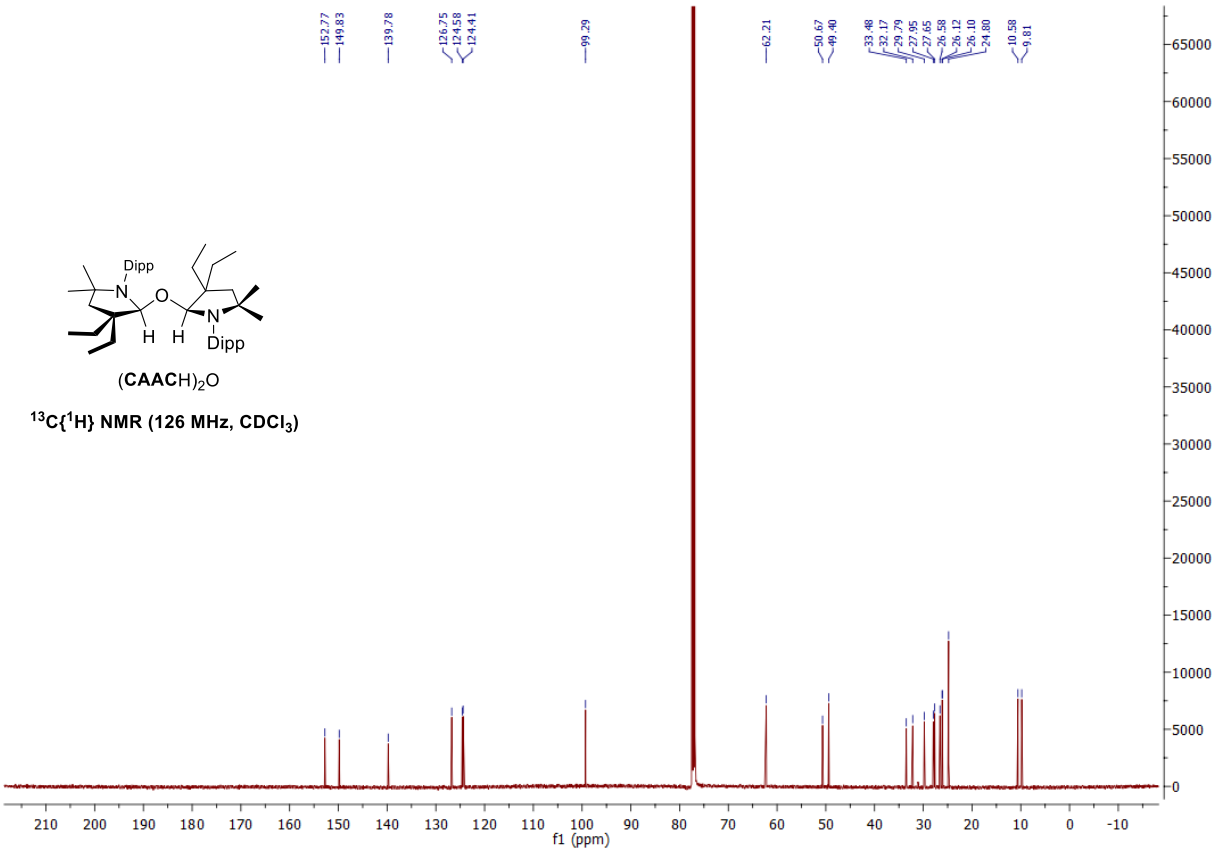

Dipp
N
O
N
Dipp
Ph
c-1
HSQC NMR (500 MHz ($^1$H), 126 MHz ($^{13}$C), CDCl$_3$)
f1 (ppm)
f2 (ppm)
2.724
2.501
X-ray


Dipp
N
O
N
Dipp
Ph
c-1
HSQC NMR (500 MHz ($^1$H), 126 MHz ($^{13}$C), CDCl$_3$)
f1 (ppm)
f2 (ppm)



