

Supporting Information for:

**Ruthenium-Tris(bipyridine) Complexes with Multiple Redox-Active
Amine Substituents: Tuning of Spin Density Distribution and
Deep-Red to NIR Electrochromism and Electrofluorochromism**

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Synthesis. NMR spectra were recorded in the designated solvent on a Bruker Avance 400 MHz spectrometer. Spectra are reported in ppm values from residual protons of deuterated solvent. Mass spectra were obtained with a Bruker Daltonics Inc. Apex II FT-ICR or Autoflex III MALDI-TOF mass spectrometer. The matrix for MALDI-TOF measurement is α -cyano-4-hydroxycinnamic acid. Microanalysis was carried out using Flash EA 1112 or Carlo Erba 1106 analyzer at the Institute of Chemistry, Chinese Academy of Sciences. Ligand NNbpy and complex **1**(PF₆)₂ were prepared according to known procedures.¹

Synthesis of 2(PF₆)₂, [Ru(NNbpy)₂(bpy)](PF₆)₂. To 10 mL DMF were added ligand NNbpy (50 mg, 0.082 mmol), RuCl₃·3H₂O (11 mg, 0.041 mmol) and LiCl (17 mg, 0.41 mmol). The mixture was heated at 140 °C for 20 h under a N₂ atmosphere. After cooling to room temperature, DMF was removed under reduced pressure. To the residue were added 20 mL ethanol, 10 mL water, and 2,2'-bipyridine (11 mg, 0.07 mmol). The mixture was stirred and refluxed for 4 h. After cooling to room temperature, ethanol was removed under reduced pressure, followed by the addition of an excess of aq. KPF₆. The resulting precipitate was collected by filtering and washing with water and Et₂O. The obtained solid was subjected to flash column chromatography on silica gel (eluent: saturated aq. KNO₃/H₂O/CH₃CN, 1/20/500) to give 42 mg **2**(PF₆)₂ as an orange solid in 58% yield. ¹H NMR (400 MHz, CD₃CN): δ 3.79 (s, 12H), 3.83 (s, 12H), 6.30 (dd, J = 6.6, 2.4 Hz, 2H), 6.51 (dd, J = 6.6, 2.4 Hz, 2H), 6.90 (overlapping, 2H), 6.91 (d, J = 8.8 Hz, 8H), 6.95 (s, 4H), 6.98 (d, J = 8.7 Hz, 8H), 7.10 (d, J = 8.8 Hz, 8H), 7.20 (overlapping, 2H), 7.21 (d, J = 8.9 Hz, 8H), 7.40 (t, J = 6.6 Hz, 2H), 7.90-8.00 (m, overlapping, 4H), 8.38 (d, J = 8.1 Hz, 2H). MALDI-MS: 1623.1 for [M – PF₆]⁺, 1477.1 for [M – 2PF₆]⁺. ¹³C NMR (100 MHz, D₆-acetone): δ 54.9, 55.1, 107.9, 108.0, 112.5, 115.3, 115.4, 123.8, 127.3, 128.4, 128.6, 136.0, 136.2, 150.0, 150.2, 151.7, 154.7, 154.8, 156.6, 156.8, 158.1, 158.8, 158.9. Anal. Calcd for C₈₆H₇₆F₁₂N₁₀O₁₂₀P₂Ru·4H₂O: C, 56.12; H, 4.60; N, 7.61. Found: C, 55.72; H, 4.20; N, 7.61.

Synthesis of 3(PF₆)₂, [Ru(NNbpy)₃](PF₆)₂. To 10 mL ethylene glycol were added ligand NNbpy (60 mg, 0.098 mmol) and RuCl₃·3H₂O (8.6 mg, 0.033 mmol). The mixture was heated under microwave conditions (power = 375 W) for 30 min. After

¹ Nie, H.-J.; Yang, W.-W.; Zheng, R.-H.; Shi, Q.; Chen, H.; Yao, J.; Zhong, Y.-W. *Inorg. Chem.* **2015**, *54*, 1272.

cooling to room temperature, an excess of aq. KPF_6 was added. The resulting precipitate was collected by filtering and washing with water and Et_2O . The obtained solid was subjected to flash column chromatography on silica gel (eluent: saturated aq. $\text{KNO}_3/\text{H}_2\text{O}/\text{CH}_3\text{CN}$, 1/20/1000) to give 50 mg of complex $\mathbf{3}(\text{PF}_6)_2$ as an orange solid in 69% yield. ^1H NMR (400 MHz, CD_3CN): δ 3.81 (s, 36H), 6.43 (d, $J = 6.5$ Hz, 6H), 6.89 (s, 6H), 6.93 (d, $J = 8.7$ Hz, 24H), 7.13 (d, $J = 8.6$ Hz, 24H), 7.19 (d, $J = 6.6$ Hz, 6H). MALDI-MS: 2077.6 for $[\text{M} - \text{PF}_6]^+$, 1931.5 for $[\text{M} - 2\text{PF}_6]^+$. ^{13}C NMR (100 MHz, D_6 -acetone): δ 55.2, 106.5, 113.8, 115.6, 119.2, 128.6, 142.2, 150.2, 154.8, 162.1. Anal. Calcd for $\text{C}_{114}\text{H}_{102}\text{F}_{12}\text{N}_{12}\text{O}_{12}\text{P}_2\text{Ru} \cdot 5\text{H}_2\text{O}$: C, 59.19; H, 4.88; N, 7.27. Found: C, 59.04; H, 4.52; N, 7.43.

Electrochemical Measurements

All electrochemical measurements were performed using a CHI 660D potentiostat with one-compartment electrochemical cell under an atmosphere of nitrogen. All measurements were carried out in 0.1 M Bu_4NClO_4 in CH_2Cl_2 at a scan rate of 100 mV/s. The working electrode was a glassy carbon with a diameter of 3 mm. The electrode was polished prior to use with 0.05 μm alumina and rinsed thoroughly with water and acetone. A large area platinum wire coil was used as the counter electrode. All potentials are referenced to a Ag/AgCl electrode in saturated aqueous NaCl without compensation for the liquid junction potential. The potential versus ferrocene⁺⁰ can be calculated by subtracting 0.45 V.

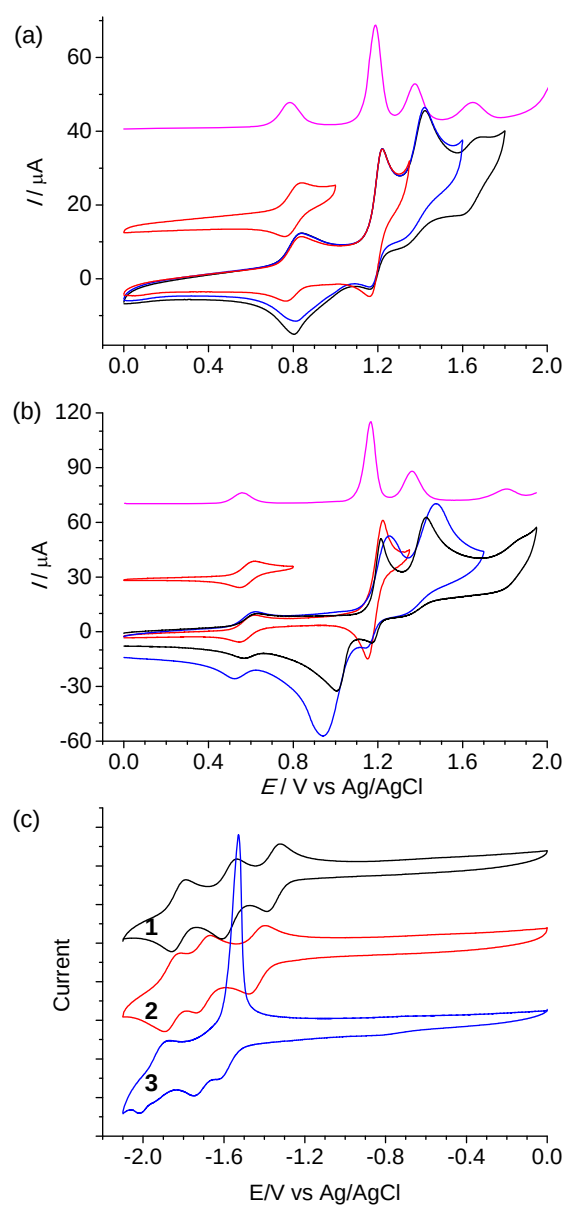


Figure S1. Anodic CVs and DPVs (pink curves) of $2(\text{PF}_6)_2$ (a) and $3(\text{PF}_6)_2$ (b) and cathodic CVs of $1(\text{PF}_6)_2$ - $3(\text{PF}_6)_2$ in CH_2Cl_2 .

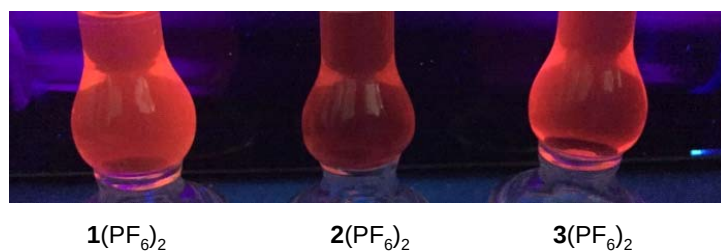


Figure S2. Emission images of $1(\text{PF}_6)_2$ - $3(\text{PF}_6)_2$ in CH_2Cl_2 ($c = 1 \times 10^{-4}$ M) under the illumination at 465 nm.

Spectroscopic Measurements

Absorption spectra were recorded on a PE Lambda 750 UV/vis/NIR spectrophotometer at room temperature. Spectroelectrochemical measurements were performed in a thin layer cell (optical length = 0.2 cm), in which an ITO glass electrode ($< 10\Omega/\text{square}$) working electrode was set in CH_2Cl_2 containing the compound to be studied (concentration around $5 \times 10^{-5} \text{ M}$) and 0.1 M Bu_4NClO_4 as the supporting electrolyte. A platinum wire and Ag/AgCl in saturated aqueous NaCl was used as the counter electrode and reference electrode, respectively. The cell was put into the spectrometer to monitor the spectral change during electrolysis.

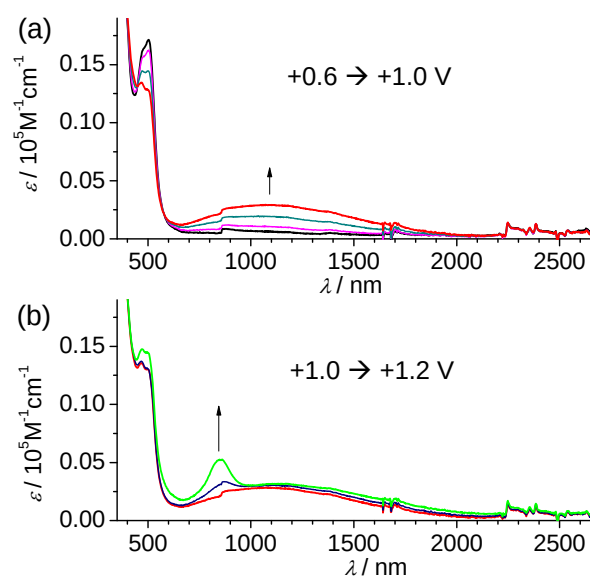


Figure S3. Absorption spectral changes of $2(\text{PF}_6)_2$ upon electrolysis at ITO in CH_2Cl_2 . The potentials were applied vs Ag/AgCl .

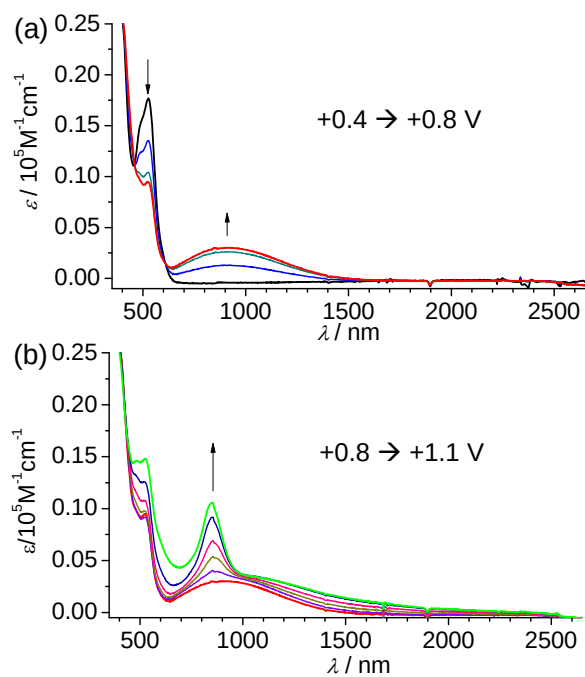


Figure S4. Absorption spectral changes of $3(\text{PF}_6)_2$ upon electrolysis at ITO in CH_2Cl_2 . The potentials were applied vs Ag/AgCl.

