Electronic Supplementary Material (ESI) for ChemComm.

Electronic Supplementary Information

An air-stable radical with a redox-chameleonic amide.

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General methods and materials

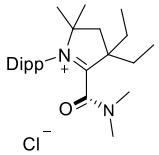
All manipulations were performed -unless otherwise noted- under an atmosphere of dry argon using standard Schlenk or dry box techniques. Solvents were dried by standard methods (Na for ethers and toluene, and CaH_2 for the rest) and distilled under argon. ^{1}H and ^{13}C NMR spectra were recorded on the NMR-ICMG platform of Grenoble with Bruker Avance 400 and 500 MHz spectrometers or at UCSD on Bruker Advance 300 MHz, Varian INOVA 500 MHz, or ECA JEOL 400 MHz spectrometers at 298 K. Chemical shifts are given in ppm and are referenced to $SiMe_4$ (^{1}H, ^{13}C). 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 and an electrothermal MEL-TEMP apparatus. Infrared (IR) data were recorded on Perkin-Elmer GS2000 IR spectrophotometer with a Golden-Gate ATR unit in the solid state and a Bruker Alpha 2 spectrometer, equipped with a platinum ATR using a monolithic diamondoid crystal in an Argon filled glovebox. 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 on a Rigaku XCallibur S instrument, at DCM-UMR 5250 on a Bruker-AXS-Enraf-Nonius KappaAPEXII apparatus and at UCSD on a Bruker Apex II diffractometer.

Cyclic (alkyl)(amino)carbene **1**,[1] carbazole-9-carbonyl chloride[2] and *N*-formyl carbazole[3] were prepared according to reported procedures; 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. A silver reference electrode (0.01 M $AgNO_3$ in 0.1 M $[^{n}Bu_4N]PF_6$ in CH_3CN) was used. Cyclic voltammetry experiments were performed in 0.1 M $[^{n}Bu_4N]PF_6$ 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 were monitored with a Zeiss MCS 501 UV-NIR spectrophotometer (1 mm cell). EPR spectra were obtained using an X-band Bruker EMX Plus spectrometer and fitted with the EasySpin simulation package.[4]

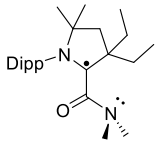
Experimental procedures and characterization data

2aCl



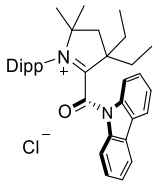
In a Schlenk, dimethyl carbamyl chloride (0.28 mL, 2.98 mmol) was added to a hexane solution of carbene **1** (0.94 g, 2.98 mmol) and a pale-yellow precipitate formed. The solution was stirred overnight and then filtered and washed twice with hexanes (20 mL). The solid was then dried under vacuum to afford a pale white powder (0.77 g, 61%).
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.47 (t, *J* = 7.8 Hz, 1H), 7.33 (d, *J* = 7.7 Hz, 1H), 7.29 (d, *J* = 7.7 Hz, 1H), 3.52 (s, 3H), 3.50-3.41 (m, 2H), 2.84 (s, 3H), 2.76-2.62 (m, 2H), 2.36-2.14 (m, 3H), 1.93 (dq, J = 14.7, 7.3 Hz, 1H), 1.84 (s, 3H), 1.47 (s, 3H), 1.42 (d, *J* = 6.2 Hz, 3H), 1.32-1.30 (m, 6H), 1.12 (d, *J* = 6.4 Hz, 3H), 1.07 (t, *J* = 7.3 Hz, 3H), 0.95 (t, *J* = 7.4 Hz, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 193.6, 158.6, 147.2, 146.4, 131.6, 128.0, 126.4, 126.3, 84.2, 59.7, 43.2, 39.8, 35.1, 32.2, 29.9, 29.2, 29.1, 28.0, 27.0, 26.3, 25.3, 24.4, 8.4, 8.4.
HRMS: m/z calculated for $C_{25}H_{41}ON_2$ $[M]^+$ 385.32134 found 385.32019.
Mp: 172 °C.
IR: 1658 (s, ν_{CO}) cm^{-1}.

2a$^\bullet$



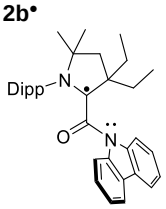
2aCl (150 mg, 0.356 mmol) was dissolved in THF (2 mL). Subsequently, zinc dust (11.6 mg, 0.177 mmol) was added to the suspension and stirred overnight to afford an orange solution. Afterwards, the solvent was removed under vacuum, the solid was washed with pentane (2x1 mL) and extracted with ether (10 mL). The solvent was removed under vacuum to engender a yellow solid (121 mg, 88% yield).
Mp: 80 °C
IR: 1564 (s, ν_{CO}) cm^{-1}.

2bCl



In a Schlenk, carbene **1** (1.2 g, 3.82 mmol) and carbazole-N-carbamoyl chloride (0.88 g, 383 mmol) were dissolved in diethyl ether (40 mL) and stirred overnight. The precipitate was filtered and washed with THF (3 mL), and then washed with toluene (3x5 mL). The precipitate was dried under vacuum to afford a pale white powder (1.95 g, 94%). *NMR analysis shows broad peaks at 25 °C. Therefore, NMR analysis for characterization was done at -20 °C.*
^{1}H NMR (400 MHz, $CDCl_3$, -20 °C) δ 8.34 (d, *J* = 7.8 Hz, 1H), 8.19 (t, *J* = 7.1 Hz, 1H), 7.95 (t, *J* = 7.3 Hz, 3H), 7.56 (t, *J* = 7.3 Hz, 1H), 7.49-7.39 (m, 3H), 7.32 (d, *J* = 8.4 Hz, 1H), 7.10 (d, *J* = 7.5 Hz, 1H), 3.63 (d, *J* = 13.7 Hz, 1H), 2.92-2.81 (m, 3H), 2.65-2.46 (m, 3H), 2.18-2.05 (m, 2H), 2.02 (s, 3H), 1.87-1.77 (m, 1H), 1.67 (s, 3H), 1.44 (d, *J* = 5.9 Hz, 3H), 1.37 (d, *J* = 6.2 Hz, 3H), 1.19-1.14 (m, 4H), 0.56 (t, *J* = 6.7 Hz, 3H), -0.23 (d, *J* = 5.7 Hz, 3H).
^{13}C NMR (101 MHz, $CDCl_3$, -20 °C) δ 189.3, 156.8, 146.6, 146.4, 137.4, 134.2, 132.1, 129.4, 128.4, 127.4, 127.1, 127.0, 126.9, 126.6, 121.2, 120.4, 118.3, 113.8, 86.2, 61.6, 42.9, 32.6, 30.5, 30.3, 29.6, 29.0, 27.4, 26.7, 26.0, 25.4, 23.9, 8.5, 8.0.
HRMS: m/z calculated for $C_{35}H_{43}ON_2$ $[M]^+$ 507.33699 found 507.33499.
Mp: 123 °C.
IR: 1661 (s, ν_{CO}) cm^{-1}.

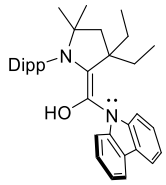
2b$^\bullet$



2bCl (150 mg, 0.276 mmol) was dissolved in THF (2 mL). Subsequently, zinc dust (9.0 mg, 0.138 mmol) was added to the suspension and stirred overnight to afford an orange solution. Afterwards, the solvent was removed under vacuum, the solid was washed with pentane (2x1 mL) and extracted with ether (10 mL). The solvent was removed under vacuum to engender a pale white solid (118 mg, 84% yield).

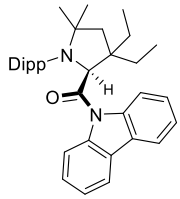
HRMS: m/z calculated for $C_{35}H_{43}ON_2$ $[M]^+$ 507.33699 found 507.33521.
Mp: 177 °C.
IR: 1564 (s, ν_{CO}) cm^{-1}.

3



2bCl (150 mg, 0.276 mmol) was dissolved in THF (2 mL). Subsequently, zinc dust (18 mg, 0.276 mmol) was added to the suspension, and stirred for 3 hours. The resulting enolate was stirred overnight. Afterwards, the solvent was removed under vacuum to afford a pale white solid. Then, single-crystals were grown from slow diffusion of pentane into a saturated solution of benzene (< 5% yield).
^{1}H NMR (500 MHz, THF-d8) *δ* 7.99 (d, *J* = 7.7 Hz, 2H), 7.56 (d, *J* = 8.2 Hz, 2H), 7.34 (t, *J* = 7.6 Hz, 2H), 7.16-7.11 (m, 5H), 5.22 (s, 1H), 3.72 (sept, *J* = 6.7 Hz, 2H), 2.05 (s, 2H), 1.58-1.51 (m, 2H), 1.40 (d, *J* = 6.7 Hz, 12H), 1.37-1.32 (m, 2H), 1.23 (s, 6H), 0.91 (t, *J* = 7.3 Hz, 6H).
^{13}C NMR (126 MHz, THF-d8) δ 150.7, 143.8, 138.6, 136.2, 127.6, 125.8, 124.8, 123.8, 120.6, 120.4, 114.4, 112.9, 64.4, 49.6, 45.2, 32.7, 30.7, 29.9, 26.7, 24.3, 11.0.

4



Carbene **1** (50 mg, 0.159 mmol) and *N*-formyl carbazole (31 mg, 0.159 mmol) were dissolved in THF (2 mL) and stirred for 2 hours. Afterwards, the solvent was removed under vacuum to afford a pale white solid (76 mg, 94% yield).
^{1}H NMR (500 MHz, C_6D_6) *δ* 7.68 (d, *J* = 7.8 Hz, 2H), 7.28 (dd, *J* = 7.7, 1.8 Hz, 1H), 7.24 (t, *J* = 7.6 Hz, 2H), 7.17-7.10 (m, 4H), 7.06 (t, *J* = 7.2 Hz, 2H), 5.27 (s, 1H), 4.39 (sept, *J* = 6.8 Hz, 1H), 3.71 (sept, *J* = 6.8 Hz, 1H), 2.34 (d, *J* = 12.7 Hz, 1H), 1.99-1.90 (m, 1H), 1.88 (s, 3H), 1.82 (d, J = 12.7 Hz, 1H), 1.79-1.71 (m, 1H), 1.61-1.54 (m, 1H), 1.42 (d, *J* = 6.8 Hz, 3H), 1.32-1.27 (m, 1H), 1.30 (d, *J* = 6.8 Hz, 3H), 1.28 (d, *J* = 6.8 Hz, 3H), 1.16 (s, 3H), 0.98 (d, *J* = 6.7 Hz, 3H), 0.51 (t, *J* = 7.4 Hz, 3H), 0.24 (t, *J* = 7.3 Hz, 3H).
^{13}C NMR (126 MHz, C_6D_6) δ 179.0, 154.0, 151.1, 146.2, 139.8, 139.0, 127.1, 126.1, 125.9, 125.8, 125.2, 123.8, 123.2, 120.3, 115.2, 77.4, 64.9, 53.8, 52.6, 32.6, 31.8, 29.0, 28.0, 27.0, 26.5, 25.6, 25.2, 25.2, 9.3, 9.1.
HRMS: m/z calculated for $C_{35}H_{45}ON_2$ $[M+H]^+$ 509.35264 found 509.35014.
Mp: 143 °C.
IR: 1703 (s, ν_{CO}) cm^{-1}.

Electrochemical studies

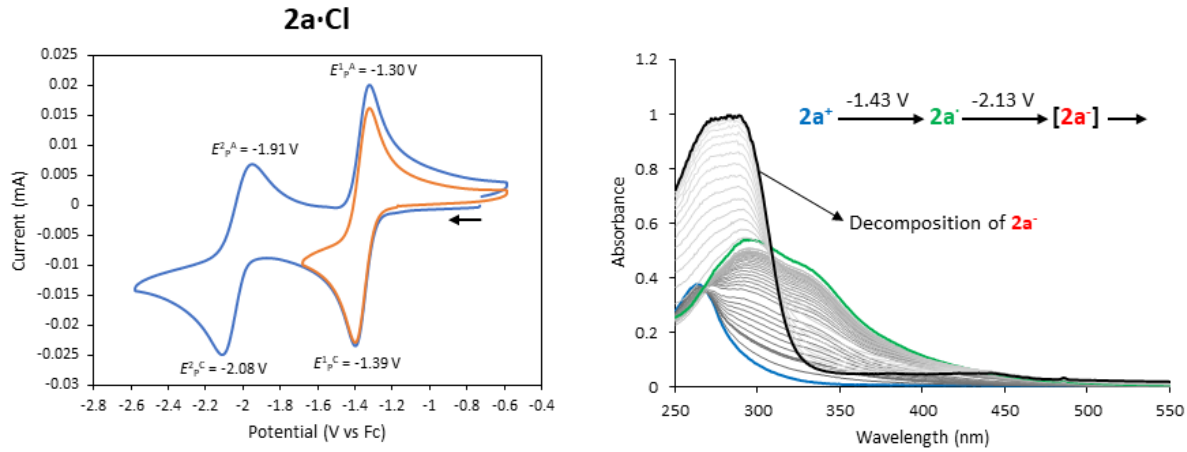


Figure S1: Left: Cyclic voltammogram of compound **2aCl** (1 mM solution employing 0.1 M of ^{n}Bu$_4$NPF$_6$ in acetonitrile electrolyte; 100 mV/s rate). Right: UV-vis monitoring of consecutive electrochemical reductions at given potentials on a reticulated vitreous carbon electrode.

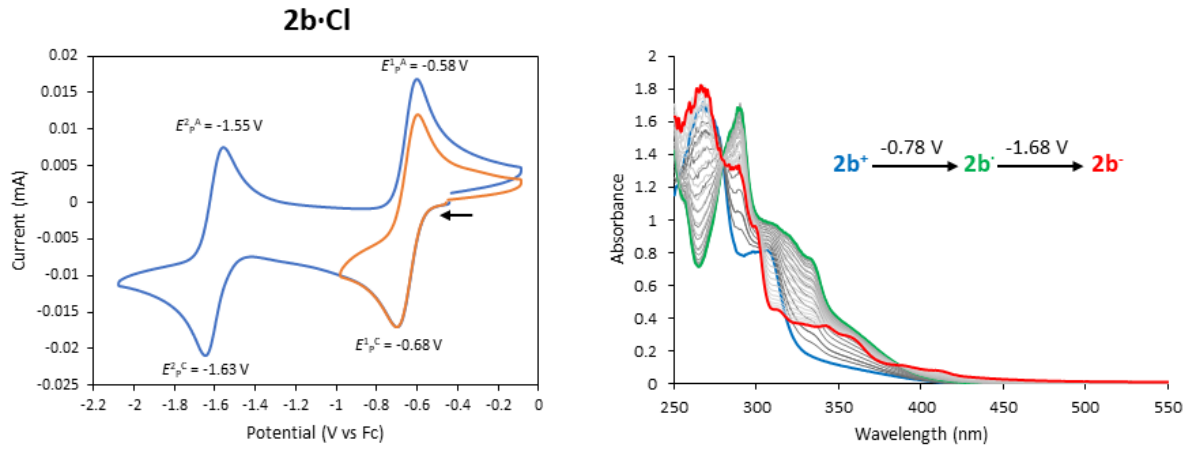


Figure S2: Left: Cyclic voltammogram of compound **2bCl** (1 mM solution employing 0.1 M of ^{n}Bu$_4$NPF$_6$ in acetonitrile electrolyte; 100 mV/s rate). Right: UV-vis monitoring of consecutive electrochemical reductions at given potentials on a reticulated vitreous carbon electrode.