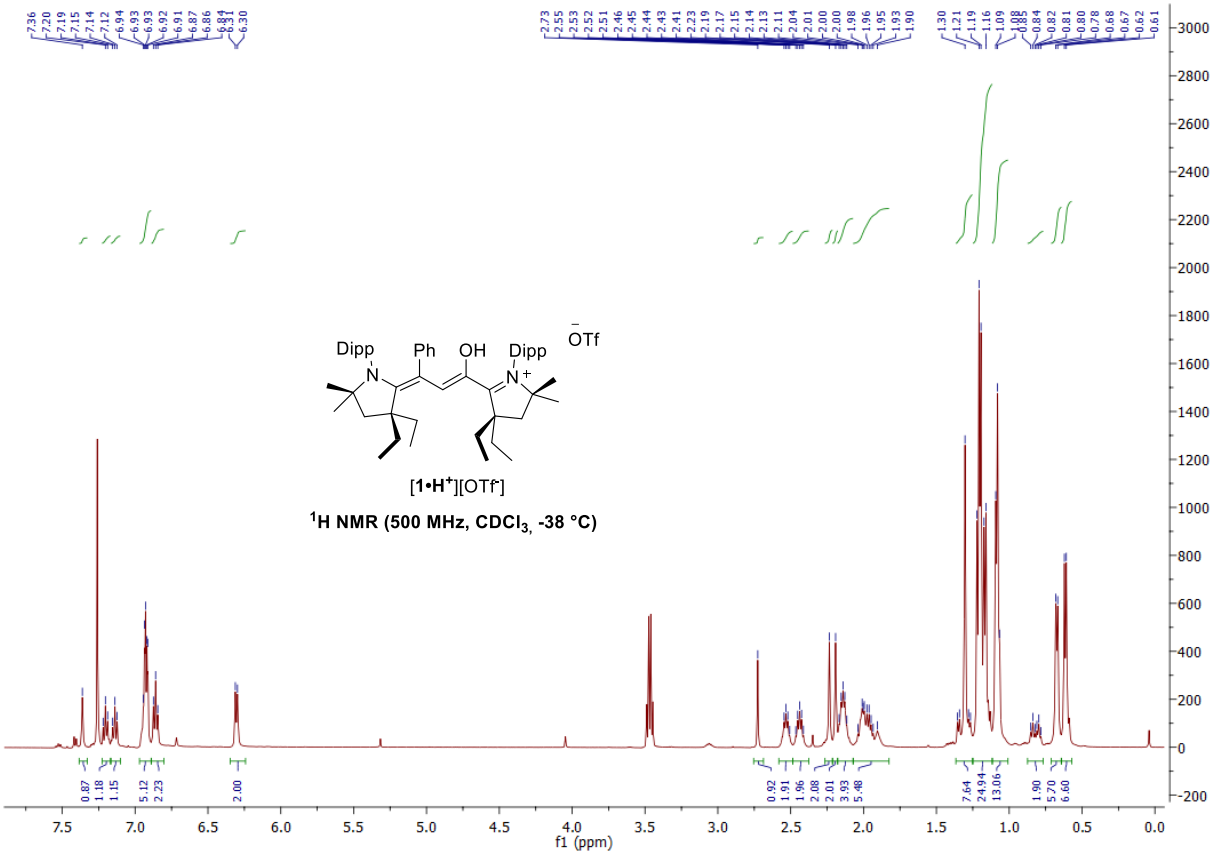

(**CAAC**H)$_2$O

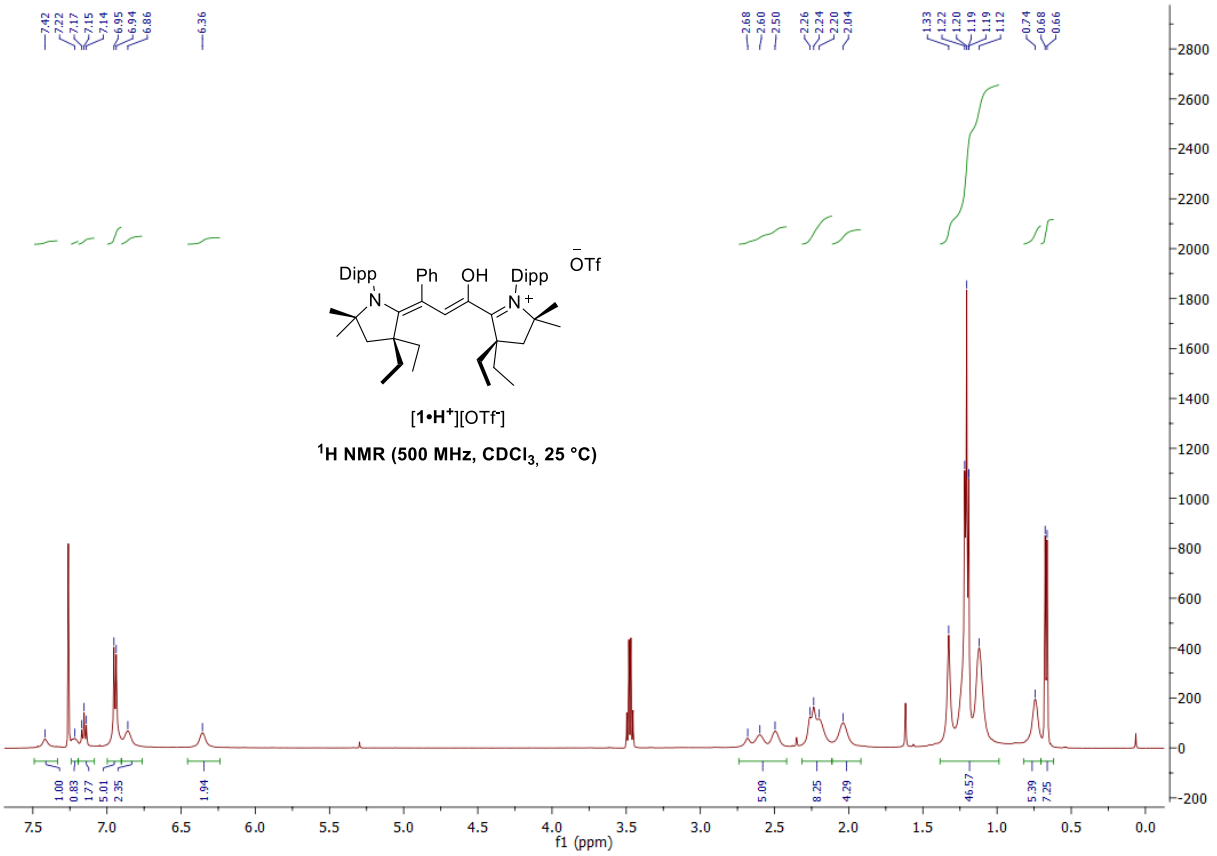
**$^1$H NMR (500 MHz, CDCl$_3$)**




(**CAAC**H)$_2$O

**$^{13}$C{$^1$H} NMR (126 MHz, CDCl$_3$)**


Dipp
Ph
OH
Dipp
OTf
[1•H+][OTf-]