DFT and TDDFT Calculations

DFT calculations are carried out using the B3LYP exchange correlation functional and implemented in the *Gaussian 09* package. The electronic structures are optimized using a general basis set with the Los Alamos effective core potential LANL2DZ basis set for Ru and 6-31G* for other atoms.² The solvation effects in CH₂Cl₂ are included for all calculations with the conductor-like polarizable continuum model (CPCM).³ No symmetry constraints are used in the optimization (nosymm keyword was used). Frequency calculations are performed with the same level of theory to ensure the optimized geometries to be local minima. All orbitals are computed at an isovalue of 0.02 e/bohr³.

² Hay, P. J.; Wadt, W. R. *J. Chem. Phys.* **1985**, 82, 270.

³ Barone, V.; Cossi, M. *J. Phys. Chem. A* **1998**, 102, 1995.

Table S1. TDDFT Results of 1^{2+} - 3^{2+} ^a

	S_n	λ/nm	f	dominant transitions (percent contribution ^b)
1^{2+}	S_1	503.8	0.0068	HOMO $\rightarrow$ LUMO (53%)
	S_2	500.4	0.0014	HOMO $\rightarrow$ LUMO+1 (43%)
	S_3	489.6	0.0227	HOMO-1 $\rightarrow$ LUMO (47%)
	S_4	485.4	0.0168	HOMO-1 $\rightarrow$ LUMO+1 (44%)
	S_5	445.7	0.0697	HOMO-2 $\rightarrow$ LUMO (47%)
	S_6	435.9	0.2033	HOMO $\rightarrow$ LUMO+2 (66%)
	S_7	429.5	0.0870	HOMO-2 $\rightarrow$ LUMO+1 (26%), HOMO-1 $\rightarrow$ LUMO+2 (37%)
	S_8	417.8	0.0884	HOMO-1 $\rightarrow$ LUMO+2 (41%)
2^{2+}	S_1	541	0.0021	HOMO $\rightarrow$ LUMO (63%)
	S_2	524.7	0.0042	HOMO-1 $\rightarrow$ LUMO (51%)
	S_3	477.4	0.1092	HOMO-2 $\rightarrow$ LUMO (69%)
	S_4	466.8	0.0732	HOMO $\rightarrow$ LUMO+1 (77%)
	S_5	455.8	0.1686	HOMO-1 $\rightarrow$ LUMO+1 (58%)
	S_6	452.6	0.0238	HOMO-1 $\rightarrow$ LUMO+2 (30%), HOMO $\rightarrow$ LUMO+2 (38%)
	S_7	438.5	0.0140	HOMO-2 $\rightarrow$ LUMO+1 (24%), HOMO-1 $\rightarrow$ LUMO+2 (30%), HOMO $\rightarrow$ LUMO+2 (24%)
	S_8	428.5	0.0884	HOMO-2 $\rightarrow$ LUMO+2 (49%)
	S_9	425.7	0.0447	HOMO-2 $\rightarrow$ LUMO+1 (34%), HOMO-2 $\rightarrow$ LUMO+2 (27%)
3^{2+}	S_1	500.0	0.0195	HOMO-2 $\rightarrow$ LUMO (62%)
	S_2	488.8	0.1241	HOMO $\rightarrow$ LUMO (83%)
	S_3	488.0	0.1145	HOMO-1 $\rightarrow$ LUMO (72%)
	S_4	481.8	0.0055	HOMO-2 $\rightarrow$ LUMO+1 (57%)
	S_5	481.2	0.0037	HOMO-2 $\rightarrow$ LUMO+2 (59%)
	S_6	473.6	0.0062	HOMO $\rightarrow$ LUMO+1 (41%)
	S_7	467.5	0.1600	HOMO $\rightarrow$ LUMO+2 (31%), HOMO-1 $\rightarrow$ LUMO+1 (20%), HOMO-1 $\rightarrow$ LUMO+2 (21%),
	S_8	467.4	0.1766	HOMO-1 $\rightarrow$ LUMO+2 (23%), HOMO $\rightarrow$ LUMO+1 (27%), HOMO-2 $\rightarrow$ LUMO+2 (18%), HOMO-1 $\rightarrow$ LUMO+1 (16%),
	S_9	441.5	0	HOMO-1 $\rightarrow$ LUMO+1 (35%), HOMO $\rightarrow$ LUMO+2 (35%)

^aCalculation method: B3LYP/LANL2DZ/6-31G*/CPCM. The involved molecular orbitals are displayed in Figures S5 - S7.

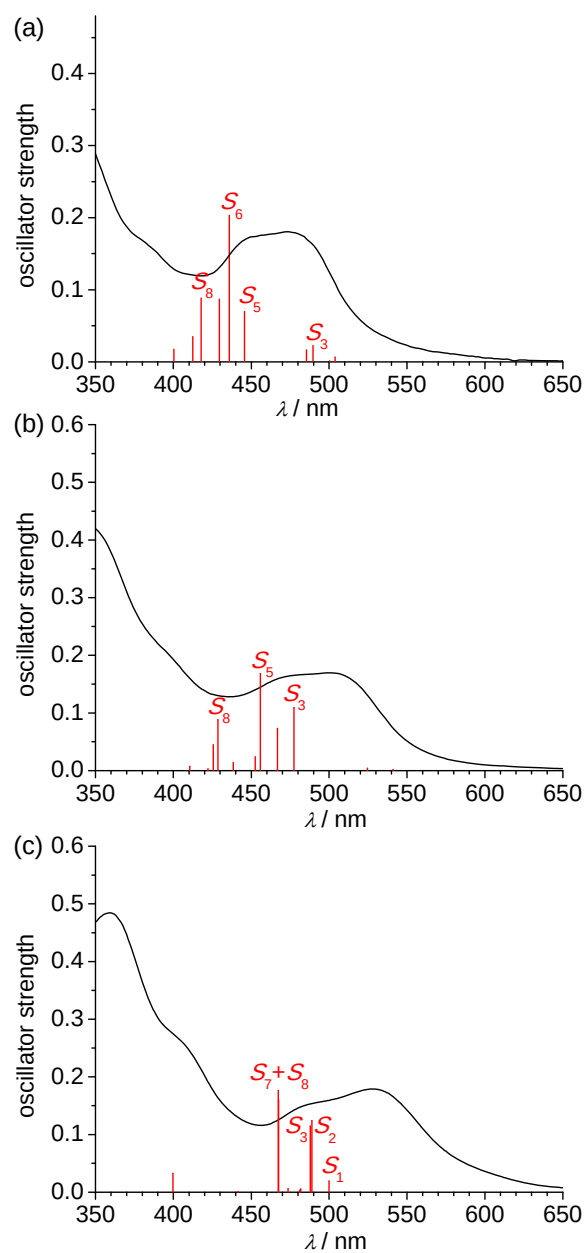


Figure S5. TDDFT calculated vertical excitations of 1^{2+} (a), 2^{2+} (b), and 3^{2+} (c). See Table S1 for details.

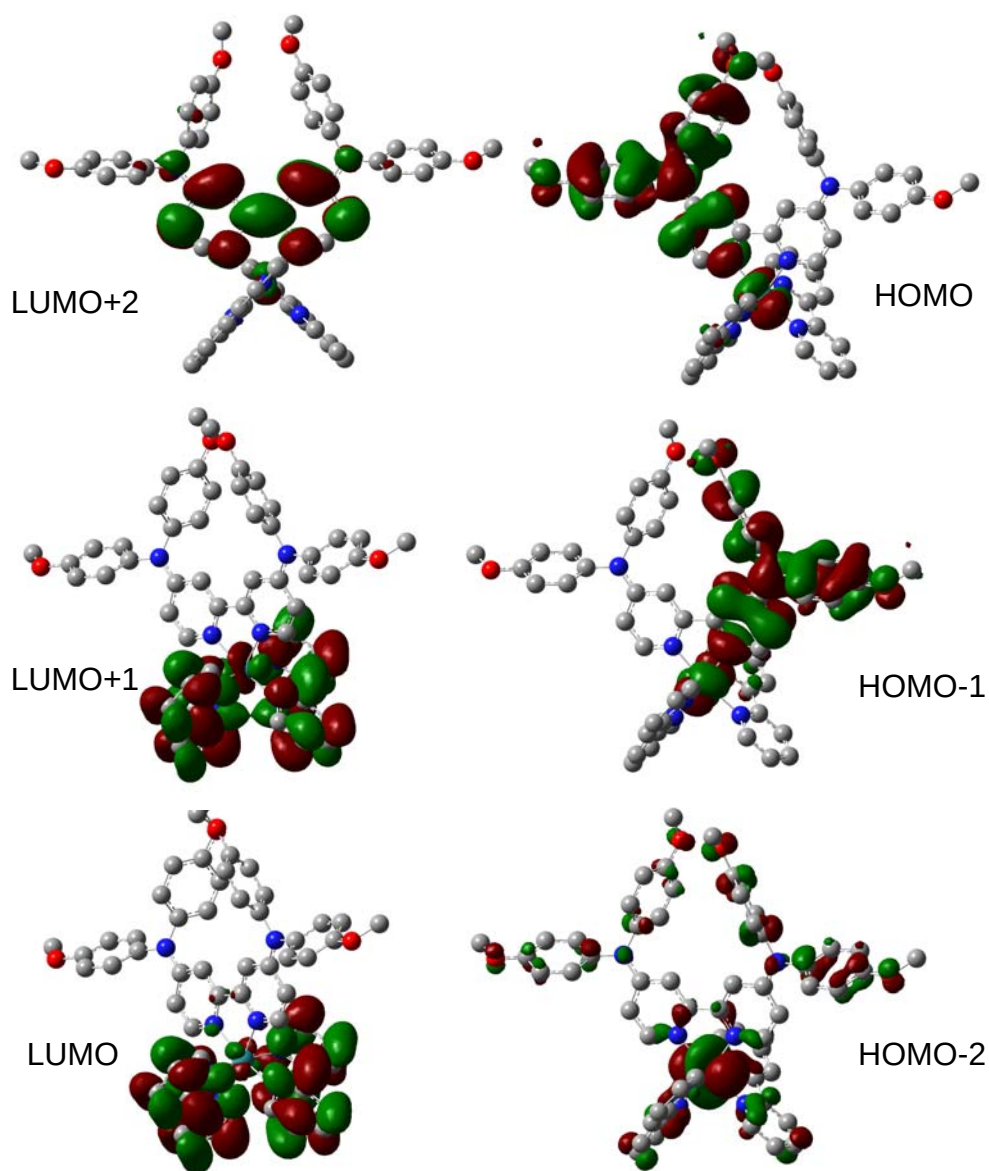


Figure S6. Frontier molecular orbitals of $\mathbf{1}^{2+}$.

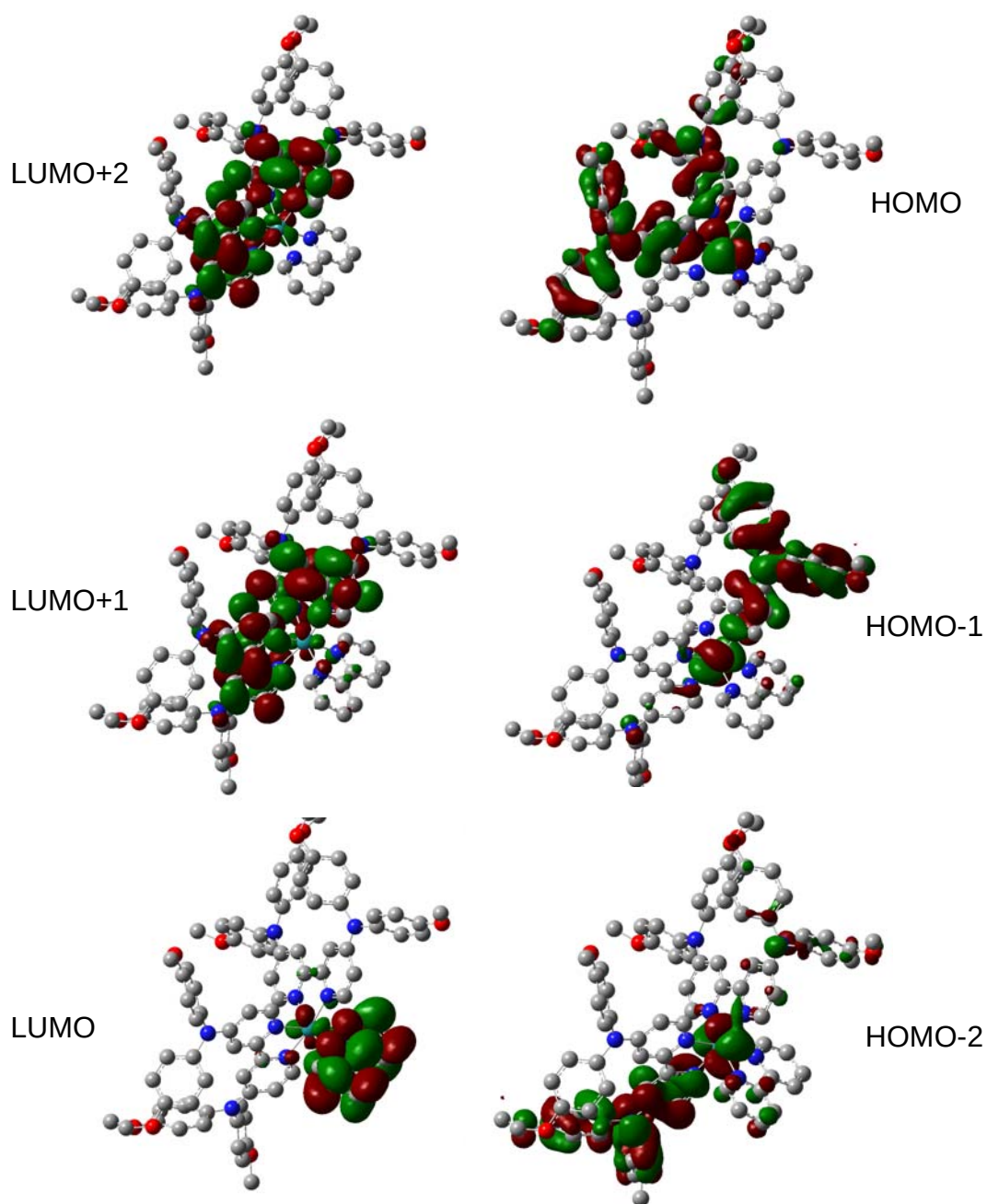


Figure S7. Frontier molecular orbitals of 2^{2+} .