Monitoring of the decay of radical 2b$^\bullet$ in technical ethanol at 60°

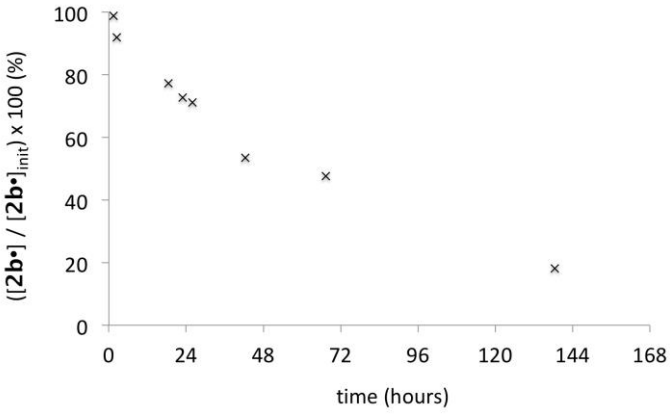


Figure S3: Decay of radical **2b$^\bullet$** in an aerated solution of technical ethanol at 60 °C, according to EPR monitoring.

X-ray diffraction studies

Single crystals of **2a•** were grown from a saturated solution of pentane at -36 °C. Crystals of **2bCl** were grown by the slow diffusion of diethyl ether into a saturated solution of dichloromethane. Crystals of **2b•** were grown by the slow evaporation of a saturated solution of diethyl ether. Crystals of **3** were grown from the slow diffusion of pentane into a saturated solution of benzene. Crystals of **4** were grown from the slow evaporation of a saturated solution of THF.

The X-Ray structure of **2a•** was collected on a Bruker diffractometer fitted with Photon 3 detector using Mo-Kα radiation (λ = 0.71073 Å). A crystal was selected under Paratone oil, mounted on nylon loops then immediately placed in a cold stream of N_2 at 100K. The space group was determined from systematic absences. The structure was solved by intrinsic phasing method using ShelXT software, in Olex1.2 environment.[5,6] All non-hydrogen atoms were refined anisotropically, all CH hydrogens were placed in calculated positions with isotropic U values 1.2 times greater than U(eq) value of corresponding non-hydrogen atom.

For structures **2bCl**, **2b•** and **4** diffraction data were collected using a Rigaku XCallibur S Kappa area detector four-circle diffractometer (Mo-Kα radiation λ = 0.71073 Å, graphite monochromator), controlled by the Rigaku CrysAlis CCD software.[7] 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.[5,6] All the atoms were found by difference Fourier syntheses. All non-hydrogen atoms were anisotropically refined on F^2 using ShelXL program.[8] Hydrogen atoms were fixed in ideal positions for compounds **2bCl** and **2b•** and found by Fourier transform and refined isotropically with a riding model for compound **4**.

Crystals of compound **3** was selected, damped in a paraffin mixture, mounted on a nylon cryo-loop then centred on a Bruker-AXS-Enraf-Nonius KappaAPEXII goniometer equipped with a high brilliance micro-source at Mo Kα radiation (λ = 0.71073 Å) at 200 K. The data was collected with an APEXII 2D detector, then integrated and corrected for Lorentz and polarization effects using the EVAL14[9] software. Final cell parameters were obtained post-refining the whole data. The data was then reintegrated and corrected for absorption using the SADABS[10] program and finally merged with the software XPREP.[11] The structure was solved by direct methods and refined by full-matrix least square methods with respectively, the SHELXT-2016 and SHELXL-2013 programs[12] implemented in Olex2 software.[6] C, N, O atoms were refined with anisotropic thermal parameters. H atoms were set geometrically, riding on the carrier atoms, with isotropic thermal parameters.

CCDC 2191398, 2191542-2191545 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 **2a•** and **2bCl**.

	2a•	**2bCl**
CCDC	2191398	2191543
Empirical formula	$C_{25}H_{41}N_2O$	$C_{37}H_{48.5}ClN_2O_{1.75}$
Formula weight	385.60	584.73
Temperature/K	273.15	150.05(10)
Crystal system	triclinic	monoclinic
Space group	P-1	$P2_1/c$
a/Å	9.3426(7)	17.5309(4)
b/Å	13.6019(9)	14.9228(3)
c/Å	19.5752(13)	25.1286(5)
α/°	75.524(2)	90
β/°	76.840(2)	95.6541(18)
γ/°	89.604(2)	90
Volume/Å^3	2342.0(3)	6542.0(2)
Z	4	8
ρ_{calc}g/cm^3	1.094	1.187
μ/mm^{-1}	0.066	0.150
F(000)	852.0	2524.0
Crystal size/mm^3	0.22 × 0.15 × 0.125	0.368 × 0.36 × 0.079
Radiation	MoKα (λ = 0.71073)	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.238 to 50.91	3.848 to 52.744
Index ranges	-11 ≤ h ≤ 11, -16 ≤ k ≤ 16, -23 ≤ l ≤ 23	-21 ≤ h ≤ 21, -18 ≤ k ≤ 18, -31 ≤ l ≤ 31
Reflections collected	16889	107550
Independent reflections	8638 [R_{int} = 0.0534, R_{sigma} = 0.0907]	13377 [R_{int} = 0.0665, R_{sigma} = 0.0407]
Data/restraints/parameters	8638/0/525	13377/100/803
Goodness-of-fit on F^2	0.979	1.099
Final R indexes [I>=2σ (I)]	R_1 = 0.0626, wR_2 = 0.1315	R_1 = 0.0965, wR_2 = 0.2468
Final R indexes [all data]	R_1 = 0.1265, wR_2 = 0.1566	R_1 = 0.1207, wR_2 = 0.2620
Largest diff. peak/hole / e Å^{-3}	0.23/-0.22	1.02/-0.98

[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 **2b•** and **3**.

	2b•	**3**
CCDC	2191544	2191542
Empirical formula	$C_{35}H_{43}N_2O$	$C_{35}H_{44}N_2O$
Formula weight	507.71	508.72
Temperature/K	150.00(10)	200
Crystal system	monoclinic	triclinic
Space group	$P2_1/c$	P-1
a/Å	17.8022(15)	10.721(2)
b/Å	20.9612(13)	10.918(2)
c/Å	7.8163(6)	13.573(3)
α/°	90	76.14(3)
β/°	96.965(9)	83.20(3)
γ/°	90	69.57(3)
Volume/Å^3	2895.2(4)	1444.4(6)
Z	4	2
ρ_{calc}g/cm^3	1.165	1.170
μ/mm^{-1}	0.069	0.069
F(000)	1100.0	552.0
Crystal size/mm^3	0.231 × 0.21 × 0.082	0.3 × 0.25 × 0.25
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.518 to 52.738	4.074 to 59.998
Index ranges	-21 ≤ h ≤ 22, -26 ≤ k ≤ 15, -9 ≤ l ≤ 9	-15 ≤ h ≤ 15, -15 ≤ k ≤ 15, -19 ≤ l ≤ 19
Reflections collected	12977	31205
Independent reflections	5917 [R_{int} = 0.0633, R_{sigma} = 0.1348]	8388 [R_{int} = 0.0246, R_{sigma} = 0.0220]
Data/restraints/parameters	5917/1044/619	8388/0/353
Goodness-of-fit on F^2	0.956	1.065
Final R indexes [I>=2σ (I)]	R_1 = 0.0609, wR_2 = 0.0494	R_1 = 0.0451, wR_2 = 0.1159
Final R indexes [all data]	R_1 = 0.1898, wR_2 = 0.0715	R_1 = 0.0573, wR_2 = 0.1283
Largest diff. peak/hole / e Å^{-3}	0.15/-0.14	0.34/-0.19

[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 **4**.

	4
CCDC	2191545
Empirical formula	$C_{17.5}H_{22}NO_{0.5}$
Formula weight	254.36
Temperature/K	150.00(14)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	15.9008(7)
b/Å	10.0800(3)
c/Å	18.4449(6)
α/°	90
β/°	101.381(4)
γ/°	90
Volume/Å^3	2898.21(19)
Z	8
ρ_{calc}g/cm^3	1.166
μ/mm^{-1}	0.069
F(000)	1104.0
Crystal size/mm^3	0.648 × 0.199 × 0.026
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.506 to 61.014
Index ranges	-22 ≤ h ≤ 22, -14 ≤ k ≤ 14, -26 ≤ l ≤ 26
Reflections collected	29188
Independent reflections	8836 [R_{int} = 0.0791, R_{sigma} = 0.1003]
Data/restraints/parameters	8836/0/519
Goodness-of-fit on F^2	1.007
Final R indexes [I>=2σ (I)]	R_1 = 0.0634, wR_2 = 0.1035
Final R indexes [all data]	R_1 = 0.1377, wR_2 = 0.1291
Largest diff. peak/hole / e Å^{-3}	0.22/-0.24

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

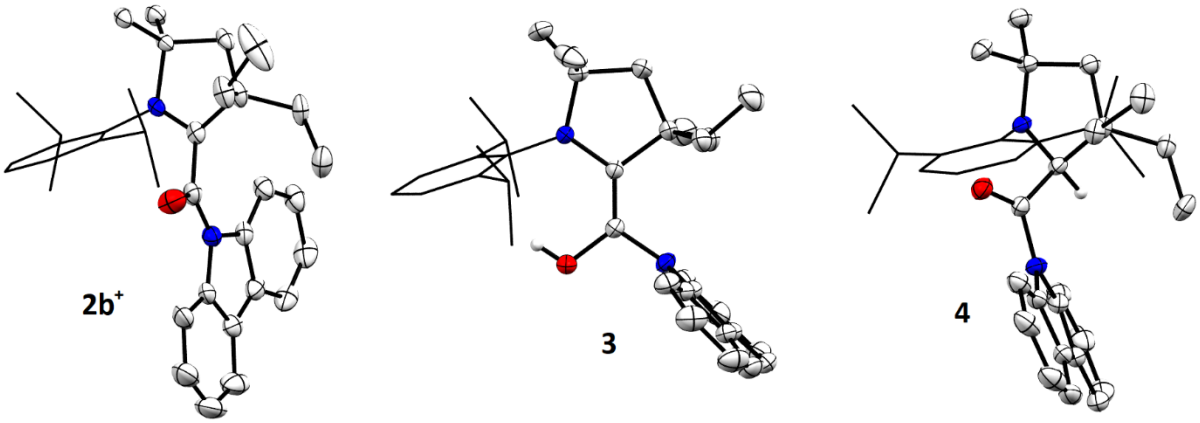


Figure S4: Solid state structures of **2b**$^{+}$, **3** and **4**. Thermal ellipsoids are set at 50% probability. Molecules of solvent, counter anions, selected hydrogen atoms and ellipsoids on 2,6-diisopropylphneyl groups are omitted for clarity.

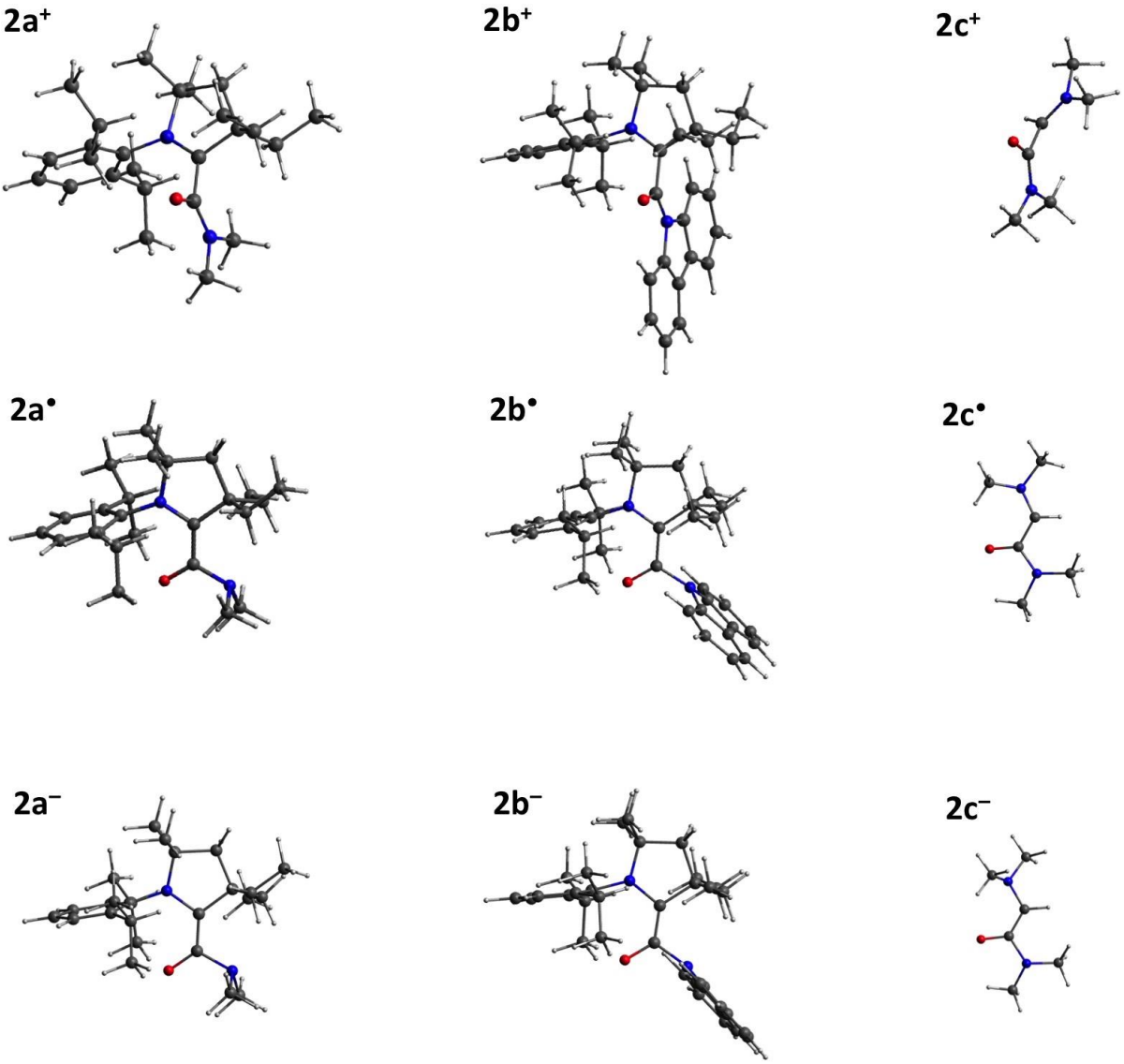


Figure S5: representation of optimized structures of **2a-c**$^{+}$, **2a-c**$^{•}$ and **2a-c**$^{-}$.