1H NMR (500 MHz, CDCl3, -38 °C)
f1 (ppm)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Ph
OH
Dipp
OTf
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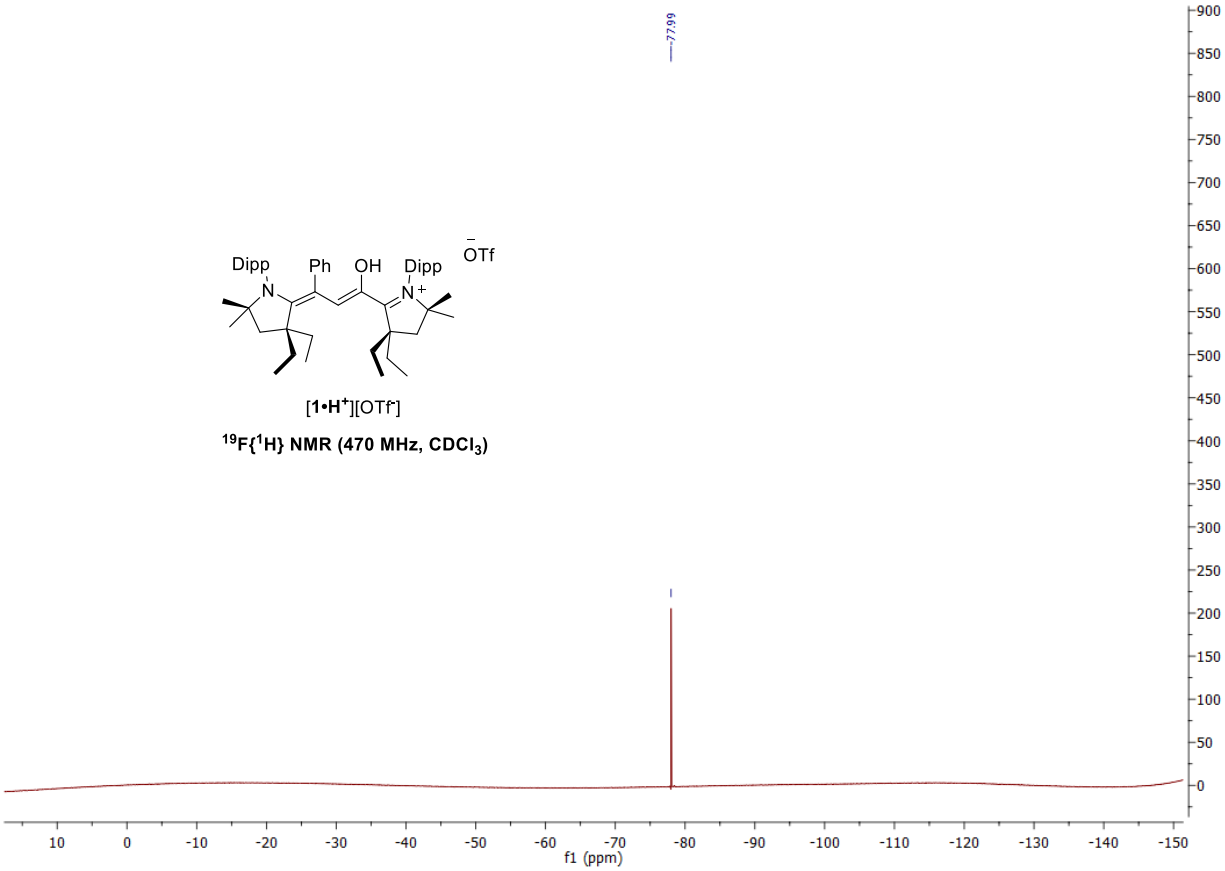
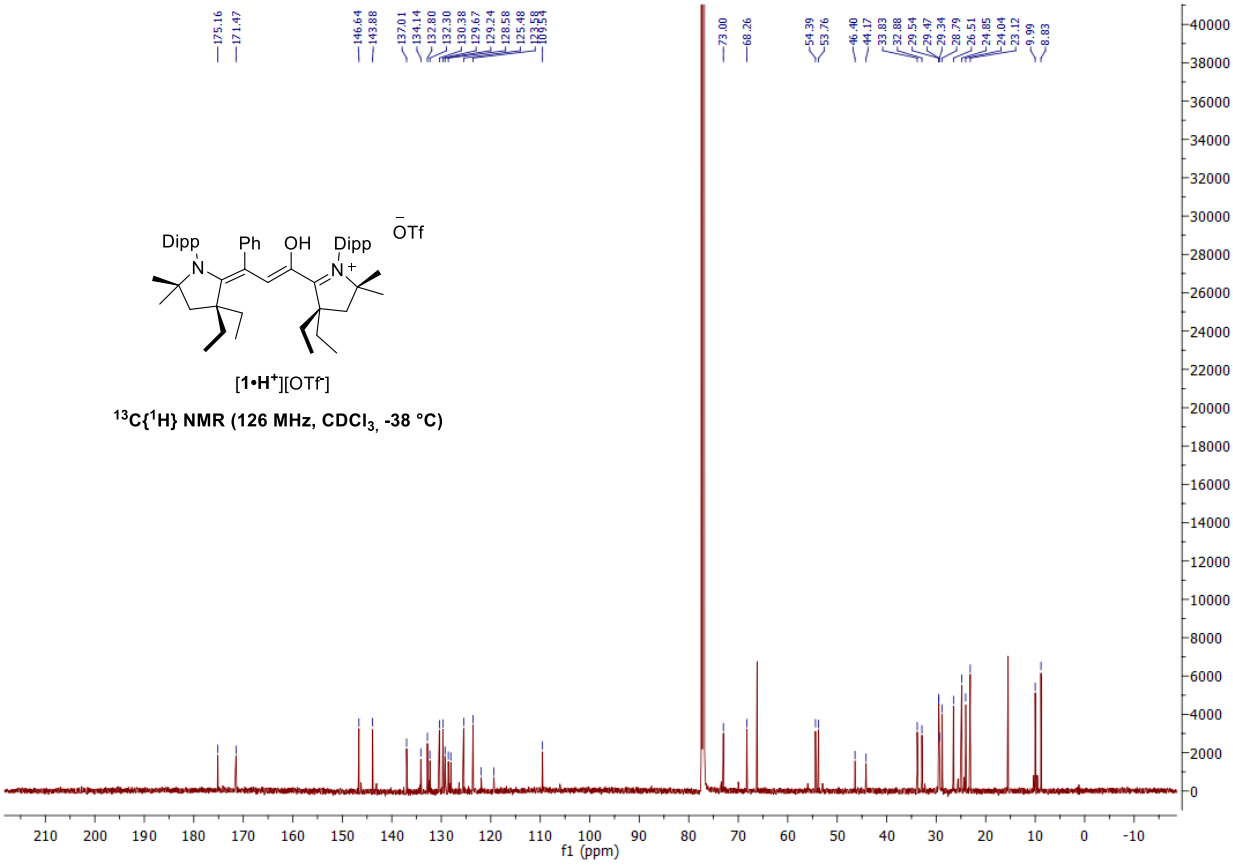
f1 (ppm)



