Electronic Supplementary Information for:

Organic-Inorganic Mixed-Valence System with Strongly-Coupled Triarylamine and Cyclometalated Osmium

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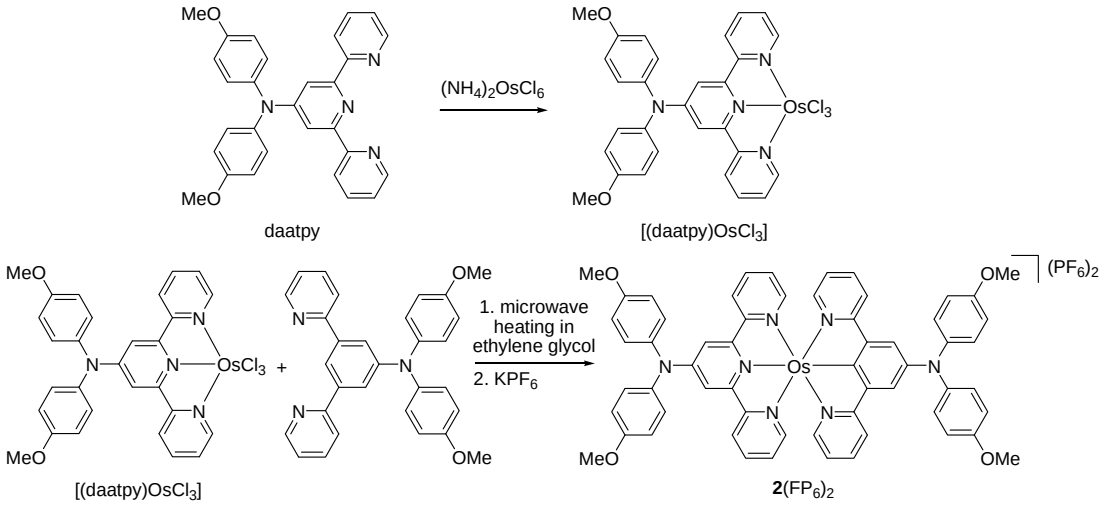
Synthetic Procedures and Characterization

General. NMR spectra were recorded in the designated solvent on Bruker Avance 400 MHz spectrometer. Spectra are reported in ppm values from residual protons of deuterated solvent. Mass data were obtained with a Bruker Daltonics Inc. ApexII 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. 4'-Di-*p*-anisylamino-2,2':6',2''-terpyridine [1] (daatpy), 1-di-*p*-anisylamino-3,5-di(2-pyridyl)benzene (daadpb), [2] and [(ttpy)$OsCl_3$] (ttpy = 4'-tolyl-2,2':6',2''-terpyridine)[3] were prepared according to known procedures.



To 10 mL dry *N*,*N*-dimethylformamide were added $(NH_4)_2OsCl_6$ (131 mg, 0.3 mmol) and daatpy (138 mg, 0.3 mmol). The mixture was refluxed for 2 h before cooling to room temperature. The solution was then poured into 50 mL ethyl ether. The resulting precipitate was collected by filtering and washing with ethyl ether to give 179 mg of [(daatpy)$OsCl_3$] as a black solid in 73% yield. This crude product was used for next transformation without any further purification and characterization.

To 5 mL dry ethylene glycol were added [(daatpy)$OsCl_3$] (50 mg, 0.066 mmol) and 1-di-*p*-anisylamino-3,5-di(2-pyridyl)benzene (36 mg, 0.079 mmol). The resulting mixture was refluxed under microwave heating (power 375 W) for 40 min. After

(1) Yao, C.-J.; Yao, J.; Zhong, Y.-W. *Inorg*. *Chem*. **2011**, *50,* 6847.
(2) Yao, C.-J.; Zheng, R.-H.; Shi, Q.; Zhong, Y.-W.; Yao, J. *Chem*. *Commun.* **2012**, *48,* 5680.
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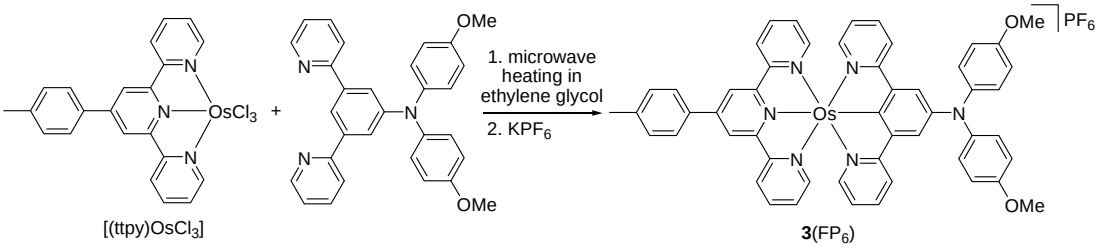
cooling to room temperature, the system was treated with an excess of aq. KPF_6. The resulting precipitate was collected by filtering and washing with water and Et_2O. The obtained solid was subjected to flash column chromatography on silica gel (eluent: saturated aq. $KNO_3/H_2O/CH_3CN$, 1/20/3000), followed by anion exchange using KPF_6, to give 10 mg of **2**(PF_6) (minor, 12%) and 40 mg of **2**$(PF_6)_2$ (major, 43%) as black solids.

Data for **2**$(PF_6)_2$: MALDI-MS: 1110.2 for $[M - 2PF_6]^+$. Anal. Calcd for $C_{59}H_{48}F_{12}N_7O_4P_2Os$: C, 50.64; H, 3.46; N, 7.01. Found: C, 50.66; H, 3.57; N, 7.32.

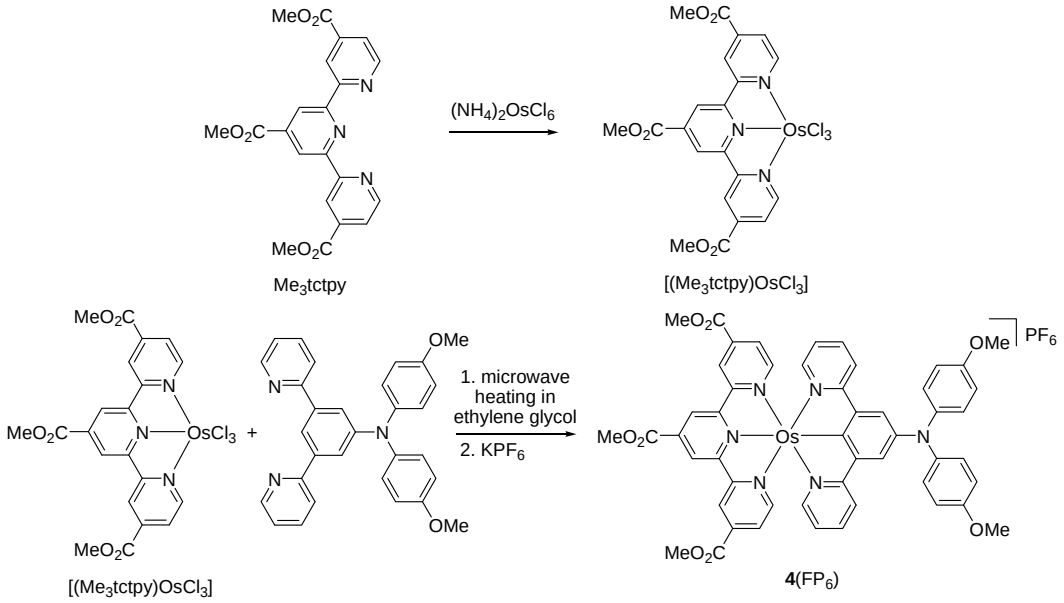
Data for **2**(PF_6): 1110.5 for $[M - PF_6]^+$. The isolated minor product of **1**$(PF_6)_2$ has identical cyclic voltammogram as **2**$(PF_6)_2$. However, it always contain small amount of the oxidized form (judging by TLC and absorption spectrum) and no satisfactory NMR and microanalysis dada have been obtained.



To 5 mL dry ethylene glycol were added $[(ttpy)OsCl_3]$ (50 mg, 0.081 mmol) and 1-di-*p*-anisylamino-3,5-di(2-pyridyl)benzene (45 mg, 0.097 mmol). The resulting mixture was refluxed under microwave heating (power 375 W) for 40 min. After cooling to room temperature, the system was treated with an excess of aq. KPF_6. 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. $KNO_3/H_2O/CH_3CN$, 1/20/3000), followed by anion exchange using KPF_6, to give 32 mg of **3**(PF_6) (major, 35%) and 22 mg of **3**$(PF_6)_2$ (minor, 22%) as black solids.

Data for **3**(PF_6): ^{1}H NMR (400 MHz, acetone-D_6, in the presence of small amount of $NH_2NH_2{\cdot}H_2O$): δ 3.74 (s, 3H), 3.82 (s, 6H), 6.65 (t, J = 6.4 Hz, 2H), 6.94 (d, J = 8.8 Hz, 4H), 7.09 (m, 4H), 7.20 (d, J = 8.8 Hz, 4H), 7.33 (d, J = 5.6 Hz, 2H), 7.52 (m, 4H), 7.73 (t, J = 7.4 Hz, 2H), 8.19 (d, J = 8.0 Hz, 4H), 8.26 (s, 2H),8.92 (d, J = 8.0 Hz, 2H), 9.33 (s, 2H). MALDI-MS: 971.5 for $[M - PF_6 - 2H]^+$. Anal. Calcd for $C_{52}H_{41}F_6N_6O_2POs$: C, 55.91; H, 3.70; N, 7.52. Found: C, 56.05; H, 3.73; N, 7.59.

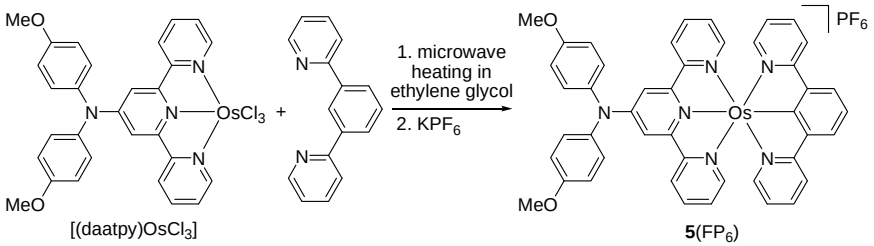
Data for **3**$(PF_6)_2$: MALDI-MS: 973.2 for $[M - 2PF_6]^+$. Anal. Calcd for $C_{52}H_{41}F_{12}N_6O_2P_2Os \cdot H_2O$: C, 48.79; H, 3.39; N, 6.57. Found: C, 48.79; H, 3.41; N, 6.56.



To 10 mL dry *N*,*N*-dimethylformamide were added $(NH_4)_2OsCl_6$ (203.5 mg, 0.5 mmol) and Me_3tctpy (220 mg, 0.5 mmol). The mixture was refluxed for 2 h before cooling to room temperature. The solution was then poured into 50 mL ethyl ether. The resulting precipitate was collected by filtering and washing with ethyl ether to give 303 mg of $[(Me_3tctpy)OsCl_3]$ as a black solid in 86% yield. This crude product was used for next transformation without any further purification and characterization.

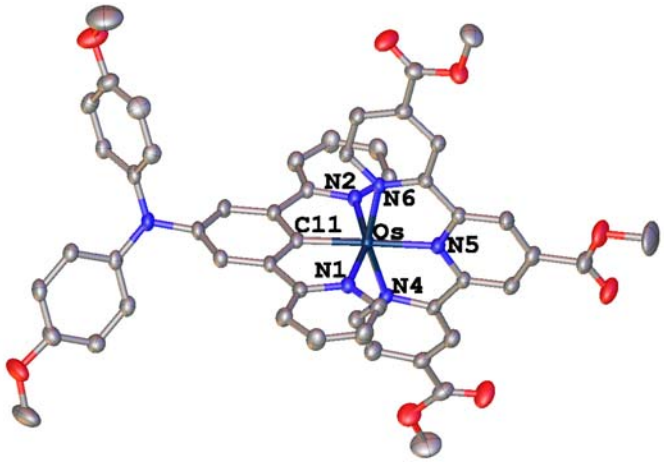
To 5 mL dry ethylene glycol were added $[(Me_3tctpy)OsCl_3]$ (50 mg, 0.071 mmol) and 1-di-*p*-anisylamino-3,5-di(2-pyridyl)benzene (39 mg, 0.085 mmol). The resulting mixture was refluxed under microwave heating (power 375 W) for 40 min. After cooling to room temperature, the system was treated with an excess of aq. KPF_6. 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. $KNO_3/H_2O/CH_3CN$, 1/20/1500), followed by anion exchange using KPF_6, to give 18 mg of **4**(PF_6) as a black solid in 22% yield. ^{1}H NMR (400 MHz, CD_3CN) : δ 3.81 (s, 6H), 3.93 (s, 6H), 4.16 (s, 3H), 6.46 (t, J = 6.4 Hz, 2H), 6.57 (d, J = 5.6 Hz, 2H), 6.95 (d, J = 8.8 Hz, 4H), 7.20 (d, J = 8.8 Hz, 4H), 7.41 (t, J = 7.8 Hz, 2H), 7.44 (d, J = 6.4 Hz, 2H), 7.55 (d, J = 6.0 Hz, 2H), 7.95 (d, J = 8.0 Hz, 2H), 8.17 (s, 2H), 9.08 (s, 2H), 9.35 (s, 2H). MALDI-MS: 1057.4 for $[M - PF_6]^+$. Anal. Calcd for $C_{51}H_{41}F_6N_6O_8POs$: C,

51.00; H, 3.44; N, 7.00. Found: C, 50.89; H, 3.93; N, 6.88.