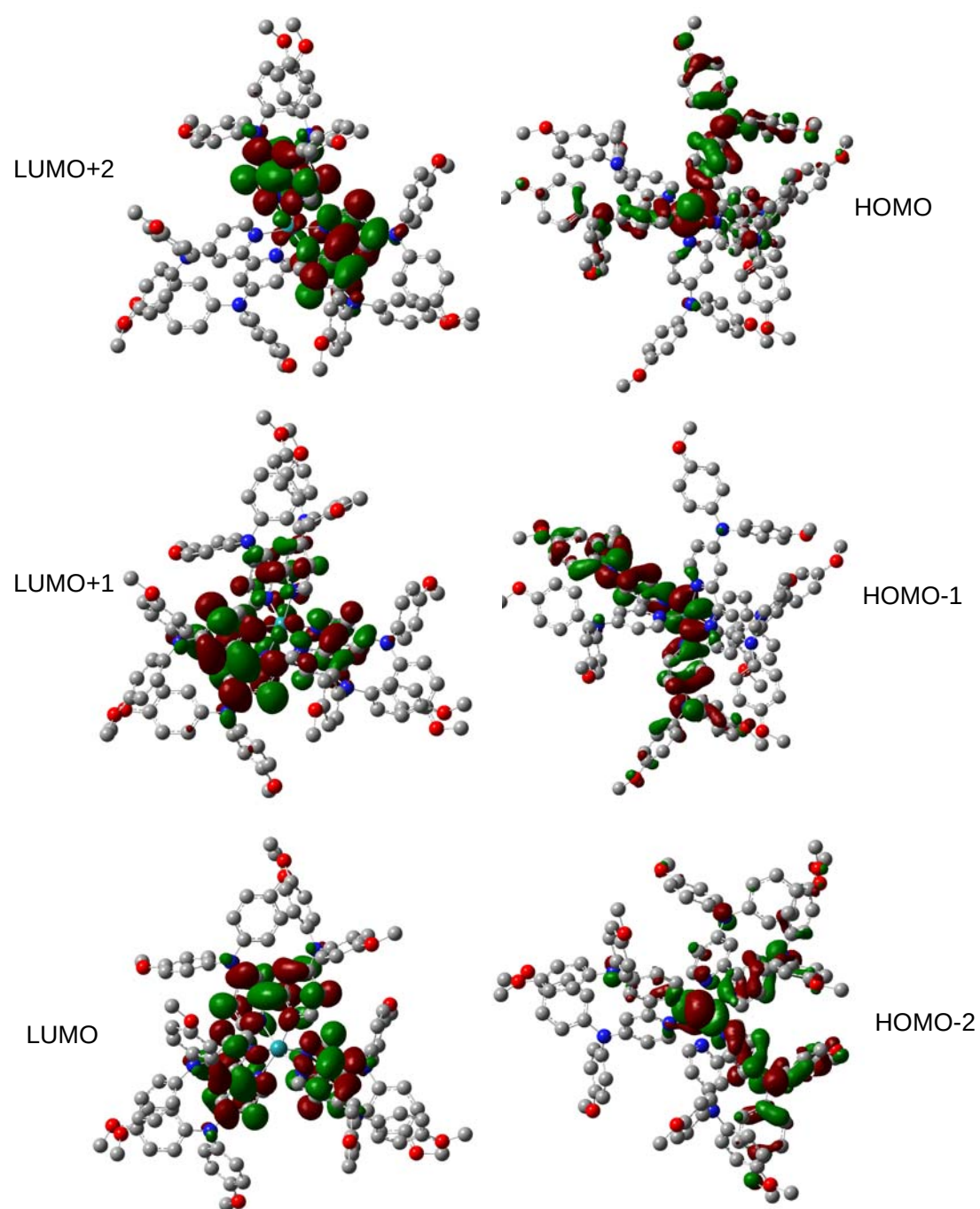
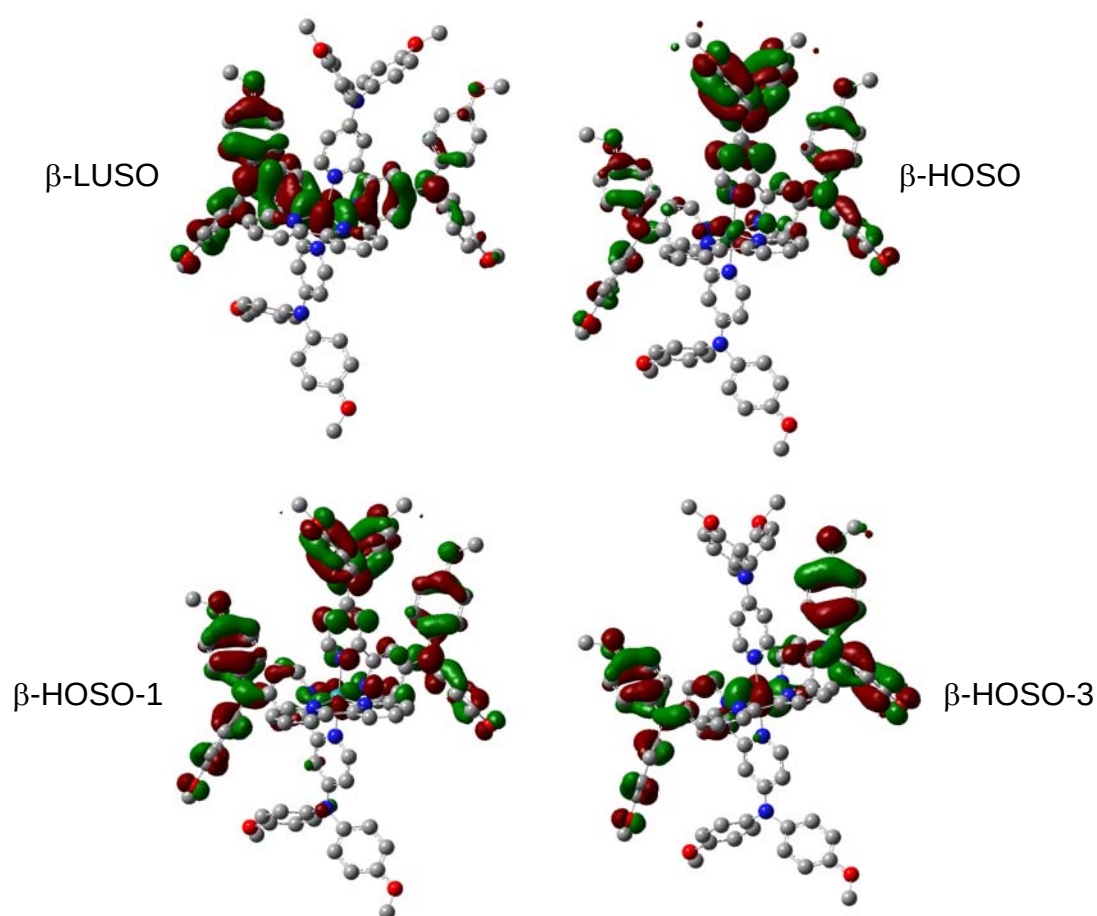


Figure S8. Frontier molecular orbitals of 3^{2+} .

Table S2. TDDFT-predicted Excitations of 2^{3+} and 3^{3+}

	D_1	λ/nm	f	dominant transitions (percent contribution)
2^{3+}	2	3667.1	0.0024	$\beta\text{-HOSO-1} \rightarrow \beta\text{-LUSO}$ (46%)
	3	2106.1	0.2991	$\beta\text{-HOSO-1} \rightarrow \beta\text{-LUSO}$ (51%), $\beta\text{-HOSO} \rightarrow \beta\text{-LUSO}$ (49%)
	4	1655.8	0.0458	$\beta\text{-HOSO-3} \rightarrow \beta\text{-LUSO}$ (30%), $\beta\text{-HOSO} \rightarrow \beta\text{-LUSO}$ (14%)
3^{3+}	3	1532.2	0.0771	$\beta\text{-HOSO} \rightarrow \beta\text{-LUSO}$ (43%)
	4	1518.3	0.069	$\beta\text{-HOSO-1} \rightarrow \beta\text{-LUSO}$ (44%)
	5	1480.8	0.0663	$\beta\text{-HOSO-2} \rightarrow \beta\text{-LUSO}$ (68%)

^aCalculation method: UB3LYP/LANL2DZ/6-31G*/CPCM. The involved spin orbitals are displayed in Figures S8 and S9. HOSO is the highest occupied spin orbital and LUSO is the lowest unoccupied spin orbital.

**Figure S9.** Frontier spin orbitals of 2^{3+} .

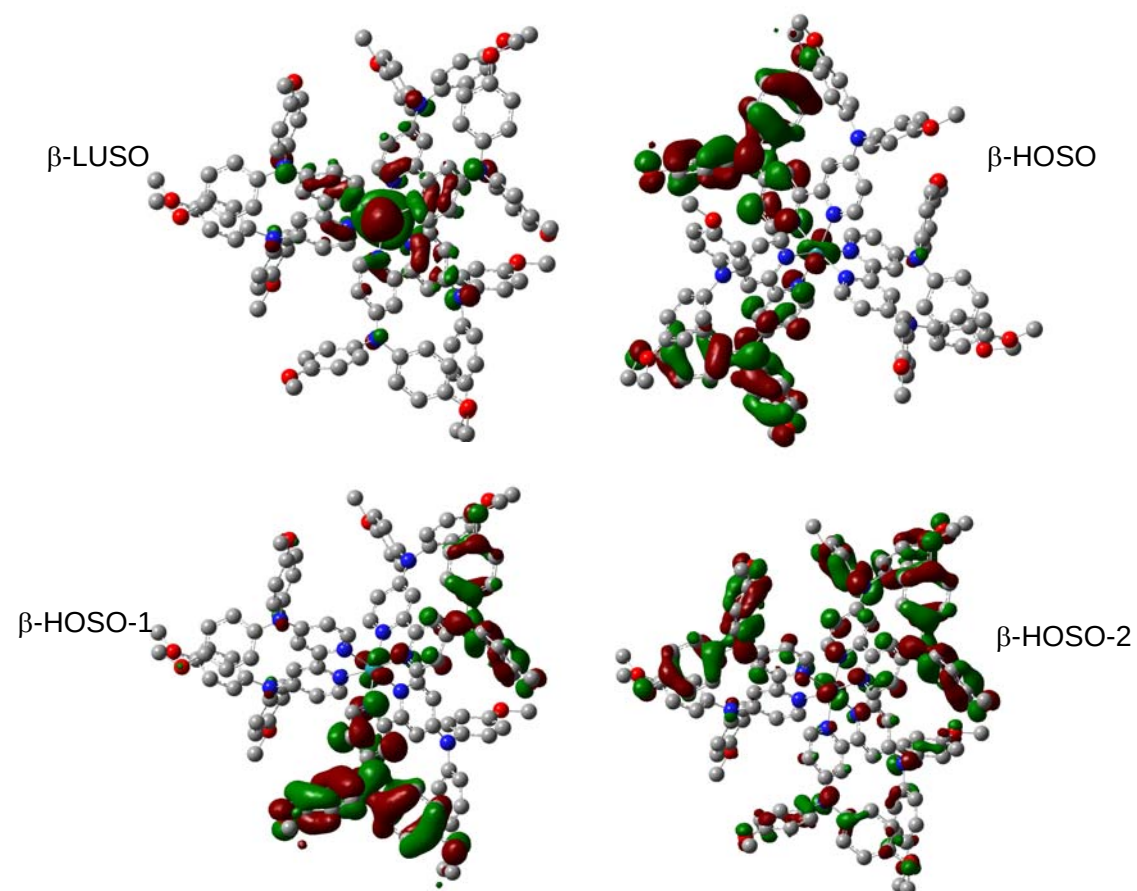
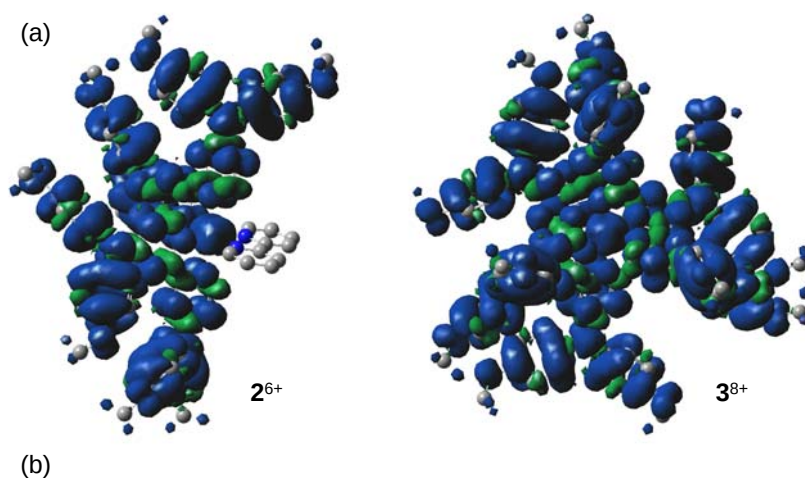


Figure S10. Frontier spin orbitals of 3^{3+} .



