

The Serendipitous Discovery of a Readily Available Redox-Bistable Molecule Derived from Cyclic(alkyl)(amino)carbenes

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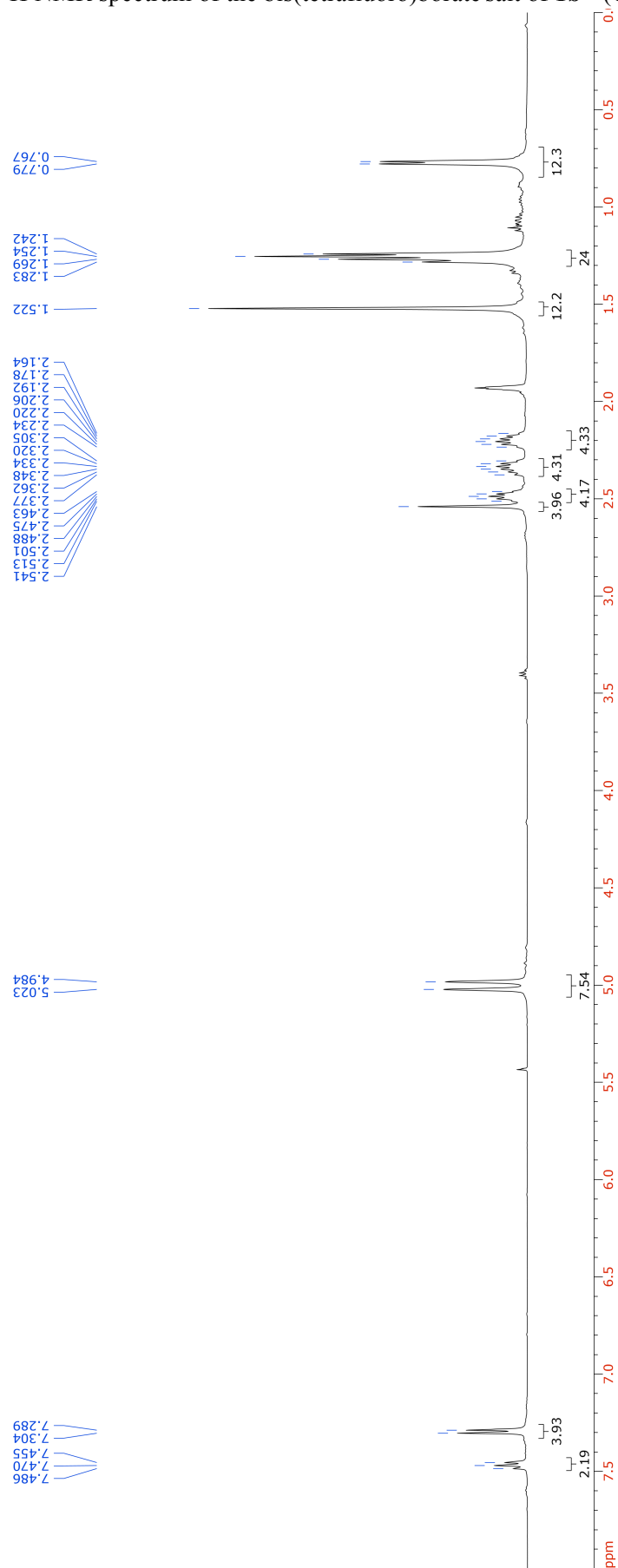
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SUPPORTING INFORMATION

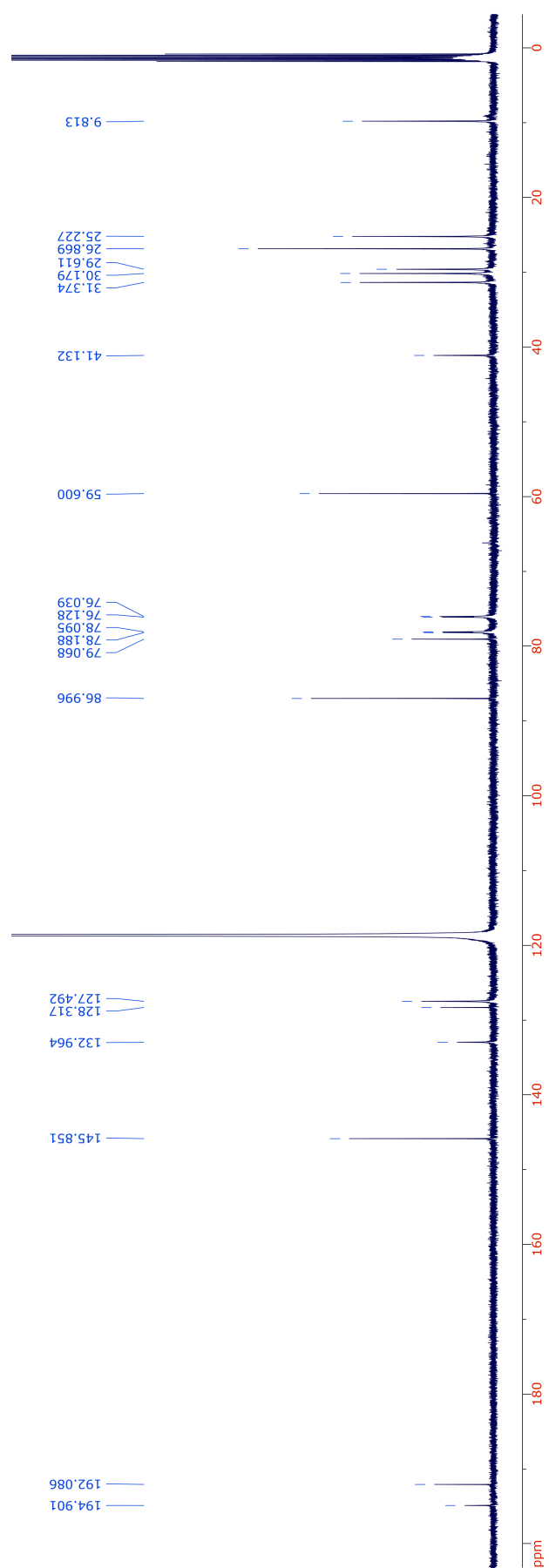
I. ¹ H and ¹³ C NMR spectra of new compounds	S2
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I. ^1H and ^{13}C NMR spectra of new compounds