To 5 mL dry ethylene glycol were added [(daatpy)$OsCl_3$] (92 mg, 0.12 mmol) and 1,3-di(2-pyridyl)benzene (42 mg, 0.18 mmol). The resulting mixture was refluxed under microwave heating (power 375 W) for 40 min. After cooling to room temperature, the system was treated with an excess of aq. KPF_6. 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. $KNO_3/H_2O/CH_3CN$, 1/20/3000), followed by anion exchange using KPF_6, to give 51 mg of **5**(PF_6) as a black solid in 42% yield. ^{1}H NMR (400 MHz, acetone-D_6) : δ 3.90 (s, 6H), 6.74 (t, J = 6.4 Hz, 2H), 6.92 (t, J = 6.2 Hz, 2H), 7.04 (d, J = 5.6 Hz, 2H), 7.14 (d, J = 8.8 Hz, 4H), 7.28 (m, 3H), 7.47 (d, J = 8.8 Hz, 4H), 7.51 (t, J = 8.0 Hz, 2H), 7.57 (t, J = 7.6 Hz, 2H), 8.29 (t, J = 8.0 Hz, 4H), 8.34 (s, 2H), 8.45 (m, 2H). MALDI-MS: 883.2 for $[M - PF_6]^+$. Anal. Calcd for $C_{45}H_{35}F_6N_6O_2POs \cdot 2H_2O$: C, 50.84; H, 3.70; N, 7.91. Found: C, 51.23; H, 3.54; N, 7.71.

X-ray Crystallography. The X-ray diffraction data were collected using a Rigaku Saturn 724 diffractometer on a rotating anode (Mo-K radiation, 0.71073 Å) at 173 K. The structure was solved by the direct method using SHELXS-97[4] and refined with Olex2.[5] Bond lengths [Å] and angles [°] for **4**(PF_6):



Os1-N1	2.096(3)
Os1-N2	2.090(3)
Os1-N4	2.048(3)
Os1-N5	2.010(3)
Os1-N6	2.055(3)
Os1-C11	1.990(4)
N2-Os1-N1	155.07(13)
N4-Os1-N1	96.97(13)
N4-Os1-N2	89.88(13)
N4-Os1-N6	155.55(13)
N5-Os1-N1	97.45(13)
N5-Os1-N2	107.43(13)
N5-Os1-N4	78.00(13)
N5-Os1-N6	78.07(13)
N6-Os1-N1	91.02(13)
N6-Os1-N2	92.52(13)
C11-Os1-N1	77.51(15)
C11-Os1-N2	77.56(15)
C11-Os1-N4	104.90(14)
C11-Os1-N5	174.39(14)
C11-Os1-N6	99.37(14)

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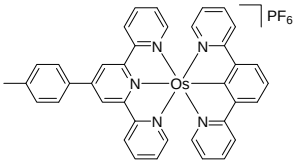
Electrochemical Measurement. All electrochemical measurements were taken using a CHI 660D potentiostat with one-compartment electrochemical cell under an atmosphere of nitrogen. All measurements were carried out in 0.1 M Bu_4NClO_4 in indicated solvents at a scan rate of 100 mV/s. The working electrode 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 regard for the liquid junction potential. The potential versus ferrocene$^{+/0}$ can be subtracted by 0.45 V.

Table S1. Electrochemical Data in CH_3CN[a]

Compound	$E_{1/2}$ (anodic)	ΔE (mV)[b]	K_c[c]	$E_{1/2}$ (cathodic)
1	+0.27, +0.68, +1.69[d]	410	8.9×10^6	–1.50
2	+0.03, +0.58, +1.12	550	2.1×10^9	–1.53
3	+0.18, +0.59, +1.50[d]	410	8.9×10^6	–1.48
4	+0.32, +0.64, +1.62[d]	320	2.6×10^5	–1.08, –1.42
5	+0.20, +1.02[d]	--	--	–1.53
 [Os(dpb)(ttpy)](FP$_6$)	+0.36, +1.27[d]	--	--	–1.48

[a]The electrochemical potential is reported as the $E_{1/2}$ value vs Ag/AgCl unless otherwise noted. Potential versus ferrocene$^{+/0}$ can be estimated by subtracting 0.45 V. [b]ΔE is the potential difference between the first and second oxidative waves. [c]K_c is the comproportionation constant determined by $10^{\Delta E(\text{mV})/59}$. [d]Irreversible, peak potential.

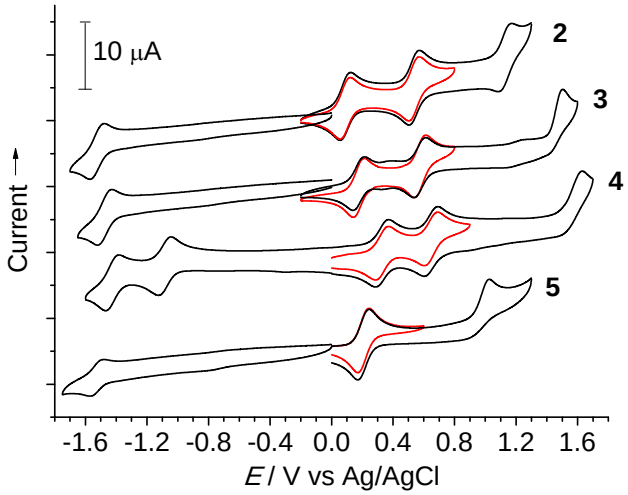


Figure S1. CVs of **2**(PF_6) - **5**(PF_6) in CH_3CN.

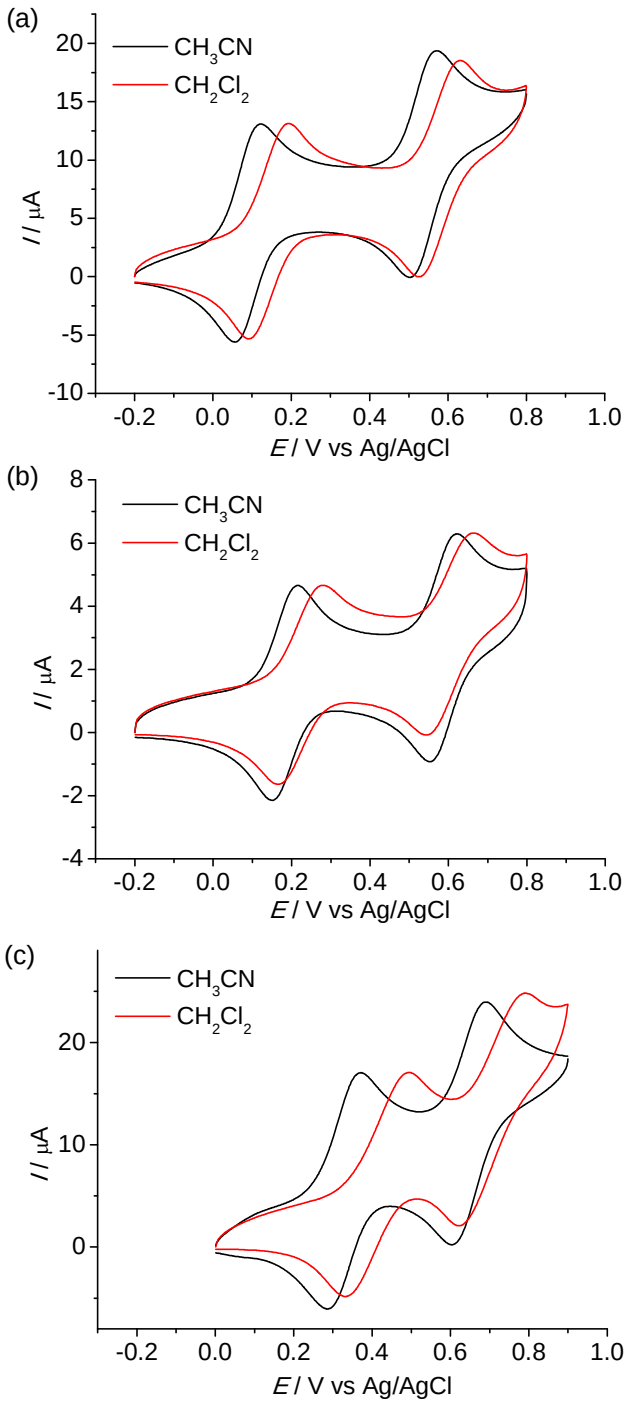


Figure S2. A comparison of the anodic CVs of (a - c) **2 - 4** in CH_3CN versus CH_2Cl_2.

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 (< 10Ω/square) working electrode was set in the indicated solvent containing the compound to be studied (concentration around 5×10^{-5} 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.

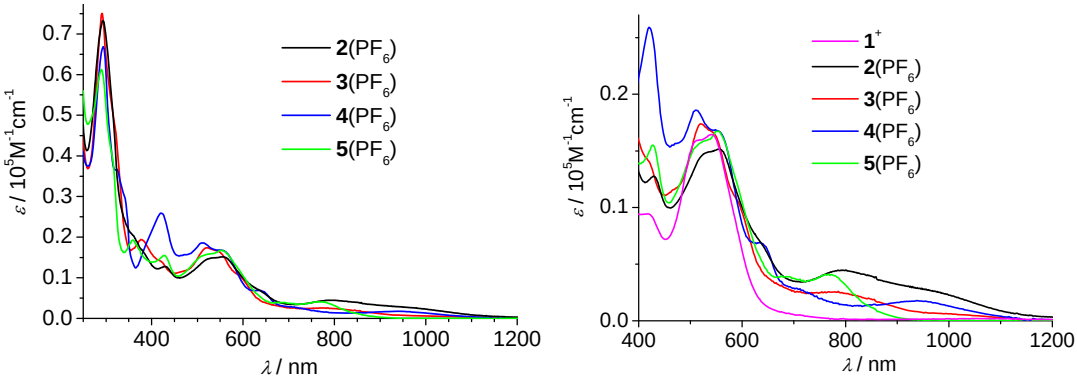


Figure S3. Absorption spectra of **2**(PF_6) - **5**(PF_6) in CH_2Cl_2.

Table S2. Absorption Data in CH_2Cl_2

	$\lambda_{abs,max}$ [nm] ($\varepsilon \times 10^5$ $M^{-1}cm^{-1}$)
$\mathbf{1}^{+}$	292 (0.70), 418 (0.096), 505 (0.16), 547 (0.16)
$\mathbf{1}^{2+}$	468 (0.14), 1050 (0.20)
$\mathbf{1}^{3+}$	712 (0.82)
$\mathbf{2}^{+}$	293 (0.82), 432 (0.14), 522 (0.16), 560 (0.15), 793 (0.046), 970 (0.026)
$\mathbf{2}^{2+}$	476 (0.15), 513 (0.15), 912 (0.13), 2465 (0.025)
$\mathbf{2}^{3+}$	714 (0.33), 2147 (0.018)
$\mathbf{3}^{+}$	290 (0.75), 376 (0.19), 520 (0.17), 776 (0.026), 1010 (0.0056)
$\mathbf{3}^{2+}$	500 (0.13), 972 (0.12), 1957 (0.029)
$\mathbf{3}^{3+}$	726 (0.51), 1830 (0.015)
$\mathbf{4}^{+}$	293 (0.67), 419 (0.26), 509 (0.19), 554 (0.17), 640 (0.068), 945 (0.018)
$\mathbf{4}^{2+}$	515 (0.18), 1012 (0.21), 1544 (0.070)
$\mathbf{4}^{3+}$	733 (0.85), 1645 (0.019)
$\mathbf{5}^{+}$	288 (0.61), 357 (0.19), 426 (0.16), 551 (0.17), 686 (0.039), 770 (0.041)
$\mathbf{5}^{2+}$	426 (0.15), 600 (0.033), 772 (0.022)

Computational Method

DFT and TDDFT calculations are carried out using the B3LYP exchange correlation functional[6] and implemented in the *Gaussian* 03 program package.[7] The electronic structures of complexes were determined using a general basis set with the Los Alamos effective core potential LanL2DZ basis set for Os, and 6-31G* for other atoms.[8] No symmetry constraints were used in the optimization (nosymm keyword was used). Solvation effects in CH_2Cl_2 are included for all calculations with the conductor-like polarizable continuum model (CPCM).[9] Frequency calculations have been performed with the same level of theory to ensure the optimized geometries to be local minima. All orbitals have been computed at an isovalue of 0.02 e/bohr^3.

(6) (a) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648. (b) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785.