	Ru	pyridine	N _{amine}	phenyl	oxygen	pyridine + N _{amine} + phenyl + oxygen
2⁶⁺	0.354	0.452	0.909	1.823	0.489	3.673
3⁸⁺	0.399	0.692	1.297	2.850	0.792	5.631

Figure S11. DFT-calculated spin density distributions (a) and segmental analysis (b) of **2⁶⁺** and **3⁸⁺** on the level of theory of UB3LYP/LANL2DZ/6-31G*/CPCM.

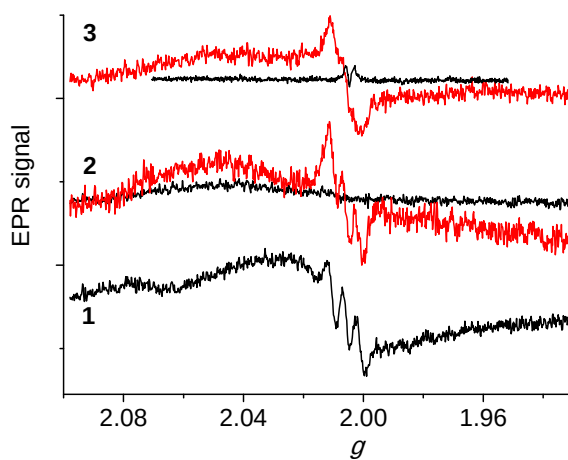


Figure S12. EPR spectra of **1**(PF₆)₂, **2**(PF₆)₂, and **3**(PF₆)₂ upon addition of 0.5 equiv (black curves) or 2 equiv (red curves) of CAN in CH₃CN at rt. $g = 2.006$ for all available data. The weak signal in the black curve of **3** is from impurities.

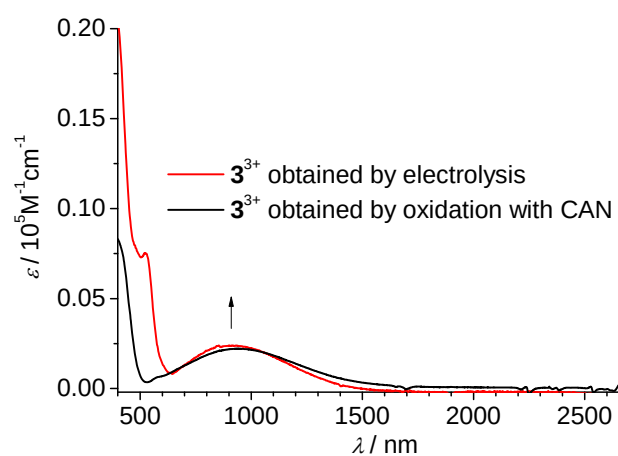


Figure S13. A comparison of the NIR absorption spectrum of 3^{3+} obtained by electrolysis or oxidation with CAN in CH_3CN .

Cartesian coordinates of DFT-optimized structure of **1**²⁺:

Charge = 2; multiplicity=1

N	-1.26508016	-2.86699795	2.19568319
C	-4.62047504	-4.44446153	2.01582753
C	-5.45892286	-4.89875699	1.00229352
C	-5.04558876	-4.77025929	-0.32309282
C	-3.80782616	-4.19273648	-0.58334410
N	-2.99201269	-3.74918674	0.39168855
C	-3.38770381	-3.86974554	1.69039467
C	-2.43387369	-3.35950473	2.69473631
C	-2.68029461	-3.36973698	4.07133136
C	-1.71933994	-2.87455086	4.94788154
C	-0.52492970	-2.37752390	4.42801256
C	-0.33960847	-2.39086627	3.04993930
C	0.58567747	-6.90360400	0.71220105
C	0.05931995	-5.63180406	0.90925847
C	0.77478616	-7.35461976	-0.59348656
N	-0.27413507	-4.81584731	-0.10863318
C	0.43144471	-6.51757777	-1.65093464
C	-0.09267233	-5.24768699	-1.38856181
Ru	-1.09184316	-2.88080934	0.09387662
N	0.73553716	-1.81603296	0.00577312
C	0.63476753	-0.45549671	0.00194197
C	-0.48361294	-4.29125521	-2.44293901
N	-1.00504783	-3.11193187	-2.00092479
C	-0.34462781	-4.54813855	-3.81069240
C	-1.38909744	-2.18924287	-2.90320191
C	-0.74471056	-3.58973310	-4.73708457
C	-1.27822594	-2.38742541	-4.27508473
H	-4.92505485	-4.54041006	3.05035735
H	-6.41691339	-5.34581371	1.24607709
H	-3.44660224	-4.07175198	-1.59711907
H	-3.61345410	-3.75869124	4.45907433
H	-1.90255086	-2.87848459	6.01718581
H	0.57205808	-2.01636032	2.60137337
H	0.83784354	-7.51870757	1.56863371
H	-0.10248448	-5.23934104	1.90560438
H	1.18190961	-8.34111389	-0.78861433
H	0.56970808	-6.85442925	-2.67055883
H	0.07410245	-5.48596736	-4.15356126
H	-1.79784046	-1.27152150	-2.49921969
H	-0.64017085	-3.78117654	-5.79984356
H	-1.60425300	-1.61057852	-4.95747183
H	0.25434919	-1.98321088	5.07042919
H	-5.66342177	-5.10937012	-1.14692559
H	3.14350752	3.67048318	3.45359597
C	3.50921355	3.47994179	2.44947796
H	3.30045698	1.34707395	2.57979857
O	3.78242322	5.79586108	2.23400448
C	3.59849091	2.18527983	1.95699790
H	-0.92596164	3.92936206	1.66805817
H	-3.76986269	-1.18915042	0.21143967
C	-3.00722747	-0.42560325	0.11304976
H	4.04335514	7.79549061	2.15071929

C	3.90889728	4.56956145	1.65716468
C	-3.36871968	0.90418554	0.02847336
H	-4.41693817	1.16800536	0.07281156
N	-1.73187776	-0.86329511	0.07525071
C	4.19432540	6.94244344	1.48761035
H	-4.06760797	4.74680366	1.42449122
H	0.80290268	5.71303007	1.51076775
H	-8.69254193	5.32161899	0.90818156
C	-0.82262355	4.50878022	0.75538977
H	-6.36925817	5.57495339	1.14872254
C	-4.63246576	4.47482912	0.53788959
H	6.33848789	0.56188929	1.72647546
C	-0.74880395	0.07624600	-0.02538345
C	-5.93771561	4.94559186	0.37963333
C	-2.36885564	1.89258464	-0.13418014
C	0.14180045	5.50700803	0.67474651
H	5.25393379	6.87776142	1.21378048
C	-1.03352845	1.42941557	-0.15124275
C	4.07294697	1.95200929	0.65613306
C	1.97392948	-2.35057494	-0.00433245
N	-2.67887991	3.22719997	-0.26808901
C	-8.60113471	5.82222029	-0.06305644
C	6.52169668	0.16861165	0.73128553
C	-4.04149027	3.66423526	-0.43292718
C	1.75586844	0.36112827	0.04643150
C	3.13627387	-1.60409976	0.01392626
C	3.05450000	-0.19419766	0.06997100
H	3.58086069	7.06537174	0.58907362
C	4.39861070	4.34068963	0.36341168
H	8.59306233	-0.21741849	1.12898912
C	-1.66148470	4.24412349	-0.33817268
H	-9.59578712	6.01255551	-0.46818356
C	-6.66960712	4.59226811	-0.76279733
N	4.17333691	0.60894345	0.15366744
H	-0.22785956	2.13797457	-0.27446748
C	7.80207564	-0.27274265	0.39055478
H	4.09221590	-2.11164485	0.01865169
O	-7.94613192	4.98821150	-1.01730250
C	4.47146042	3.03545459	-0.12938710
C	5.47650980	0.11652421	-0.19401483
H	-8.07119212	6.77348678	0.06530523
C	-4.77373483	3.32131924	-1.57980083
H	10.16428076	-1.83074190	0.46040067
C	-6.07716408	3.77407025	-1.73985764
C	0.26868344	6.27696929	-0.49360646
H	4.71219350	5.16257037	-0.26891984
O	1.23191843	7.24039050	-0.47209636
H	-4.31878000	2.69881433	-2.34460472
C	8.04278937	-0.78792213	-0.89072460
C	10.35234913	-1.21423903	-0.42667655
C	-1.52790367	5.00831553	-1.49965565
H	-6.65282775	3.51403529	-2.62259365
H	4.84330370	2.86107233	-1.13454606
C	5.72589151	-0.38756227	-1.48037662
H	10.58046432	-0.18779882	-0.11545335

C	-0.57617276	6.02587993	-1.58313271
O	9.24686860	-1.24980915	-1.32694370
C	6.99207016	-0.84422422	-1.82195551
H	11.19941453	-1.62257573	-0.97943400
H	4.92432083	-0.41749681	-2.21235239
H	-2.17748103	4.81371886	-2.34743051
C	1.38802797	8.06949504	-1.62342645
H	2.19375431	8.76365923	-1.38225032
H	-0.50022711	6.60380202	-2.49629155
H	7.19348677	-1.23560294	-2.81421116
H	1.66603041	7.47967234	-2.50477156
H	0.47111557	8.63216355	-1.83415949
H	2.02328707	-3.43298755	-0.00576525
H	1.64266453	1.43566459	0.06896009

Cartesian coordinates of DFT-optimized structure of 2^{2+} :

Charge = 2; multiplicity=1

N	0.46857375	-1.16778996	3.82879054
C	-0.40134253	1.56254042	6.18804989
C	-0.84493293	2.87667106	6.07606355
C	-1.03637588	3.41675571	4.80459910
C	-0.77971850	2.61990955	3.69456721
N	-0.35069379	1.34705372	3.79421269
C	-0.15711274	0.81195469	5.03312166
C	0.31878593	-0.58456929	5.05193497
C	0.60469111	-1.28954956	6.22585183
C	1.04625347	-2.60688642	6.14959368
C	1.19398585	-3.19596625	4.89417567
C	0.89657749	-2.44325883	3.76371560
C	-2.74329142	0.32501592	1.10933527
Ru	0.02546480	0.05639498	2.17322131
N	0.62077721	-1.32540118	0.68434679
C	1.94090372	-1.30272853	0.34156288
C	-1.96383836	1.34340052	0.36566513
H	-0.24919491	1.12665356	7.16757301
H	-1.03723817	3.46589024	6.96655710
H	-0.91372458	2.99640993	2.68809894
H	0.48630300	-0.81596779	7.19244440
H	1.27055116	-3.16097566	7.05503887
H	0.99467840	-2.85931347	2.76873329
H	1.53399937	-4.21956585	4.78335135
H	-1.37965910	4.43588387	4.66607777
H	6.01895400	-5.59886982	0.20890146
C	5.55908341	-5.23703525	-0.70539802
H	3.59136016	-5.06333233	0.13554829
O	7.67163064	-5.41311823	-1.70128696
C	4.20465475	-4.93703974	-0.75169712
H	6.78836798	-1.32253707	1.23511590
H	2.25438068	1.95493154	3.38395517
C	2.79381234	1.41016367	2.61787406
H	9.51162142	-5.64202078	-2.49825815
C	6.35758124	-5.09169124	-1.85257751
C	4.12049553	1.70044275	2.36693053
H	4.61100457	2.46791944	2.95089899
N	2.08963837	0.47050383	1.95448917
C	8.53132121	-5.30363818	-2.83698470
H	8.25191520	1.29740794	2.62346468
H	8.09571641	-2.64427091	-0.41861952
H	9.64057652	5.23319258	4.75747562
C	7.14414348	-0.85340601	0.32259719
H	9.45488696	3.25844614	3.50065211
C	7.90316051	2.29536733	2.37538927
H	2.03511783	-6.83330132	-2.10054350
C	2.74655087	-0.24666924	0.99936435
C	8.58612958	3.40834738	2.87075458
C	4.80754241	1.00575224	1.34336085
C	7.87764601	-1.59566320	-0.59588824
H	8.18833444	-5.94526702	-3.65713013
C	4.07089765	0.00807420	0.66643888