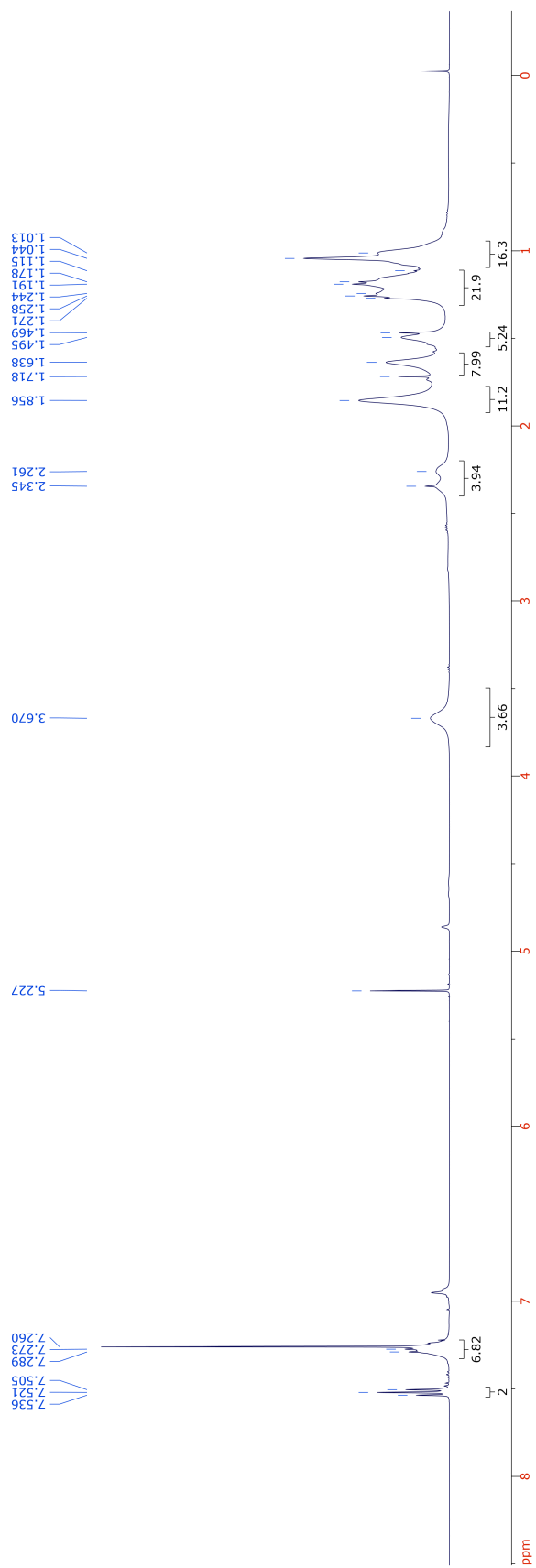
^1H NMR spectrum of the bis(tetrafluoro)borate salt of **1b** $^{2+}$ (CD_3CN , 500 MHz)



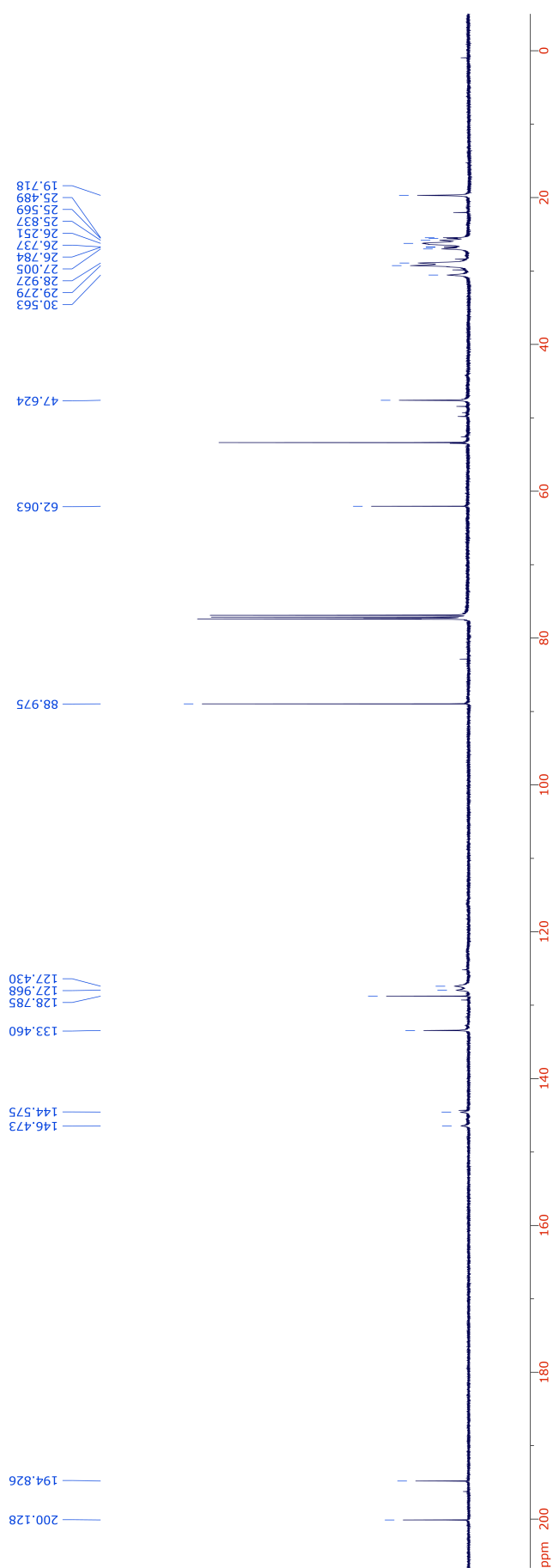
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum the bis(tetrafluoro)borate salt of **1b**²⁺ (CD_3CN , 125 MHz)