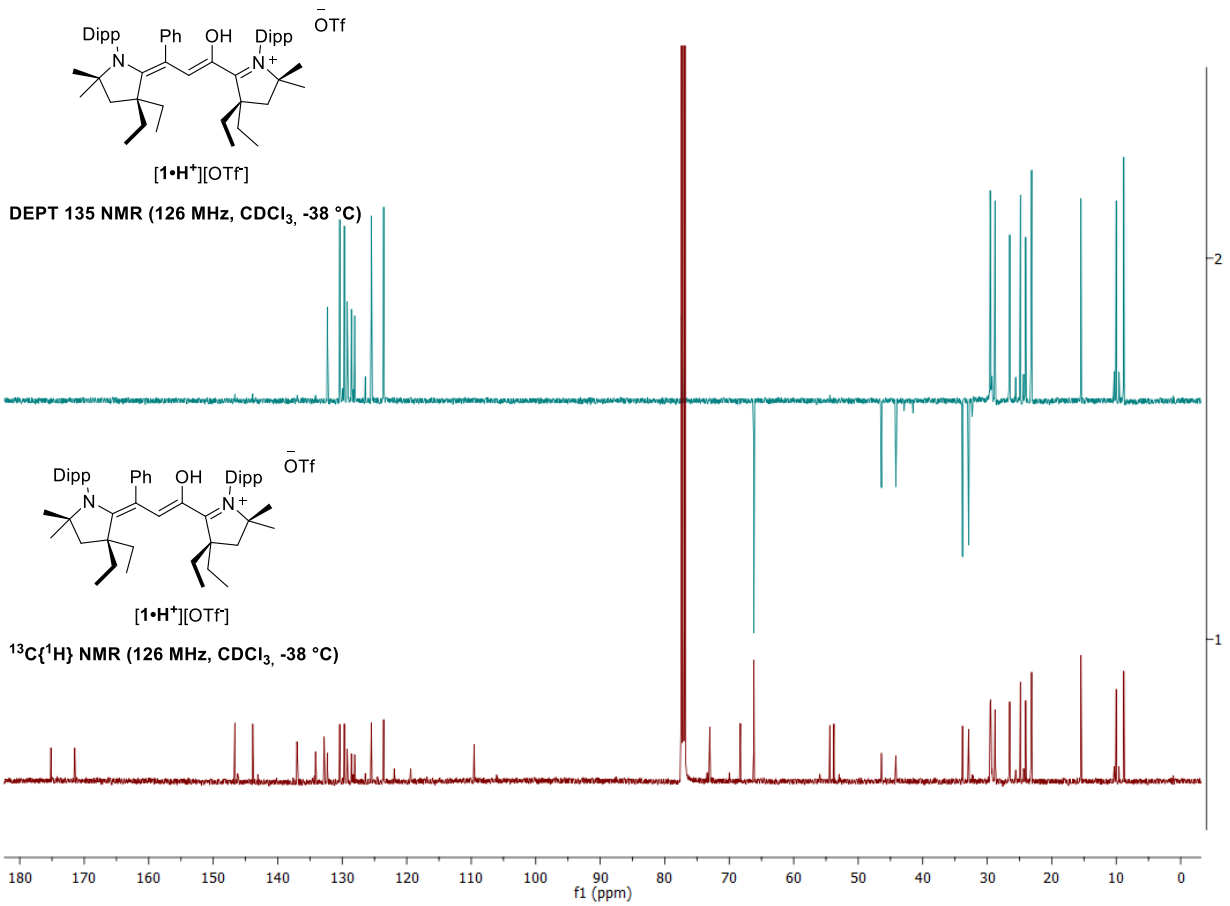

[1•H$^+$][OTf$^-$]

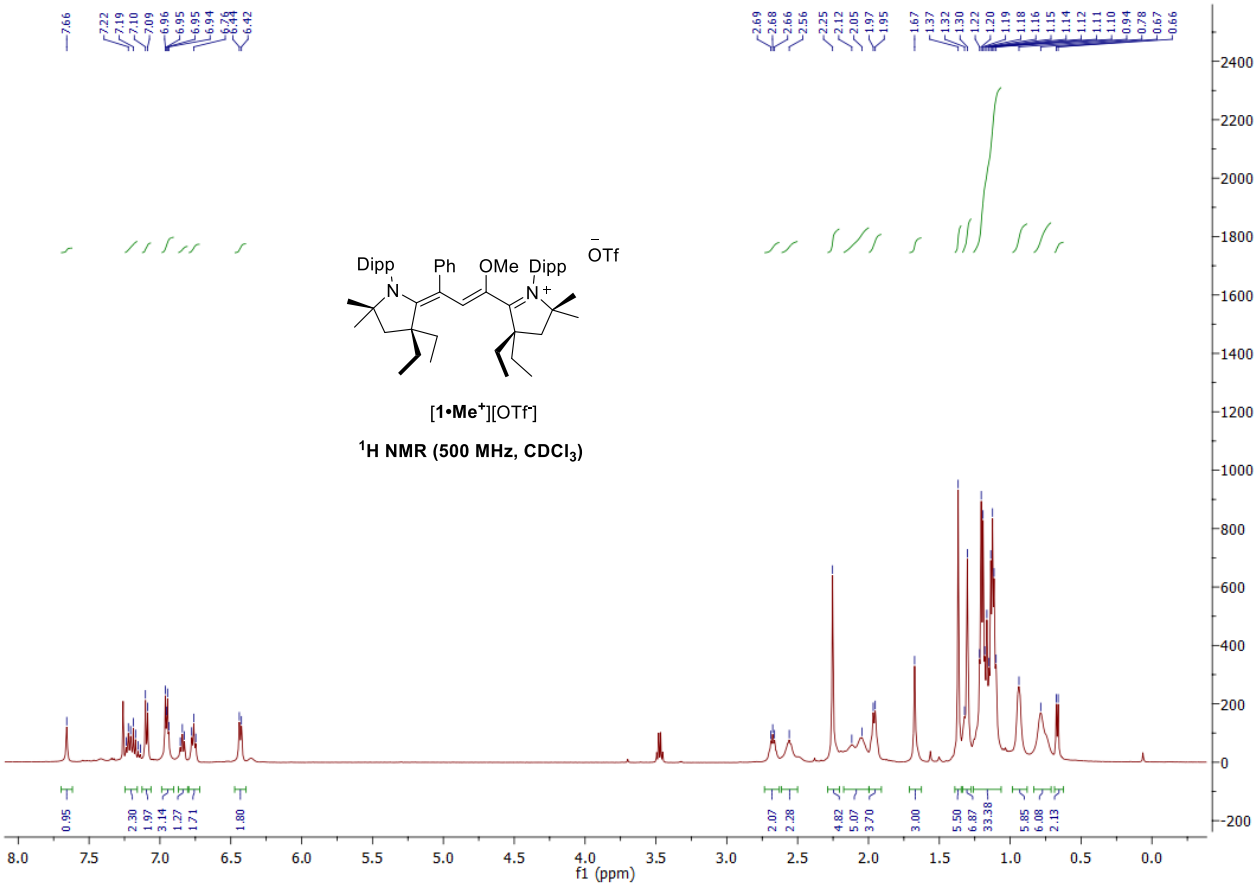
**$^{19}$F{$^1$H} NMR (470 MHz, CDCl$_3$)**