DFT studies

General considerations: The DFT calculations were performed with the program package Gaussian09.[13] 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 B3LYP/6-311g(d,p) level of theory.
EPR hyperfine constants were calculated on previously optimized structures, with a single point calculation at the B3LYP/EPRII level of theory.

xyz coordinates of optimized structure of $2a^+$
(E = -1161.556999)

	x	y	z		x	y	z
C	-1.04159400	-0.02720400	0.16294200	H	1.38812600	4.17994400	-2.11749100
C	-2.35995200	-0.40891000	-0.50945000	H	1.97207900	2.64354900	-2.76560200
C	-1.86119700	-0.98356700	-1.85815000	H	2.99463400	3.59567100	-1.69856300
H	-1.88930900	-2.07205400	-1.83277700	C	1.51923000	-2.55754300	0.42740100
H	-2.48635700	-0.66542800	-2.69051800	H	0.46236000	-2.53577700	0.15773300
C	-0.40952300	-0.51581400	-2.06470200	C	1.60538000	-2.97478200	1.91160400
C	-3.16552600	-1.44310700	0.34002400	H	2.64620200	-3.08844000	2.22492700
H	-4.11013400	-1.59043600	-0.18770700	H	1.11572600	-3.94266300	2.04924800
H	-3.42597200	-0.96987900	1.29231600	H	1.12115500	-2.25201800	2.56360800
C	-3.24761100	0.86920800	-0.69545300	C	2.21843800	-3.63487900	-0.43119700
H	-3.50898300	1.25139100	0.29346800	H	2.28642400	-3.36756800	-1.48592100
H	-2.65898700	1.64799600	-1.18927500	H	1.67491600	-4.57993000	-0.35240700
C	0.47466200	-1.60996200	-2.65078800	H	3.23480000	-3.81985600	-0.07630900
H	1.52197600	-1.30863300	-2.69599300	C	-0.92951200	0.18577500	1.66756800
H	0.13848200	-1.79852300	-3.67310500	N	-0.00361600	-0.15004300	-0.60760700
H	0.39117400	-2.54185500	-2.09733000	O	-0.64711700	-0.84902800	2.25664100
C	-0.31334500	0.73455400	-2.94565000	N	-1.20190400	1.36277800	2.26232900
H	0.71772100	1.06557000	-3.05309900	C	-1.17816900	1.41825500	3.72957300
H	-0.91531700	1.56399600	-2.57330500	H	-0.45572500	2.16946800	4.05665300
H	-0.68094900	0.47575200	-3.94080300	H	-2.16874000	1.69029700	4.10348000
C	1.41433300	-0.00499900	-0.21086300	H	-0.89615100	0.44516700	4.12064900
C	2.05489000	1.25211900	-0.32351400	C	-1.61858100	2.59263100	1.59875500
C	3.42573100	1.30651400	-0.05227000	H	-2.67959600	2.78773400	1.77865500
H	3.93949300	2.25581900	-0.13523500	H	-1.04447900	3.42873800	1.99850000
C	4.13909000	0.18390300	0.33119000	H	-1.44190500	2.54075600	0.52791500
H	5.20138300	0.25464100	0.53286100	C	-4.54522200	0.67096300	-1.48988700
C	3.48110200	-1.02626600	0.47280700	H	-5.03828000	1.63808600	-1.61081000
H	4.03862600	-1.89460400	0.79936500	H	-4.36982900	0.27225700	-2.49107900
C	2.11545900	-1.16591400	0.20768400	H	-5.25028300	0.01226000	-0.98180000
C	1.37116400	2.58058800	-0.64314500	C	-2.54536900	-2.81676500	0.61212200
H	0.31436000	2.39306200	-0.84215300	H	-2.35324800	-3.37850200	-0.30512800
C	1.46640600	3.53064500	0.57024600	H	-1.62324200	-2.74638000	1.18747600
H	2.49681200	3.85507900	0.72916500	H	-3.25106600	-3.41000900	1.19812400
H	1.13367700	3.04741300	1.49011100				
H	0.86383200	4.42747800	0.40330800				
C	1.96474300	3.28180700	-1.88140200				

xyz coordinates of optimized structure of 2a˙
(E = -1161.737922)

	x	y	z
C	-0.98865300	-0.07986600	0.05843900
C	-2.19130600	-0.29996100	-0.86564400
C	-1.50855800	-0.67526500	-2.20741700
H	-1.54473100	-1.75628200	-2.35207100
H	-2.01369900	-0.22689400	-3.06362800
C	-0.03645700	-0.22592600	-2.14248600
C	-3.12924100	-1.44591200	-0.39029000
H	-3.85924600	-1.62585100	-1.18689200
H	-3.68362800	-1.08283600	0.47647000
C	-3.01874000	1.01642000	-0.98903800
H	-3.38191000	1.26410100	0.00882400
H	-2.34542300	1.82624900	-1.28800900
C	0.88756600	-1.26452300	-2.79058700
H	1.93894400	-0.98755400	-2.69383200
H	0.65267100	-1.32543400	-3.85666200
H	0.74477000	-2.25461600	-2.35930400
C	0.18598300	1.11848100	-2.85814500
H	1.22089800	1.44696100	-2.75582500
H	-0.46793200	1.90352400	-2.47777300
H	-0.02149200	0.99424200	-3.92444200
C	1.52637200	0.09912500	-0.13715800
C	2.04470600	1.40547800	0.01090200
C	3.39525300	1.54809400	0.34492100
H	3.80965600	2.54313100	0.45887000
C	4.20929500	0.44678800	0.56073000
H	5.25535900	0.58176900	0.81312000
C	3.66498300	-0.82762000	0.49355900
H	4.28927200	-1.68339300	0.72223100
C	2.32330000	-1.02976100	0.16158400
C	1.18088700	2.66323700	-0.03548300
H	0.19190800	2.38129000	-0.39694200
C	1.00288100	3.22431800	1.39250000
H	1.95101600	3.61147200	1.77761900
H	0.65381600	2.45066400	2.07671600
H	0.28293000	4.04911700	1.39066700
C	1.72913600	3.76005800	-0.96601600
H	1.03375900	4.60412700	-1.00094500
H	1.87573700	3.40303400	-1.98721600
H	2.68751800	4.14636900	-0.60894500
C	1.75597600	-2.44317300	0.26090500
H	0.75102100	-2.43109000	-0.16218300
C	1.61876500	-2.84980900	1.74395000
H	2.60335900	-2.94137100	2.21266900
H	1.11804000	-3.82000500	1.82639900
H	1.04829700	-2.10492900	2.29940700
C	2.58074000	-3.49355400	-0.50462800
H	2.72814600	-3.21993500	-1.55157700
H	2.07403800	-4.46283200	-0.47477100
H	3.56819700	-3.63305500	-0.05642200
C	-1.00535900	0.07474500	1.48301700
N	0.18535900	-0.10411400	-0.65587500
O	0.01612300	0.04873000	2.18747000
N	-2.31498300	0.26315100	2.09768300
C	-2.49323100	-0.62901900	3.25094300
H	-1.76477800	-0.43867300	4.05045300
H	-3.50186900	-0.49028900	3.64904100
H	-2.39329200	-1.66894900	2.93419900
C	-2.49222400	1.66104400	2.51603600
H	-3.51062500	1.79770800	2.89043000
H	-1.78598700	1.95349500	3.30786500
H	-2.34852600	2.33106700	1.66653700
C	-4.21545900	0.98593900	-1.94947600
H	-4.67735600	1.97617500	-1.99435500
H	-3.93140600	0.71658100	-2.97063200
H	-4.98556100	0.28454900	-1.62167900
C	-2.45959600	-2.77704900	-0.03382800
H	-1.93852400	-3.22646700	-0.88420400
H	-1.73407700	-2.66414400	0.77488100
H	-3.21301900	-3.49785900	0.29576200

xyz coordinates of optimized structure of 2a$^-$

(E = -1161.774663)

	x	y	z		x	y	z
O	0.01682700	0.23031900	2.22489100	H	3.66837800	-1.09717600	0.47006000
N	-0.23257500	-0.21056800	-0.65940500	C	2.54268000	-0.67385800	3.15056900
N	2.37851700	0.29189800	2.06304300	H	1.77033300	-0.56276800	3.92735300
C	-2.39816300	-1.00953500	0.15023200	H	3.53118400	-0.54698200	3.60976500
C	-3.74702100	-0.77626700	0.42872800	H	2.47983300	-1.69055900	2.75458000
H	-4.39851700	-1.61395100	0.65659100	C	1.47247500	-0.72207600	-2.19001300
C	1.01535400	-0.05091500	0.08502600	H	1.96746100	-0.30945800	-3.07369300
C	-3.40457500	1.58708500	0.25226600	H	1.49358500	-1.80866900	-2.30110700
H	-3.79216800	2.59711700	0.34201000	C	4.23833700	0.89889800	-2.02266100
C	-1.82548200	-2.40790800	0.34410500	H	5.00903300	0.20670800	-1.67312000
H	-0.84208400	-2.40595000	-0.12612400	H	4.70770600	1.88445800	-2.12009600
C	-4.26220100	0.51340800	0.44957800	H	3.94211000	0.58220300	-3.02839400
H	-5.31491300	0.68226600	0.65719200	C	2.44751800	-2.79165500	-0.03765500
C	-2.04705600	1.39947600	-0.03051600	H	3.17498900	-3.48825700	0.39406300
C	-0.00037600	-0.26419200	-2.11628700	H	2.00309600	-3.28852700	-0.90645400
C	-1.13419200	2.62140100	-0.03795300	H	1.65343400	-2.62638300	0.69303700
H	-0.15094300	2.29111800	-0.37088300	C	-1.54475000	0.08035700	-0.16172200
C	2.18370500	-0.31595600	-0.86827300	C	1.02567500	0.14401900	1.44294400
C	2.53494800	1.64510600	2.59728300	C	-1.60435100	-2.64894400	1.85212600
H	2.43750900	2.37166500	1.78673500	H	-1.01546200	-1.82861900	2.27455000
H	3.53267100	1.75584200	3.04143400	H	-1.08097600	-3.59880300	2.01695900
H	1.78081700	1.88609100	3.36457400	H	-2.56332600	-2.69519800	2.38221400
C	3.04545500	0.97140700	-1.05417100	C	-0.96325000	3.13581200	1.40784900
H	2.38191800	1.78232300	-1.37020300	H	-1.90731200	3.54318300	1.78940700
H	3.41071900	1.24150100	-0.06127600	H	-0.21477200	3.93674100	1.44020200
C	-1.61099900	3.75919300	-0.95866300	H	-0.64363000	2.31195900	2.05135400
H	-1.74357500	3.42968500	-1.99201400	C	-2.66272200	-3.53072200	-0.28763000
H	-0.87903000	4.57443700	-0.95668400	H	-3.64496600	-3.62663000	0.18748200
H	-2.56255800	4.18032600	-0.61794700	H	-2.15317100	-4.49341000	-0.16953200
C	-0.91867900	-1.28620400	-2.81470800	H	-2.82523500	-3.36286600	-1.35647000
H	-1.97082800	-1.00602100	-2.71793100	C	-0.18880100	1.08806200	-2.84978900
H	-0.78937000	-2.28266000	-2.38909000	H	0.05093000	0.97569400	-3.91370400
H	-0.67916400	-1.33581300	-3.88275000	H	0.45769800	1.86449900	-2.43975400
C	3.12620000	-1.46711800	-0.40273100	H	-1.22443300	1.42631200	-2.77460000
H	3.86844700	-1.66052700	-1.18994100				

xyz coordinates of optimized structure of $2b^+$

(E = -1543.824991)

	x	y	z		x	y	z
O	0.07101400	-1.91291200	0.95752300	H	0.03518500	3.50690200	1.66540300
N	-1.59688000	0.46911600	0.26842200	H	1.23684800	3.72193700	2.92871800
C	-0.58317800	0.24929700	1.05375500	H	-0.46826100	3.69447200	3.34251200
N	1.76600100	-0.53280700	0.32665800	C	-4.05720100	0.75973200	0.86697900
C	-0.75691300	0.78712900	2.47582000	H	-4.38750700	0.62144500	-0.16265100
C	-2.14642800	1.47124800	2.39417300	H	-4.75262500	1.45054600	1.34940500
H	-2.84694200	0.97764000	3.06587700	H	-4.11237100	-0.18957100	1.39469700
H	-2.09320200	2.51214200	2.70270400	C	-2.68920500	2.73920800	0.23961000
C	-2.66512000	1.37993500	0.94060300	H	-1.71834300	3.23439600	0.24632900
C	0.48696400	-0.78969300	0.72677600	H	-3.39488800	3.38059600	0.77198400
C	2.72682500	-1.59519600	0.13695200	H	-3.03681000	2.64817700	-0.78801900
C	2.58110600	-2.97499700	0.26165300	C	-1.82958300	-0.08917200	-1.09366100
H	1.64580900	-3.42560200	0.54593100	C	-1.44478600	0.65347200	-2.23880000
C	3.70338500	-3.76457300	0.01001900	C	-1.81952100	0.15619500	-3.49155500
H	3.61325900	-4.84037600	0.10053200	H	-1.53477900	0.70928100	-4.37698300
C	4.93042000	-3.20351400	-0.35181900	C	-2.52788400	-1.02304500	-3.63235300
H	5.78090200	-3.84746900	-0.53972500	H	-2.80780700	-1.38015800	-4.61634400
C	5.06604000	-1.82490100	-0.47043000	C	-2.85781000	-1.75176700	-2.50350300
H	6.01636900	-1.38522900	-0.74846600	H	-3.38783000	-2.68846200	-2.61646000
C	3.95707000	-1.01801100	-0.22401900	C	-2.53084800	-1.32033300	-1.21454200
C	3.78270000	0.42145500	-0.26144000	C	-0.58051700	1.91238700	-2.25758000
C	4.66685700	1.46035400	-0.54985900	H	-0.37937300	2.21656700	-1.23133900
H	5.69776400	1.24688700	-0.80507900	C	0.77270000	1.61096800	-2.93776900
C	4.20808200	2.77209100	-0.50312600	H	1.27657200	0.75441200	-2.48860400
H	4.88424100	3.58952900	-0.72153900	H	1.43755200	2.47371800	-2.86128100
C	2.87649500	3.04242200	-0.17896100	H	0.63142200	1.39243100	-3.99861600
H	2.52656500	4.06743700	-0.15154500	C	-2.94180500	-2.25640900	-0.07778700
C	1.98244400	2.01136000	0.10535600	H	-2.65337600	-1.80311400	0.86790200
H	0.95711600	2.24883700	0.33236200	C	-2.20677700	-3.61053800	-0.18516600
C	2.44527300	0.70532600	0.06869100	H	-2.54961500	-4.17310400	-1.05700600
C	-0.75351800	-0.38620400	3.53071100	H	-2.41901900	-4.21732400	0.69933300
H	-0.87700800	0.13065100	4.48703700	H	-1.12941300	-3.48271100	-0.25949500
H	0.24876000	-0.82348700	3.55210400	C	-4.46262200	-2.52326200	-0.04553200
C	-1.79383200	-1.50202700	3.45010900	H	-5.05880800	-1.61110700	-0.04739600
H	-1.62067100	-2.16470100	2.60588700	H	-4.71724200	-3.09394200	0.85145500
H	-2.81783300	-1.12217100	3.40653500	H	-4.77648800	-3.12031200	-0.90461300
H	-1.72400100	-2.10501300	4.35876400	C	-1.25282200	3.10157800	-2.97360000
C	0.41302000	1.73340200	2.93970900	H	-1.37449000	2.90503500	-4.04089200
H	0.50932600	1.59200400	4.01799800	H	-0.62682300	3.99264300	-2.87928500
H	1.35182700	1.36606000	2.52279800	H	-2.23795400	3.33819100	-2.57002300
C	0.28465300	3.24126300	2.69447500				