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Table S3. TDDFT results.[a]

	S_n	E/eV	E/nm	f	dominant transitions (percent contribution[b])
2$^+$	3	2.06	603	0.0214	HOMO-1 → LUMO (89%)
	4	2.17	572	0.0896	HOMO-1 → LUMO+1 (73%)
	5	2.19	567	0.0839	HOMO → LUMO+2 (96%)
	6	2.24	553	0.0738	HOMO-2 → LUMO+1 (88%)
	7	2.47	503	0.1940	HOMO-2 → LUMO (49%); HOMO → LUMO+3 (39%)
	10	2.55	486	0.1138	HOMO → LUMO+3 (48%); HOMO-2 → LUMO (24%)
3$^+$	3	2.11	589	0.0104	HOMO-2 → LUMO (89%)
	4	2.20	564	0.0799	HOMO → LUMO+2 (96%)
	5	2.27	545	0.0492	HOMO-2 → LUMO+1 (40%); HOMO-1 → LUMO (55%)
	6	2.31	538	0.0749	HOMO-1 → LUMO+1 (91%)
	8	2.49	497	0.0680	HOMO → LUMO+3 (81%)
	10	2.63	471	0.2983	HOMO-2 → LUMO+1 (40%); HOMO-1 → LUMO (30%)
4$^+$	3	1.92	647	0.0419	HOMO-3 → LUMO (78%)
	6	2.17	570	0.0249	HOMO → LUMO+3 (80%)
	7	2.18	570	0.0279	HOMO-2 → LUMO (52%)
	8	2.20	564	0.0434	HOMO → LUMO+4 (78%)
	9	2.35	528	0.1250	HOMO-2 → LUMO+1 (72%)
	10	2.42	512	0.0109	HOMO-1 → LUMO+1 (83%)
5$^+$	2	2.05	605	0.0202	HOMO → LUMO (89%)
	4	2.17	573	0.0675	HOMO → LUMO+1 (67%)
	5	2.24	554	0.0782	HOMO-2 → LUMO+1 (88%)
	6	2.50	497	0.2616	HOMO-2 → LUMO (73%)
	8	2.56	485	0.0959	HOMO-1 → LUMO+2 (92%)

[a] The involved molecular orbitals are shown in Figure S5.

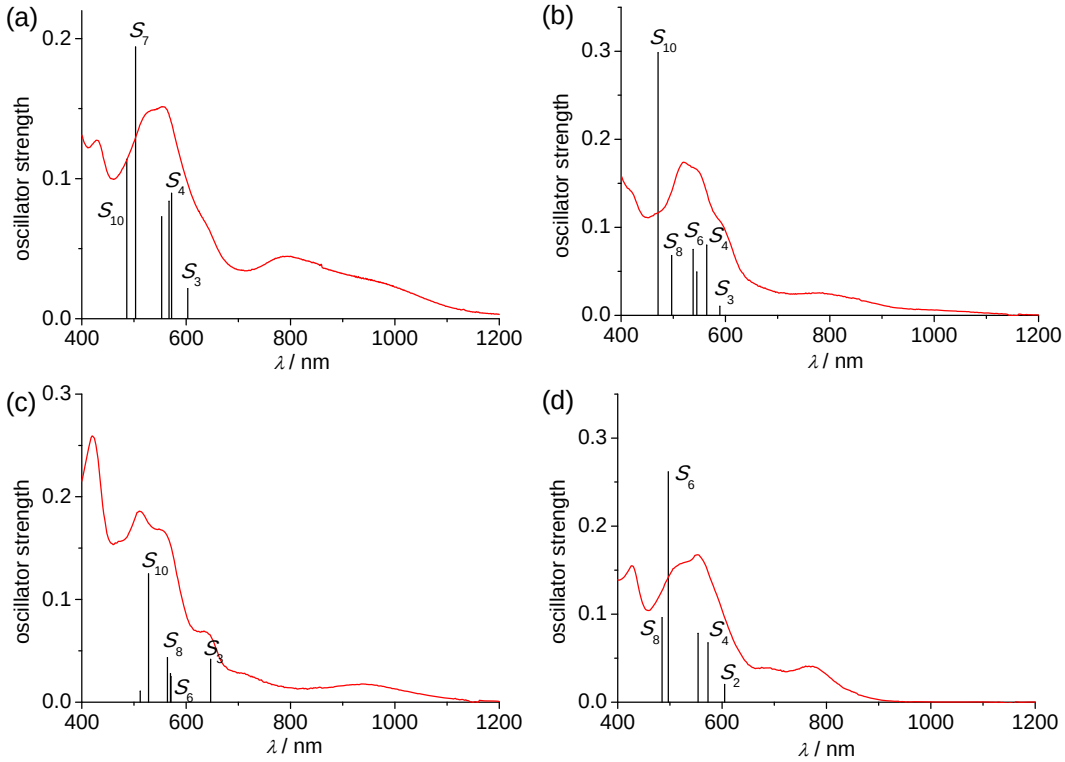


Figure S4. TDDFT-predicted excitations of (a) $\mathbf{2}^{+}$, (b) $\mathbf{3}^{+}$, (c) $\mathbf{4}^{+}$, and (d) $\mathbf{5}^{+}$. The observed absorption spectra of $\mathbf{2}(PF_6)$ - $\mathbf{5}(PF_6)$ are included for comparison (red curves).

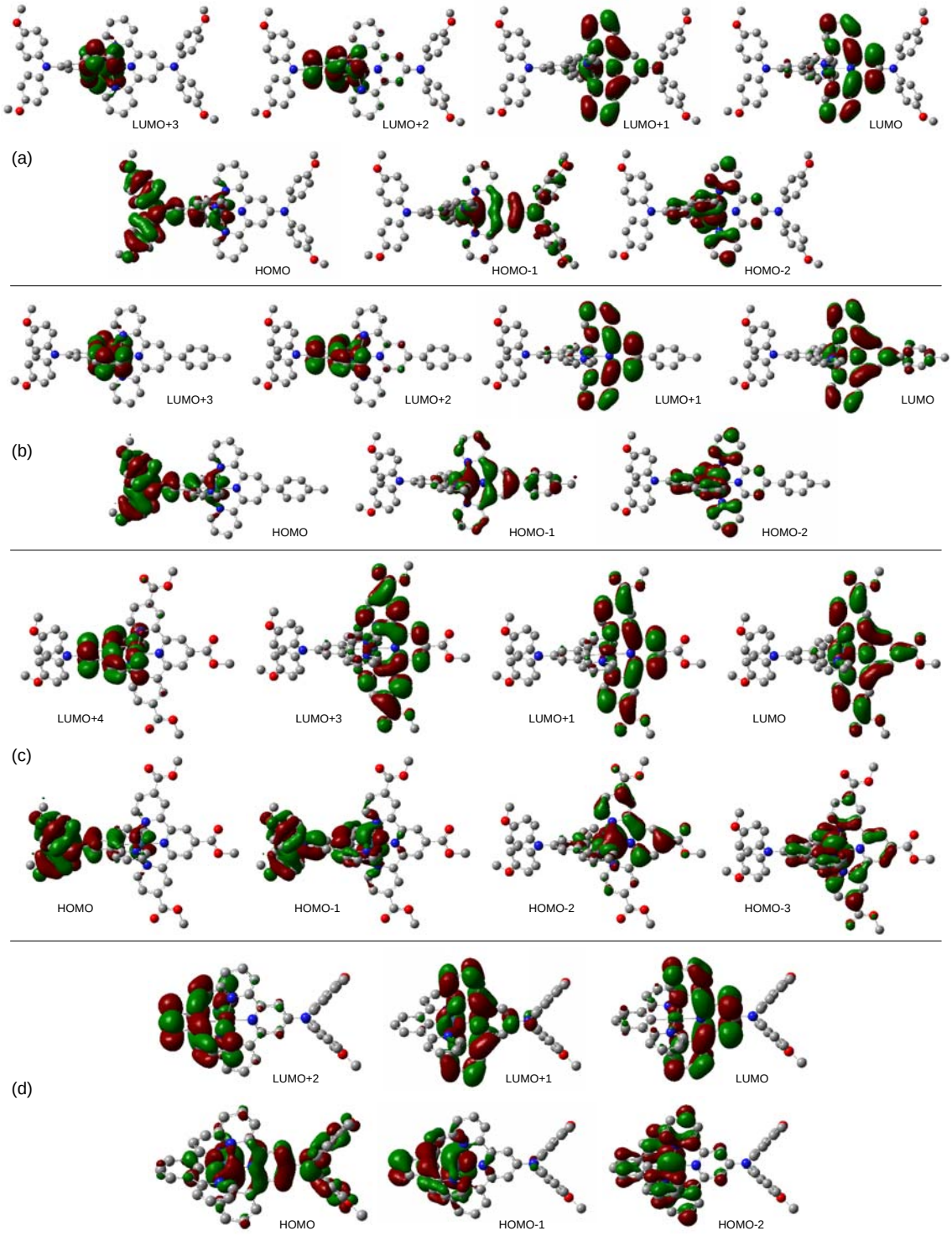


Figure S5. Frontier molecular orbitals of (a) $\mathbf{2}^{+}$, (b) $\mathbf{3}^{+}$, (c) $\mathbf{4}^{+}$, and (d) $\mathbf{5}^{+}$ involved in the TDDFT-predicted excitations in Table S3 and Figure S4.

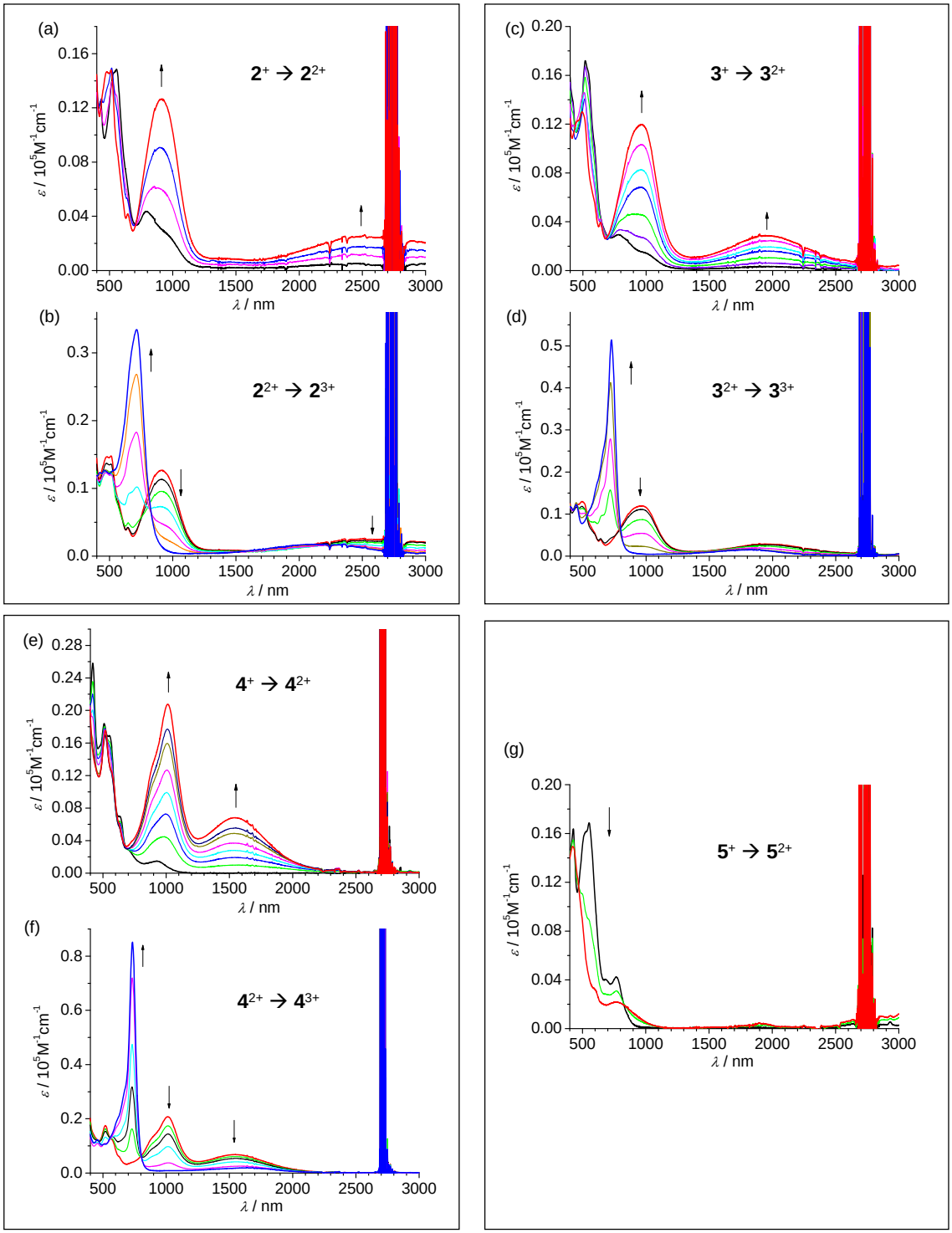


Figure S6. Absorption spectral changes of $\mathbf{2}^{+}$ - $\mathbf{5}^{+}$ upon stepwise oxidations in CH_2Cl_2.