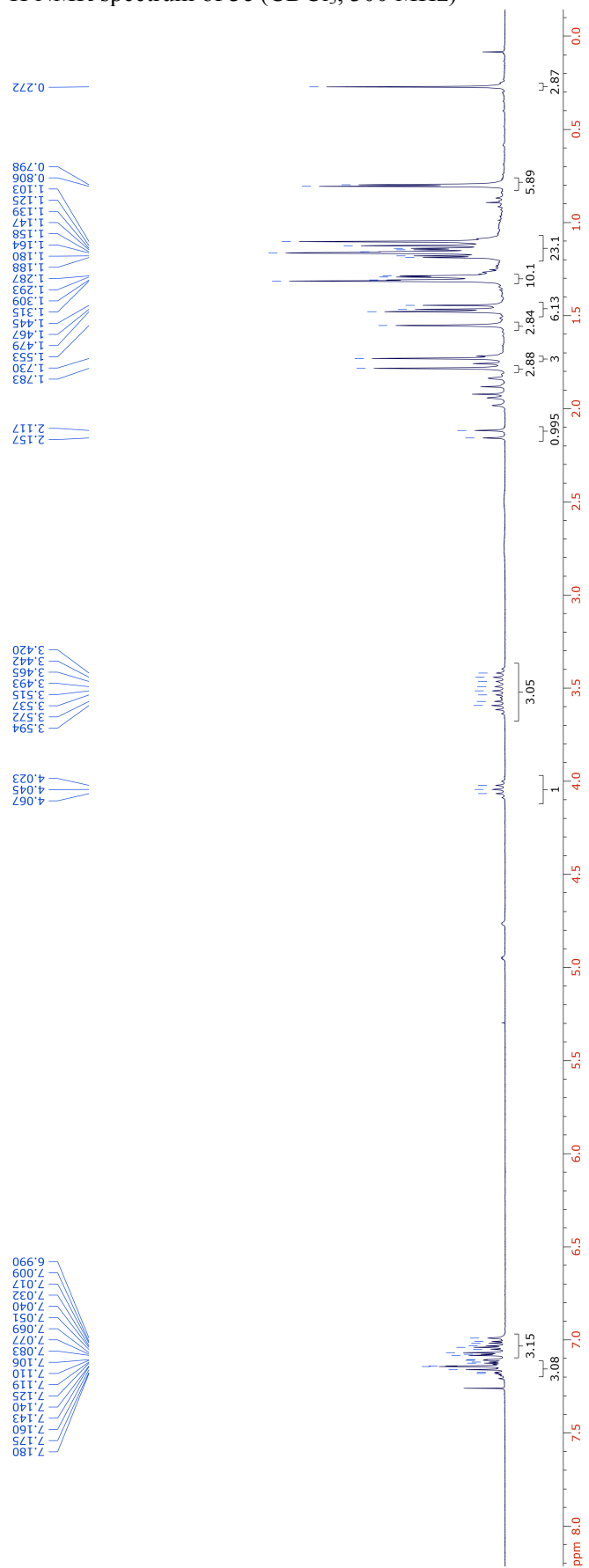
^1H NMR spectrum of the bis(tetrafluoro)borate salt of **2b**²⁺ (CDCl_3 , 500 MHz)



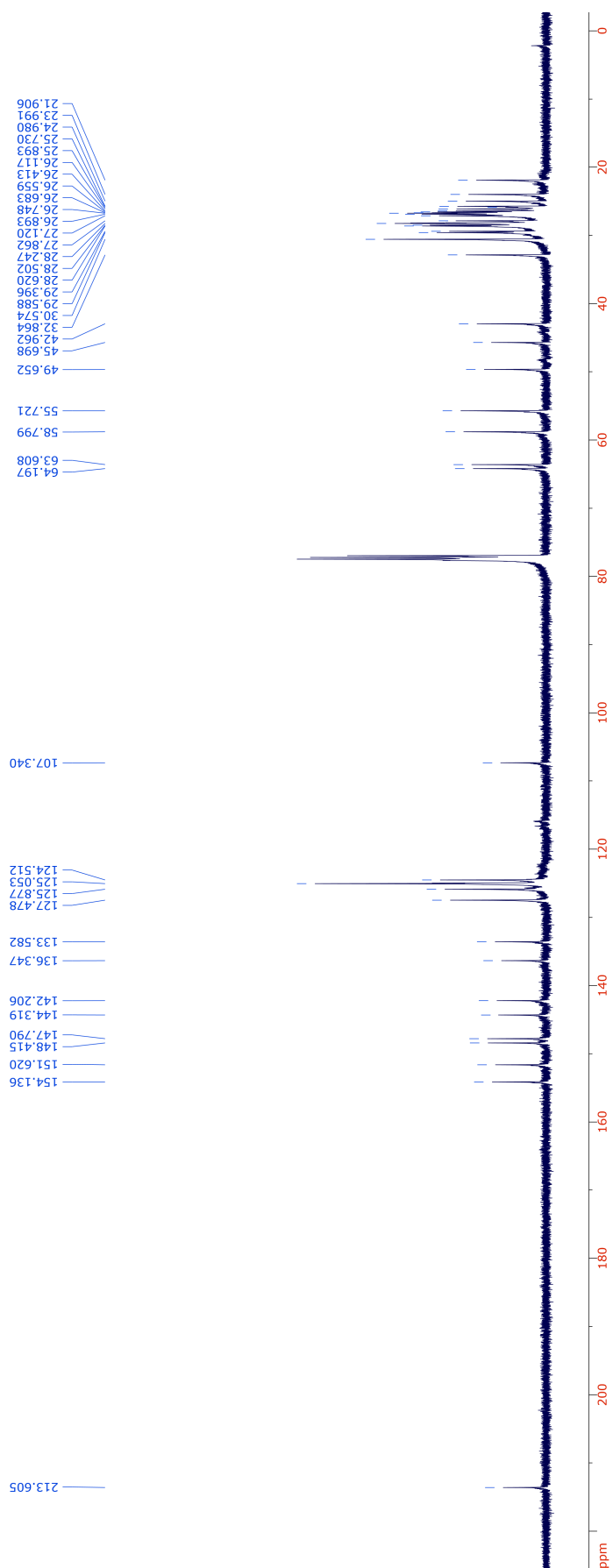
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of the bis(tetrafluoro)borate salt of **2b**²⁺ (CDCl_3 , 125 MHz)



¹H NMR spectrum of **3c** (CDCl₃, 300 MHz)