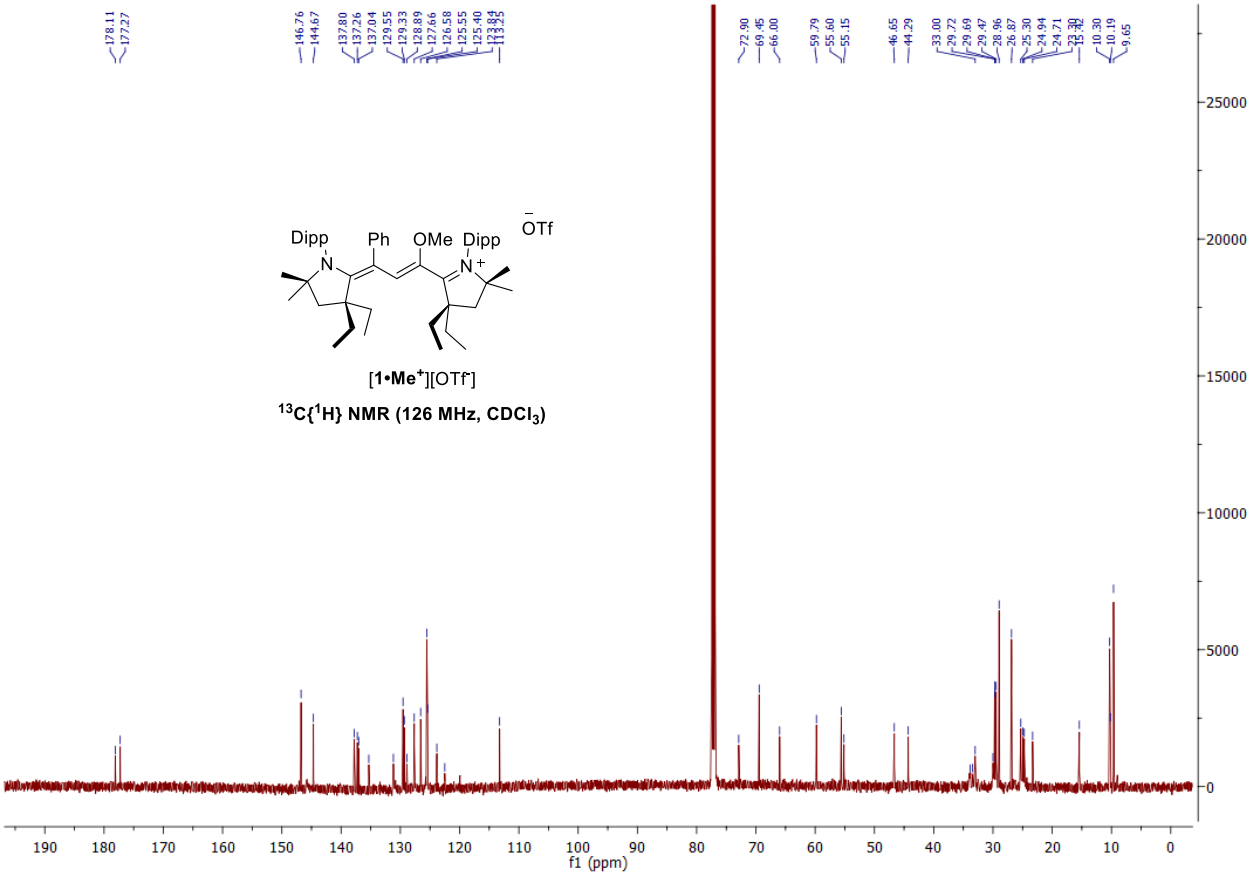


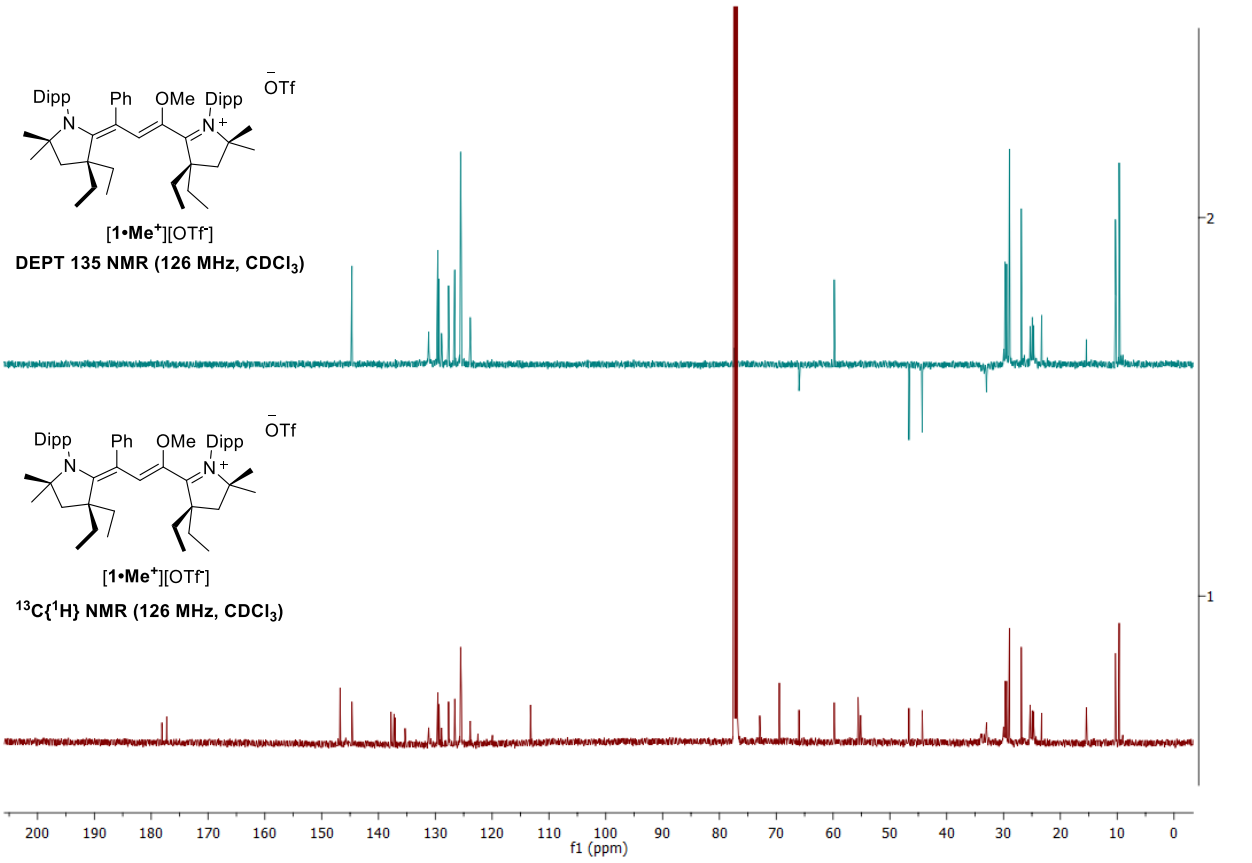

[1•H$^+$][OTf$^-$]

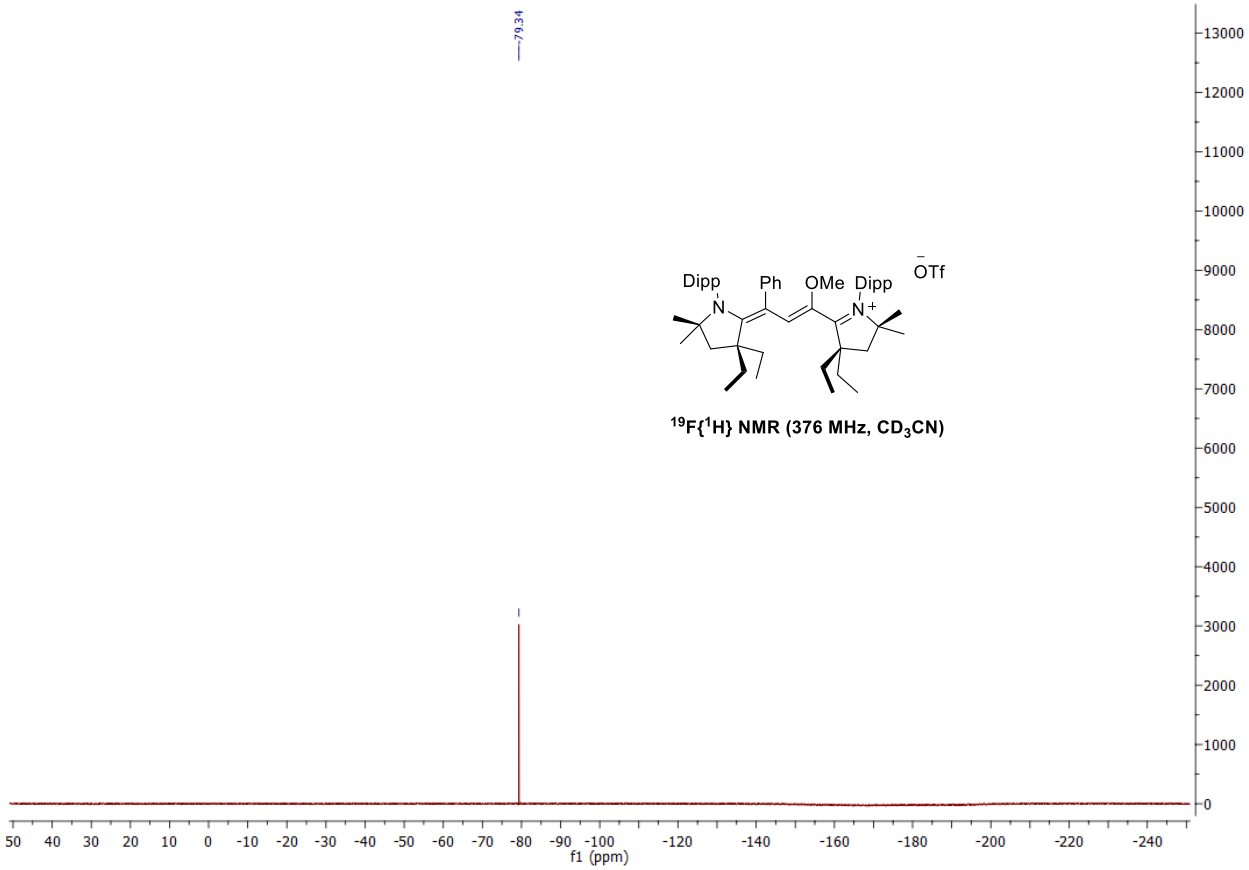
**$^{13}$C{$^1$H} NMR (126 MHz, CDCl$_3$, -38 °C)**


Dipp
Ph
OH
Dipp
OTf
[1•H+][OTf-]
DEPT 135 NMR (126 MHz, CDCl3, -38 °C)
[1•H+][OTf-]
13C{1H} NMR (126 MHz, CDCl3, -38 °C)
f1 (ppm)