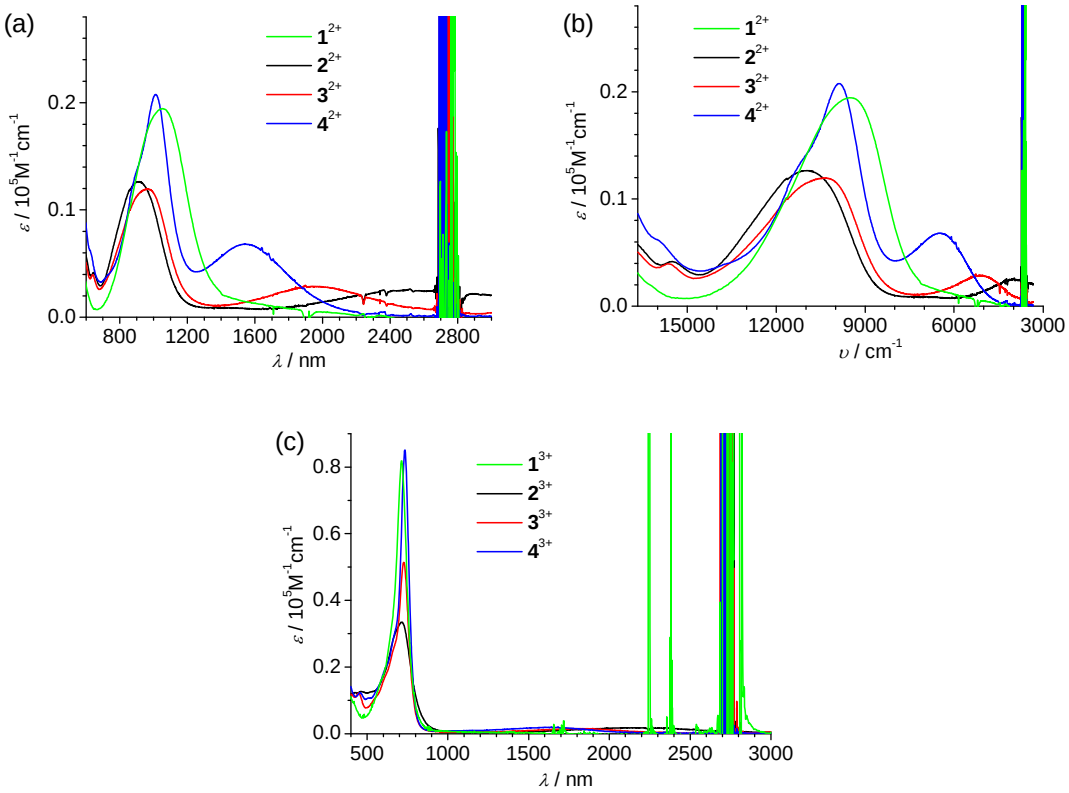


Figure S7. A comparison of the absorption spectra of (a,b) $\mathbf{1}^{2+}$ - $\mathbf{4}^{2+}$ and (c) $\mathbf{1}^{3+}$ - $\mathbf{4}^{3+}$ in CH_2Cl_2. The x axis of (a,c) is wavelength in nm and that of (b) is wavenumbers in cm^{-1}.

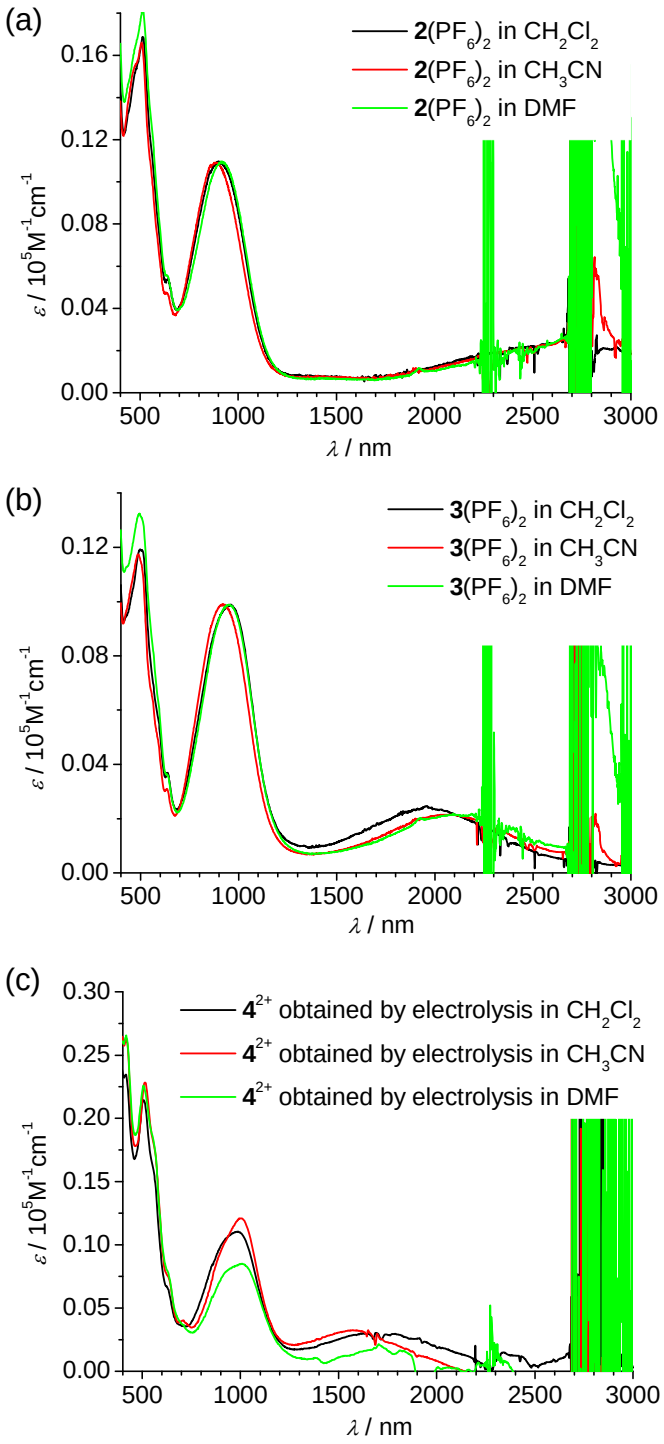


Figure S8. A comparison of the absorption spectra of (a - c) $\mathbf{2}^{2+}$ - $\mathbf{4}^{2+}$ in different solvents. Complexes $\mathbf{2}(PF_6)_2$ and $\mathbf{3}(PF_6)_2$ were obtained by synthesis and measured directly in different solvents. $\mathbf{4}^{2+}$ was obtained by electrolysis at an ITO electrode in different solvents.

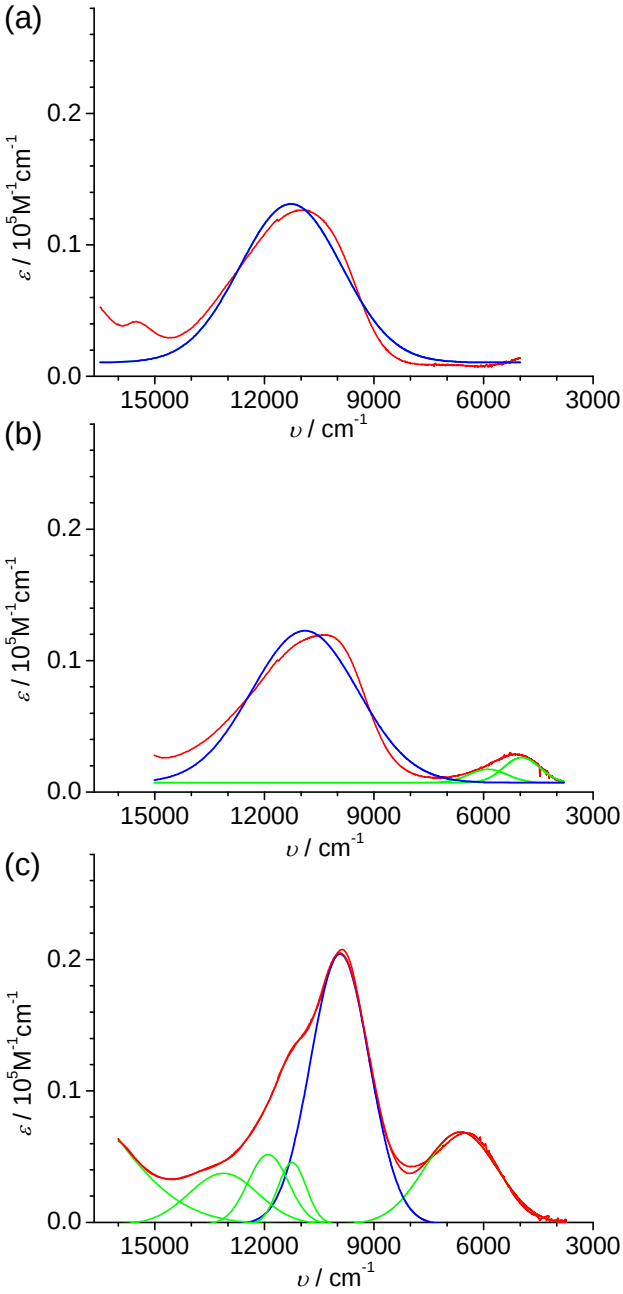


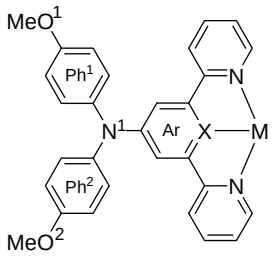
Figure S9. Gaussian-fitting of the NIR transitions of (a - c) $\mathbf{2}^{2+}$ - $\mathbf{4}^{2+}$ in CH_2Cl_2. The blue cure is the IVCT band.

Table S4. Parameters for the IVCT transitions of $\mathbf{1}^{2+}$ - $\mathbf{4}^{2+}$ in CH_2Cl_2.

	$\mathbf{1}^{2+}$	$\mathbf{2}^{2+}$	$\mathbf{3}^{2+}$	$\mathbf{4}^{2+}$
ν_{max} [cm^{-1}]	9500	11270	10890	9940
$\Delta\nu_{1/2}$ [cm^{-1}]	3580	4460	3570	1920
ε_{max} [$M^{-1}cm^{-1}$]	20000	13200	12300	20370
r_{ab} [a]	6.16	6.22	6.22	6.23
H_{ab} [cm^{-1}][b]	2760	2700	2290	2060
$\nu_{max}/2$ [cm^{-1}]	4750	5635	5445	4970

[a]r_{ab} is taken by the DFT-calculated metal ion-nitrogen atom geometrical distance. [b]H_{ab} was calculated by the Hush formula, $H_{ab} = 0.0206(\varepsilon_{max}\nu_{max}\Delta\nu_{1/2})^{1/2}/(r_{ab})$, where $\Delta\nu_{1/2}$ (in cm^{-1}) is the full width at half intensity.

Table S5. DFT-Calculated Spin Distribution.

		$\mathbf{1}^{2+}$	$\mathbf{2}^{2+}$	$\mathbf{3}^{2+}$	$\mathbf{4}^{2+}$	$\mathbf{5}^{2+}$
 M = Ru for $\mathbf{1}^{2+}$; Os for $\mathbf{2}^{2+}$ - $\mathbf{5}^{2+}$ X = C for $\mathbf{1}^{2+}$ - $\mathbf{4}^{2+}$, N for $\mathbf{5}^{2+}$	M	0.268	0.356	0.305	0.213	0.804
	Ar	0.216	0.176	0.224	0.185	0.028
	N^1	0.238	0.202	0.226	0.269	0.102
	Ph^1	0.103	0.104	0.093	0.140	0.030
	MeO^1	0.020	0.021	0.020	0.030	0.006
	Ph^2	0.104	0.104	0.098	0.140	0.028
	MeO^2	0.020	0.021	0.021	0.030	0.006

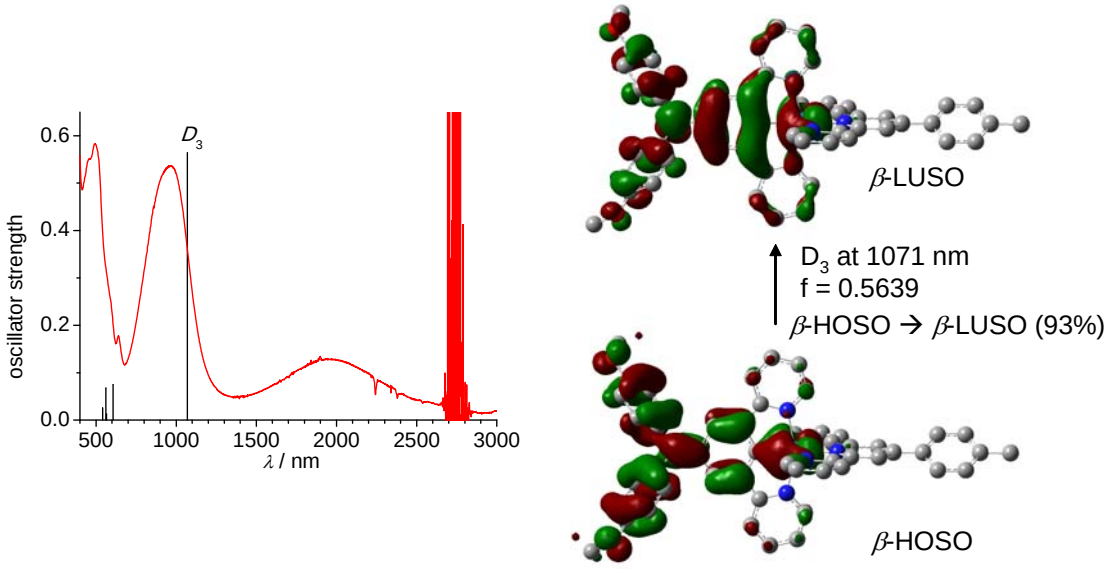


Figure S10. TDDFT-predicted doublet excitations for $\mathbf{3}^{2+}$. The observed absorption spectrum of $\mathbf{3}^{2+}$ (red plot) is included for comparison.