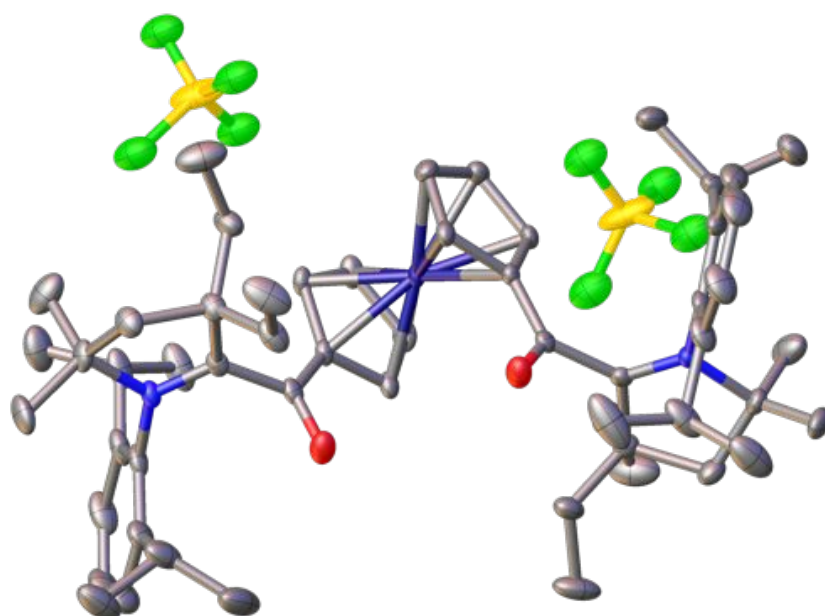
^{13}C NMR spectrum of **3c** (CDCl_3 , 125 MHz)



II. X-ray Diffraction Tables

X-ray Collection Parameter for $1b^{2+}BF_4^{2-}$

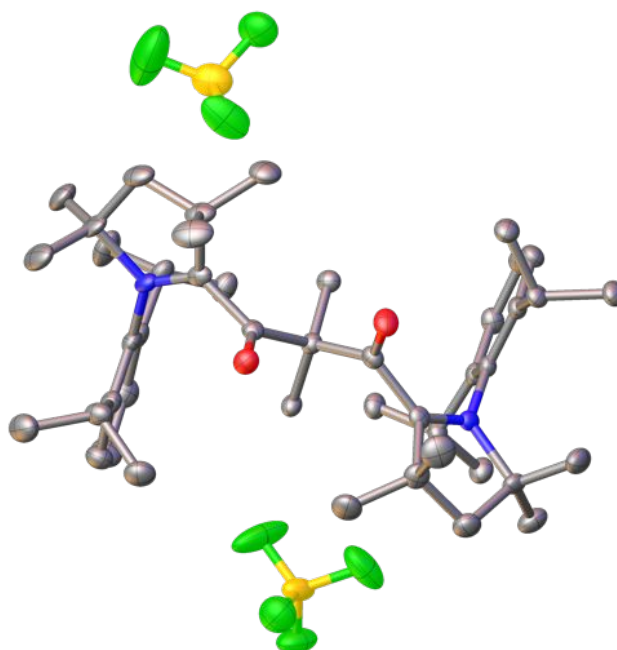
CCDC 1825142	Copy_sq
Identification code	
Empirical formula	$C_{56}H_{78}B_2F_8FeN_2O_2$
Formula weight	1040.67
Temperature/K	100.0
Crystal system	monoclinic
Space group	C2/c
a/Å	21.6194(8)
b/Å	10.6383(4)
c/Å	26.8304(10)
$\alpha/^\circ$	90
$\beta/^\circ$	95.299(2)
$\gamma/^\circ$	90
Volume/Å ³	6144.5(4)
Z	4
$\rho_{calc}/\text{g}/\text{cm}^3$	1.125
μ/mm^{-1}	0.307
F(000)	2208.0
Crystal size/mm ³	0.2 × 0.1 × 0.1
Radiation	MoK α ($\lambda = 0.71073$)
2 θ range for data collection/ $^\circ$	3.048 to 52.854
Index ranges	-26 ≤ h ≤ 27, -12 ≤ k ≤ 13, -32 ≤ l ≤ 33
Reflections collected	27629
Independent reflections	6295 [$R_{int} = 0.0468$, $R_{sigma} = 0.0407$]
Data/restraints/parameters	6295/0/324
Goodness-of-fit on F ²	1.039
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0546$, $wR_2 = 0.1126$
Final R indexes [all data]	$R_1 = 0.0680$, $wR_2 = 0.1185$
Largest diff. peak/hole / e Å ⁻³	0.47/-0.38



X-ray Collection Parameter for $1c^{2+}BF_4^{2-}$

CCDC 1820818

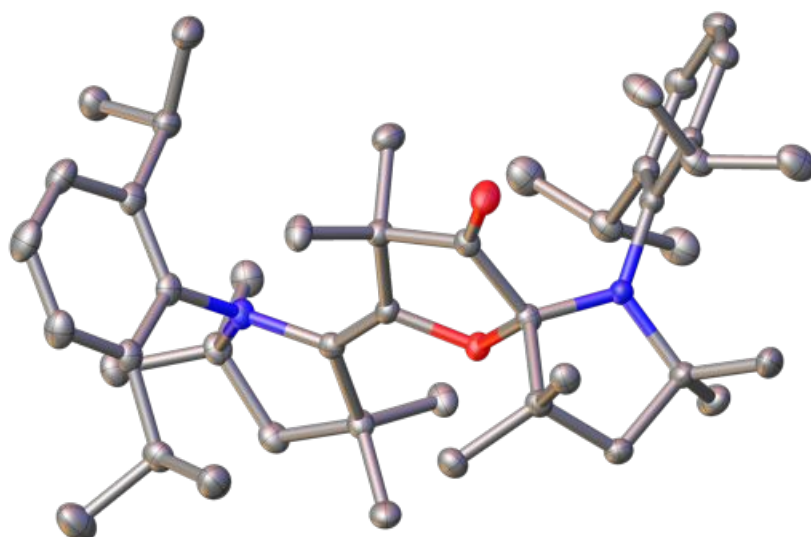
Identification code	GB_JKM20b_0m_a_sq
Empirical formula	$C_{47}H_{71}B_2F_8N_3O_2$
Formula weight	883.68
Temperature/K	100.0
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	21.3381(5)
b/Å	10.2919(3)
c/Å	24.6126(6)
$\alpha/^\circ$	90
$\beta/^\circ$	111.6150(10)
$\gamma/^\circ$	90
Volume/Å ³	5025.1(2)
Z	4
$\rho_{\text{calc}}/\text{g/cm}^3$	1.168
μ/mm^{-1}	0.753
F(000)	1888.0
Crystal size/mm ³	$0.13 \times 0.12 \times 0.05$
Radiation	$\text{CuK}\alpha$ ($\lambda = 1.54178$)
2θ range for data collection/ $^\circ$	4.698 to 136.932
Index ranges	$-25 \leq h \leq 23, -12 \leq k \leq 12, -29 \leq l \leq 29$
Reflections collected	58527
Independent reflections	9239 [$R_{\text{int}} = 0.0548, R_{\text{sigma}} = 0.0328$]
Data/restraints/parameters	9239/60/615
Goodness-of-fit on F^2	1.030
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0515, wR_2 = 0.1361$
Final R indexes [all data]	$R_1 = 0.0641, wR_2 = 0.1447$
Largest diff. peak/hole / $e \text{ \AA}^{-3}$	0.54/-0.41