xyz coordinates of optimized structure of 2b$^{\bullet}$
(E = -1544.031898)

	x	y	z		x	y	z
O	-0.05779300	-0.00026900	-1.58510400	H	-0.04231800	-2.79213200	1.39112700
N	1.66486200	0.00013300	0.66625800	H	-1.12247300	-3.40312700	2.63611700
C	0.29687800	0.00010100	0.75018100	H	0.46292300	-2.78671700	3.08272700
N	-1.96725400	-0.00015000	-0.27598900	C	3.23936900	1.24326700	2.19395200
C	-0.16368100	0.00009300	2.21482400	H	4.04472900	1.27088000	1.45868900
C	1.17332200	0.00019200	3.00771400	H	3.69383800	1.20720400	3.18761600
H	1.23305500	0.87257100	3.65832600	H	2.66401600	2.16557600	2.12042300
H	1.23330100	-0.87230800	3.65814200	C	3.24014700	-1.24173500	2.19419800
C	2.35565800	0.00046800	2.01165400	H	2.66539400	-2.16442800	2.12077600
C	-0.51068700	-0.00009100	-0.43393400	H	3.69453100	-1.20522100	3.18788600
C	-2.77554400	1.12957900	-0.45532800	H	4.04557400	-1.26893800	1.45899700
C	-2.42005100	2.47739700	-0.50579200	C	2.48041300	0.00010000	-0.54368000
H	-1.38606200	2.78836200	-0.44720400	C	2.90146600	-1.22696800	-1.10547900
C	-3.43438900	3.41625900	-0.66272800	C	3.83494700	-1.19630600	-2.14520300
H	-3.17656800	4.46840600	-0.71050400	H	4.16857100	-2.13024700	-2.58172300
C	-4.77812900	3.02963700	-0.77088500	C	4.32257700	0.00020800	-2.64770200
H	-5.54530900	3.78598600	-0.88945200	H	5.05182900	0.00025600	-3.45020600
C	-5.12745900	1.68525600	-0.74684300	C	3.83441600	1.19664400	-2.14554200
H	-6.16421100	1.38524900	-0.85339200	H	4.16761700	2.13061100	-2.58232700
C	-4.12454200	0.72272000	-0.60206500	C	2.90091500	1.22717800	-1.10582700
C	-4.12442500	-0.72335900	-0.60209200	C	2.29478200	-2.57639300	-0.73188700
C	-5.12718900	-1.68605400	-0.74688100	H	1.67834800	-2.43395500	0.15542600
H	-6.16399200	-1.38621300	-0.85340900	C	1.36435100	-3.06121600	-1.86493700
C	-4.77763900	-3.03037700	-0.77095700	H	0.62213800	-2.30355000	-2.11786900
H	-5.54469500	-3.78684900	-0.88953200	H	0.84913800	-3.98019700	-1.56709600
C	-3.43383400	-3.41678300	-0.66281800	H	1.93880800	-3.28283000	-2.76900500
H	-3.17584300	-4.46888700	-0.71061900	C	2.29358800	2.57640600	-0.73259100
C	-2.41964700	-2.47776100	-0.50587200	H	1.67702800	2.43383300	0.15461500
H	-1.38560400	-2.78855900	-0.44730600	C	1.36316900	3.06064400	-1.86590300
C	-2.77536400	-1.13000300	-0.45538100	H	1.93770400	3.28236600	-2.76989400
C	-1.02216000	1.24616200	2.59142200	H	0.84749000	3.97944500	-1.56831100
H	-1.29891500	1.12501700	3.64523900	H	0.62133100	2.30261900	-2.11887300
H	-1.95580100	1.20767600	2.02972800	C	3.33880700	3.65972300	-0.40936100
C	-0.38676500	2.62699100	2.41347000	H	4.02780700	3.34872000	0.37821600
H	-0.04292800	2.79235700	1.39102500	H	2.83879900	4.57509500	-0.07911100
H	0.46247500	2.78705900	3.08257700	H	3.93460900	3.91775500	-1.28904200
H	-1.12308500	3.40314200	2.63611200	C	3.34052900	-3.65922600	-0.40875300
C	-1.02196600	-1.24612200	2.59139800	H	3.93622400	-3.91714300	-1.28854100
H	-1.29884200	-1.12499400	3.64518500	H	2.84097900	-4.57475800	-0.07825200
H	-1.95556100	-1.20782400	2.02961000	H	4.02959600	-3.34783500	0.37860800
C	-0.38628700	-2.62683300	2.41353600				

xyz coordinates of optimized structure of 2b$^-$
(E = -1544.086344)

	x	y	z		x	y	z
O	-0.08304400	0.16352400	-1.62367100	H	-0.11305100	-2.77886600	1.47177200
N	1.70877400	0.00887800	0.66493300	H	-1.24951500	-3.36759900	2.68609000
C	0.25433100	-0.02765300	0.72807100	H	0.34512300	-2.79797400	3.17747200
N	-1.98838000	0.06604800	-0.27353100	C	3.39791700	0.96339000	2.26176700
C	-0.17074600	-0.00822300	2.20205200	H	4.20735400	0.93835700	1.52830000
C	1.17842700	-0.03678200	2.98139900	H	3.83876700	0.82185400	3.25481200
H	1.28753900	0.86989100	3.57964100	H	2.93597500	1.95117400	2.23280400
H	1.20425900	-0.86922600	3.68798800	C	3.09338200	-1.49728200	2.15879000
C	2.36001100	-0.14591300	1.98407800	H	2.41280900	-2.33976900	2.03837900
C	-0.48594400	0.06921600	-0.42489200	H	3.53297900	-1.55677200	3.16094600
C	-2.78201300	1.18744500	-0.46530300	H	3.90277300	-1.59874000	1.43218400
C	-2.40965400	2.53402300	-0.52834800	C	2.51569300	-0.03708800	-0.52342100
H	-1.36836100	2.81696700	-0.46651300	C	2.84353600	-1.26248300	-1.15632500
C	-3.40705600	3.48517300	-0.70093900	C	3.80916000	-1.27647000	-2.16772300
H	-3.13186900	4.53368100	-0.75691500	H	4.06520800	-2.21793900	-2.64263500
C	-4.76009600	3.12101900	-0.81561200	C	4.42701500	-0.11001200	-2.59615200
H	-5.51454000	3.88992700	-0.94602600	H	5.18230400	-0.14211700	-3.37571500
C	-5.12993000	1.78229300	-0.78182300	C	4.03039400	1.10305800	-2.05046000
H	-6.17194500	1.49717300	-0.89158400	H	4.45781900	2.02378700	-2.43405100
C	-4.14294800	0.80452900	-0.62112800	C	3.06931200	1.16326200	-1.03758200
C	-4.15781100	-0.63816400	-0.59981000	C	2.07671400	-2.54777600	-0.87095200
C	-5.16448400	-1.59936200	-0.73422200	H	1.48070600	-2.37065800	0.02331400
H	-6.19994900	-1.29553900	-0.85532300	C	1.09300100	-2.81984600	-2.02906200
C	-4.82359700	-2.94639400	-0.72782400	H	0.46074500	-1.94399800	-2.19549100
H	-5.59409000	-3.70246900	-0.83770900	H	0.46351800	-3.68818000	-1.80134400
C	-3.47934800	-3.33544600	-0.59610400	H	1.63724000	-3.03779200	-2.95501400
H	-3.22619400	-4.39079100	-0.61686700	C	2.52725800	2.52387800	-0.62050900
C	-2.46289900	-2.40048800	-0.44711900	H	1.94771800	2.36418200	0.28748800
H	-1.42901200	-2.70307600	-0.36244300	C	1.55108800	3.02702700	-1.70435900
C	-2.80443300	-1.04465700	-0.42964100	H	2.08566200	3.24699500	-2.63558500
C	-0.96897800	1.27302500	2.60213800	H	1.05593700	3.94938400	-1.37731400
H	-1.20281900	1.20320000	3.67445700	H	0.79888400	2.26059600	-1.91269700
H	-1.92795300	1.25343500	2.08091600	C	3.60931300	3.57343100	-0.31863700
C	-0.29010600	2.61805100	2.33467000	H	4.30886200	3.22898600	0.44803700
H	0.03967500	2.68463300	1.29707800	H	3.14546400	4.49928300	0.03849900
H	0.58211400	2.77990100	2.97553200	H	4.19066100	3.82827200	-1.21085100
H	-0.98771000	3.44092500	2.51876600	C	2.97192100	-3.77420100	-0.62111400
C	-1.06624200	-1.20797800	2.63729200	H	3.53770500	-4.04999600	-1.51674300
H	-1.33543900	-1.05732400	3.69258200	H	2.35687500	-4.63914800	-0.35025800
H	-2.00138900	-1.15513800	2.07756600	H	3.68801300	-3.60375500	0.18648100
C	-0.48172800	-2.61400300	2.48539300				

xyz coordinates of optimized structure of C^+
(E = -1296.743679)

	x	y	z		x	y	z
O	-0.44822700	-0.07868900	-2.31377400	H	-5.10189700	1.49614900	-0.40439000
N	0.52112600	0.69252900	0.48122300	H	-5.38761500	2.98477300	0.47971000
C	0.37471000	1.81951700	1.54627300	C	-2.34681000	-3.66552200	0.23885700
C	-2.50506600	-4.43084000	-0.91560300	C	4.33143900	-0.96736800	-0.45028000
C	-2.07884900	-3.94028800	-2.15260500	H	5.31172800	-1.36998100	-0.67634800
C	-0.95851400	2.44849800	1.10875700	C	3.54938300	-1.54853800	0.53304000
H	-1.51759900	2.80302000	1.97307300	H	3.92507300	-2.41242100	1.06613000
H	-0.76279900	3.31336300	0.47125900	C	2.59373700	0.68140000	-0.88566800
C	-0.76332700	-0.56012500	-1.24335700	C	1.50067100	-1.81757600	1.92455000
C	-1.50489600	-2.68165100	-2.23823600	H	0.52790000	-1.34028700	2.05674400
C	-1.34394100	-1.90085200	-1.07923000	C	-1.73756700	1.37782100	0.29872700
C	-4.01783100	1.62226400	1.45972300	C	-2.85839000	0.67040500	1.12290800
H	-3.67868700	2.40268400	2.14978300	H	-2.44786700	0.24711400	2.04375300
H	-4.78337300	1.05539600	1.99650400	H	-3.25411000	-0.16222100	0.53568400
C	0.29191200	1.19273500	2.94253800	C	-2.38846900	1.98205400	-0.98282700
H	-0.50997400	0.45910300	3.02830300	H	-2.79381600	1.17327300	-1.59821100
H	1.23111700	0.72301200	3.22589600	H	-1.62362000	2.47885100	-1.58500000
H	0.09316900	1.99133600	3.66040300	C	3.84836700	0.12532900	-1.15134900
C	1.82135600	0.07526100	0.13962700	H	4.45812600	0.56422700	-1.93053400
C	1.53703800	2.80264800	1.50078100	C	3.16799300	3.06053100	-1.59887900
H	2.49277800	2.31167600	1.69058600	H	3.36600800	3.33103100	-0.56137200
H	1.58763500	3.33121900	0.55236600	H	4.12837000	2.82290500	-2.06141600
H	1.38231900	3.54468400	2.28757400	H	2.77232300	3.94032500	-2.11288000
C	2.18085400	1.88058800	-1.74321300	C	2.07775500	1.50269200	-3.23653600
H	1.19263800	2.22004400	-1.42530200	H	3.05816100	1.23886100	-3.64086900
C	-0.61358300	0.42774100	-0.08573700	H	1.39896100	0.66943000	-3.40034900
C	-1.76236800	-2.40716400	0.15985800	H	1.70933200	2.35964700	-3.80678900
C	-3.52461600	2.95321700	-0.63159500	C	1.25063900	-3.27798600	1.49275600
H	-3.94651700	3.34506400	-1.56081300	H	2.18597200	-3.84034500	1.45239600
H	-3.12819900	3.81831900	-0.08743300	H	0.60045400	-3.77819400	2.21541900
C	2.22379500	-1.80817500	3.28761700	H	0.78230100	-3.34096600	0.51061100
H	3.14441000	-2.39463600	3.24510800	H	-1.17874800	-2.27947000	-3.18900900
H	2.49753800	-0.80375000	3.61469000	H	-2.20149400	-4.54074500	-3.04567600
H	1.58760200	-2.25485600	4.05597500	H	-2.95988500	-5.41251400	-0.85254300
C	2.28048700	-1.05564000	0.85440500	H	-2.67374800	-4.05253500	1.19619000
C	-4.61172900	2.26679100	0.20267900	H	-1.63112400	-1.82739400	1.06451900

xyz coordinates of optimized structure of D^+
(E = -1676.353283)