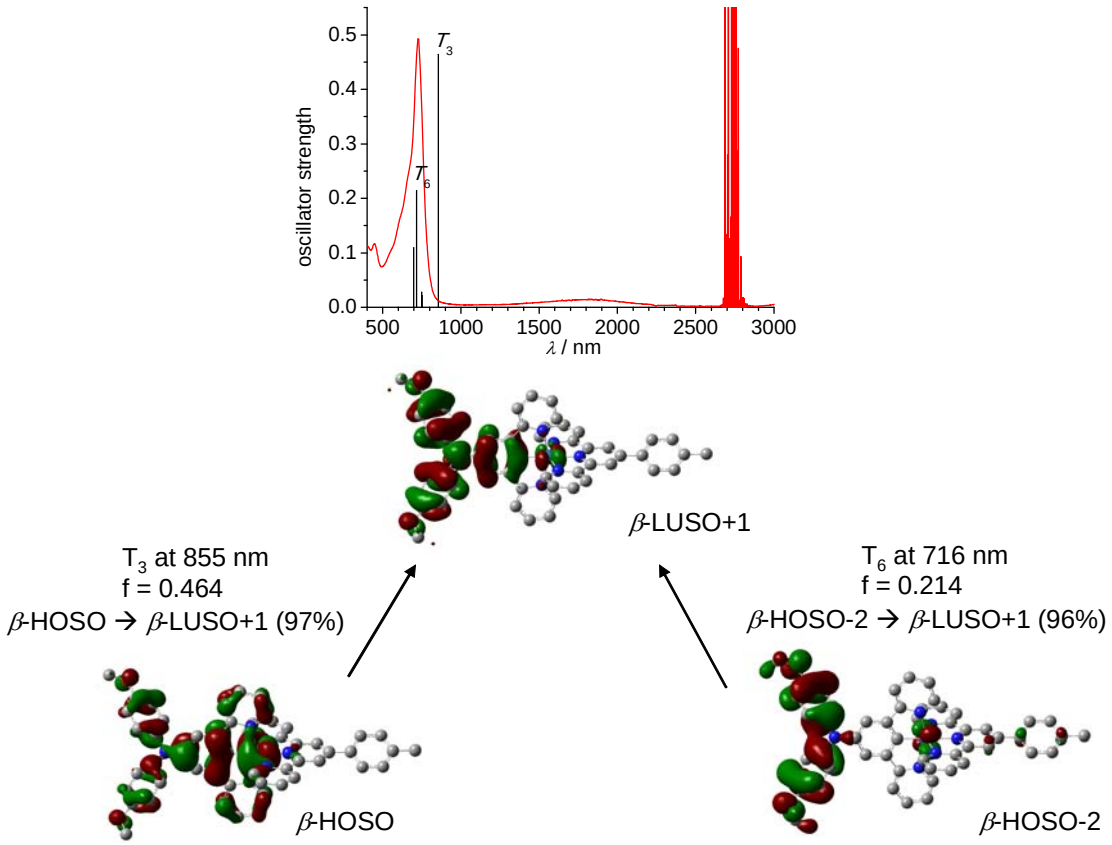


Figure S11. TDDFT-predicted triplet excitations for $\mathbf{3}^{3+}$. The observed absorption spectrum of $\mathbf{3}^{3+}$ (red plot) is included for comparison.

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

Charge = 1 multiplicity = 1

C	2.68792332	-1.01478589	0.62015631
C	4.07770204	-1.04286963	0.61124931
N	2.01047043	-0.02011656	-0.00707474
C	1.78763228	-1.98340097	1.27210133
C	4.79633279	-0.03234103	-0.06903901
C	2.66833107	0.96934594	-0.66305836
N	0.43598537	-1.73054241	1.13741692
C	2.23765545	-3.09590673	1.98742665
H	4.61582624	-1.82818230	1.12467817
C	4.05734285	0.98558533	-0.71568509
C	1.74817400	1.94430985	-1.27674273
C	-0.43816398	-2.58630099	1.71625008
C	1.32677089	-3.96587744	2.57687269
N	0.40141535	1.69569821	-1.09330818
C	-2.03134620	-0.01830099	0.05852129
N	-0.47526912	1.11376660	1.77094406
N	-0.52712898	-1.15176801	-1.69877615
N	6.18632028	-0.04146056	-0.10226739
H	3.30219587	-3.27736181	2.07996447
C	-0.03751908	-3.70284140	2.43680653
C	2.17563654	3.05927988	-2.00196842
C	-0.49015047	2.55765088	-1.63521394
C	-2.72756429	0.65176562	1.09402892
C	-2.75788728	-0.68873711	-0.95521090
C	-1.82130589	1.28550338	2.05216872
C	-1.88099082	-1.32364704	-1.93920316
C	0.43922930	1.66290055	2.60126779
C	0.36199950	-1.70414667	-2.55415848
C	6.93206739	1.14840623	-0.39496130
C	6.92650515	-1.24394257	0.15074670
H	4.57926509	1.76549017	-1.25360962
H	-1.48441846	-2.34236029	1.58021865
H	1.67445851	-4.83005087	3.13308027
C	1.24701913	3.93563206	-2.55304378
C	-0.11217670	3.67651027	-2.36434101
C	-4.12691177	0.63486149	1.12194637
C	-4.15779042	-0.67289545	-0.94071595
C	0.09661023	2.39489767	3.72863657
C	-2.21084975	2.01923043	3.18090384
C	-2.30431606	-2.05976654	-3.05420739
C	-0.01432409	-2.43908624	-3.66876500
C	6.71032842	-2.39549386	-0.62436921
C	7.90239701	-1.27382536	1.15037391
C	6.78297937	2.29931681	0.38488229
C	7.85164092	1.15926098	-1.45561863
H	-0.78779197	-4.35046115	2.87712273
H	3.23675251	3.23783838	-2.13173558
H	-1.53157117	2.31678473	-1.46178584
H	1.47612815	1.49671544	2.33216642
H	1.40665170	-1.53834098	-2.31667973
C	-4.84291093	-0.01963674	0.10130513
C	-1.25870755	2.57690099	4.02415893

C	-1.37793649	-2.62043529	-3.92372571
C	7.44391953	-3.55049284	-0.38822808
C	8.65841005	-2.42530495	1.38218312
C	7.52024425	3.45369727	0.10958842
C	8.60223276	2.29581166	-1.72458940
H	1.57729096	4.80163238	-3.11697827
H	-0.87576184	4.32900783	-2.77347486
H	-4.68929956	1.12044226	1.91491411
H	-4.74285024	-1.15995160	-1.71607869
H	0.87695095	2.81079058	4.35652349
H	-3.26814583	2.14632833	3.38735538
H	-3.36730639	-2.18693957	-3.22895113
H	0.74676275	-2.85766766	-4.31812526
H	5.96528961	-2.38052734	-1.41437288
H	8.08001985	-0.38703263	1.75116961
H	6.08469533	2.29756521	1.21670624
H	7.97811836	0.26925763	-2.06445154
N	-6.27063594	-0.02130684	0.12680766
C	8.42782488	-3.57514407	0.61481554
C	8.44036342	3.45540502	-0.94759030
H	-1.56465463	3.14462079	4.89744896
H	-1.70999336	-3.19026212	-4.78603618
H	7.28285121	-4.44406644	-0.98321654
H	9.41067044	-2.41500936	2.16208359
H	7.38069905	4.32986041	0.73173138
H	9.31718350	2.31102308	-2.54131269
C	-6.97243483	-1.24540922	-0.03541228
C	-6.97179643	1.20714265	0.25790545
O	9.09857170	-4.75146508	0.75812847
O	9.21809215	4.51678374	-1.29807063
C	-6.52564529	2.36629488	-0.39124343
C	-8.12719066	1.29913172	1.05813240
C	-8.12893297	-1.32571812	-0.82356200
C	-6.51576894	-2.42065661	0.59182997
C	10.11690839	-4.83281076	1.75223968
C	9.11010210	5.71677305	-0.53667603
C	-7.19487015	3.58491063	-0.24623196
C	-8.80985582	2.50137294	1.18798083
C	-8.82288543	-2.52939056	-0.97485759
C	-7.18742176	-3.62495816	0.42633262
H	-5.64012982	2.32027278	-1.01745722
H	-8.49010550	0.41817970	1.57807395
H	-8.49843961	-0.43648568	-1.32441585
H	-5.62573641	-2.38395877	1.21220628
H	10.91960248	-4.11042260	1.56106632
H	10.51693289	-5.84550764	1.68666274
H	9.70897845	-4.66639525	2.75654825
H	8.09673661	6.13315945	-0.58803185
H	9.81340428	6.41898131	-0.98631872
H	9.38239063	5.54976746	0.51247110
C	-8.34915416	3.65941802	0.54162383
C	-8.35199246	-3.69239580	-0.35432367
H	-6.81317904	4.45781225	-0.76337882
H	-9.70130930	2.56763163	1.80474446
H	-9.71557200	-2.54582074	-1.58956377

H	-6.83099247	-4.52901183	0.91128071
O	-9.08705479	4.79310648	0.74493992
O	-8.94430362	-4.92219957	-0.44345860
C	-8.66588722	5.98973596	0.10123194
C	-10.12684909	-5.03961264	-1.22595489
H	-7.66097688	6.28871941	0.42551062
H	-9.38335738	6.75757310	0.39536742
H	-8.67529213	5.88356622	-0.99097352
H	-10.93156200	-4.40354720	-0.83599712
H	-10.42887891	-6.08607754	-1.15864067
H	-9.94112322	-4.78211884	-2.27637231
Os	-0.05499581	-0.01773336	0.02883490

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

Charge = 1 multiplicity = 1

C	2.67931653	-1.03760169	0.60473098
C	4.07205486	-1.05417957	0.58770686
N	2.00078945	-0.03216004	-0.01191233
C	1.78407568	-2.01476114	1.24464113
C	4.78431465	-0.03560975	-0.07265591
C	2.65430860	0.97191775	-0.65705711
N	0.43290532	-1.76228736	1.11352793
C	2.23638311	-3.13558932	1.94644355
H	4.61383441	-1.83883282	1.10203086
C	4.04654402	0.98494021	-0.70111276
C	1.73439543	1.95112243	-1.25755552
C	-0.44123103	-2.62527783	1.68061769
C	1.32579185	-4.01297475	2.52441167
N	0.38946040	1.69790933	-1.07392753
C	-2.03159481	-0.03363396	0.06129218
N	-0.47282590	1.07376711	1.78589044
N	-0.53222679	-1.14338628	-1.71350966
H	3.30101748	-3.31706786	2.03749824
C	-0.03910610	-3.75012482	2.38714958
C	2.15855413	3.07545714	-1.97123451
C	-0.50632447	2.56332917	-1.60218024
C	-2.72492570	0.62307396	1.10515496
C	-2.75969044	-0.68820030	-0.95948725
C	-1.81712339	1.24275055	2.07133068
C	-1.88548809	-1.31106904	-1.95375498
C	0.44468745	1.60962955	2.62134853
C	0.35631802	-1.68458435	-2.57645465
H	4.56735636	1.76768895	-1.23948730
H	-1.48768690	-2.38073643	1.54725228
H	1.67398826	-4.88347654	3.07029215
C	1.22590327	3.95534440	-2.50877849
C	-0.13250063	3.69140586	-2.31898613
C	-4.12434346	0.60975928	1.13435149
C	-4.15968404	-0.67022949	-0.94430260
C	0.10465626	2.32602510	3.75947033
C	-2.20416246	1.96066796	3.21067474
C	-2.31109812	-2.03213587	-3.07734187
C	-0.02221310	-2.40481457	-3.69986489
H	-0.78831001	-4.40438289	2.81925525
H	3.21878529	3.25789084	-2.10260360
H	-1.54668026	2.31819349	-1.42840378
H	1.48115013	1.44676514	2.34909740
H	1.40155340	-1.52279221	-2.33939456
C	-4.84322145	-0.02918500	0.10606102
C	-1.24963071	2.50525040	4.05985443
C	-1.38600857	-2.58197685	-3.95517683
H	1.55228740	4.82857526	-3.06370614
H	-0.89825841	4.34742824	-2.71814855
H	-4.68395966	1.08674952	1.93423503
H	-4.74518011	-1.14560626	-1.72632402
H	0.88673854	2.73201893	4.39150899
H	-3.26086400	2.08581076	3.42080380