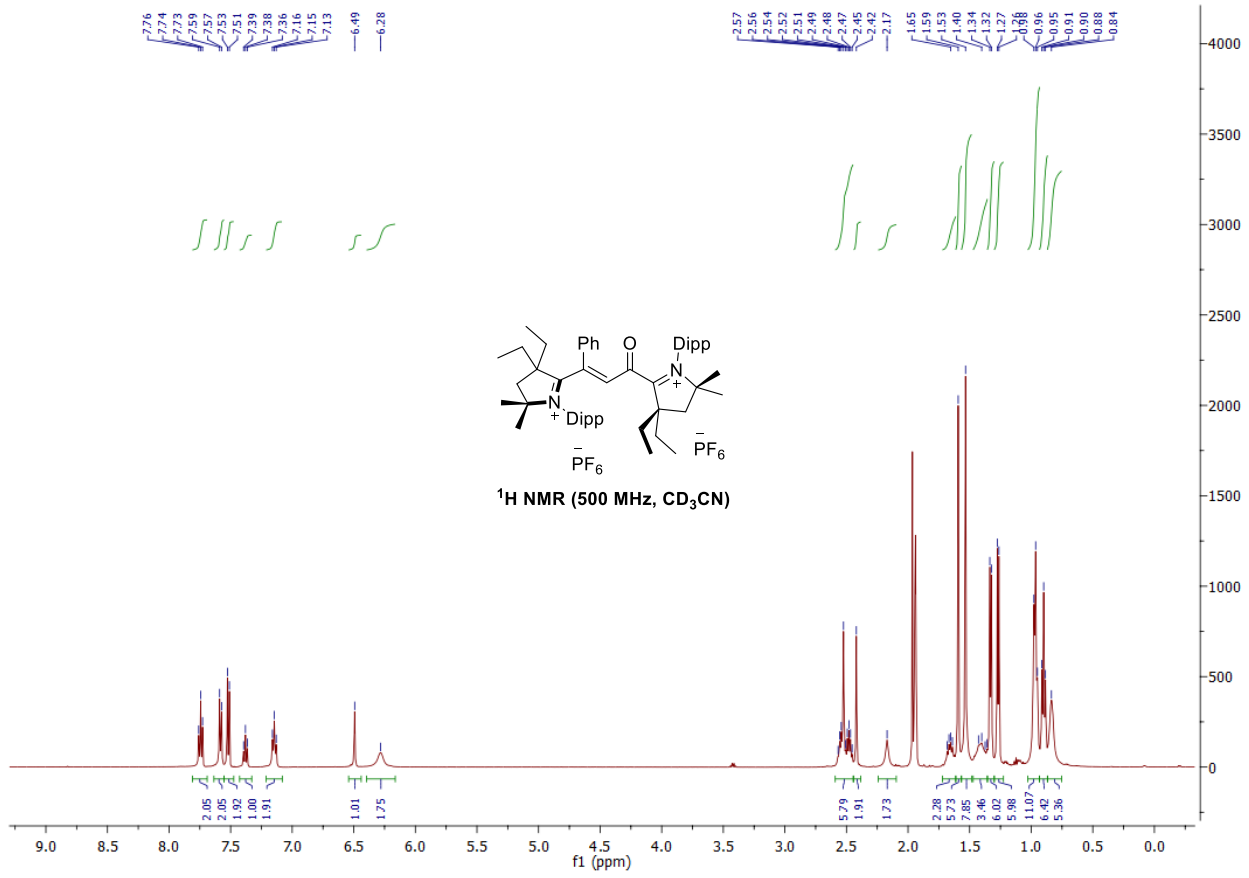

Dipp
Ph
OMe
Dipp
OTf
[1•Me+][OTf-]
1H NMR (500 MHz, CDCl3)
f1 (ppm)


Dipp
Ph
OMe
Dipp
OTf
[1•Me+][OTf-]
13C{1H} NMR (126 MHz, CDCl3)
f1 (ppm)