	x	y	z		x	y	z
F	2.31882700	-2.80748600	-0.98444900	C	-1.20890600	1.51939700	-1.52383600
F	1.47447200	1.27865200	1.29589800	C	3.58763300	0.83690100	0.42441200
F	5.69870600	0.36879900	-0.49066000	C	-2.17607500	0.62167400	-3.56720200
F	4.83080700	-2.03170200	-1.40175000	H	-2.35064000	0.70704500	-4.63320100
F	4.00471000	2.02327700	0.85240200	C	-1.45373800	1.59535200	-2.89860100
O	0.00180400	-2.36422500	0.15883800	H	-1.06289000	2.43908200	-3.45292900
N	-1.54373700	0.27432900	0.63445500	C	-2.47591600	-0.61162700	-1.48871100
C	-2.51792600	0.89937400	1.68591900	C	-0.37892800	2.64430700	-0.91041000
C	4.45323800	-0.00524600	-0.27083100	H	-0.24435700	2.44328100	0.15005200
C	4.00215700	-1.23693000	-0.73906700	C	-0.85011100	-0.65171900	2.70495700
C	-2.25907100	-0.02752200	2.88699000	C	0.22615200	0.01716400	3.59123300
H	-2.33712000	0.51772000	3.82756200	H	0.27436000	1.09680500	3.46197800
H	-3.00779800	-0.82175500	2.90270100	H	1.21764300	-0.39910600	3.40348500
C	0.40591200	-1.25983000	0.44684300	C	-0.87130100	-2.16463500	3.03072700
C	2.68924400	-1.62912400	-0.51238300	H	0.11715500	-2.61736800	2.93884700
C	1.78642800	-0.80045400	0.18996000	H	-1.55954900	-2.71598900	2.38961100
C	-2.10063900	2.34547200	1.97689300	C	-2.67259400	-0.46403300	-2.86492600
H	-1.05505300	2.43065800	2.27293400	H	-3.23254600	-1.22350500	-3.39493000
H	-2.28098000	2.99719700	1.12522900	C	-4.63468900	-1.86490800	-0.99414300
H	-2.71417500	2.70951500	2.80388500	H	-5.10587900	-0.93683400	-0.66946100
C	-1.72878500	0.40144000	-0.83027200	H	-4.92038000	-2.02516200	-2.03612700
C	-3.96125400	0.86479500	1.20330100	H	-5.05913400	-2.68708400	-0.41237400
H	-4.09163600	1.41899300	0.27243700	C	-2.53051800	-3.15847300	-1.43761200
H	-4.32222400	-0.15188700	1.06842500	H	-2.82898700	-3.27214100	-2.48240100
H	-4.58387100	1.34123500	1.96409500	H	-1.44521600	-3.20163000	-1.38360700
C	-3.09697300	-1.85199300	-0.84075400	H	-2.93129300	-4.01538700	-0.88997900
H	-2.86189700	-1.85176600	0.22594800	C	1.02571700	2.71531900	-1.54587400
C	-0.62873300	-0.43470400	1.21103500	H	0.97907400	3.08218500	-2.57361400
C	2.28447700	0.43108900	0.63959600	H	1.66192000	3.40126300	-0.98090900
C	-1.07526400	4.01365500	-1.05121400	H	1.51041000	1.73784600	-1.57475100
H	-1.12673600	4.32295100	-2.09762900	H	-1.19729000	-2.27935200	4.06715300
H	-2.09753900	4.00523200	-0.66749900	H	-0.02252800	-0.19040300	4.63397600
H	-0.51404200	4.77954700	-0.50994500				

xyz coordinates of optimized structure of C•
(E = -1296.936678)

	x	y	z		x	y	z
O	0.22205500	-1.97483000	-0.59732100	H	-4.80677500	1.73390900	0.21906800
N	0.87597200	0.68873000	-0.00185800	H	-4.82236400	3.49125100	0.18012400
C	0.95575400	2.17830400	0.20886300	C	-4.02906500	-2.58091000	0.85056800
C	-4.57861000	-3.03591900	-0.34448000	C	4.55822300	-1.38272300	0.34472000
C	-3.87631000	-2.85842500	-1.53664600	H	5.52868200	-1.85655500	0.44382800
C	-0.44973700	2.62185500	-0.22785200	C	3.71833900	-1.27447700	1.44240400
H	-0.77498700	3.49815700	0.33279400	H	4.03105100	-1.69199400	2.39246400
H	-0.41796200	2.91004500	-1.28224800	C	2.88814100	-0.29795100	-1.04605700
C	-0.69219200	-1.15663600	-0.35640800	C	1.53595400	-0.72670700	2.55547300
C	-2.63935500	-2.22207600	-1.53111100	H	0.66020100	-0.11283500	2.34388900
C	-2.09418300	-1.72574400	-0.34025100	C	-1.40389900	1.40878000	-0.06438200
C	-3.19574100	2.63811100	1.33808300	C	-2.19313700	1.47329100	1.27789400
H	-2.66586300	3.59775700	1.35999300	H	-1.50107600	1.53125900	2.12242300
H	-3.75287800	2.57965100	2.27884000	H	-2.74844900	0.54104700	1.39309000
C	1.25308700	2.52983900	1.67809500	C	-2.42973700	1.38333200	-1.22857800
H	0.51402500	2.11618100	2.36296800	H	-3.01311800	0.46219800	-1.17886100
H	2.23862600	2.16531000	1.97095400	H	-1.89060700	1.36397400	-2.18161100
H	1.25061700	3.61698400	1.79372000	C	4.12945100	-0.91891800	-0.89100500
C	2.08024500	-0.11754900	0.09995300	H	4.76207000	-1.06230800	-1.75916500
C	2.03151700	2.84375700	-0.65814700	C	3.42764400	0.84867000	-3.27743600
H	3.03195500	2.48757800	-0.40670000	H	3.73248700	1.76337000	-2.76497400
H	1.85430200	2.67484000	-1.71929100	H	4.33146800	0.27007700	-3.48674000
H	2.00500400	3.92241100	-0.48064200	H	2.99409800	1.12811300	-4.24241300
C	2.41211800	0.03046800	-2.45913500	C	2.05383800	-1.27134000	-3.20793500
H	1.49440800	0.61488300	-2.37579900	H	2.94816400	-1.87924500	-3.37534400
C	-0.41760100	0.23294700	-0.11352700	H	1.34232000	-1.86433800	-2.63344300
C	-2.79459700	-1.93090300	0.85197600	H	1.62035300	-1.03803200	-4.18606600
C	-3.39945400	2.57408600	-1.18337300	C	1.03864300	-2.17565000	2.75188200
H	-4.10243600	2.49827300	-2.01905400	H	1.86251300	-2.83198700	3.04757800
H	-2.85418100	3.51525300	-1.32621200	H	0.28241500	-2.21471300	3.54273800
C	2.17180900	-0.20349800	3.85590600	H	0.60923900	-2.57298100	1.83169800
H	3.01036000	-0.82885300	4.17381400	H	-2.08413400	-2.10594100	-2.45502500
H	2.54152100	0.81866000	3.75213500	H	-4.28958800	-3.22489800	-2.47000200
H	1.43534800	-0.21555800	4.66508400	H	-5.53952200	-3.53816000	-0.34691600
C	2.46599200	-0.65922700	1.34661000	H	-4.55487400	-2.73903700	1.78592800
C	-4.16196900	2.61870000	0.14683100	H	-2.36167100	-1.60711600	1.79133800

xyz coordinates of optimized structure of D˙
(E = -1676.572070)

	x	y	z		x	y	z
F	-2.16743800	2.41342200	-0.25542500	C	2.79517300	-1.18580900	-1.03910600
F	-2.17546200	-2.31798200	-0.33644700	C	-4.19921600	-1.14791500	-0.49587900
F	-6.22029200	0.06051700	-0.66542100	C	4.23603800	0.09391300	-2.51928300
F	-4.86200100	2.41659400	-0.50578800	H	4.95725400	0.12125700	-3.32865100
F	-4.86766900	-2.30432900	-0.57035500	C	3.72327200	-1.11835100	-2.08242400
O	-0.10426700	0.13427500	-1.50206400	H	4.02924300	-2.03283300	-2.57683800
N	1.58820100	-0.01562600	0.78600600	C	2.86612700	1.26795300	-0.89370500
C	2.22946200	-0.10996300	2.15159700	C	2.14352500	-2.53312500	-0.73700700
C	-4.89023900	0.05628900	-0.54535900	H	1.52632700	-2.41909800	0.15424700
C	-4.19475600	1.25791400	-0.46532200	C	-0.26334400	-0.10633500	2.28414800
C	1.03508600	0.20935100	3.06738400	C	-0.78654200	-1.52532800	2.61043800
H	1.08531500	-0.34246900	4.00820100	H	-0.05347100	-2.29869100	2.37776400
H	1.05144500	1.27475100	3.31173100	H	-1.69280000	-1.75602800	2.05070800
C	-0.57158300	0.05833800	-0.34835500	C	-1.34428300	0.92187100	2.67497000
C	-2.81234000	1.23771100	-0.34055100	H	-2.32480000	0.66080700	2.27802600
C	-2.09255000	0.04859000	-0.27511600	H	-1.08812900	1.92592600	2.33017300
C	2.81416600	-1.50948000	2.40900600	C	3.78769300	1.27413700	-1.94355600
H	2.06958900	-2.29933200	2.31926800	H	4.14506700	2.22187200	-2.32866600
H	3.62879200	-1.72130000	1.71592700	C	3.38468000	3.63675600	-0.05951000
H	3.22147100	-1.54315300	3.42288100	H	4.10077300	3.25267500	0.67031100
C	2.41581400	0.01971200	-0.40870000	H	3.94840000	3.94591700	-0.94380900
C	3.35677000	0.91310900	2.33743300	H	2.92263200	4.53622000	0.35798200
H	4.17575100	0.74291000	1.63661600	C	1.34002000	3.18108600	-1.47538600
H	2.99854300	1.93449100	2.21725300	H	1.88796100	3.46229000	-2.37973000
H	3.75473000	0.81390000	3.35082800	H	0.57908200	2.45295700	-1.75517300
C	2.30042700	2.60271100	-0.41390300	H	0.84497300	4.07765800	-1.08995600
H	1.70964100	2.41741600	0.48484200	C	1.19833700	-2.93240300	-1.89141500
C	0.22149500	-0.00967400	0.83369400	H	1.76655300	-3.14295200	-2.80238500
C	-2.81504900	-1.13461300	-0.37254100	H	0.63989000	-3.83565900	-1.62736300
C	3.15609700	-3.66153700	-0.47002200	H	0.48915800	-2.13504300	-2.11258400
H	3.75040500	-3.88473000	-1.36018800	H	-1.02458600	-1.59253100	3.67650400
H	3.84950200	-3.41504800	0.33685000	H	-1.43185800	0.94961700	3.76550600
H	2.62995800	-4.58006400	-0.19405000				

xyz coordinates of optimized structure of O_2[3]

(E = -150.361053)

	x	y	z
O	0.00000000	0.00000000	0.60283800
O	0.00000000	0.00000000	-0.60283800

xyz coordinates of optimized structure of the C-adduct of O_2[3] on 2a$^{\bullet}$

(E = -1312.102721)

	x	y	z
O	1.26869400	-2.21246600	0.69722200
N	-0.26156700	0.17782200	0.62097700
N	2.02639300	-2.00483200	-1.41707700
C	0.95553100	-0.01413100	-0.14350400
C	2.08617400	0.76531000	0.66289900
C	1.54263900	0.59814700	2.10251300
H	1.87767000	1.40873900	2.75245100
H	1.92216800	-0.33800600	2.51527700
C	-0.00029100	0.53125000	2.05362500
C	1.40991300	-1.51524000	-0.30264500
C	2.36657000	-3.42798900	-1.42967500
C	2.46550800	-1.28470400	-2.61063200
C	2.15912100	2.27646300	0.28641000
H	2.64600800	2.77533300	1.13014000
H	1.15301700	2.68977200	0.25104800
C	2.89741200	2.68151800	-0.99721900
H	3.94607700	2.37518700	-0.98934000
H	2.42612000	2.27043500	-1.88943000
H	2.88350000	3.77117800	-1.09219900
C	3.49631100	0.12599400	0.55251900
H	3.42835000	-0.92591400	0.83435700
H	3.83995800	0.15105900	-0.48537700
C	4.56595700	0.77878500	1.44002300
H	4.74549900	1.82535900	1.18477900
H	5.51475200	0.24793700	1.32568100
H	4.29537500	0.73385700	2.49788800
C	-0.50185400	-0.54547900	3.03284600
H	-0.05914100	-1.51351600	2.80527100
H	-0.21999300	-0.26590500	4.05292500
H	-1.59041100	-0.62889400	3.00331700
C	-0.64803500	1.86408400	2.46975000
H	-0.44171600	2.05107300	3.52708600
H	-1.73201600	1.81980100	2.34934600
H	-0.26960000	2.71202600	1.90083200
C	-1.61366800	0.08349000	0.08983000
C	-2.35199600	-1.13307000	0.15361000
C	-3.68619400	-1.14967500	-0.26509200
H	-4.24012300	-2.07913100	-0.20902600
C	-4.31419200	-0.01941900	-0.75867800
H	-5.35133700	-0.05765600	-1.07413200
C	-3.59142800	1.15623600	-0.85918700
H	-4.07118600	2.03738000	-1.26863900
C	-2.25570500	1.23910600	-0.45485900
C	-1.76798600	-2.47088200	0.59038000
H	-0.78715300	-2.29091200	1.01231600
C	-1.56935600	-3.38471700	-0.63665700
H	-2.52773500	-3.65256700	-1.09263200
H	-1.06499900	-4.31016600	-0.34259500
H	-0.96548800	-2.89161800	-1.40125300
C	-2.61132000	-3.19145000	1.65832600
H	-3.58085600	-3.51960400	1.27220600
H	-2.79737500	-2.55439000	2.52585600
H	-2.08199100	-4.08375100	2.00584200
C	-1.57687300	2.58681100	-0.68807900
H	-0.57004500	2.51547800	-0.29107500
C	-2.29198800	3.75309400	0.02390100
H	-1.70720700	4.67206000	-0.08379300
H	-3.27588900	3.94363400	-0.41328700
H	-2.43395600	3.56593100	1.08886100
C	-1.45599000	2.90826200	-2.19323700
H	-0.96399000	2.10301700	-2.73742600
H	-0.87989900	3.82833900	-2.33477100
H	-2.44186500	3.06569900	-2.64071900
H	3.42848000	-1.69928500	-2.91990800
H	1.75205700	-1.40002000	-3.43212300
H	2.59971400	-0.22614100	-2.42018400
H	1.88227200	-3.92026000	-0.59243400
H	2.02931800	-3.87367400	-2.36983200
H	3.45058800	-3.56588700	-1.34589400
O	0.75727300	0.62783000	-1.44614000
O	-0.07225500	-0.07132700	-2.21354700

xyz coordinates of optimized structure of the C-adduct of O_2[3] on 2b$^{\bullet}$