C	3.62110816	-4.46891434	-1.94006366
C	-0.16167381	-2.24782907	0.08794389
N	6.11839704	1.28790667	1.02454970
C	9.87032533	5.75431907	3.82055616
C	1.40904357	-6.32814766	-2.82959437
C	6.78107619	2.44912485	1.55904450
C	2.48541419	-2.22613003	-0.54075765
C	0.30183932	-3.18533629	-0.81557467
C	1.67692274	-3.21678555	-1.13956545
H	8.60087552	-4.26491668	-3.17640682
C	5.77657653	-4.64060366	-3.04625942
H	0.67262270	-8.16510959	-3.65459431
C	6.85961614	0.49882633	0.07610552
H	10.16438379	6.78169262	4.03911538
C	8.13531612	4.69748112	2.55397609
N	2.21714935	-4.16582641	-1.98548484
H	4.54080559	-0.55139908	-0.12908453
C	0.63568508	-7.08384749	-3.71352852
H	-0.39047070	-3.90274885	-1.23688454
O	8.71866996	5.84917108	2.98422382
C	4.41548353	-4.32702972	-3.07965309
C	1.39192371	-4.93196164	-2.87554263
H	10.69290771	5.24009053	3.30951215
C	6.33991328	3.74149649	1.23543766
H	-1.35974123	-8.89114141	-4.59357116
C	7.00491864	4.85438781	1.73398051
C	8.36355239	-0.99233313	-1.76803011
H	6.36903513	-4.51933890	-3.94525401
O	9.08621462	-1.79625681	-2.59787115
H	5.47422931	3.87089627	0.59259373
C	-0.18072494	-6.43735048	-4.65164053
C	-1.00072104	-8.49844141	-5.55243330
C	7.33883340	1.09232162	-1.09415907
H	6.67139431	5.85824213	1.49046854
H	3.96976092	-3.96912308	-4.00286734
C	0.58436417	-4.28963029	-3.82760521
H	-0.00869209	-8.91332860	-5.76738324
C	8.09384884	0.36085477	-2.01253026
O	-0.97862016	-7.07258660	-5.55387536
C	-0.20125271	-5.03319267	-4.69852553
H	-1.69351192	-8.78608364	-6.34436282
H	0.57576999	-3.20521339	-3.88342949
H	7.12822974	2.13925247	-1.28958474
C	9.63990727	-1.22497740	-3.78273678
H	10.18429456	-2.03162476	-4.27492119
H	8.45518054	0.85141628	-2.90838322
H	-0.82923511	-4.54409715	-5.43661767
H	8.85467666	-0.85375006	-4.45176879
H	10.33178218	-0.40908995	-3.54313576
H	-1.20698814	-2.23806185	0.37328805
H	3.54130183	-2.19771796	-0.76980512
H	-6.18770132	-1.61790483	-3.29248671
C	-6.62317673	-1.19558265	-2.39228915
H	-5.21721952	-2.11905918	-1.05865701
O	-8.20454875	-0.16505128	-3.77886840

C	-6.08547285	-1.47238555	-1.14304581
H	-9.55236336	0.65378558	-5.03809262
C	-7.75608252	-0.37258395	-2.51050008
H	-7.42171446	-3.50999899	0.90302685
H	-3.56070709	1.99503037	-3.41902122
H	-1.67187176	4.38423612	-4.72684519
H	-0.40860692	6.25240922	-5.71369080
C	-9.35765535	0.65748398	-3.96462855
H	1.49913551	7.59253203	-6.00769554
H	-5.95608182	1.93456372	-4.08958861
H	-8.88994479	-4.67874650	2.49155087
C	-1.29102134	5.17232480	-4.08422454
C	-4.20683310	2.84171117	-3.20707709
C	-0.57549508	6.23338615	-4.64334097
C	-7.56982493	-3.09742107	1.89624933
H	-10.22675092	0.24818893	-3.43629480
C	-6.65648558	-0.91964093	0.01475637
C	-5.54321196	2.80445110	-3.58823420
C	0.12950681	2.25020466	-0.03630728
C	0.90475796	8.43935184	-5.64441033
C	-8.40426167	-3.76022085	2.79892097
H	1.18825256	2.24157780	0.19448939
C	-0.36595205	3.12775236	-0.98094994
N	-0.63091098	1.37296359	0.64979932
H	-9.34866071	-5.81994594	4.49406292
H	-0.02247412	8.50999118	-6.22535678
C	-8.33990705	0.16883492	-1.35642587
H	0.31747673	3.79529361	-1.48866230
C	-4.08166369	0.06190738	0.85031146
C	-4.78118547	-0.91893003	1.58639227
N	-2.04599081	-0.36147067	2.05989579
N	-6.10096981	-1.21658102	1.30634622
C	-1.75368937	3.14940762	-1.25626235
C	-2.71915659	-1.27554237	2.78805038
C	-4.05539143	-1.57677311	2.60475197
H	-9.16391636	1.68266285	-3.63229225
C	-2.54239351	2.21509524	-0.54826447
N	-2.30380736	4.03207912	-2.16135686
C	-1.52919216	5.11461131	-2.70973256
H	-2.14153375	-1.80180669	3.53890089
H	1.47698705	9.36063165	-5.76079287
C	-6.92844835	-1.90858364	2.25296930
C	-7.78314623	-0.10333705	-0.10418157
C	-3.68857879	3.96706078	-2.54727437
H	-4.51692662	-2.33691793	3.22169509
C	-0.07884006	7.24909219	-3.81442581
H	-10.75298658	-4.88242990	3.90004758
C	-10.05578349	-5.01736050	4.73564736
O	0.63478471	8.32334666	-4.24859182
C	-6.38183206	3.90420311	-3.34066372
O	-7.67121011	3.77918968	-3.76397778
H	-9.21284636	0.80757712	-1.41861488
C	-8.59248473	-3.23766831	4.08583059
C	-1.04076560	6.13991868	-1.88524847
H	-10.61380217	-5.28379666	5.63424309

C	-0.31577136	7.19188257	-2.43039327
O	-9.37587693	-3.80282220	5.04556239
C	-4.52775663	5.05580870	-2.29854564
C	-7.13275008	-1.38126710	3.53819233
H	-8.23238131	0.32428107	0.78714212
C	-5.86545609	5.03658393	-2.69674232
C	-7.94653351	-2.04356677	4.44791048
C	-8.55928034	4.87886245	-3.56666179
H	-9.51564973	4.56749439	-3.98823477
H	-8.20337313	5.77453745	-4.08900535
H	-1.22999237	6.10931901	-0.81628870
H	0.06758124	7.98919123	-1.80143423
H	-6.65280161	-0.44908562	3.82095059
H	-4.13283094	5.93294121	-1.79532374
H	-6.48902009	5.89887236	-2.49333730
H	-8.68608523	5.10306777	-2.50102450
H	-8.10879746	-1.64282650	5.44362578
H	-4.59961082	0.60479887	0.07236664
H	-3.60940138	2.18895930	-0.71337917

Cartesian coordinates of DFT-optimized structure of $\mathbf{3}^{2+}$:

Charge = 2; multiplicity=1

N	1.81077088	0.04309405	-1.11787261
N	1.24004630	-1.37588226	1.03920411
C	-2.07234733	-2.07694949	-0.59567527
Ru	0.00440068	-0.02120388	-0.01749524
N	-0.98531316	1.52145141	-1.07325672
C	-0.76420596	2.79010629	-0.62409186
C	-2.53384047	-1.42944319	0.65492051
H	1.23409029	7.57808809	-3.43649745
C	0.17904037	7.47481147	-3.20284799
H	0.09313451	5.38187068	-3.67135113
O	0.18766968	9.75933385	-2.68439508
C	-0.46289807	6.25099267	-3.33275020
H	2.01109201	6.57249092	0.83880574
H	1.80708750	0.81891608	2.45137814
C	1.38072840	1.76334608	2.13392572
H	0.26595086	11.74035037	-2.30684833
C	-0.53451062	8.60904052	-2.77984567
C	1.65821689	2.91998663	2.83704412
H	2.31043493	2.86897490	3.69889161
N	0.58643967	1.71434950	1.04507169
C	-0.48628433	10.95074605	-2.27563462
H	3.59516621	6.48794829	3.76453210
H	1.17181542	8.77376974	0.03887170
H	5.66917975	5.61964844	7.87656236
C	1.28208307	7.12287108	1.42610427
H	4.66259710	6.57103325	5.98104660
C	3.12215551	5.99054539	4.60597585
H	-2.45222635	5.58666747	-5.73767634
C	0.05508270	2.89052215	0.60641771
C	3.72637942	6.03829882	5.86432756
C	1.07482591	4.14285630	2.43015727
C	0.82000548	8.35461987	0.97650978
H	-1.30356341	11.20003208	-2.96267344
C	0.26166342	4.09005042	1.27693266
C	-1.82775220	6.12787339	-3.02572226
C	-1.75612231	1.37602426	-2.17028337
N	1.28714375	5.31848800	3.12084066
C	4.85117338	6.04435313	8.47051377
C	-3.41201157	5.19529706	-5.41469735
C	1.91378536	5.31730323	4.41650521
C	-1.25655994	3.90229323	-1.29467920
C	-2.29970160	2.43170416	-2.87852449
C	-2.03218201	3.75541664	-2.46418605
H	-0.87029017	10.85239195	-1.25490637
C	-1.90159602	8.49625152	-2.49001355
H	-4.31692419	5.48840518	-7.33610919
C	0.80921464	6.58491595	2.63337371
H	5.05783718	5.89608132	9.53120680
C	3.11973535	5.39277555	6.95087482
N	-2.48760385	4.85911656	-3.16290872
H	-0.21610280	4.99154197	0.92236503
C	-4.47234695	5.14018411	-6.32191792

H	-2.89402151	2.22904121	-3.76027484
O	3.62072287	5.36939972	8.21612239
C	-2.53594120	7.25688887	-2.60849876
C	-3.57208467	4.76044615	-4.09647042
H	4.76792095	7.11756243	8.26160131
C	1.30469694	4.68183697	5.50971657
H	-5.95027600	4.38541847	-8.61590294
C	1.90491647	4.71202990	6.76194071
C	-0.10551016	9.08583017	1.73985045
H	-2.47606218	9.35408345	-2.16133941
O	-0.48865416	10.28816882	1.22450210
H	0.35964882	4.16411749	5.37458391
C	-5.71188790	4.62895177	-5.91389755
C	-6.70430553	4.96203022	-8.06681132
C	-0.11494782	7.31362355	3.38598066
H	1.44216186	4.22303205	7.61345131
H	-3.59245989	7.17039242	-2.37307320
C	-4.82047170	4.26265681	-3.68935108
H	-6.45835681	6.02923708	-8.12289326
C	-0.56861558	8.56101752	2.95369469
O	-6.80926239	4.52421720	-6.71387554
C	-5.87477770	4.18736796	-4.59009760
H	-7.68563786	4.79199607	-8.51174477
H	-4.96239434	3.93749924	-2.66307190
H	-0.48116143	6.90802385	4.32405600
C	-1.41326039	11.08069018	1.96857102
H	-1.56610632	11.98751001	1.38238741
H	-1.28209777	9.10271802	3.56295221
H	-6.84251986	3.80347396	-4.28261465
H	-2.37095565	10.56224782	2.09518759
H	-1.00782071	11.34488949	2.95227501
H	-1.91967880	0.35678809	-2.49999468
H	-1.03852651	4.89555968	-0.92853050
H	-7.30527345	-2.70558965	-3.27727188
C	-6.68122600	-3.56957973	-3.07110416
H	-4.83916370	-2.58784485	-3.57192325
O	-8.64898604	-4.71585134	-2.52327851
C	-5.30426531	-3.50930159	-3.23460875
H	-10.39282749	-5.64660912	-2.11623646
C	-7.29424614	-4.76200861	-2.65041755
H	-3.78786618	-4.82909640	-5.70905510
H	-6.67346789	-1.52755821	0.97871279
H	-7.30800919	-0.12630689	3.94822629
H	-7.84229750	0.74157474	6.18956350
C	-9.33202417	-5.90142114	-2.11309921
H	-7.44395261	2.05826752	8.09734548
H	-8.22137103	-3.31001721	0.19299056
H	-2.81367513	-6.35661555	-7.37062060
C	-6.62586823	-0.31323164	4.77216302
C	-6.79902207	-2.43498316	1.56184633
C	-6.92886312	0.17720205	6.04433927
C	-2.96679040	-5.47825000	-5.42072547
H	-9.15378653	-6.72512548	-2.81442307
C	-4.50631101	-4.63296786	-2.96435643
C	-7.66875742	-3.42540226	1.12029417