H	-3.37432498	-2.15637126	-3.25214356
H	0.73787646	-2.81519442	-4.35546316
N	-6.26996066	-0.02651746	0.13205693
H	-1.55327819	3.06087607	4.94161545
H	-1.71950536	-3.14038274	-4.82430902
C	-6.97709212	-1.24292563	-0.06476268
C	-6.96750380	1.20098563	0.29235037
C	-6.52076966	2.37276391	-0.33303812
C	-8.12065198	1.27735553	1.09720898
C	-8.12805126	-1.29749522	-0.86285750
C	-6.53206829	-2.43478135	0.53880108
C	-7.18716818	3.58921143	-0.15981713
C	-8.80079498	2.47771022	1.25474536
C	-8.82828839	-2.49294849	-1.04686397
C	-7.20968341	-3.63073762	0.34063086
H	-5.63725157	2.33872332	-0.96284983
H	-8.48382644	0.38578340	1.59857093
H	-8.48833127	-0.39442833	-1.34538227
H	-5.64672168	-2.41783987	1.16673352
C	-8.33927649	3.64867654	0.63255932
C	-8.36892195	-3.67280529	-0.44983267
H	-6.80526022	4.47233604	-0.65910653
H	-9.69060838	2.53229960	1.87497817
H	-9.71654203	-2.48952250	-1.66813243
H	-6.86254853	-4.54792236	0.80729036
O	-9.07422007	4.77891579	0.86240197
O	-8.96786931	-4.89633374	-0.57125216
C	-8.65074693	5.98931039	0.24622285
C	-10.14587931	-4.98894196	-1.36402654
H	-7.64469944	6.27787948	0.57627231
H	-9.36590660	6.75179665	0.55922129
H	-8.66179922	5.90876845	-0.84813648
H	-10.94906019	-4.35617250	-0.96572408
H	-10.45504291	-6.03460204	-1.32127584
H	-9.95128575	-4.71023503	-2.40737906
Os	-0.04918895	-0.03316653	0.02751439
C	6.26563654	-0.03791620	-0.10597012
C	6.99405738	1.16420671	-0.07381013
C	6.98822172	-1.24258056	-0.16620697
C	8.38699367	1.15802148	-0.10122223
H	6.47032320	2.11268169	0.00605303
C	8.38094380	-1.24119505	-0.19484868
H	6.45865219	-2.18984613	-0.21600666
C	9.10863263	-0.04263288	-0.16584940
H	8.92346287	2.10295053	-0.06102523
H	8.91232052	-2.18841876	-0.24758149
C	10.61754049	-0.04486259	-0.22637535
H	10.96981252	-0.02367481	-1.26637895
H	11.03938583	0.83107980	0.27708922
H	11.03539848	-0.94361844	0.23899178

Cartesian coordinates for DFT-optimized structure of **4**$^{+}$:

Charge = 1 multiplicity = 1

C	2.70399538	-1.01946145	0.64500474
C	4.09599254	-1.04059051	0.62155619
N	2.02440664	-0.03187927	-0.00682263
C	1.80836122	-1.97132399	1.31646909
C	4.78062274	-0.03638453	-0.07773469
C	2.67228963	0.95504663	-0.69237904
N	0.45709346	-1.71867129	1.17742607
C	2.26160372	-3.06495623	2.05508197
H	4.65368472	-1.81572874	1.13078851
C	4.06200317	0.96902611	-0.73943795
C	1.74654699	1.90927964	-1.31761702
C	-0.41974844	-2.55890618	1.77757947
C	1.34798350	-3.92170860	2.66654268
N	0.40321581	1.65378310	-1.12050465
C	-2.00413859	-0.03782545	0.06922609
N	-0.44982348	1.13317722	1.75441747
N	-0.50402296	-1.20707635	-1.66531482
H	3.32362921	-3.24879078	2.15435933
C	-0.01933228	-3.65592263	2.52049926
C	2.16607695	3.00932807	-2.06633234
C	-0.49998664	2.49747813	-1.67480737
C	-2.69792113	0.65309507	1.08641958
C	-2.72953415	-0.72699819	-0.92619348
C	-1.79287043	1.30888388	2.03154298
C	-1.85520923	-1.38429262	-1.89838154
C	0.46862028	1.69951601	2.56794706
C	0.38804025	-1.77639998	-2.50570987
H	4.60920340	1.73547499	-1.27468192
H	-1.46578156	-2.31720849	1.63904283
C	1.22557165	3.86991610	-2.62978347
C	-0.13367045	3.60110798	-2.42555161
C	-4.09740899	0.64024538	1.11648170
C	-4.12972252	-0.70958802	-0.91516151
C	0.12669574	2.45582020	3.67919223
C	-2.18188182	2.06662965	3.14350830
C	-2.27945106	-2.14575759	-2.99491511
C	0.01092358	-2.53695891	-3.60253579
H	-0.75451169	-4.30277419	2.98411938
H	3.22272656	3.19530181	-2.20918023
H	-1.53867066	2.25333599	-1.49222032
H	1.50521760	1.52920419	2.30190504
H	1.43271814	-1.60486837	-2.27430434
C	-4.81708027	-0.03334779	0.11067623
C	-1.22776699	2.64285142	3.97209859
C	-1.35219406	-2.72485367	-3.85145856
H	-0.88909070	4.25102961	-2.85072440
H	-4.65480370	1.14440868	1.90054819
H	-4.71076740	-1.21124682	-1.68336474
H	0.90783495	2.88580160	4.29604841
H	-3.23861587	2.19779637	3.34866328
H	-3.34213486	-2.27825247	-3.16561664
H	0.77196166	-2.96929119	-4.24244765

N	-6.24058211	-0.02942763	0.13430175
H	-1.53247470	3.22942974	4.83309112
H	-1.68413685	-3.31457612	-4.70014609
C	-6.95468596	-1.23501569	-0.10886963
C	-6.94187744	1.19161848	0.33503860
C	-6.51861480	2.37818721	-0.27781510
C	-8.07864425	1.24038628	1.16404468
C	-8.08201411	-1.25659743	-0.94055457
C	-6.54354646	-2.44336374	0.48494784
C	-7.19181732	3.58479456	-0.06711466
C	-8.76644693	2.43087885	1.35883961
C	-8.79287410	-2.43802272	-1.16899791
C	-7.23089558	-3.62556034	0.24312417
H	-5.64873467	2.36402569	-0.92720416
H	-8.42289189	0.33503119	1.65410309
H	-8.41513881	-0.33834589	-1.41402315
H	-5.67755863	-2.45048184	1.13966856
C	-8.32777244	3.61781110	0.75023059
C	-8.36660727	-3.63553181	-0.58226528
H	-6.82887200	4.48087979	-0.55730385
H	-9.64406729	2.46539245	1.99752152
H	-9.66260337	-2.40995155	-1.81530704
H	-6.91090300	-4.55648677	0.70178952
O	-9.06740946	4.73598708	1.01684119
O	-8.97750277	-4.84747219	-0.74517408
C	-8.66696262	5.96293863	0.41746769
C	-10.13334839	-4.90947111	-1.57319909
H	-7.65791342	6.25467188	0.73515161
H	-9.38365298	6.71156944	0.75893409
H	-8.69748112	5.90397723	-0.67780504
H	-10.93910224	-4.27299163	-1.18638688
H	-10.45727122	-5.95137727	-1.55847608
H	-9.90464841	-4.61487345	-2.60514439
Os	-0.01143090	-0.03457155	0.03576048
C	1.60781311	5.06623057	-3.44055380
O	0.79715139	5.82738512	-3.93540076
O	2.93676724	5.19896391	-3.55563807
C	6.26986482	0.00960424	-0.15109661
O	6.89002172	0.86805130	-0.75348772
O	6.84518495	-1.00002743	0.52078472
C	1.76744109	-5.11048257	3.46987045
O	0.98083633	-5.86633738	4.00949073
O	3.10044254	-5.24351157	3.52360133
C	3.39463058	6.33184127	-4.32295534
H	4.48187800	6.27239397	-4.30546672
H	3.02075309	6.26924362	-5.34736695
H	3.05109934	7.26149351	-3.86374621
C	8.28687704	-1.03094996	0.50164300
H	8.56528661	-1.90251058	1.09250394
H	8.64931355	-1.12898790	-0.52419511
H	8.69052990	-0.11855147	0.94650041
C	3.59266168	-6.36968146	4.27944709
H	4.67789542	-6.31391094	4.20772402
H	3.27009448	-6.29508530	5.32037330
H	3.22441408	-7.30307123	3.84783311

Cartesian coordinates for DFT-optimized structure of $\mathbf{5}^{+}$:

Charge = 1 multiplicity = 1

C	2.68636507	-1.02049287	0.61245885
C	4.07623474	-1.04716826	0.60571192
N	2.00889753	-0.02622657	-0.01530589
C	1.78594605	-1.98998593	1.26290955
C	4.79485093	-0.03581905	-0.07337863
C	2.66668156	0.96385765	-0.67036059
N	0.43427304	-1.73646445	1.12901049
C	2.23583698	-3.10430135	1.97553000
H	4.61433356	-1.83167992	1.12037499
C	4.05574651	0.98118482	-0.72139867
C	1.74642350	1.93915061	-1.28339691
C	-0.43992927	-2.59359175	1.70589411
C	1.32492282	-3.97547494	2.56311390
N	0.39970573	1.69194600	-1.09757820
C	-2.03357230	-0.01629486	0.06083096
N	-0.46422326	1.10723140	1.77094002
N	-0.53441737	-1.15010760	-1.70440769
N	6.18494907	-0.04278778	-0.10379094
H	3.30035843	-3.28634890	2.06714495
C	-0.03936073	-3.71186078	2.42377414
C	2.17380992	3.05321086	-2.01008130
C	-0.49186733	2.55469401	-1.63832178
C	-2.72107213	0.65452273	1.10317836
C	-2.76260510	-0.68199347	-0.95630752
C	-1.80832546	1.28120219	2.05878007
C	-1.88904008	-1.31561644	-1.94338280
C	0.45619998	1.65034544	2.59885281
C	0.35208878	-1.70250850	-2.56269712
C	6.92944357	1.14792423	-0.39641194
C	6.92688103	-1.24294478	0.15504342
H	4.57762198	1.76187377	-1.25821375
H	-1.48616639	-2.34915750	1.57058593
H	1.67253756	-4.84105044	3.11718608
C	1.24519270	3.93017106	-2.56018197
C	-0.11395218	3.67264969	-2.36885889
C	-4.12319486	0.65655472	1.12268887
C	-4.16446073	-0.67347974	-0.92598856
C	0.12148935	2.37852392	3.73087573
C	-2.18978319	2.01080213	3.19339966
C	-2.31591263	-2.04515262	-3.06175587
C	-0.02790028	-2.43162713	-3.67971704
C	6.71565951	-2.39730715	-0.61723687
C	7.89965180	-1.26771416	1.15786067
C	6.77723166	2.29957850	0.38173006
C	7.85106549	1.15878019	-1.45527896
H	-0.78970852	-4.36037339	2.86265663
H	3.23489648	3.23045991	-2.14190925
H	-1.53324953	2.31525642	-1.46275262
H	1.49124605	1.48246490	2.32370320
H	1.39753388	-1.54143040	-2.32539126
C	-4.83196336	-0.00582132	0.11055104
C	-1.23199760	2.56237494	4.03403715

C	-1.39258092	-2.60601446	-3.93422934
C	7.45092552	-3.55003332	-0.37517782
C	8.65737541	-2.41684779	1.39561357
C	7.51338902	3.45467243	0.10644134
C	8.60057347	2.29605735	-1.72420863
H	1.57539811	4.79540497	-3.12533159
H	-0.87758697	4.32569831	-2.77701956
H	-4.67770526	1.16318981	1.90948218
H	-4.75030495	-1.17570614	-1.69259951
H	0.90606058	2.78977550	4.35654933
H	-3.24564165	2.13862268	3.40665965
H	-3.37954070	-2.16618645	-3.23704248
H	0.73089737	-2.85066068	-4.33147029
H	5.97308455	-2.38633835	-1.40961347
H	8.07349478	-0.37871032	1.75649061
H	6.07728696	2.29790551	1.21215579
H	7.97995603	0.26818861	-2.06274807
C	8.43163919	-3.56953260	0.63109900
C	8.43552420	3.45638849	-0.94897730
H	-1.53201519	3.12666900	4.91163809
H	-1.72765487	-3.17044027	-4.79896486
H	7.29362790	-4.44577409	-0.96791238
H	9.40714686	-2.40252851	2.17783706
H	7.37135864	4.33141393	0.72720192
H	9.31708116	2.31128477	-2.53956543
O	9.10438736	-4.74400326	0.78026130
O	9.21239275	4.51844739	-1.29930444
C	10.11916575	-4.82029635	1.77841416
C	9.10108212	5.71931024	-0.53975760
H	10.92134888	-4.09718130	1.58783095
H	10.52116514	-5.83251337	1.71768847
H	9.70722042	-4.65125189	2.78064072
H	8.08716840	6.13404032	-0.59360041
H	9.80413426	6.42200180	-0.98903556
H	9.37165256	5.55416725	0.51012867
Os	-0.05678811	-0.02138343	0.02447157
H	-5.91785781	-0.00175869	0.12974894