(E = -1694.378670)

	x	y	z		x	y	z
O	-0.78854800	0.95284700	1.70558800	H	0.55029500	2.43262100	0.98824300
N	1.65633700	0.16262000	0.61426800	C	-0.27383000	3.40585300	-0.72491600
N	-2.12601300	0.00603300	0.15381900	H	0.02313100	4.09739100	-1.51921300
C	0.45705700	-0.64359700	0.49902200	H	-1.09081100	3.86777500	-0.16436600
C	0.59794800	-1.76752100	1.61958200	H	-0.65610500	2.50085300	-1.20143200
C	1.40264600	-0.97659300	2.68036500	C	1.41716500	4.37873000	0.88205100
H	1.99291100	-1.64588800	3.30858000	H	1.69020100	5.14706600	0.15327300
H	0.70845700	-0.44154200	3.33000000	H	2.28832400	4.19555100	1.51490700
C	2.31015300	0.04660200	1.95955000	H	0.62729200	4.79841700	1.51225200
C	-0.88095200	0.16351100	0.78616000	C	3.49366600	-1.13426300	-1.44336000
C	1.43638900	-3.00019700	1.16155400	H	2.95368200	-1.62355000	-0.64059000
H	1.73209100	-3.50603800	2.08528300	C	4.99259200	-1.45576300	-1.27702500
H	2.36810800	-2.65732900	0.71728800	H	5.14120400	-2.53961500	-1.24284800
C	0.80806400	-4.04538100	0.23076700	H	5.57797400	-1.07643700	-2.11883200
H	-0.14493600	-4.42378300	0.60769000	H	5.41021300	-1.02801800	-0.36452900
H	0.65182900	-3.65830900	-0.77557100	C	2.98405800	-1.73523100	-2.77091300
H	1.48285800	-4.90227900	0.14858200	H	1.92780700	-1.51966100	-2.92890000
C	-0.75844200	-2.23871600	2.21245800	H	3.12193500	-2.82119900	-2.76954900
H	-1.30702300	-1.36842600	2.57728900	H	3.54098600	-1.33391100	-3.62270100
H	-1.37694300	-2.68907900	1.43261600	O	0.45033300	-1.23194000	-0.82711700
C	-0.64323700	-3.23122200	3.37854900	O	0.13090300	-0.33159200	-1.75238600
H	-0.20305800	-4.18470200	3.07913100	C	-3.15692300	0.99191100	0.34508500
H	-1.63832800	-3.44432500	3.77704300	C	-4.26063200	0.65570100	-0.46093700
H	-0.04443500	-2.82723100	4.19885900	C	-3.19284500	2.14018200	1.14075500
C	2.31777600	1.37421900	2.73878900	C	-5.39555700	1.46600400	-0.49700800
H	1.30987800	1.76763800	2.85438200	C	-4.33519000	2.93726200	1.09238100
H	2.73968100	1.20422600	3.73425700	H	-2.37361100	2.40024900	1.78658100
H	2.94131100	2.11904000	2.24023600	C	-5.42797300	2.61357800	0.28333300
C	3.77072300	-0.43346200	1.87144000	H	-6.23869100	1.19820200	-1.12352200
H	4.19806600	-0.47444900	2.87691800	H	-4.37156900	3.82796500	1.70940600
H	4.37198300	0.26489300	1.28634700	H	-6.30144200	3.25514500	0.27152500
H	3.86347900	-1.42344900	1.42887300	C	-2.66516300	-0.99384500	-0.72425900
C	2.25579700	0.95329200	-0.45330900	C	-3.95913700	-0.59368100	-1.11953100
C	1.99144300	2.34701100	-0.57397800	C	-2.18199200	-2.23809500	-1.12755200
C	2.69450100	3.10041000	-1.51974800	C	-4.73696600	-1.39422100	-1.95640200
H	2.49043100	4.16134300	-1.60025700	C	-2.97150900	-3.03029500	-1.95730500
C	3.62775000	2.52808600	-2.36588000	H	-1.21585900	-2.60121100	-0.83417600
H	4.16111500	3.13440400	-3.08997300	C	-4.23539500	-2.61517600	-2.38346000
C	3.85236700	1.16487600	-2.28790600	H	-5.72704000	-1.06801400	-2.25363100
H	4.55877000	0.70609300	-2.96946100	H	-2.58567700	-3.99231700	-2.27450300
C	3.18855300	0.35891200	-1.35853000	H	-4.82525600	-3.25141900	-3.03272600
C	0.91426200	3.08915500	0.20716600				

xyz coordinates of optimized structure of 2c^{+}

(E = -420.866036)

	x	y	z		x	y	z
C	-0.67580600	0.38564300	-0.56191500	H	2.38333700	2.21154800	-0.29253200
H	-0.72212200	1.10235800	-1.37845800	H	0.73209200	2.09502200	0.34939000
C	0.60134300	-0.40863200	-0.36235900	H	2.10716900	1.77834900	1.40861400
N	1.70396500	0.24300800	0.03203100	C	-3.05984300	0.71471600	-0.38994800
O	0.49360300	-1.58669400	-0.66784900	H	-2.89513900	1.38239700	-1.23227200
N	-1.78046600	0.10659200	0.03083000	H	-3.74414300	-0.08527200	-0.67709000
C	2.97676800	-0.48455200	0.10282000	H	-3.48261200	1.26612700	0.45055000
H	3.37138800	-0.43922200	1.12018000	C	-1.88901200	-0.88712100	1.12026700
H	2.80826700	-1.52017700	-0.18107200	H	-0.90789100	-1.13358000	1.51237700
H	3.69719400	-0.03052500	-0.58175000	H	-2.52140200	-0.46748400	1.90201200
C	1.73197500	1.65907700	0.38926600	H	-2.35200600	-1.78797400	0.71402400

xyz coordinates of optimized structure of 2c$^{\bullet}$
(E = -421.077587)

	x	y	z		x	y	z
C	-0.58181500	0.49850100	-0.08337400	H	1.97328500	2.14884800	-0.75814800
H	-0.43410500	1.55640700	-0.23442100	H	1.29439400	2.07987200	0.88670000
C	0.55282500	-0.39941000	-0.04865500	H	3.01197100	1.79930700	0.63177200
N	1.80590400	0.19558600	0.09637600	C	-2.91150400	1.14108600	-0.15956200
O	0.45707700	-1.63296600	-0.14574300	H	-2.53769400	2.02492400	-0.67780900
N	-1.89298300	0.10562600	-0.13580400	H	-3.79266300	0.77576500	-0.69288500
C	2.98668700	-0.62417400	-0.11992600	H	-3.22206000	1.43283800	0.85473500
H	3.70279900	-0.48624300	0.69740700	C	-2.35915900	-1.20223400	0.31435000
H	2.67642100	-1.66520400	-0.15555400	H	-1.56647400	-1.93017400	0.17281200
H	3.48762400	-0.36836500	-1.06401800	H	-2.64180000	-1.16790500	1.37692600
C	2.02000400	1.62612700	0.20908000	H	-3.24099000	-1.48420100	-0.26705600

xyz coordinates of optimized structure of 2c^{-}
(E = -421.097386)

	x	y	z		x	y	z
C	-0.56692300	0.47355200	-0.06274100	H	1.85987400	2.08543300	-0.57719800
H	-0.50659100	1.47973700	0.34689000	H	1.31709200	1.99581200	1.11059700
C	0.51152900	-0.40397400	-0.06882700	H	3.03141000	1.77748000	0.73388700
N	1.82657000	0.13271300	0.30706800	C	-2.84776500	0.99618700	-0.56884100
O	0.47477100	-1.63540200	-0.33895900	H	-2.50620000	1.55860700	-1.44404300
N	-1.90096100	-0.04064200	-0.26336700	H	-3.83546100	0.56829500	-0.78799700
C	2.93735200	-0.55121200	-0.31984200	H	-2.98871100	1.73402100	0.26082500
H	3.84570000	-0.45765800	0.29231500	C	-2.36193700	-0.91885900	0.79928400
H	2.65734100	-1.59903000	-0.41778200	H	-1.62439900	-1.71527100	0.91342700
H	3.17584300	-0.16221900	-1.33308400	H	-2.48173400	-0.39670500	1.77547800
C	2.01241600	1.56115900	0.38766800	H	-3.32962500	-1.37090200	0.53225100

xyz coordinates of optimized transition state for the rotation around N2-C2 bond of 2c^{+}
(E = -420.826001; 1 imaginary frequency)

	x	y	z		x	y	z
C	0.47960200	-0.40197800	-0.37016300	H	-1.41409000	-1.57423900	1.38448100
H	0.21043500	-1.37607700	-0.77071100	H	-1.35634800	0.02380500	2.19444000
C	-0.63835200	0.64276300	-0.23609200	H	-2.90250400	-0.69560400	1.76931500
N	-1.89411300	0.15023200	0.15468400	C	2.70497100	-1.31530100	-0.25820700
O	-0.37257900	1.79304800	-0.44847700	H	2.23741900	-2.16301600	-0.75310000
N	1.71393600	-0.23252900	-0.05935200	H	3.52015200	-0.92510700	-0.86890000
C	-2.62281300	-0.56601300	-0.90832800	H	3.09632500	-1.61410400	0.71526200
H	-3.65400400	-0.70023800	-0.58000500	C	2.28569200	1.01948000	0.49155700
H	-2.63881600	0.03733600	-1.81661700	H	1.50495900	1.68080800	0.84702800
H	-2.20435100	-1.55957100	-1.13339800	H	2.97036200	0.74596400	1.29344000
C	-1.87034700	-0.57282300	1.43913100	H	2.83981800	1.51497200	-0.30813000

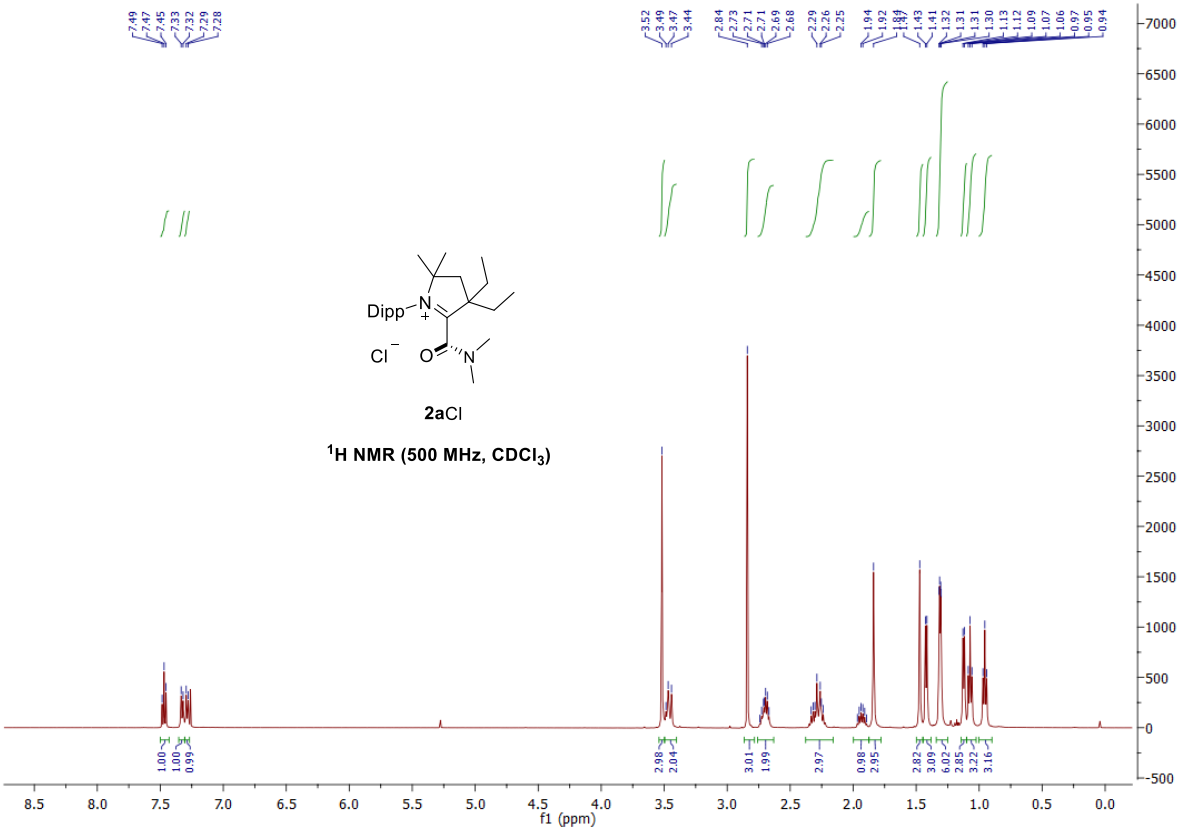
xyz coordinates of optimized transition state for the rotation around N2-C2 bond of 2c$^{\bullet}$
(E = -421.067243; 1 imaginary frequency)

	x	y	z		x	y	z
C	0.62731200	-0.56575000	-0.02756000	H	-2.90499600	0.86648300	-1.19815800
H	0.46286600	-1.63263200	-0.07155200	H	-1.99270100	-0.35761800	-2.11184300
C	-0.53254100	0.26042900	-0.00064100	H	-3.45147100	-0.83134500	-1.23069300
N	-1.76122800	-0.52813000	-0.02977500	C	2.98761400	-1.16144900	-0.04822700
O	-0.56064500	1.49883500	0.04409900	H	2.56403800	-2.16453400	-0.07043700
N	1.92616100	-0.17121500	-0.00282200	H	3.60854200	-1.02104700	-0.94095600
C	-2.52311100	-0.34346400	1.21011400	H	3.63454100	-1.07163100	0.83209500
H	-3.40405600	-0.99057100	1.18812400	C	2.36589000	1.21820200	0.04770300
H	-1.90854800	-0.63755300	2.06466800	H	1.49704000	1.86903200	0.07534600
H	-2.85097400	0.69660400	1.35872300	H	2.98332400	1.37854700	0.93925200
C	-2.57222500	-0.18220200	-1.20213400	H	2.97538900	1.44640000	-0.83470800

xyz coordinates of optimized transition state for the rotation around N2-C2 bond of 2c^{-}
(E = -421.087817; 1 imaginary frequency)