X-ray Collection Parameter for 3c

CCDC 1820817

Identification code	gb_jkm011_0m_a
Empirical formula	C ₄₅ H ₆₈ N ₂ O ₂
Formula weight	669.01
Temperature/K	100.0
Crystal system	tetragonal
Space group	I4 ₁ /a
a/Å	40.9015(14)
b/Å	40.9015(14)
c/Å	9.3338(5)
α/°	90
β/°	90
γ/°	90
Volume/Å ³	15614.8(14)
Z	16
ρ _{calc} /cm ³	1.138
μ/mm ⁻¹	0.517
F(000)	5888.0
Crystal size/mm ³	0.31 × 0.2 × 0.12
Radiation	CuKα (λ = 1.54178)
2θ range for data collection/°	4.32 to 136.492
Index ranges	-49 ≤ h ≤ 45, -49 ≤ k ≤ 48, -11 ≤ l ≤ 11
Reflections collected	63703
Independent reflections	7156 [R _{int} = 0.0710, R _{sigma} = 0.0353]
Data/restraints/parameters	7156/0/460
Goodness-of-fit on F ²	1.038
Final R indexes [I ≥ 2σ(I)]	R ₁ = 0.0390, wR ₂ = 0.0921
Final R indexes [all data]	R ₁ = 0.0530, wR ₂ = 0.1006
Largest diff. peak/hole / e Å ⁻³	0.22/-0.18



III. Cyclic Voltammograms of $1c^{2+}$

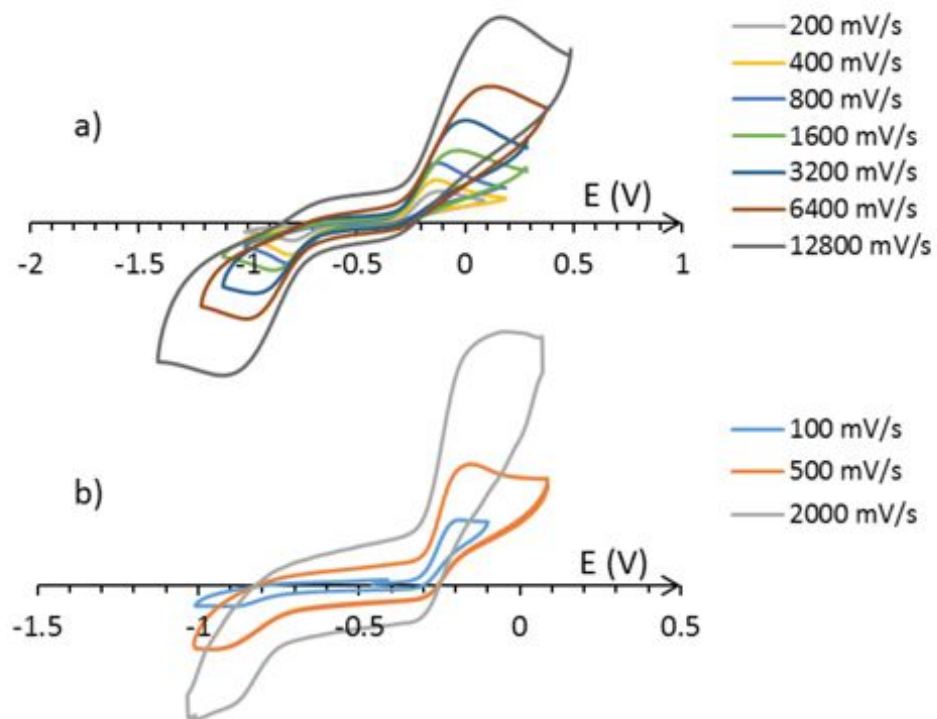


Figure S1: Cyclic voltammogram of $1c^{2+}$ in $CH_3CN + 0.1M NBu_4PF_6$ at different sweep rates; (a) at room temperature (b) at $-40\text{ }^\circ\text{C}$.

IV. VT-EPR plots

EPR spectra were recorded on a Bruker EMX+ spectrometer equipped with a previously calibrated low-temperature (T) measurement device. Samples were approx. 0.01M solution of biradical in frozen acetonitrile. I is the double integration of the EPR signal (arbitrary unit). When varying temperature, all other acquisition parameters were kept constant. The half-field band ($\Delta m = \pm 2$) was chosen for measurements, due to the saturation of the main $\Delta m = \pm 1$ transition at low temperature. A “blank” spectrum from a pure frozen acetonitrile sample was subtracted prior to integration, in order to minimize signal from triplet oxygen.

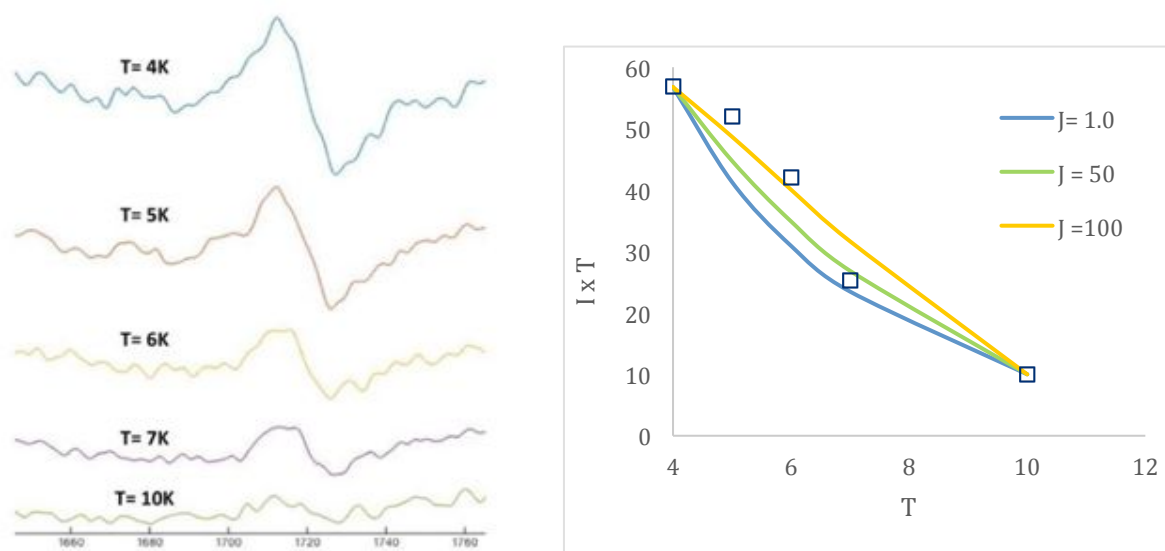


Figure S2: Left: half-field EPR band ($\Delta m = \pm 2$) of a solution of **2a** in frozen acetonitrile at different Helium temperature; right: $I \cdot T$ (arbitrary unit) as a function of temperature T (K) and fit with $C/(3+\exp(-J/T/k_B))$. C is a proportionality factor, $-2J$ is the singlet-triplet energy gap ($\text{J}\cdot\text{mol}^{-1}$), and R is molar gas constant ($8.314 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$). Any value of $J < 100 \text{ J}\cdot\text{mol}^{-1}$ could allow for a possible fit.