C	-2.16417653	0.25874324	2.19641303
C	-7.41346835	1.12712995	8.67550936
C	-2.41339961	-6.34713142	-6.36377823
H	-1.54257500	1.08966830	2.50918832
C	-3.28885856	-0.07821672	2.92435544
N	-1.76122221	-0.39312215	1.08669739
H	-1.06530542	-7.18282025	-8.70725073
H	-8.32053541	0.54424912	8.47600774
C	-6.50451270	-5.89198152	-2.39544075
H	-3.54192778	0.50269622	3.80140232
C	-2.81206783	-3.04788620	-1.25866011
C	-2.33238736	-3.63316478	-2.44980647
N	-0.87273672	-1.63409195	-1.07097322
N	-3.08210792	-4.56743208	-3.14090446
C	-4.07861060	-1.18080920	2.52201204
C	-0.39505616	-2.21715829	-2.18951605
C	-1.06225336	-3.20240174	-2.89341627
H	-9.03074367	-6.19672057	-1.10260867
C	-3.66280387	-1.84834404	1.34914225
N	-5.18926254	-1.58039625	3.23713486
C	-5.46002466	-1.04755112	4.54659924
H	0.56233786	-1.85206301	-2.54260956
H	-7.35969838	1.36207051	9.73930936
C	-2.48240943	-5.43809169	-4.11079281
C	-5.11754126	-5.81760761	-2.54807474
C	-6.08026432	-2.60212828	2.75620934
H	-0.61528783	-3.60579431	-3.79300998
C	-6.04693880	-0.05972279	7.10801919
H	-2.23025481	-8.45811535	-8.23763535
C	-1.18160409	-8.14137023	-8.18745262
O	-6.23787235	0.37387014	8.38387591
C	-7.85821373	-4.59217145	1.87951254
O	-8.74366278	-5.49633786	1.37313046
H	-6.95114550	-6.82362939	-2.06907516
C	-1.34727843	-7.18122102	-6.00041766
C	-4.58534970	-1.29114201	5.61684158
H	-0.55273164	-8.89258670	-8.66713359
C	-4.87129986	-0.79589481	6.88265298
O	-0.72805113	-8.05854076	-6.83812446
C	-6.26701584	-3.76753078	3.50376087
C	-1.42472366	-6.28752770	-3.74806667
H	-4.50753589	-6.69177287	-2.34097832
C	-7.15508718	-4.75783980	3.08012341
C	-0.85635249	-7.14111013	-4.68451459
C	-9.00035603	-6.68484176	2.11996915
H	-9.73737606	-7.24485565	1.54330169
H	-9.41079755	-6.45055763	3.10916157
H	-3.68082667	-1.86945938	5.45310826
H	-4.20112505	-0.97801216	7.71691170
H	-1.05059670	-6.27745259	-2.72869992
H	-5.71928130	-3.90270582	4.43128595
H	-7.28130501	-5.64760530	3.68531364
H	-8.09203667	-7.28797936	2.23470226
H	-0.03750436	-7.79965693	-4.41206406
H	-3.77213371	-3.35633420	-0.86935311

H	-4.22176674	-2.70293991	0.99743777
H	6.50588237	2.71581948	-8.86840071
C	7.40395729	3.09496924	-8.36621886
H	7.72826145	4.01704987	-8.85044297
C	2.04146780	0.75187549	-2.24177525
H	6.70643118	0.78334508	-7.53949588
H	3.30838733	1.26952071	-3.87783489
C	3.21067958	0.67865989	-2.97612974
C	6.52022773	1.12144568	-6.52698527
O	7.13251359	3.44218892	-7.01008881
H	8.20275108	2.34680971	-8.43435456
H	5.92432139	-0.83440778	-5.86266441
C	6.07499403	0.20161036	-5.57503599
C	6.70907199	2.46217669	-6.16459009
H	4.60954070	-2.90128367	-3.64748423
C	4.23845606	-0.19618272	-2.55855857
C	5.82763277	0.59546474	-4.25754028
C	6.45796865	2.86175955	-4.84116179
C	2.81306185	-0.76569479	-0.66870548
C	6.03258460	1.93683248	-3.89655082
N	5.40644568	-0.36599230	-3.27939316
C	0.90780965	-2.07041096	2.14644648
H	6.61782141	3.90057079	-4.56960273
C	4.00841674	-0.90739983	-1.36152517
C	5.64789550	-2.81713397	-3.34112464
C	2.51922238	-1.49908022	0.58499499
C	6.20407888	-1.54865375	-3.10917414
H	5.99354169	-4.94611268	-3.35310956
H	5.85891805	2.25193581	-2.87194532
C	6.41611232	-3.96171112	-3.17768615
H	4.77156465	-1.57759364	-0.99194466
C	1.78950120	-2.86497153	2.85367211
C	3.47332460	-2.25173463	1.25924889
H	1.43702678	-3.39199451	3.73046597
C	7.54584992	-1.45199872	-2.73413607
C	3.13673869	-2.96103484	2.43286478
C	7.76493650	-3.86247472	-2.79650211
H	4.48872051	-2.28315042	0.89234175
H	4.78199558	-5.00051955	0.86862871
H	7.98420670	-0.47428017	-2.55806659
C	8.33100883	-2.59781319	-2.58298220
O	8.42913745	-5.04368728	-2.66274040
N	4.06760476	-3.70380662	3.13019677
C	5.62516643	-4.62203074	1.43883515
H	3.97122066	-6.27331326	3.83513093
C	3.77526206	-4.21993340	4.44152321
H	7.10459177	-5.36817140	0.05404188
C	3.77542851	-5.59845785	4.66302109
C	5.40036808	-3.91778247	2.63213534
H	9.36814528	-2.49253011	-2.28795400
C	6.92063690	-4.83478672	0.98154987
C	9.80923505	-5.00761413	-2.29607766
H	10.39978511	-4.44415081	-3.02806272
C	3.52806602	-3.35293164	5.51715448
C	3.53358953	-6.11959214	5.93609897

H	3.53547993	-2.27896027	5.35644404
H	10.13937715	-6.04742003	-2.28829947
H	3.54193861	-7.19366431	6.07797018
C	3.27317445	-3.86221797	6.78405164
C	3.27638760	-5.24998497	7.00514296
H	2.23942738	-7.56432911	7.99831906
H	9.93817914	-4.57664790	-1.29772897
C	6.49626828	-3.45180979	3.36255603
C	8.01952145	-4.37048315	1.72379839
H	3.08004664	-3.20006145	7.62223634
O	3.02344171	-5.64619451	8.28241136
C	3.01615765	-7.04316159	8.57044974
H	6.33199769	-2.91087058	4.28936236
C	7.80155683	-3.68006507	2.92344113
O	9.24925990	-4.64124492	1.20225441
H	2.79878375	-7.12575843	9.63613858
H	3.99116174	-7.49885237	8.36062895
H	8.62977225	-3.31054839	3.51613238
C	10.40213572	-4.21847721	1.92947934
H	10.43035589	-3.12744175	2.03375479
H	11.26058398	-4.54931745	1.34386690
H	10.43655071	-4.68130415	2.92268021
H	-0.11996988	-1.97213677	2.47569131
H	1.23060604	1.39072275	-2.57168866

Cartesian coordinates of DFT-optimized structure of $\mathbf{1}^{3+}$:

Charge = 3; multiplicity=2

N	-2.97672362	-0.92178965	2.25712626
C	-6.46525648	0.26717815	1.81263807
C	-7.33941851	0.42627139	0.74137109
C	-6.90405195	0.09283902	-0.54008296
C	-5.60938023	-0.38836345	-0.70116156
N	-4.75889701	-0.54392314	0.33048874
C	-5.17468944	-0.22106522	1.58713636
C	-4.17841563	-0.41998911	2.65818977
C	-4.42121320	-0.12693697	4.00363833
C	-3.42389026	-0.34832977	4.94882029
C	-2.19793982	-0.86117886	4.52822419
C	-2.01633083	-1.13246534	3.17658755
C	-4.46348284	-5.22440268	1.20104701
C	-3.93428658	-3.94030426	1.27164935
C	-4.62333181	-5.81413193	-0.05178883
N	-3.56790917	-3.24416453	0.17939038
C	-4.24950315	-5.09893031	-1.18593016
C	-3.72254738	-3.81103521	-1.05015620
Ru	-2.78403745	-1.28018238	0.18265985
N	-0.75453856	-1.81046003	0.19803982
C	0.12825856	-0.77769315	0.06186068
C	-3.30076440	-2.97757072	-2.19404362
N	-2.84141022	-1.73398089	-1.87856852
C	-3.36114308	-3.40289716	-3.52447432
C	-2.44601854	-0.90989224	-2.86670904
C	-2.95012960	-2.54606890	-4.54162726
C	-2.48513110	-1.27508353	-4.20789703
H	-6.78867829	0.52099490	2.81410461
H	-8.34255749	0.80429007	0.90777582
H	-5.22866420	-0.65623695	-1.67874221
H	-5.37883728	0.27105400	4.31466385
H	-3.60418540	-0.12338432	5.99466731
H	-1.08124183	-1.53473178	2.80742303
H	-4.74091784	-5.74114616	2.11275709
H	-3.79122703	-3.44473885	2.22392221
H	-5.03307031	-6.81397821	-0.14821033
H	-4.36999243	-5.54197601	-2.16634502
H	-3.72407014	-4.39329679	-3.76851296
H	-2.09528115	0.06711971	-2.55887460
H	-2.99420237	-2.86851246	-5.57650922
H	-2.15620766	-0.57259387	-4.96519515
H	-1.39076688	-1.05111200	5.22648342
H	-7.54793303	0.19990424	-1.40559082
H	4.27983155	0.37945996	3.72986007
C	4.57161399	-0.04712175	2.77641198
H	2.88300933	-1.34946917	2.63313420
O	6.43391099	1.35132929	2.84541973
C	3.79576759	-1.00460468	2.16000676
H	1.88865245	3.48792496	1.70752550
H	-3.50747400	1.80942085	-0.03124680
C	-2.42568175	1.80682594	-0.08716695
H	8.00454727	2.60693808	3.03183630

C	5.77373215	0.39443232	2.17680016
C	-1.73761171	2.99607892	-0.22814616
H	-2.29415058	3.92265842	-0.27566289
N	-1.83117938	0.59857054	-0.01011752
C	7.64811797	1.88767534	2.29510832
H	0.34425884	6.31769398	1.08170556
H	4.37186746	3.49746844	1.85304213
H	-2.49041427	9.89990190	0.03335066
C	2.48324810	3.77686751	0.84594844
H	-0.68126410	8.49117639	0.54651835
C	-0.16347610	6.45174479	0.13131123
H	5.47727584	-3.89068726	1.20378415
C	-0.47014320	0.56795030	-0.06628491
C	-0.74435049	7.68440779	-0.17390867
C	-0.32431021	2.98539519	-0.30752027
C	3.87023944	3.78398781	0.93398335
H	8.39453889	1.09951008	2.15710303
C	0.29263422	1.71556943	-0.22268813
C	4.20752506	-1.56140111	0.92713300
C	-0.26840927	-3.06329716	0.32456304
N	0.41109570	4.13719041	-0.45602148
C	-1.98610277	10.12819685	-0.91305158
C	5.09263452	-4.26361587	0.26146578
C	-0.22416798	5.39034112	-0.77333960
C	1.50154185	-1.00056637	0.06861691
C	1.08496409	-3.35799215	0.34391471
C	1.99871645	-2.30009992	0.22268719
H	7.44235587	2.39636692	1.34879699
C	6.19371235	-0.16792629	0.95433637
H	6.52125423	-5.84409426	0.16361593
C	1.84745599	4.13682774	-0.35250800
H	-2.52440951	10.92447811	-1.42857270
C	-1.40500790	7.85676574	-1.39875561
N	3.39436432	-2.51546087	0.27365282
H	1.36870031	1.64808834	-0.28343560
C	5.67698792	-5.37297379	-0.32373749
H	1.41269508	-4.38055019	0.48346226
O	-2.01018590	9.00805535	-1.79630702
C	5.41838905	-1.14056757	0.34208753
C	3.97004780	-3.64348335	-0.33119610
H	-0.95900857	10.45392333	-0.71026613
C	-0.87554735	5.56979513	-2.00302913
H	6.56828253	-8.05744171	-0.66362322
C	-1.46671126	6.78851689	-2.30992586
C	4.64863160	4.17564718	-0.16814898
H	7.10233858	0.16651208	0.46992709
O	5.99802700	4.15622255	0.01811308
H	-0.91689522	4.75202655	-2.71644175
C	5.14978878	-5.88916190	-1.52598466
C	6.78248819	-7.64165831	-1.65303905
C	2.62403405	4.52632774	-1.44600154
H	-1.97425609	6.93887494	-3.25750329
H	5.72291785	-1.54665892	-0.61619227
C	3.44377748	-4.16623456	-1.53809413
H	7.64465483	-6.96981630	-1.60221899

C	4.01716994	4.55621536	-1.36023430
O	5.63354003	-6.95532827	-2.17469225
C	4.02642294	-5.26823877	-2.12305508
H	6.98182815	-8.44794272	-2.35774356
H	2.60510116	-3.67921346	-2.02272348
H	2.13947917	4.81349682	-2.37407483
C	6.83704721	4.58162834	-1.05607406
H	7.85891340	4.50383079	-0.68340069
H	4.59196727	4.86531310	-2.22489345
H	3.64890095	-5.66825443	-3.05767434
H	6.71842234	3.93600420	-1.93406000
H	6.62737523	5.62077125	-1.33483889
H	-1.00228481	-3.85065763	0.43779631
H	2.19150383	-0.17801003	-0.05459516

Cartesian coordinates of DFT-optimized structure of 2^{3+} :

Charge = 3; multiplicity=2

N	0.55704822	-1.12512619	3.78030295
C	-0.39140242	1.60940119	6.10075560
C	-0.89555176	2.90047919	5.97299432
C	-1.13460870	3.40920446	4.69802891
C	-0.86156933	2.60556040	3.59652049
N	-0.37322960	1.35744300	3.71518168
C	-0.13512297	0.85066736	4.95543006
C	0.39806973	-0.52442208	4.99085522
C	0.72442707	-1.19626505	6.17210261
C	1.21698083	-2.49654872	6.11147847
C	1.37309218	-3.10250457	4.86645073
C	1.03289306	-2.38273979	3.72643668
C	-2.74627421	0.26134958	1.09846457
Ru	0.04473714	0.05386723	2.07760092
N	0.64318688	-1.31619505	0.66758311
C	1.96882831	-1.27869229	0.30835376
C	-1.99680273	1.30009320	0.35532313
H	-0.20256102	1.19876708	7.08432311
H	-1.09768271	3.49614980	6.85676526
H	-1.02989864	2.96186318	2.58868698
H	0.59770149	-0.71159864	7.13165648
H	1.47281597	-3.02519990	7.02351647
H	1.13392435	-2.81728903	2.74028494
H	1.75040733	-4.11385691	4.76844111
H	-1.52590244	4.40876265	4.54772246
H	5.96961261	-5.42980457	0.38989098
C	5.52719107	-5.14666812	-0.55944942
H	3.55157286	-4.88427875	0.23080481
O	7.64828816	-5.41523182	-1.50245430
C	4.18050528	-4.83929925	-0.65252497
H	6.82012174	-1.25529619	1.29570040
H	2.22841654	2.05718069	3.26128529
C	2.78001808	1.49566214	2.51668493
H	9.51146738	-5.69989118	-2.22508526
C	6.34591389	-5.11005435	-1.70441910
C	4.10731817	1.78537719	2.27351794
H	4.58629158	2.57142478	2.84179818
N	2.09425422	0.53253745	1.86772432
C	8.54295003	-5.39230363	-2.62033163
H	8.22633381	1.37428494	2.61875678
H	8.14026155	-2.63352787	-0.30132658
H	9.59551279	5.35784620	4.67589258
C	7.17370533	-0.82162221	0.36494849
H	9.42215009	3.35113085	3.46908694
C	7.88878128	2.36720665	2.33746984
H	2.23907635	-6.77827493	-2.45894382
C	2.76611134	-0.20448102	0.93983276
C	8.56754609	3.48908526	2.81761044
C	4.81464386	1.06331114	1.28105536
C	7.91443680	-1.59481046	-0.52146474
H	8.22311811	-6.09743803	-3.39524607
C	4.09173707	0.04199652	0.61940439

C	3.62255824	-4.48377641	-1.89401699
C	-0.14568827	-2.25971151	0.09369114
N	6.12508441	1.33596051	0.97568114
C	9.84701619	5.85270847	3.73044344
C	1.55981118	-6.22670947	-3.10026751
C	6.78484975	2.50732828	1.49473731
C	2.50383620	-2.20340533	-0.56755815
C	0.31624275	-3.19560846	-0.80317730
C	1.69071807	-3.20678743	-1.14438110
H	8.61903869	-4.38165815	-3.03343443
C	5.78604007	-4.77294462	-2.94855734
H	0.91079209	-7.98250132	-4.13547193
C	6.87961603	0.51655034	0.06154167
H	10.14169648	6.88419357	3.92740264
C	8.13147276	4.77206390	2.45711190
N	2.23285966	-4.15291423	-1.98694162
H	4.57846475	-0.53921383	-0.14981892
C	0.80468994	-6.90814514	-4.04981378
H	-0.36817845	-3.93341120	-1.20076834
O	8.71262887	5.93071417	2.86853396
C	4.43066535	-4.46550059	-3.03706676
C	1.43724845	-4.83831165	-2.95273202
H	10.67676437	5.32134741	3.24959225
C	6.35771475	3.79220962	1.12686231
H	-1.09459237	-8.71937418	-5.12506415
C	7.01959574	4.91386916	1.60929441
C	8.39598471	-1.03626033	-1.71749612
H	6.39556564	-4.73409155	-3.84286323
O	9.12274991	-1.86848179	-2.51386776
H	5.50688759	3.90918505	0.46218759
C	-0.08892078	-6.19960067	-4.87055121
C	-0.79888874	-8.17339503	-6.02783174
C	7.35606357	1.06742618	-1.13006320
H	6.69797086	5.91275755	1.33200591
H	4.00258512	-4.19000139	-3.99536703
C	0.55173008	-4.12862816	-3.78534407
H	0.20910501	-8.47795516	-6.33062570
C	8.11696261	0.30428413	-2.01703695
O	-0.87013503	-6.76009029	-5.82150342
C	-0.20512055	-4.80318378	-4.72831706
H	-1.50272739	-8.38885918	-6.83196468
H	0.47475319	-3.04933065	-3.70245505
H	7.13735551	2.10380115	-1.36803312
C	9.67883969	-1.34108511	-3.71849298
H	10.22950296	-2.16365183	-4.17598335
H	8.47523688	0.76038758	-2.93202235
H	-0.88451536	-4.26712850	-5.38271086
H	8.89451391	-1.00085821	-4.40470651
H	10.36534197	-0.51289183	-3.50791309
H	-1.18325167	-2.25988500	0.40068544
H	3.55125794	-2.15832035	-0.82863364
H	-6.30163604	-1.68260566	-3.22412815
C	-6.70893451	-1.27037280	-2.30632029
H	-5.25701102	-2.20036616	-1.02723704
O	-8.33842927	-0.23451565	-3.63000551

C	-6.12961814	-1.55602893	-1.07801119
H	-9.72846043	0.58909761	-4.83912285
C	-7.84848903	-0.45113549	-2.37962595
H	-7.33322682	-3.65440085	0.97770806
H	-3.61751072	1.93493132	-3.32233346
H	-1.88717491	4.52977245	-4.67181496
H	-0.66453539	6.45194170	-5.60106093
C	-9.50032757	0.58439963	-3.77236773
H	1.23265594	7.80749103	-5.89237898
H	-6.00334560	1.83263326	-4.01610433
H	-8.73689143	-4.87367686	2.58698581
C	-1.48024294	5.28125688	-4.00238087
C	-4.27440751	2.77960541	-3.13846621
C	-0.78781948	6.37227353	-4.52784987
C	-7.47320822	-3.25274470	1.97651853
H	-10.35049251	0.16702825	-3.22033867
C	-6.66660398	-1.01642218	0.10177012
C	-5.60481216	2.71953480	-3.53377955
C	0.09427788	2.24224848	-0.07314419
C	0.65493359	8.63347776	-5.46150525
C	-8.27067998	-3.94402680	2.89084428
H	1.15641234	2.23652780	0.13607861
C	-0.42899668	3.12550642	-0.98872875
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C	-0.43786878	7.20676552	-2.27517621
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H	-8.28083055	5.64525067	-4.16348626
H	-1.28220098	6.03234785	-0.68796509
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H	-6.59244503	-0.59077532	3.90114898
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Cartesian coordinates of DFT-optimized structure of $\mathbf{3}^{3+}$:

Charge = 3; multiplicity=2

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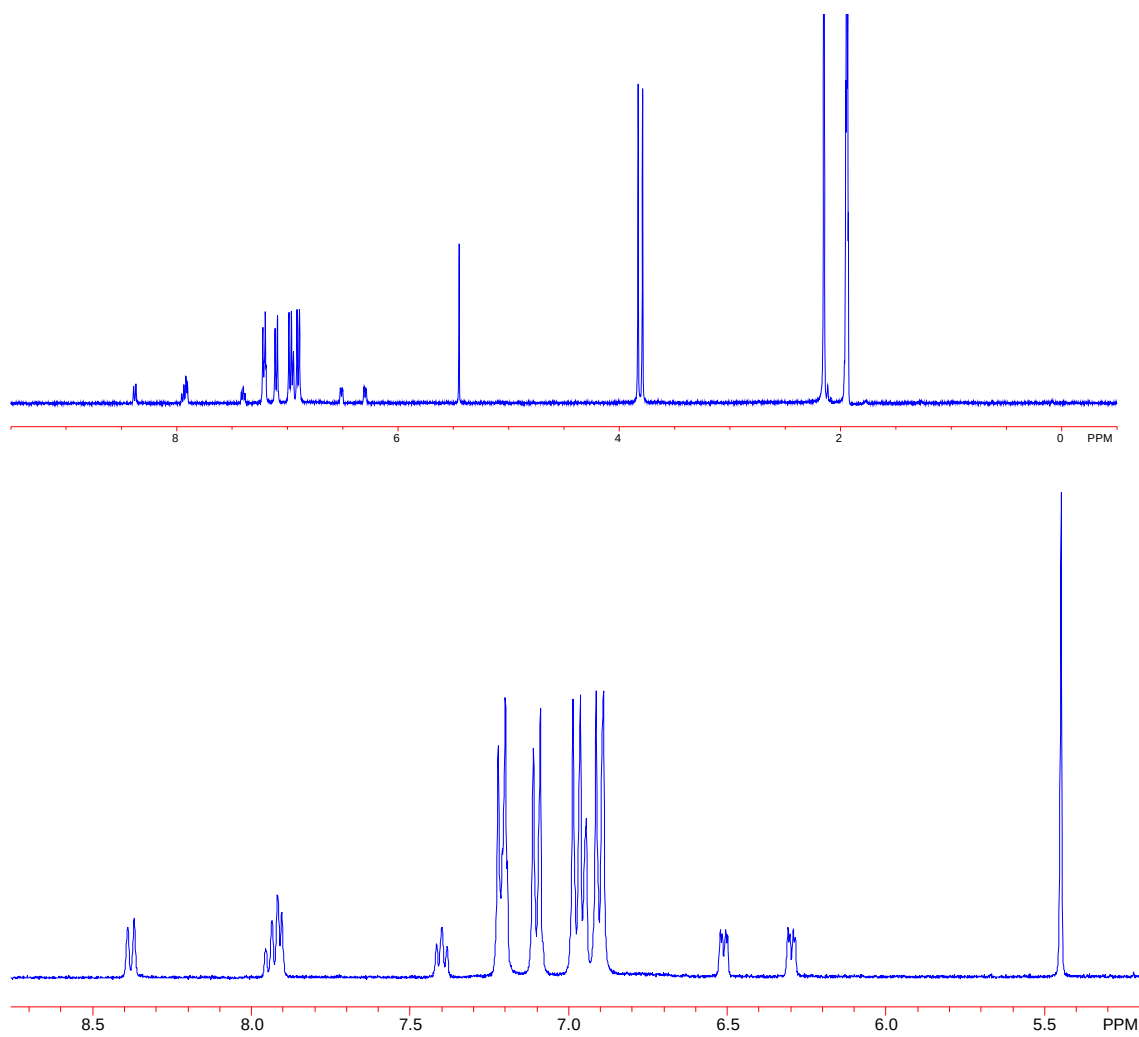
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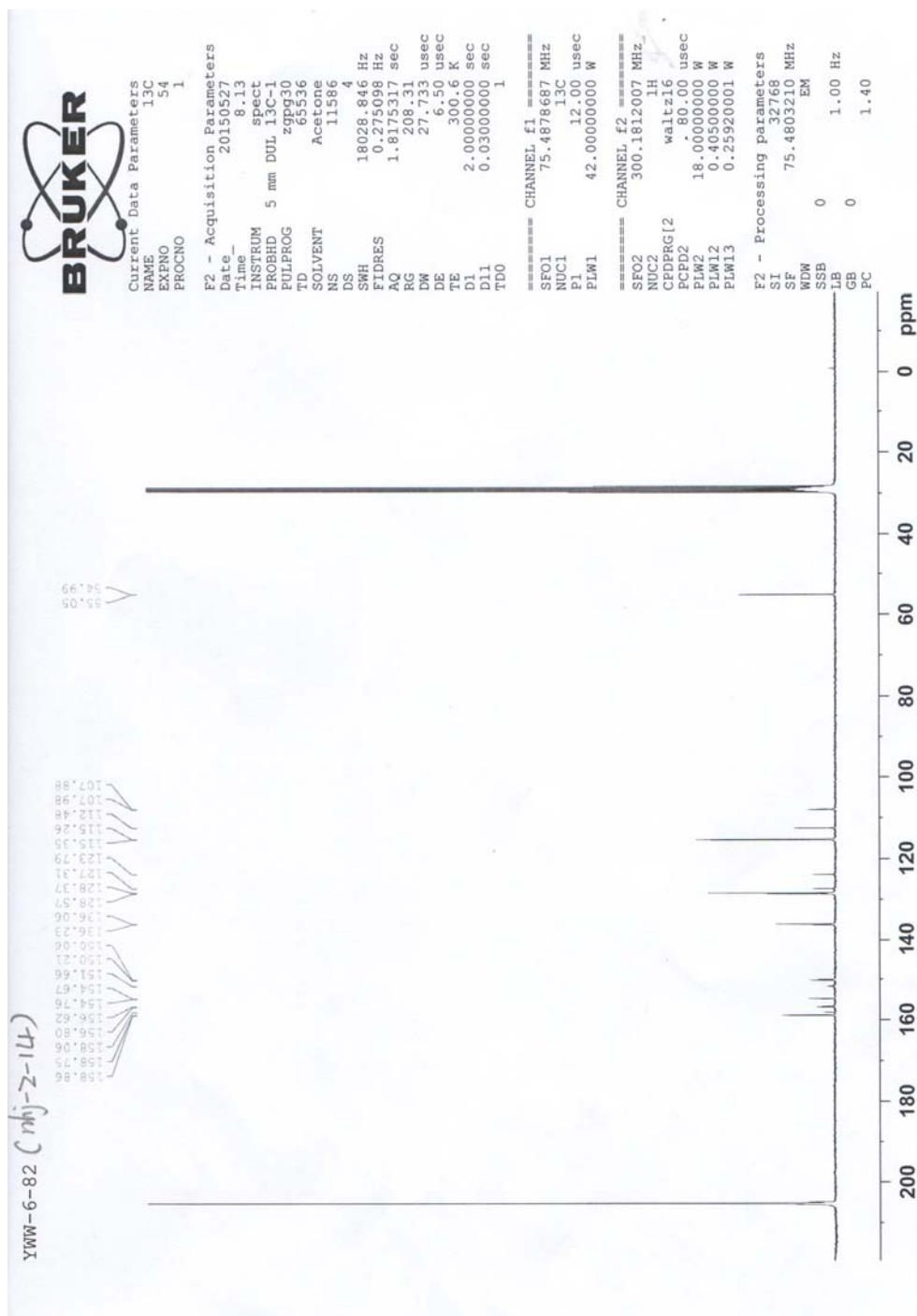
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^1H NMR spectrum of $2(\text{PF}_6)_2$ in CD_3CN :

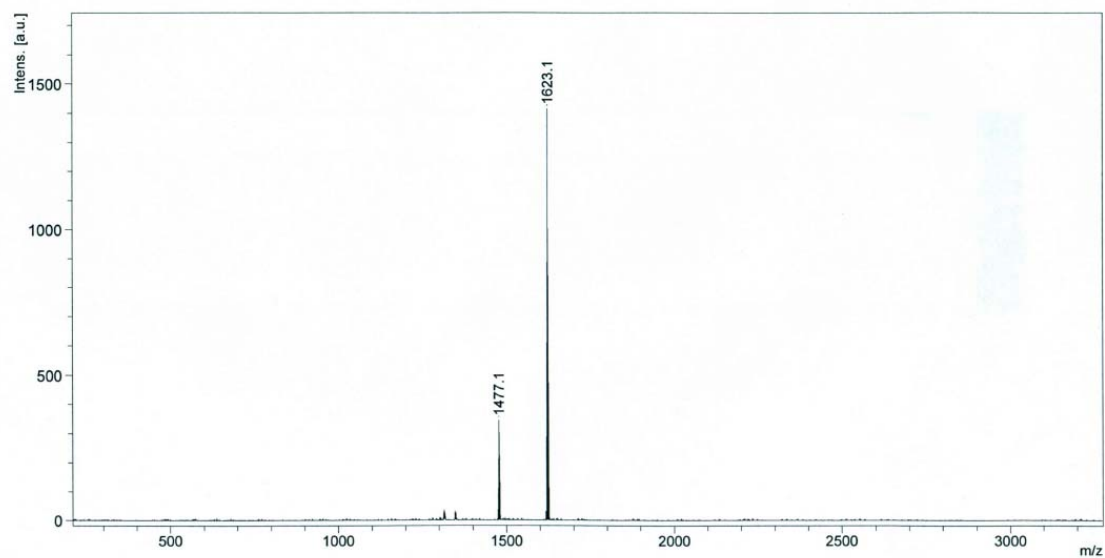


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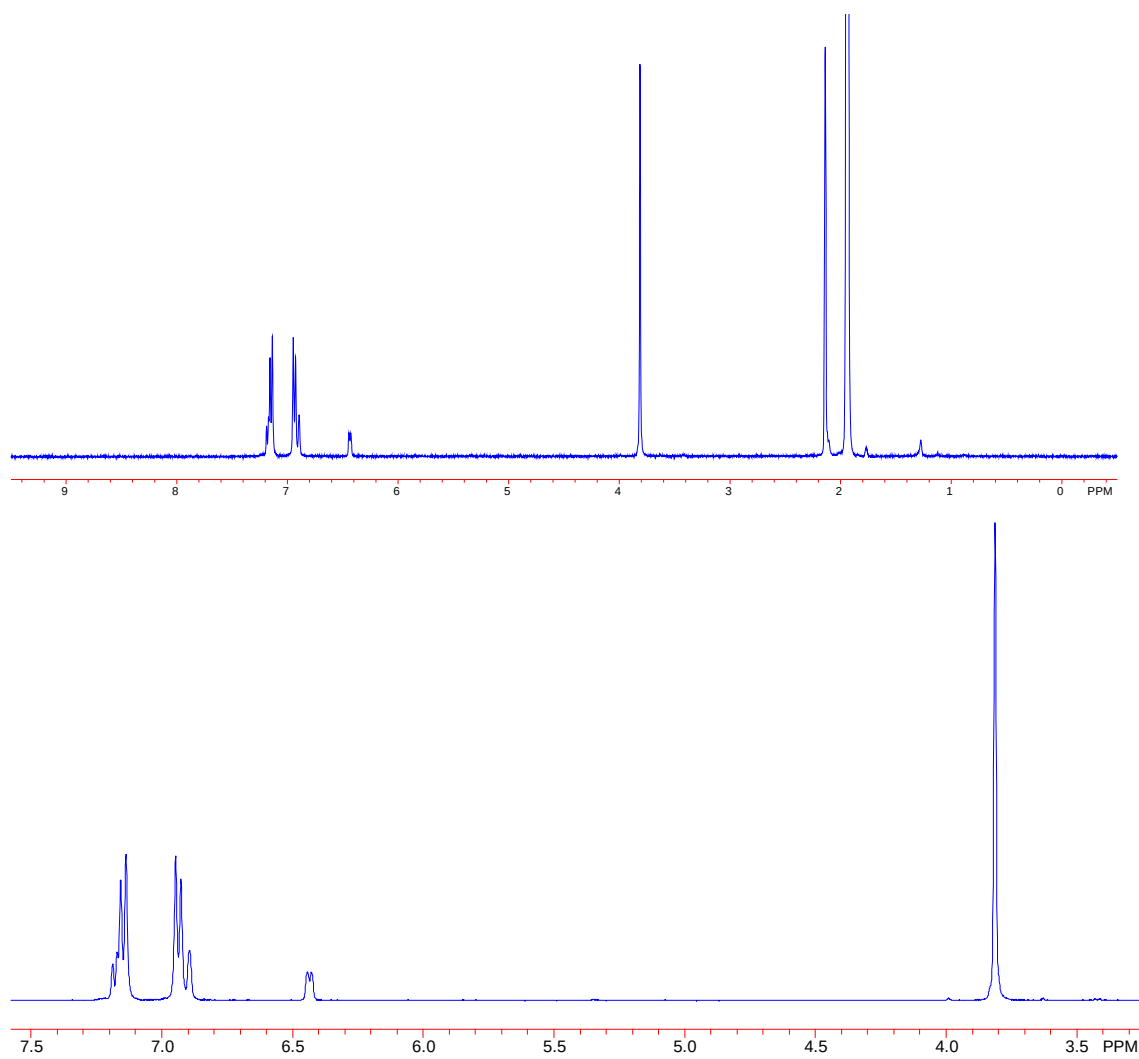


MALDI-TOF mass spectrum of $2(\text{PF}_6)_2$:

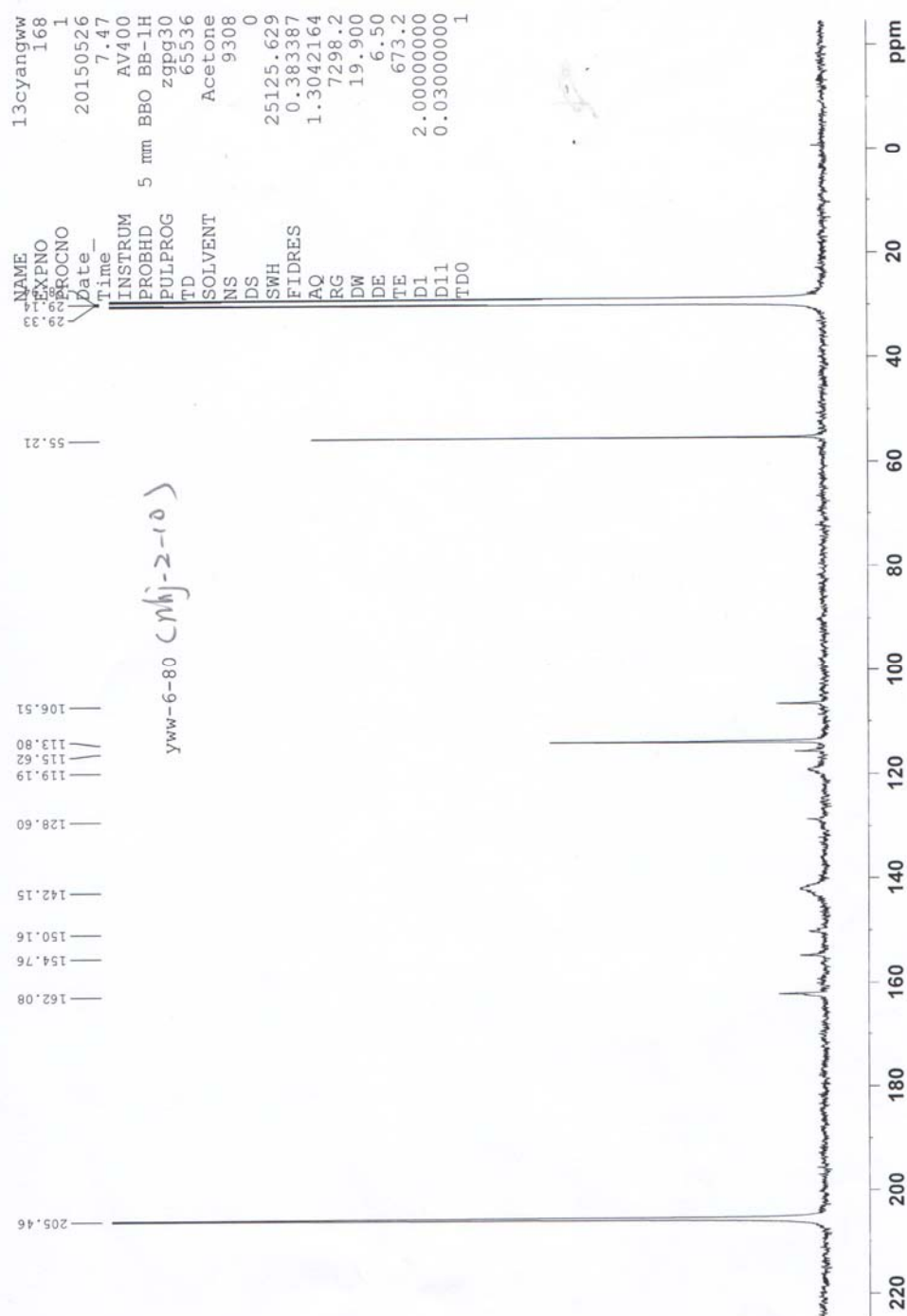
MALDI-TOF, CCA, NHJ-2-12, 2010, 04, 28



^1H NMR spectrum of $\mathbf{3}(\text{PF}_6)_2$ in CD_3CN :



^{13}C NMR spectrum of $3(\text{PF}_6)_2$ in D_6 -acetone:



MALDI-TOF mass spectrum of **3**(PF₆)₂:

MALDI-TOF,CCA,nhj-1-100-1,2011,04,02