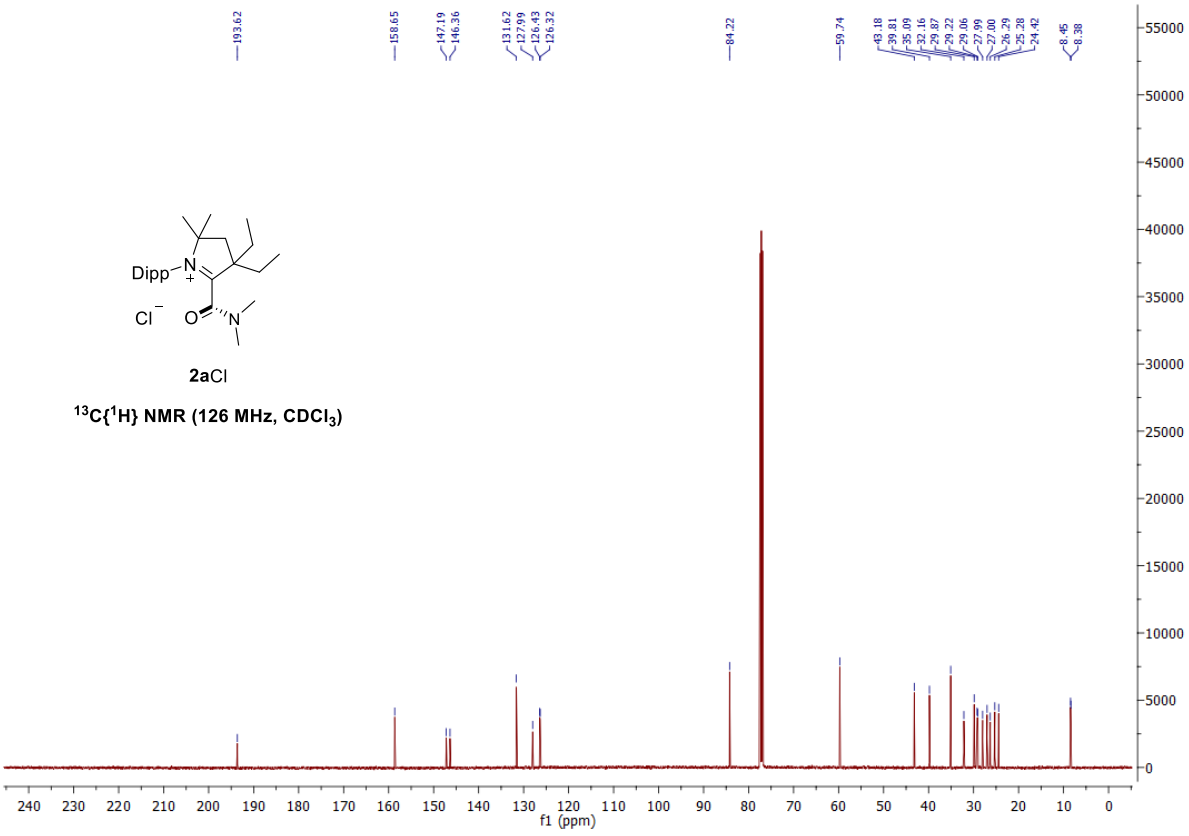
	x	y	z		x	y	z
C	0.44072700	-0.39399100	-0.04732800	H	-1.77261600	-1.10127600	1.76548300
H	0.18097300	-1.32767700	0.44819200	H	-1.73982400	0.65423700	2.02809900
C	-0.51222400	0.56668900	-0.31356500	H	-3.26767500	-0.14666000	1.60637600
N	-1.92789300	0.15321200	0.01704100	C	2.64467700	-1.34161300	-0.11266400
O	-0.36370000	1.72171100	-0.77808800	H	2.28400400	-2.11736200	-0.79707800
N	1.84988200	-0.15293800	-0.26226000	H	3.69626300	-1.13305500	-0.34799100
C	-2.46066400	-0.86481600	-0.85958800	H	2.61584800	-1.77263900	0.91831500
H	-3.55558300	-0.93332600	-0.74958500	C	2.36935900	0.96323800	0.51117400
H	-2.24368400	-0.59622300	-1.89651800	H	1.73662400	1.82929100	0.30672000
H	-2.04608500	-1.88042100	-0.68397300	H	2.36738400	0.76938900	1.60730500
C	-2.18198400	-0.13146700	1.41060700	H	3.40070900	1.19188500	0.20408600

NMR spectra



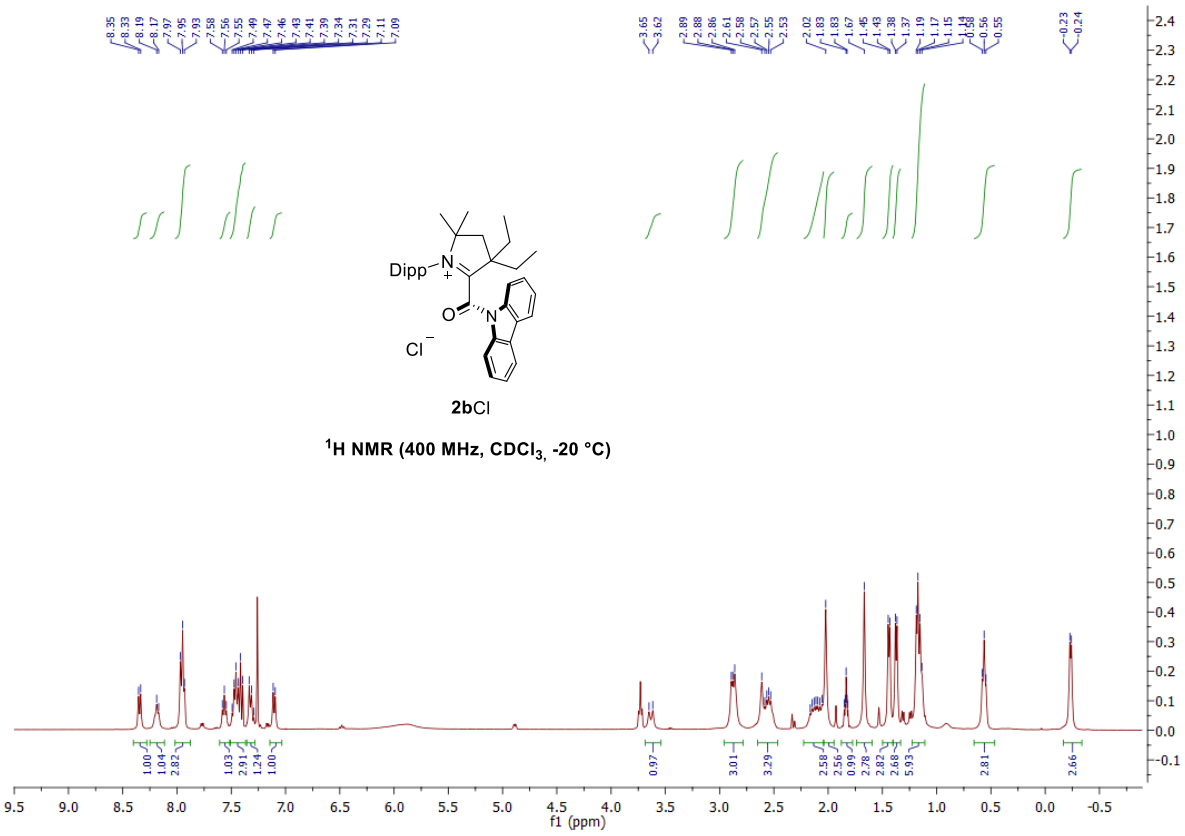
2aCl

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



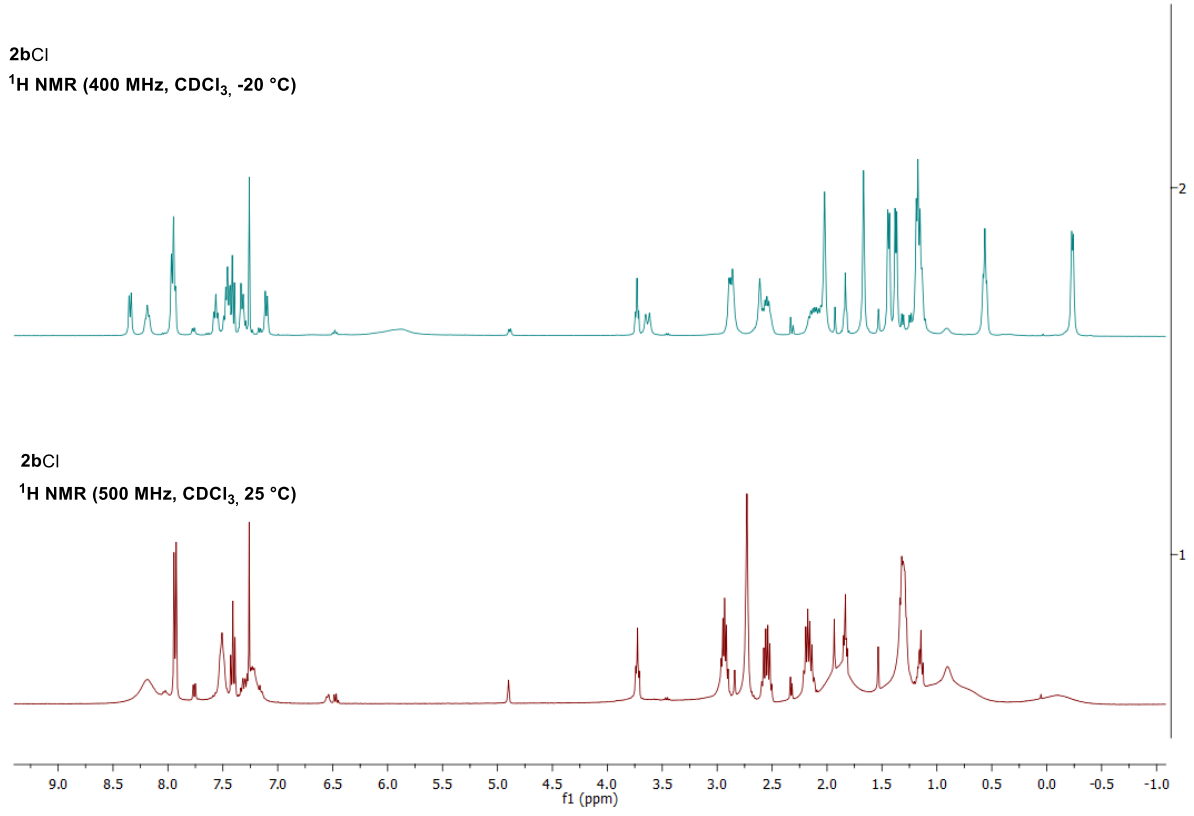
2aCl

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



2bCl

^{1}H NMR (400 MHz, $CDCl_3$, -20 °C)

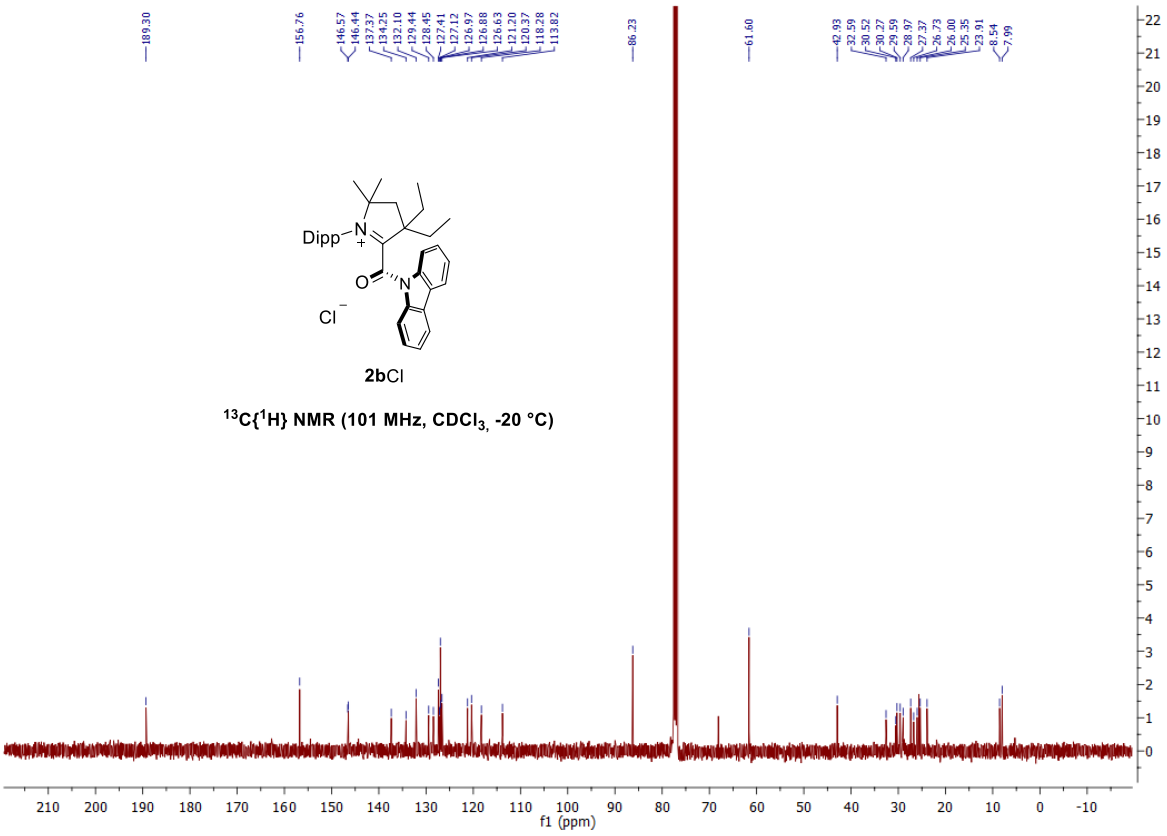


2bCl

^{1}H NMR (400 MHz, $CDCl_3$, -20 °C)

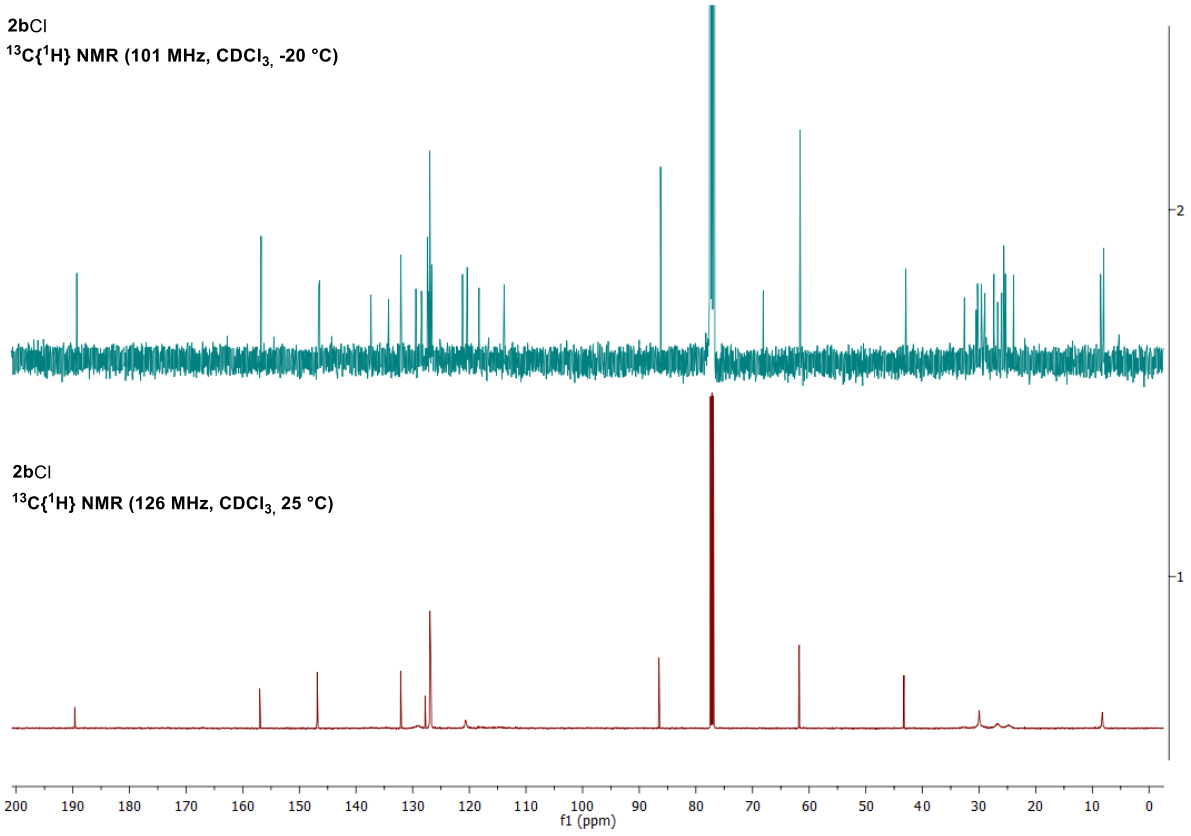
2bCl

^{1}H NMR (500 MHz, $CDCl_3$, 25 °C)