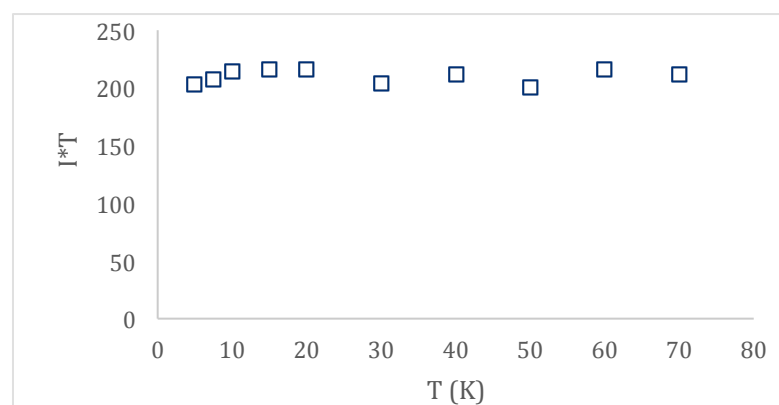


Figure S3: ($I \times T$) as a function of T for a sample of **2b** in frozen acetonitrile.

V. Computational details

Computational methods: We carried out calculations using the density functional theory as implemented in the program package Gaussian09¹ with the 6-311G(d,p) basis set and the B3LYP exchange–correlation functional.² Indeed, (amino)(carboxy)radicals, were previously studied at this level of theory and calculations well reproduced experimental data, including geometry from x-ray diffraction studies. All structures were submitted to vibrational analysis and minima were characterized by the absence of imaginary frequencies. Thermodynamic analysis was carried out for a temperature of 298.15 K, using the principal isotope for each element type.

(x,y,z) coordinates of optimized structures are provided below with corresponding zero-point energies in hartrees.

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- (1) *Gaussian 09*, Revision 4.2.0, 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, N. J. 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, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.
- (2) (a) A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648. (b) C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B*, 1988, **37**, 785. (c) S. H. Vosko, L. Wilk and M. Nusair, *Can. J. Phys.*, 1980, **58**, 1200. (d) P. J. Stephens, F. J. Devlin, C. F. Chabalowski and M. J. Frisch, *J. Phys. Chem.*, 1994, **98**, 11623.

xyz coordinate of I (UB3LYP/6-311g level of theory)**

(E = -208.554901)

	x	y	z		x	y	z
O	-1.36468100	-0.63011600	0.00180600	H	1.05704400	1.62710700	0.00361400
N	1.36232400	-0.44684900	-0.01551500	H	0.88725900	-1.33864200	0.01943800
C	0.58143400	0.65519800	0.00117800	H	2.36238500	-0.40886100	0.06123500
C	-0.83051500	0.49027200	0.00051300	H	-1.43101500	1.41644900	-0.00027200

xyz coordinate of I_{OO} (B3LYP/6-311g level of theory)**

(E = -417.059602)

	x	y	z		x	y	z
O	0.67317400	-0.30452800	0.88235500	O	-0.67331900	-0.30647500	-0.88204700
C	1.84581900	-0.51460700	0.49490400	C	-1.84589200	-0.51570200	-0.49394700
C	2.71445700	0.50463300	0.09330100	C	-2.71441300	0.50443300	-0.09432900
N	4.01298500	0.30488000	-0.27067000	H	-2.35944900	1.52771400	-0.10906100
H	2.35954300	1.52796300	0.10580600	N	-4.01280200	0.30549700	0.27045500
H	2.24004000	-1.54991500	0.42392400	H	-4.32909000	-0.63644500	0.44617000
H	4.50908500	1.03001200	-0.76102300	H	-4.50903300	1.03182800	0.75887100
H	4.32909600	-0.63747600	-0.44452700	H	-2.24014000	-1.55084100	-0.42069400

xyz coordinate of I_{CC} (B3LYP/6-311g level of theory)**

(E = -417.146248)

	x	y	z		x	y	z
C	0.36489100	-0.59670700	0.32859600	O	-2.49736200	-0.43686500	0.24351700
C	1.88424800	-0.48504700	0.23672400	H	-0.11921100	1.97569400	1.17469500
O	2.49732000	0.43693900	-0.24339200	H	-0.94430800	-2.13292900	0.06038100
H	0.13183500	-0.59017500	1.40398600	H	0.94436800	2.13284100	-0.06057800
H	0.11936100	-1.97569800	-1.17480100	N	0.02319600	-1.93038700	-0.16444700
C	-0.36491400	0.59666000	-0.32863500	N	-0.02312600	1.93034300	0.16433500
H	-0.13192000	0.59008000	-1.40403900	H	-2.40258700	1.38443700	-0.62730600
C	-1.88427000	0.48507200	-0.23666800	H	2.40258400	-1.38441100	0.62733600

xyz coordinate of I_{CO} (B3LYP/6-311g level of theory)**

(E = -417.125093)

	x	y	z		x	y	z
C	1.48078100	0.95600800	-0.43532900	H	-2.33402000	0.21686700	-1.39127900
C	1.27105500	-0.56394600	-0.42234600	H	1.84977900	-0.96260700	-1.26880600
O	2.21748900	1.53262100	0.32214100	H	0.91212200	1.48351200	-1.22525300
N	1.65144200	-1.10554900	0.84770200	H	2.09972600	-2.00819000	0.77534500
O	-0.07428600	-0.86681500	-0.80129100	H	2.24613400	-0.45262800	1.34742900
C	-1.03757700	-0.44833800	0.10781800	H	-0.80255500	-0.63183700	1.15091000
C	-2.18337400	0.08342900	-0.32496000	H	-4.14495400	0.36192200	0.12155800
N	-3.22293900	0.56615900	0.48374900	H	-3.15668300	0.27931900	1.45203600

xyz coordinate of 2c (triplet state at the B3LYP/6-311g level of theory)**
(E = -2015.083898)

	x	y	z		x	y	z
C	1.19963000	1.16042500	-0.69482900	H	4.44781400	4.23730200	0.56902300
O	0.89298500	0.11809300	-1.28530500	C	5.77345400	0.47466800	0.70348100
C	-0.00171600	2.13068600	-0.38890200	H	5.74809300	-0.54381200	1.09425800
C	-1.11535900	1.21926500	0.26429700	H	6.80989500	0.70609900	0.44373000
O	-0.73448200	0.25253000	0.92981000	H	5.46938500	1.15467500	1.49596700
C	-2.56840100	1.43990600	0.15193400	C	5.53488300	-0.30877000	-1.62812900
C	-3.37861900	2.71991100	0.47365600	H	6.53716700	0.06439800	-1.85894300
C	-4.82643400	0.70789600	0.64924700	H	5.63743600	-1.33305700	-1.26951600
C	-4.82872100	2.20749100	0.32919700	H	4.95184600	-0.31049000	-2.54853300
H	-5.14802100	2.34899200	-0.70758400	C	3.08870300	-1.02247400	0.24686500
H	-5.52110900	2.76437900	0.96454600	C	2.89530100	-2.15704400	-0.58385100
N	-3.41143400	0.33660800	0.28406800	C	2.99726700	-1.15240900	1.65789600
C	-3.10911800	-1.00813700	-0.17951600	C	2.71128200	-3.40225800	0.02679600
C	-2.87657600	-2.05680300	0.74425400	C	2.78794800	-2.42185000	2.20489800
C	-3.13869300	-1.28482600	-1.57109700	C	2.66920100	-3.54576900	1.40393200
C	-2.74839300	-3.36158100	0.25746300	H	2.57051000	-4.27580000	-0.59889100
C	-2.99531800	-2.60920100	-1.99628800	H	2.71568200	-2.52690300	3.28104600
C	-2.81875200	-3.64699600	-1.09607400	H	2.52068100	-4.52352100	1.84932700
H	-2.57350500	-4.16811500	0.95968200	C	-3.26477800	-0.22330200	-2.66296800
H	-3.01895200	-2.82686700	-3.05760100	C	-4.45337000	-0.46415400	-3.61576200
H	-2.71788200	-4.66777600	-1.44835800	C	-1.96169700	-0.15376800	-3.48581400
C	-5.87348000	-0.03581000	-0.18748400	H	-3.40509200	0.74627500	-2.18287300
H	-5.75966400	0.17205400	-1.24956300	H	-5.40341600	-0.56598700	-3.08849700
H	-5.82114600	-1.11530400	-0.03594900	H	-4.54390700	0.36921400	-4.31933000
H	-6.86880700	0.30032200	0.11638500	H	-4.30983100	-1.37292100	-4.20657800
C	-5.14861400	0.44718300	2.13552700	H	-1.08645700	-0.06407500	-2.84244200
H	-5.24418600	-0.61744100	2.33565100	H	-1.83699100	-1.05844400	-4.08820200
H	-4.39584300	0.85371900	2.80810200	H	-1.98946300	0.69808700	-4.17301000
H	-6.10746800	0.91510900	2.37744300	C	-2.70221800	-1.86384000	2.24766100
C	-3.23767900	3.95042600	-0.44326100	C	-1.28063000	-2.26084100	2.69297100
H	-4.00236800	4.68017400	-0.15686600	C	-3.73234100	-2.66917500	3.06717900
H	-2.27258300	4.44768600	-0.35111200	H	-2.82161400	-0.80346500	2.46310000
H	-3.40318900	3.69607900	-1.49230000	H	-0.53072300	-1.72706400	2.11513400
C	-3.09906200	3.18708400	1.92910600	H	-1.14252000	-2.02249100	3.75283600
H	-3.11661700	2.36310700	2.64076800	H	-1.11596400	-3.33596600	2.57301500
H	-2.12153700	3.66129500	2.01425900	H	-4.75916900	-2.51667800	2.72818700
H	-3.85073600	3.92177100	2.23535700	H	-3.52991200	-3.74221800	3.00331900
C	0.30474800	3.24625500	0.62403700	H	-3.67874200	-2.39065400	4.12409800
H	-0.58239300	3.84921500	0.81304300	C	3.06893200	0.01992900	2.63638700
H	0.63863000	2.83118900	1.57722100	C	4.12217300	-0.17972500	3.74381800
H	1.06524900	3.93079000	0.25751200	C	1.69172100	0.29169100	3.27233700
C	-0.41906200	2.70831200	-1.75884000	H	3.33866900	0.91071200	2.07377000
H	-0.46119000	1.91328900	-2.49966600	H	5.11079200	-0.40939000	3.34283300
H	-1.38920100	3.19067400	-1.72874900	H	4.20370400	0.72798300	4.35006100
H	0.30483200	3.44977700	-2.10137700	H	3.84186000	-0.99291800	4.41851200
C	2.61656600	1.37854900	-0.38958800	H	0.92085800	0.41949100	2.51258000
C	3.48098500	2.64906300	-0.55540500	H	1.38884500	-0.53964900	3.91582700
C	4.90391300	0.59434400	-0.56132700	H	1.73590000	1.19218100	3.89471700
C	4.80236300	2.03335000	-1.08292200	C	2.77951400	-2.12145200	-2.10858200
H	5.67002600	2.63276900	-0.79750200	C	1.36937100	-2.56862400	-2.55181600
H	4.76623800	2.00936000	-2.17542300	C	3.81927500	-3.00908500	-2.82338000
N	3.45274900	0.26871000	-0.31834900	H	2.90215200	-1.08702500	-2.42725300
C	2.99002200	3.64882700	-1.62096900	H	0.59925200	-2.00959500	-2.02786700
H	3.80244400	4.34364100	-1.85670600	H	1.24961800	-2.40268800	-3.62750100
H	2.70880600	3.13575400	-2.54325300	H	1.22035700	-3.63660700	-2.36496700
H	2.14368900	4.25048900	-1.29292900	H	4.84796700	-2.77261800	-2.55195300
C	3.75193800	3.41453600	0.76446500	H	3.65443700	-4.06627400	-2.59626900
H	2.84464200	3.84042800	1.18872900	H	3.72320000	-2.89392700	-3.90758300
H	4.20134300	2.77761700	1.52543400				