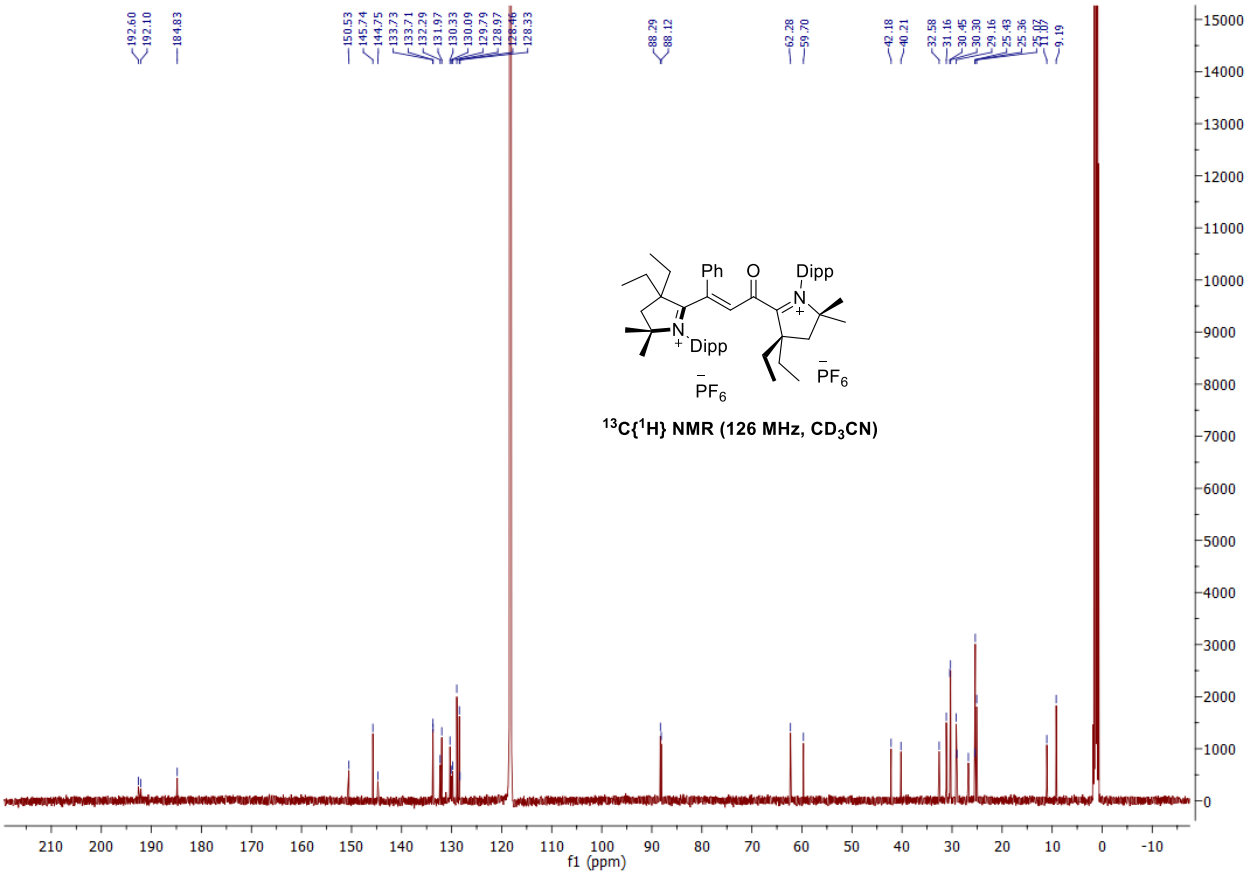

Dipp
Ph
OMe
Dipp
OTf
[1•Me+][OTf-]
DEPT 135 NMR (126 MHz, CDCl3)
13C{1H} NMR (126 MHz, CDCl3)
f1 (ppm)



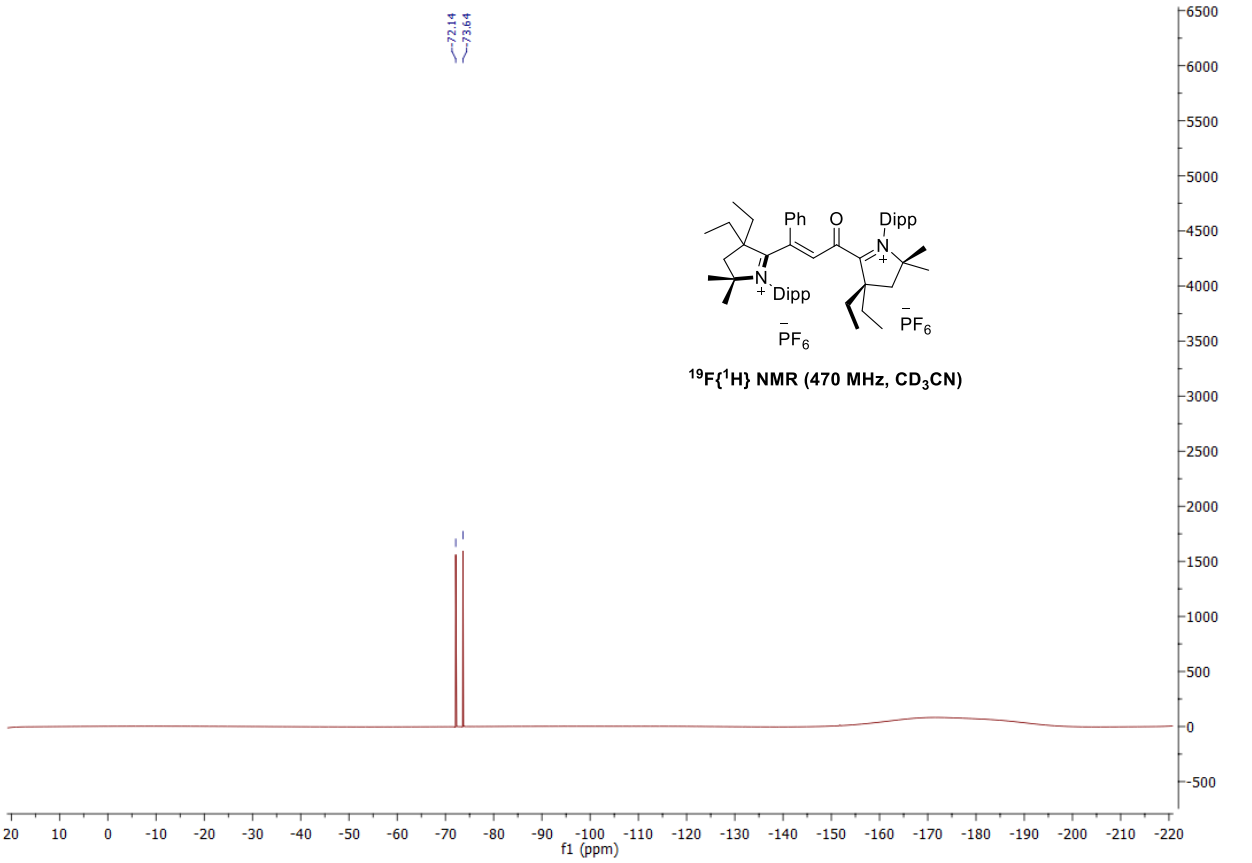

**$^{19}F\{^{1}H\}$ NMR (376 MHz, $CD_3CN$)**




**$^{1}H$ NMR (500 MHz, $CD_3CN$)**




$^{13}C\{^{1}H\}$ NMR (126 MHz, $CD_3CN$)




$^{19}F\{^{1}H\}$ NMR (470 MHz, $CD_3CN$)

## References


[1] a) J. K. Mahoney, D. Martin, C. E. Moore, A. L. Rheingold and G. Bertrand, *J. Am. Chem. Soc.*, 2013, **135**, 18766-18769. b) L. Zhou, D. Zhang, J. Hu, Y, Wu, J. Geng and X. Hu, *Organometallics*, 2021, **40**, 2643-2650.

[2] Experimental EPR spectra were fitted with the EasySpin simulation package: S. Stoll and A. Schweiger, *J. Magn. Reson.*, 2006, **178**, 42-55.

[3] CrysAlisPro 1.171.39.46 (Rigaku OD, 2018)

[4] ShelXT: G.M. Sheldrick, *Acta Cryst.*, 2015, **A71**, 3-8.

[5] Olex2: O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, *J. Appl. Cryst.*, 2009, **42**, 339-341.

[6] ShelXL: G.M. Sheldrick, *Acta Cryst.*, 2015, **C71**, 3-8.

[7] Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K., Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

[8] S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys.,* 2010, **132**, 154104.

[9] NBO (Version 3.1), E. D. Glendening, A. E. Reed, J. E. Carpenter and F. Weinhold, Theoretical Chemistry Institute, University of Wisconsin, Madison, WI, 2001.