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

Charge = 2 multiplicity = 2

C	2.69585391	-0.94584043	0.71825159
C	4.08885290	-0.96004427	0.71869022
N	2.02456267	-0.04417744	-0.03633121
C	1.79813404	-1.83054643	1.48268431
C	4.80232119	-0.03903009	-0.07071096
C	2.67360314	0.85975497	-0.80747788
N	0.45015791	-1.60507542	1.31166891
C	2.25045389	-2.84231064	2.33118955
H	4.62799156	-1.66189762	1.34285218
C	4.06599790	0.87897866	-0.84250376
C	1.75419117	1.74207417	-1.54846342
C	-0.42726663	-2.38307675	1.98416304
C	1.33796487	-3.63726083	3.01742030
N	0.41171656	1.51552681	-1.34002065
C	-2.00624654	-0.04267653	0.02468365
N	-0.45401334	1.30387187	1.59480894
N	-0.50609071	-1.39077784	-1.59362088
H	3.31464767	-3.00569988	2.45195288
C	-0.02493034	-3.40090677	2.83905244
C	2.18192232	2.75209358	-2.41169448
C	-0.48471662	2.29082218	-1.99020206
C	-2.70387183	0.75773514	0.97444624
C	-2.73458396	-0.84333096	-0.90142595
C	-1.79428774	1.50697969	1.85600859
C	-1.85419560	-1.59336110	-1.81152837
C	0.46242320	1.94826225	2.34399428
C	0.38548010	-2.03541233	-2.37202329
H	4.58692280	1.58342281	-1.47914680
H	-1.47428628	-2.16536304	1.81790103
H	1.68561692	-4.42464276	3.67750619
C	1.25007062	3.54433073	-3.07461557
C	-0.10715937	3.30691867	-2.85833689
C	-4.08789265	0.75613938	1.00151063
C	-4.11898979	-0.84195331	-0.88294168
C	0.11771702	2.81307713	3.37626014
C	-2.18939528	2.36792544	2.88207077
C	-2.28258270	-2.45448429	-2.82396961
C	0.00722830	-2.90042596	-3.39234477
H	-0.77536924	-3.99223937	3.35147211
H	3.24222755	2.91596687	-2.56239864
H	-1.52649708	2.07230112	-1.79460633
H	1.49954973	1.75479064	2.09653439
H	1.43017075	-1.84183485	-2.15874809
C	-4.81231804	-0.04315064	0.07100814
C	-1.23354605	3.02646284	3.65036115
C	-1.35222881	-3.11359088	-3.62245221
H	1.57867470	4.33028932	-3.74606424
H	-0.87205045	3.89607608	-3.35153033
H	-4.64461419	1.33082977	1.73296522
H	-4.69942124	-1.41691687	-1.59551216
H	0.89834155	3.30364093	3.94668175
H	-3.24577045	2.51890060	3.07440379

H	-3.34467475	-2.60539948	-2.98173215
H	0.76877349	-3.39145526	-3.98762219
N	-6.20488032	-0.04423258	0.09544646
H	-1.53910890	3.69472106	4.44890950
H	-1.68358648	-3.78222774	-4.41031810
C	-6.94545002	-1.19010768	-0.32156453
C	-6.93016034	1.10361729	0.53472325
C	-6.61183176	2.37820400	0.04724863
C	-7.99075776	0.96131270	1.44824756
C	-8.04652399	-1.04485830	-1.17562913
C	-6.59663696	-2.47384064	0.13842309
C	-7.32339296	3.50000398	0.46841499
C	-8.70378658	2.07238746	1.86667470
C	-8.78774600	-2.15393593	-1.57655566
C	-7.32709985	-3.58082346	-0.26209863
H	-5.81284089	2.49335070	-0.67820899
H	-8.24195010	-0.02127168	1.83379377
H	-8.31969777	-0.05924818	-1.53791201
H	-5.76234288	-2.59444875	0.82190333
C	-8.37657872	3.35408883	1.38464568
C	-8.42953465	-3.43407478	-1.12461231
H	-7.06135285	4.47163341	0.06766335
H	-9.51757134	1.97584091	2.57799911
H	-9.62959520	-2.01209333	-2.24331603
H	-7.07276990	-4.57376438	0.09420294
O	-9.13354693	4.37228233	1.85972805
O	-9.07660269	-4.57787168	-1.45397319
C	-8.85610115	5.70031659	1.41333766
C	-10.21193888	-4.49883744	-2.31746972
H	-7.83644999	6.00276695	1.67854612
H	-9.57203992	6.34075933	1.92919028
H	-8.99721584	5.79208122	0.33031319
H	-11.00657790	-3.88958587	-1.87190131
H	-10.56283409	-5.52405410	-2.43832177
H	-9.93764361	-4.08779868	-3.29576778
Os	-0.06243443	-0.04392013	-0.00602627
C	6.28257291	-0.03490630	-0.08920963
C	7.00024828	1.16786325	-0.21211262
C	7.01141323	-1.23192796	0.01934877
C	8.39266417	1.16919440	-0.22407562
H	6.46883801	2.11385117	-0.26446383
C	8.40414483	-1.22287019	0.00073283
H	6.48856484	-2.18133698	0.09223122
C	9.12242706	-0.02467585	-0.12314969
H	8.92254581	2.11506176	-0.30444857
H	8.94288601	-2.16390290	0.07840498
C	10.63131788	-0.02049549	-0.17045311
H	10.99077365	-0.07528565	-1.20665323
H	11.04220878	0.89527794	0.26687815
H	11.05134841	-0.87745075	0.36566663

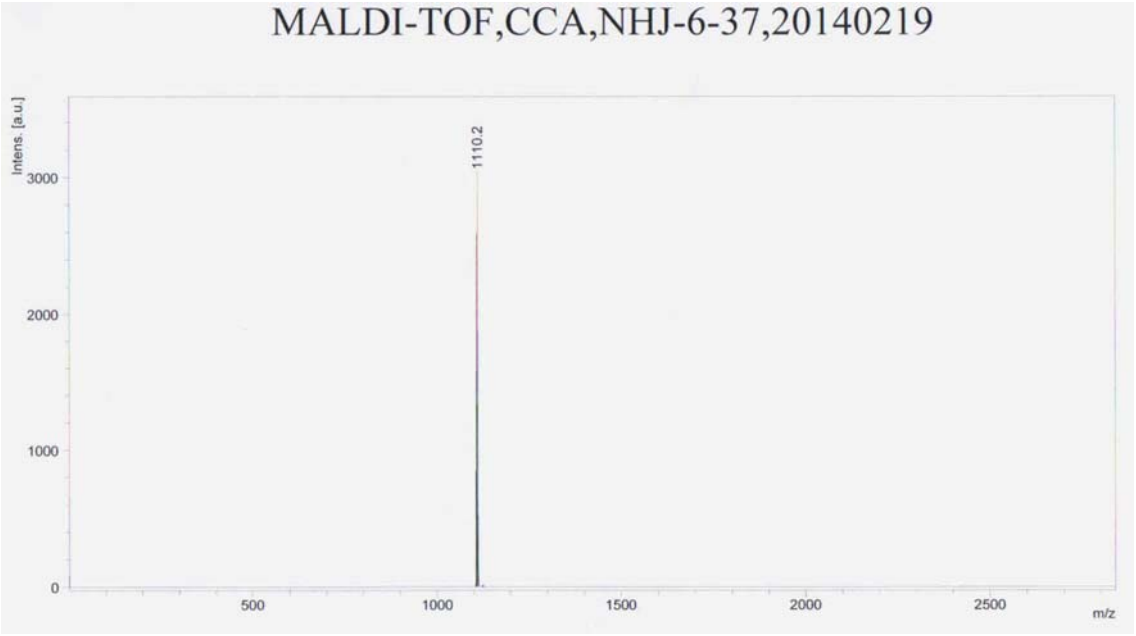
Cartesian coordinates for DFT-optimized structure of $\mathbf{3}^{3+}$:

Charge = 3 multiplicity = 3

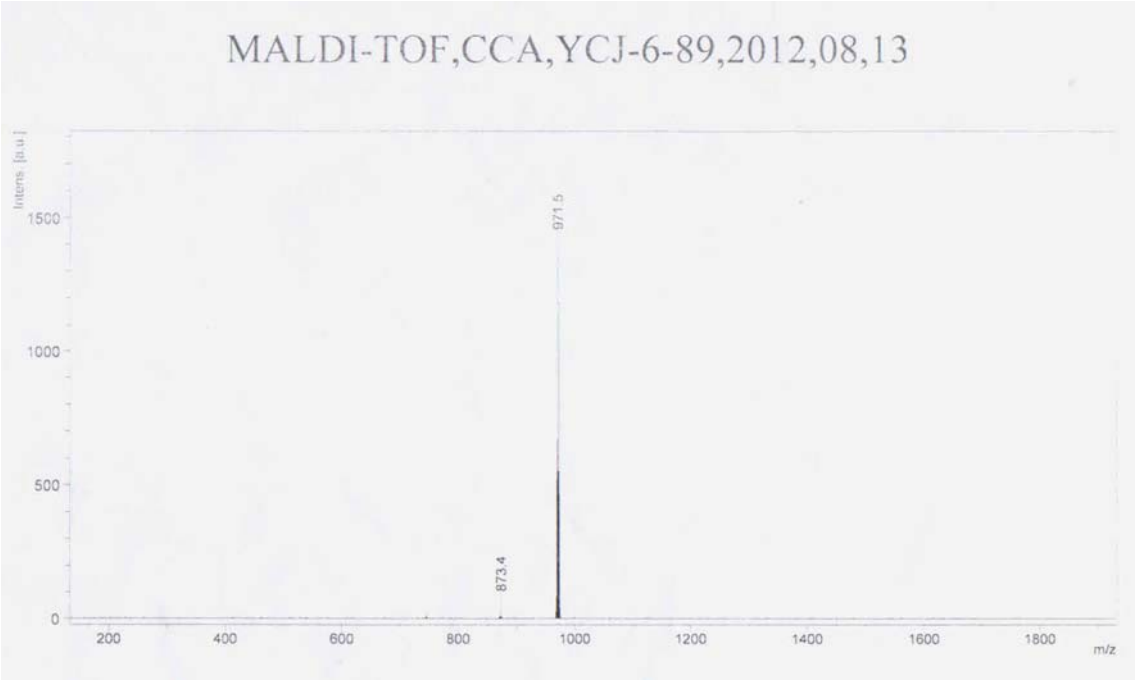
C	2.62464018	-0.98522631	0.63734831
C	4.00816622	-1.06270764	0.66869085
N	2.02601946	0.00418440	-0.06813836
C	1.66384444	-1.88949140	1.32251418
C	4.78466276	-0.10915648	-0.03271573
C	2.72312611	0.93920746	-0.75657215
N	0.32702725	-1.61442059	1.14022657
C	2.06382524	-2.96348504	2.11107955
H	4.50226926	-1.83050983	1.24944857
C	4.11307414	0.90087016	-0.75250936
C	1.85551910	1.91047194	-1.45812613
C	-0.59181137	-2.39896704	1.73402083
C	1.10424746	-3.77157800	2.72330939
N	0.49873061	1.72763749	-1.30438054
C	-2.03368922	0.07664993	-0.06017058
N	-0.49201959	1.39638062	1.51024963
N	-0.53756314	-1.03495550	-1.82214476
H	3.11737260	-3.17223423	2.25047100
C	-0.24391729	-3.48511573	2.53150966
C	2.34916881	2.95647412	-2.23570253
C	-0.34801265	2.57690570	-1.91739921
C	-2.72455423	0.78538412	0.94757437
C	-2.75161109	-0.66129024	-1.02755930
C	-1.82336029	1.52280408	1.83796292
C	-1.87642495	-1.28579360	-2.02358969
C	0.43795767	2.06576708	2.22574893
C	0.37160360	-1.52424447	-2.69312724
H	4.68247620	1.62455845	-1.32081934
H	-1.62651347	-2.13530270	1.55596920
H	1.41292188	-4.60960366	3.33883751
C	1.46484497	3.82943037	-2.86624863
C	0.09535517	3.63557631	-2.70378333
C	-4.11442408	0.73616005	1.00860844
C	-4.14229033	-0.70915630	-0.97890469
C	0.10445090	2.86609415	3.30881448
C	-2.20451959	2.32067794	2.91837228
C	-2.28668791	-2.05801918	-3.11221340
C	0.00877558	-2.29766643	-3.78619960
H	-1.02347343	-4.08489537	2.98657714
H	3.41840599	3.08833683	-2.34877017
H	-1.40297202	2.38884712	-1.76322464
H	1.46823786	1.94052961	1.91622903
H	1.40928691	-1.28981760	-2.49024570
C	-4.82290482	-0.01775786	0.04718444
C	-1.24055085	2.99377236	3.66176659
C	-1.34444660	-2.56977401	-3.99817548
H	1.84337362	4.64503310	-3.47267928
H	-0.63028745	4.28881857	-3.17448106
H	-4.66868038	1.24594411	1.78871603
H	-4.72086904	-1.24045687	-1.72650935
H	0.88789387	3.37754541	3.85575537
H	-3.25500186	2.41435424	3.16850416