2bCl

$^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$, -20 °C)

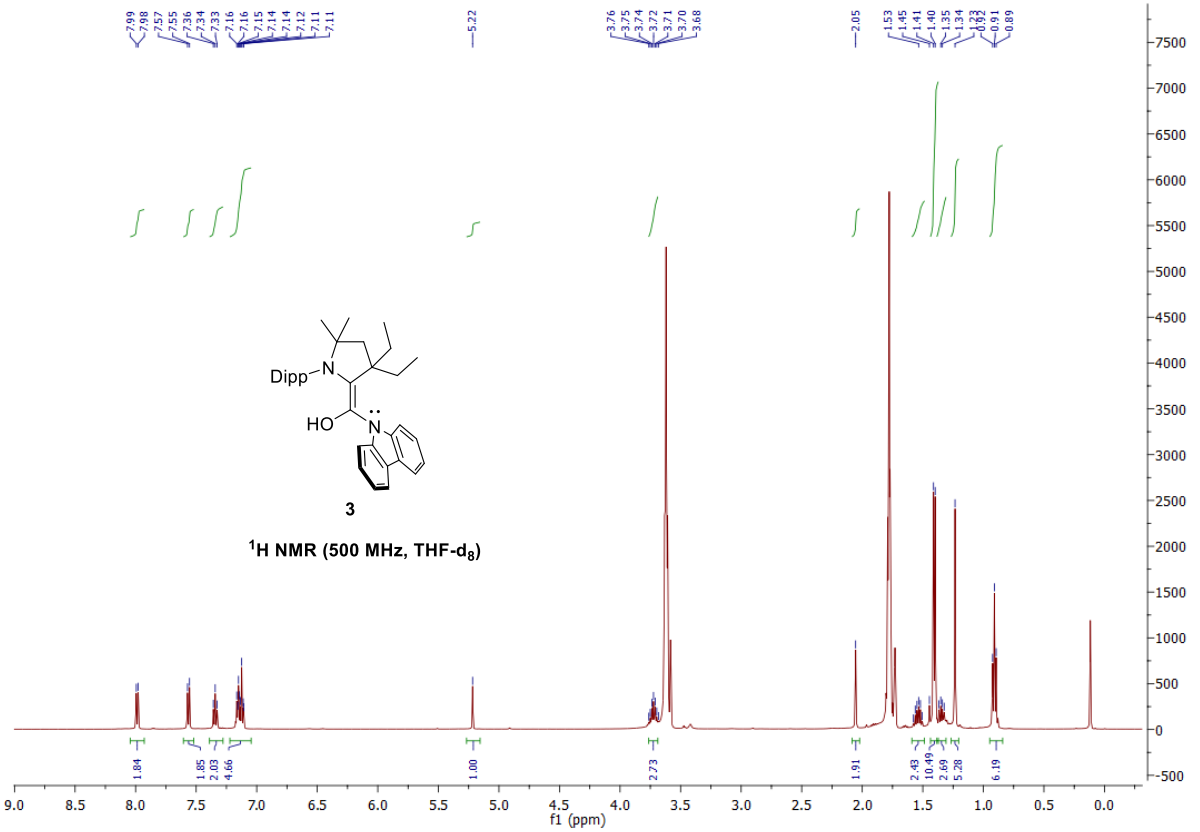


2bCl

$^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$, -20 °C)

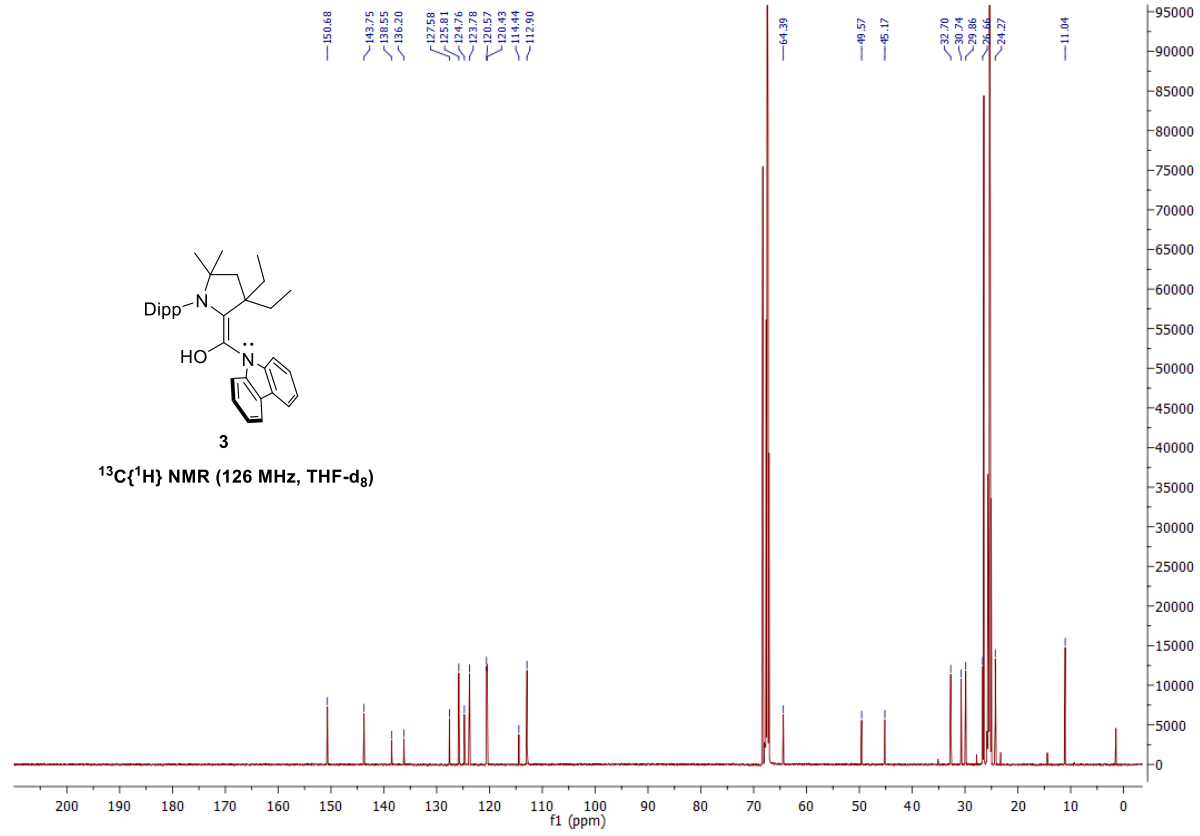
2bCl

$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 25 °C)



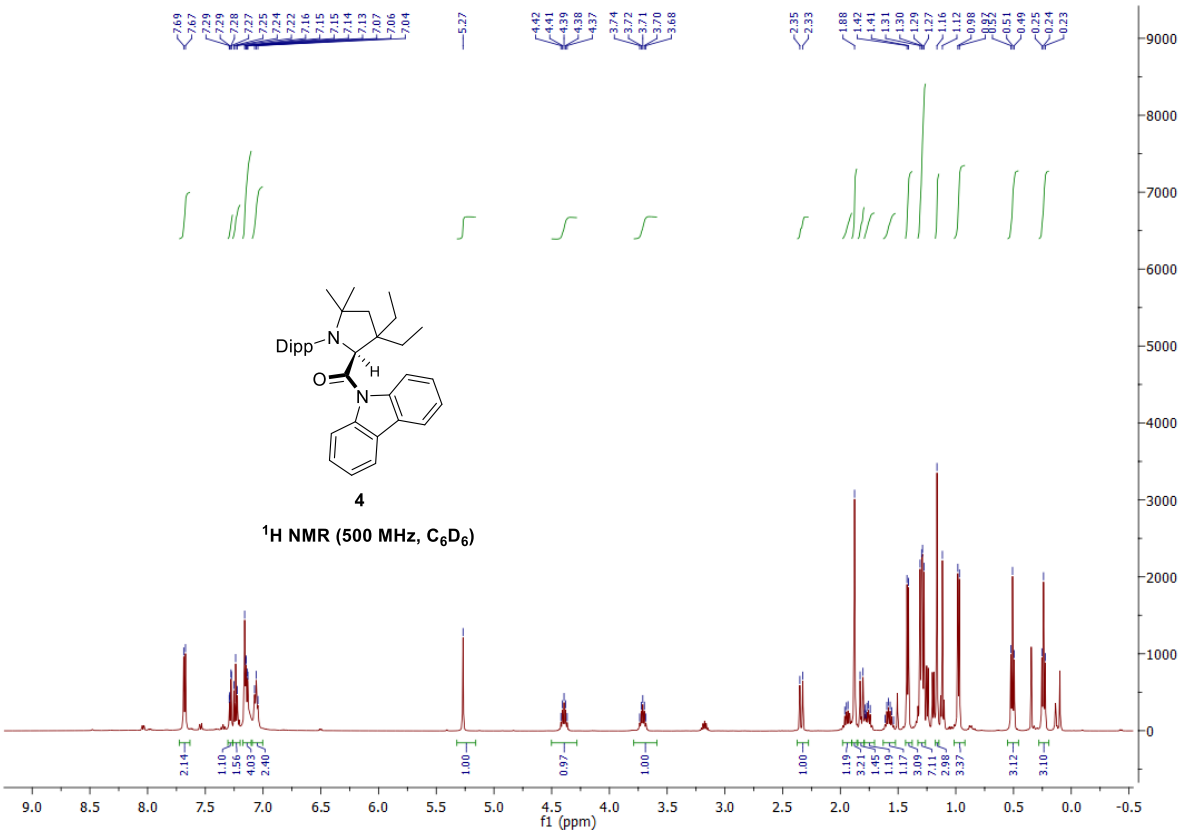
3

^{1}H NMR (500 MHz, THF-d_8)



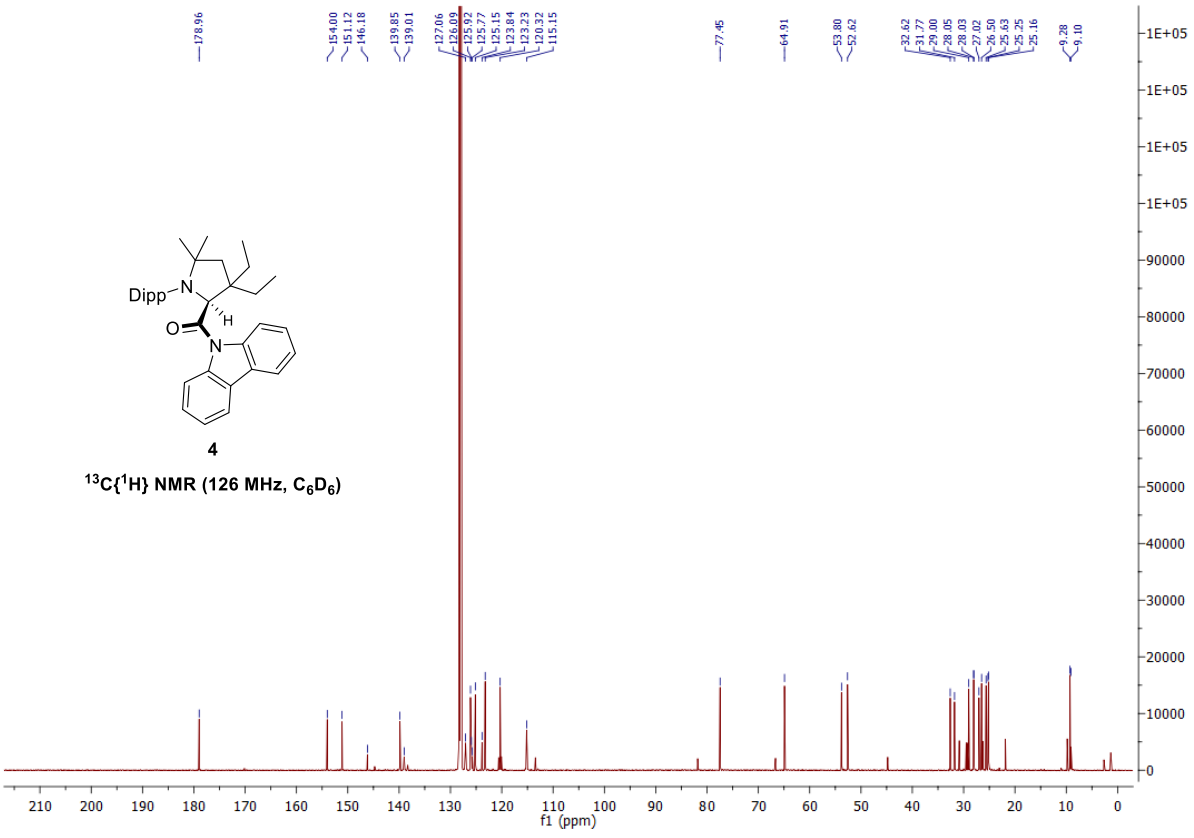
3

^{13}C{^{1}H} NMR (126 MHz, THF-d_8)



4

^{1}H NMR (500 MHz, C_6D_6)



4

^{13}C{^{1}H} NMR (126 MHz, C_6D_6)

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] Allenmark, S. *Tetrahedron Lett.,* 1990, **131**, 1455–1458.
[3] D. J. Dixon and A. C. Lucas, *Synlett,* 2004, **6**, 1092–1094.
[4] Experimental EPR spectra were fitted with the EasySpin simulation package: S. Stoll and A. Schweiger, *J. Magn. Reson.*, 2006, **178**, 42-55.
[5] ShelXT: G.M. Sheldrick, *Acta Cryst.*, 2015, **A71**, 3-8.
[6] Olex2: O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, *J. Appl. Cryst.*, 2009, **42**, 339-341.
[7] CrysAlisPro 1.171.39.46 (Rigaku OD, 2018)
[8] ShelXL: G.M. Sheldrick, *Acta Cryst.*, 2015, **C71**, 3-8.
[9] A. J. M. Duisenberg, L. M. J. Kroon-Batenburg and M. M. Schreurs, *J. Appl. Crystallogr.,* 2003, **36**, 220-229.
[10] SADABS v2.10, Program for empirical absorption correction of area detector data, G. M. Sheldrick, University of Gçttingen, Germany, 2003.
[11] XPREP v2005/3 ©Bruker AXS.
[12] G. M. Sheldrick, *Acta Cryst.,* 2008, **A64**, 112-122.
[13] 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, D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.