xyz coordinate of 3c (B3LYP/6-311g** level of theory)
(E= -2015.129391)

	x	y	z		x	y	z
O	-0.69316000	0.72651500	0.66842100	C	2.96658700	3.28010600	-1.59767800
C	0.18808900	-0.54191600	-1.13310400	C	4.81883800	3.16504100	0.09957600
C	-1.77272100	0.85250100	-0.34858400	H	2.91254000	2.19464100	0.23482100
C	-3.09573900	2.78922800	0.38586500	H	2.15553100	2.75346300	-2.10233600
C	-3.96202600	1.51928200	0.43118100	H	2.54872700	4.17600900	-1.12937000
H	-4.42876600	1.38612400	1.41238100	H	3.67407500	3.61078100	-2.36301900
H	-4.77162300	1.57405800	-0.30646600	H	5.30008600	2.59703300	0.89775400
C	0.50771400	0.18523600	0.16619700	H	5.58492000	3.40493500	-0.64320200
C	1.64738600	0.90233800	2.35342200	H	4.46403600	4.10806100	0.52715300
C	3.10479900	0.66681100	2.79729900	C	3.79824300	-2.80941400	-0.72820500
C	3.64929100	-0.50209800	1.96161900	C	4.98701500	-3.62466000	-0.17917000
H	3.70447500	1.55557800	2.58170600	C	3.15211100	-3.61206900	-1.87833400
H	3.17769200	0.47789000	3.87134800	H	3.05821700	-2.70489700	0.06488800
C	1.63215100	0.28457700	0.91993600	H	5.47976900	-3.13932600	0.66391500
N	2.92344700	-0.30420800	0.65079500	H	4.64759400	-4.61014100	0.15453100
C	-2.48614400	3.05017300	1.77767500	H	5.74372400	-3.78265600	-0.95326300
H	-1.83587400	3.92812700	1.77108200	H	2.32834500	-3.07447900	-2.34758100
H	-3.28898700	3.24519000	2.49479700	H	3.88192600	-3.84633300	-2.65799900
H	-1.90934500	2.19983400	2.13637300	H	2.76252700	-4.56187900	-1.49959900
C	-3.93559600	4.02059700	0.00782600	C	-2.01161100	2.38906300	-0.69554400
H	-4.65935100	4.22936900	0.80150600	C	-2.57965100	2.57569300	-2.12027700
H	-3.30875500	4.91097900	-0.09868600	H	-1.90621500	2.16742000	-2.87239600
H	-4.49499900	3.88469200	-0.91835900	H	-3.55416300	2.11240000	-2.26839800
C	0.67443100	0.19930500	3.32183700	H	-2.68683300	3.64358900	-2.32145800
H	-0.35553700	0.36629600	3.01957300	C	-0.72971300	3.22516700	-0.62828800
H	0.84220300	-0.87459800	3.37230200	H	-0.18654700	3.09936100	0.30126500
H	0.80625100	0.60708900	4.32965200	H	-0.05763400	2.96102800	-1.44798700
C	1.33103100	2.41046700	2.42259600	H	-0.97589300	4.28463500	-0.74641100
H	1.52761100	2.76859800	3.43891500	N	-3.04826200	0.41190700	0.13293600
H	1.94776200	3.00008200	1.74268000	C	-3.56979600	-0.93891400	0.16378700
H	0.28442400	2.60389900	2.20145300	C	-3.39524300	-1.73246400	1.32755400
C	5.17470400	-0.39503000	1.85577600	C	-4.35796800	-1.44176500	-0.90707300
H	5.59537400	-0.48094300	2.86179900	C	-3.92611200	-3.02594300	1.35793900
H	5.61068300	-1.18338000	1.24408000	C	-4.86447900	-2.74295800	-0.82196400
H	5.48922200	0.56153000	1.43977800	C	-4.64185500	-3.54023400	0.28844800
C	3.29159100	-1.86610100	2.59418600	H	-3.79045400	-3.63540600	2.24274900
H	3.82817300	-2.68057000	2.10809100	H	-5.45573400	-3.13151800	-1.64260700
H	3.56539800	-1.87719000	3.65350400	H	-5.04183200	-4.54767700	0.32992200
H	2.22539500	-2.07729000	2.51607200	C	-4.76490400	-0.61790600	-2.12417000
C	1.07509100	-0.31541700	-2.36784000	C	-6.24988800	-0.20724900	-2.02795000
H	2.03493800	-0.81183000	-2.28386000	C	-4.50529500	-1.33654800	-3.46080100
H	0.54905400	-0.70807300	-3.24042800	H	-4.15538800	0.28013800	-2.12922300
H	1.26129200	0.74702300	-2.53365700	H	-6.47281800	0.31120800	-1.09219800
C	0.00424700	-2.05841400	-0.85113700	H	-6.51652100	0.45639100	-2.85661500
H	0.94613900	-2.48530700	-0.51117900	H	-6.90296800	-1.08366400	-2.08078000
H	-0.74751400	-2.22900400	-0.07824300	H	-3.46675200	-1.65520100	-3.54071600
H	-0.31779900	-2.57217100	-1.76013500	H	-5.15242900	-2.20939600	-3.58702100
C	-1.19520900	-0.00087700	-1.48809100	H	-4.71247600	-0.65618900	-4.29233300
O	-1.75996900	-0.22629800	-2.52819000	C	-2.73534000	-1.19899500	2.59338700
C	3.70768800	-0.20715000	-0.55720000	C	-1.80105800	-2.22042200	3.26379700
C	4.08725600	1.04734600	-1.10857100	C	-3.80628900	-0.73421200	3.60285700
C	4.19526600	-1.39881400	-1.16721800	H	-2.14092200	-0.33414700	2.30508000
C	4.93008100	1.07896300	-2.22323900	H	-1.03576700	-2.58075200	2.57233600
C	5.05713000	-1.30367900	-2.26469300	H	-1.29680400	-1.76382600	4.11822900
C	5.42834600	-0.08006700	-2.79724900	H	-2.34835900	-3.08804800	3.64189500
H	5.21973500	2.03832800	-2.63700700	H	-4.47746800	0.00938700	3.16793200
H	5.43237100	-2.21294600	-2.72058700	H	-4.41901900	-1.57750300	3.93640400
H	6.09426300	-0.02965600	-3.65162900	H	-3.33543100	-0.28968800	4.48518500
C	3.64776100	2.39223300	-0.53877800				