H	-3.34269247	-2.25112695	-3.26202286
H	0.77638808	-2.67256434	-4.45306487
N	-6.23537585	-0.07650684	0.10951642
H	-1.53464266	3.61484624	4.50135742
H	-1.66125729	-3.16874838	-4.84551745
C	-6.90364660	-1.28973142	-0.15429795
C	-6.97556444	1.07675890	0.44639888
C	-6.59898084	2.33811356	-0.05556357
C	-8.10367508	0.97679756	1.29286229
C	-8.12260703	-1.28831318	-0.86168774
C	-6.36297060	-2.51885752	0.28932975
C	-7.32447550	3.47428813	0.27137092
C	-8.82304990	2.10648994	1.62389173
C	-8.79098727	-2.47497847	-1.12224343
C	-7.02822678	-3.70012361	0.03424137
H	-5.75373751	2.41918869	-0.73032880
H	-8.38433640	0.01484987	1.70705873
H	-8.52830415	-0.35373098	-1.23280176
H	-5.44119177	-2.52984591	0.86018385
C	-8.44573732	3.36987175	1.11781629
C	-8.25059601	-3.69615312	-0.67426049
H	-7.02766559	4.42894376	-0.14481034
H	-9.67790384	2.04777373	2.28892241
H	-9.71612234	-2.44747352	-1.68424258
H	-6.63671875	-4.64800504	0.38752810
O	-9.21455799	4.40303547	1.50038333
O	-8.81409982	-4.89967236	-0.86916520
C	-8.89716800	5.72344873	1.04130686
C	-10.06797399	-4.98452690	-1.56007754
H	-7.89834801	6.02350154	1.37495182
H	-9.64627153	6.37517644	1.48990282
H	-8.96180748	5.78320300	-0.05007123
H	-10.84571209	-4.42895251	-1.02610763
H	-10.31873135	-6.04466455	-1.57794704
H	-9.97490621	-4.60955994	-2.58449705
Os	-0.04014283	0.08633483	-0.09393089
C	6.25577082	-0.17150920	-0.00893420
C	7.03133808	1.00181348	-0.09296318
C	6.92639217	-1.40456462	0.10174656
C	8.41947081	0.93907943	-0.06193972
H	6.54836700	1.97305357	-0.14081092
C	8.31631421	-1.45831319	0.11801147
H	6.36292800	-2.33186807	0.13998721
C	9.09065198	-0.29084671	0.03702203
H	8.99435320	1.86017034	-0.10766098
H	8.81011739	-2.42346390	0.19090936
C	10.59722802	-0.35255168	0.03440038
H	10.98525687	-0.30097944	-0.99149619
H	11.03171170	0.48761836	0.58599161
H	10.96114570	-1.28445709	0.47720320

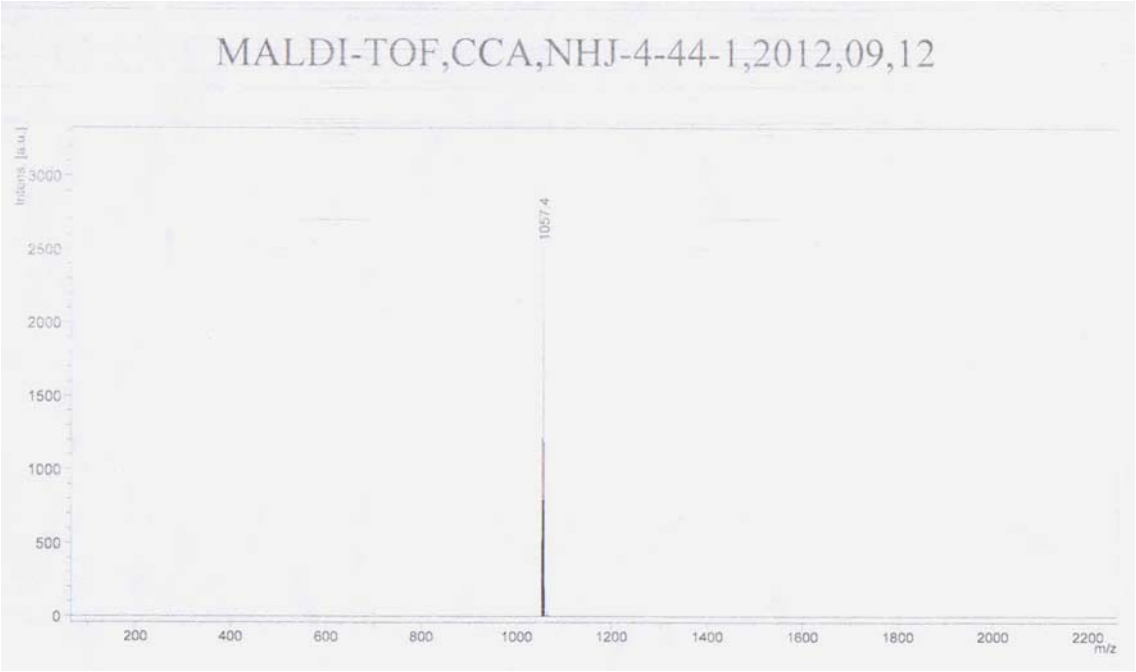
TOF-MALDI mass spectrum of **2**$(PF_6)_2$:



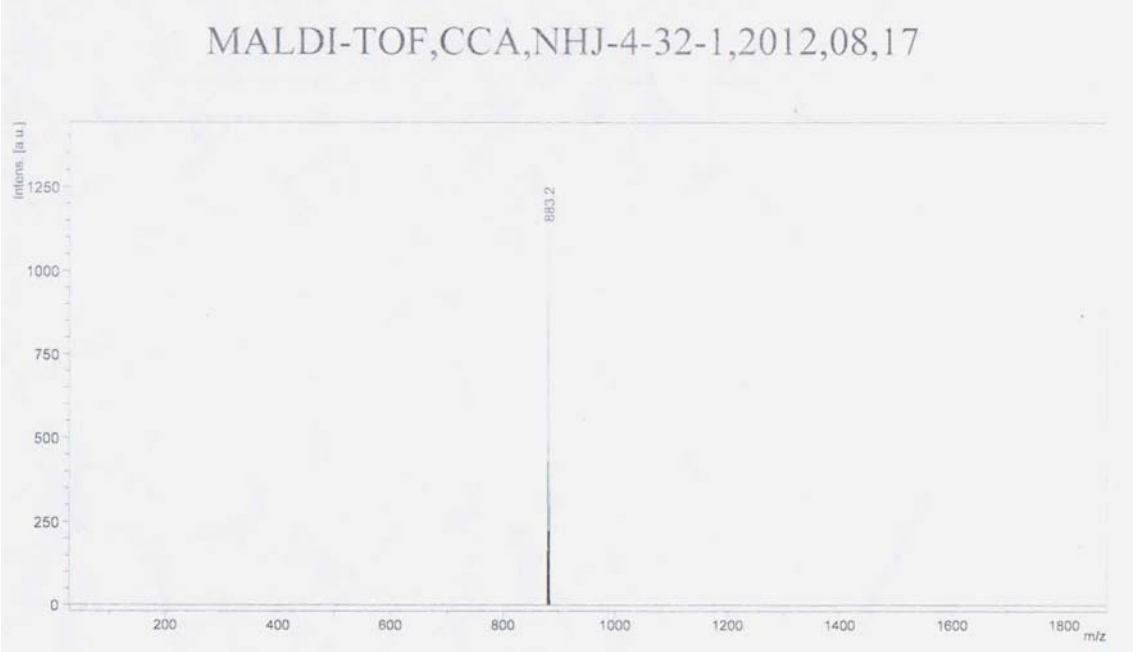
TOF-MALDI mass spectrum of **3**(PF_6):



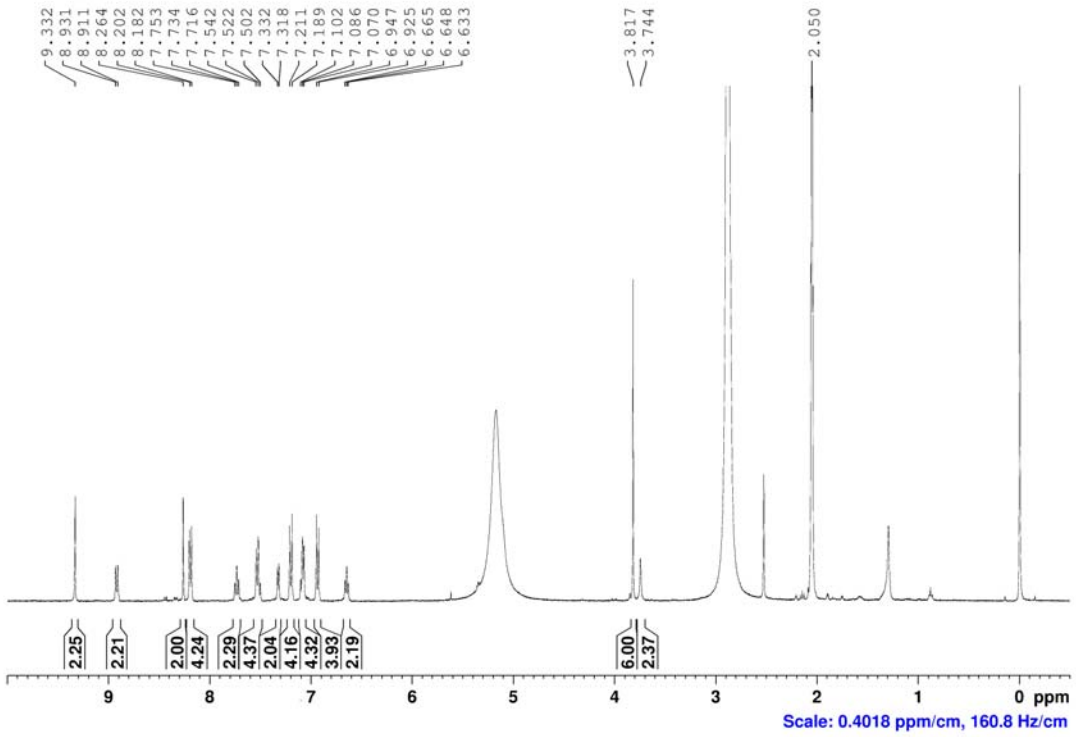
TOF-MALDI mass spectrum of **4**(PF_6):



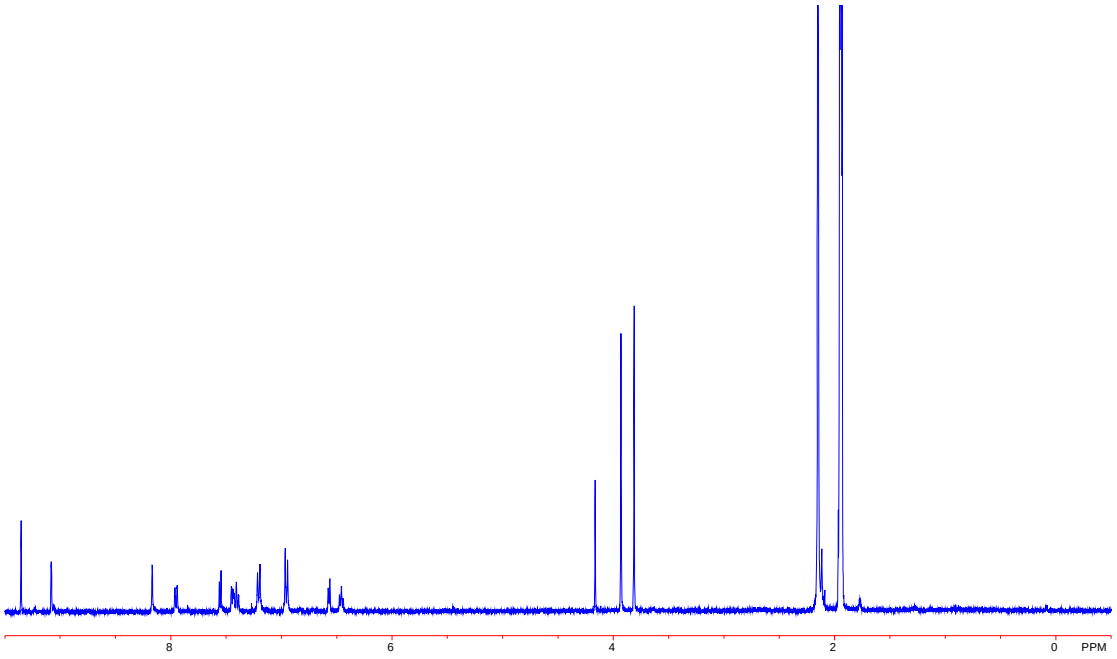
TOF-MALDI mass spectrum of **5**(PF_6):



^{1}H NMR spectrum of **3**(PF_6) in acetone-D_6 in the presence of small amount of $NH_2NH_2 \cdot H_2O$:



^{1}H NMR spectrum of **4**(PF_6) in CD_3CN:



^{1}H NMR spectrum of **5**(PF_6) in acetone-D_6: