

A Mesoionic Carbene Complex of Manganese in Five Oxidation States

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1. Methods and Materials

General remarks: If not otherwise mentioned, all transformations were carried out under inert conditions using the Schlenk technique or an argon filled glovebox. Solvents were dried by a MBraun SPS system and stored over activated molecular sieves (3 Å) for at least 24 h. The deuterated solvents CDCl_3 and MeCN-d_3 were dried by storage over activated molecular sieves (3 Å) for at least 24 h. DMSO- d_6 was used as received. Manganese iodide, NOPF_6 , LiHMDS , and potassium hexafluorophosphate were used as received. The proligand **1-I**₂ was synthesized following our previously reported procedure.¹ Potassium graphite was prepared by stirring potassium and dried graphite (molar ratio 1:8) at 250°C for 2h and subsequently stored in an argon filled glovebox. IR spectra were recorded at room temperature under inert conditions using a Bruker Vertex 70 with ATR equipment. If not otherwise stated, the NMR spectra were collected at 300 K on a Bruker Ascent 400 or 700 spectrometer using a J-Young tube. Elemental analyses were performed using an Elementar vario microcube instrument. Cyclic voltammograms at room temperature were performed with the PAR101 potentiostat from Metrohm in DCM / 0.1 M $[\text{NBu}_4]\text{PF}_6$ (analyte conc. = 0.001 mol/l) with the following three electrode arrangement: Pt working electrode (1 mm diameter), Ag/ 0.01 M AgNO_3 , 0.1 M NBu_4PF_6 in DCM as reference and Pt wire counter electrode. Ferrocene was added as internal standard after the measurements and all potentials are referenced relative to the $\text{Fc}/[\text{Fc}]^+$ couple. All measurements were carried out under argon atmosphere, with absolute and vented solvents. UV-Vis spectra were recorded on a Cary 50 Scan instrument.

Magnetometry: DC magnetometric measurements on **2(PF₆)** and **2(PF₆)₂** powder samples were performed using a Quantum Design MPMS3 equipped with a Superconducting Quantum Interference Device (SQUID). The sample was grinded, enveloped in a Teflon matrix and pressed to form a pellet. The temperature dependence of the magnetization was recorded with a constant applied magnetic field of 10 kOe for **2(PF₆)₂** and 1 kOe (1.8-50 K) and 10 kOe (40-300 K) for **2(PF₆)**. The diamagnetic response was corrected for the sample mass and sample-holder. The molar susceptibility was calculated by dividing the molar magnetization to the magnetic field applied. The field dependence of isothermal magnetization was recorded up to 7 T at 1.8, 5 and 10 K. The fits were done using the PHI program.² Alternate current SQUID measurements were performed at different field and temperature values, but no peaks in the real and imaginary part of the susceptibility were found.

High-field EPR: Measurements in the range 320-500 GHz were performed in Stuttgart on a home-built spectrometer.³ A synthesizer generates microwave radiation up to 20 GHz that is fed through an amplifier-multiplier chain (VDI) to obtain the required frequency. The setup further consists of a quasi-optical bridge (Thomas Keating) to propagate the radiation from the source to the sample and then to the detector. The detector used is a magnetically tuned InSb hot electron bolometer (QMC instruments). The detection is done in induction mode. The sample is inserted in an Oxford Instruments 15/17 T cryomagnet equipped with a variable temperature insert (1.5–300 K). The spectra were collected on the same pressed pellet of polycrystalline powder used for SQUID measurements. The data were simulated using EasySpin (v. 5.2.30) in Matlab.⁴

EPR: Electron Paramagnetic Resonance (EPR) and EPR spectroelectrochemical (SEC) measurements at X-band (9.45 GHz) were performed using a Magnettech MS5000 benchtop EPR spectrometer with a rectangular TE 102 cavity, equipped with a liquid N₂ temperature control system. Synthetic quartz EPR tubes (outer diameter 3 mm) were used for measurements. EPR spectra of a solid sample and MeCN solution of **2(PF₆)₂** were acquired, and SEC measurements were performed with the compound dissolved in 0.1 M NBu_4PF_6 solution in MeCN. A three electrode electrochemical setup consisting of two Teflon-coated Pt wires (0.005" bare, 0.008" coated) as working and counter electrodes and an Ag wire (0.005" bare, 0.007" coated) as pseudo-reference electrode was employed. SEC measurements were performed using a PalmSens4 potentiostat. The data were simulated using EasySpin (v. 5.2.30) in Matlab.⁴

MCD: MCD spectra were acquired on a home built set-up, that combines an Aviv 42 CD spectrometer with an Oxford Instruments Spectromag SM400 optical cryomagnet. Measurements can be carried out from 250 nm to 2000 nm at temperatures down to 1.5 K and at fields up to 10 T. Samples were dissolved in a 1:1 mixture of DCM/toluene and frozen to LN₂ temperature before being mounted in the cryostat. Spectra were recorded with the magnetic field parallel (plus field) and antiparallel (minus field) to the propagation direction of the light. The resulting MCD spectra were obtained by subtraction of spectra recorded at positive and negative fields, in order to remove field independent CD signals.

X-Ray crystallography: Single crystals for X-ray diffraction experiments were performed at the analytical facility of the University of Paderborn or at the University of Göttingen. All crystals were kept at 120(2) K throughout data collection. Data collection was performed using either the Apex III or the Smart software package. Data refinement and reduction were performed with Bruker Saint (V8.34A). All structures were solved with SHELXT and refined using the OLEX 2 software package.⁵ All non-hydrogen atoms were refined anisotropically, and hydrogen atoms were included at the geometrically calculated positions and refined using a riding model. The structure of contained four rotational disordered and only partially occupied THF molecules, which have been removed using the SQUEEZE algorithm.⁶ The presence of THF in the crystals can be explained from insufficient drying of the compound prior to crystallization. CCDC 1953710 and 1993282 contain the CIF-Files for complexes **2(PF₆)₂** and **2(PF₆)**. For further crystallographic details, please check Tables S1 and S2.

2. Experimental Section

Synthesis of **2(PF₆)₂**

In an argon filled glove box, bis-triazolium salt **1** (2 eq, 0.5 mmol, 393 mg) was dissolved in dry THF (5 mL) cooled to -40 °C and stirred for five minutes. To this solution a cold solution (-40°C) of LiHMDS (6 eq, 3 mmol, 501 mg) in THF (2 mL) was added dropwise over one minutes. The solution was stirred for one minute and then added to cold (-40 °C) solution of MnI₂ (1 eq, 0.25 mmol, in THF (5 mL)). The solution turns dark brown instantly and was left to stir overnight, while slowly warming to room temperature. The dark brown solution is removed from the glove box and the vial is opened to air. The solution was stirred like this for 5 minutes, resulting in no observable color change. The THF is then removed from the reaction on the rotary evaporator and the brown mixture is redissolved in acetone (5 mL). To this solution a concentrated solution of KPF₆ (2 g) in water (50 mL) was added causing the precipitation of a brownish green solid. The solids are filtered off, dissolved in acetone (5 mL) again and the procedure is repeated twice, resulting in the formation of a dark green precipitate, which is dried in air overnight. The crude complex **2(PF₆)₂** was then dissolved in dichloromethane and subjected to silica gel column chromatography using dichloromethane /methanol (99:1). The green fractions are collected and concentrated to dryness. Yield: 200 mg (0.144 mmol, 72 %) The material at this step was sufficiently pure for further use as determined elemental analysis. However, for further investigations by magnetometry and EPR, the material was recrystallized by vapour diffusion of pentane in to a saturated acetone solution (10 mL) of the complex. This resulted in the formation of large green blocks (X-ray quality) after 3 days. Crystalline yield: 100 mg (0.072 mmol, 36%) Evans Method: 3.71 μB; mass spectrometry (ESI): found 1240.5433 m/z calcd. 1240.5399 m/z for [C₆₄H₇₇N₁₄Mn₁(P₁F₆)]⁺; found 547.7909 m/z calcd. 547.7879 m/z for [C₆₄H₇₇N₁₄Mn₁]²⁺; elemental analysis: calcd. (%) for C₆₄H₇₆N₁₄Mn₁ 2(P₁F₆) C 55.45 H 5.53 N 14.15 found C 55.24 H 5.74 N 14.31.

Synthesis of **2(PF₆)**

In an argon filled glovebox, **2(PF₆)₂** (1 eq, 0.025 mmol, 34 mg) was dissolved in 10 mL of THF at room temperature. To this solution was added solid potassium graphite KC₈ (1.2 eq, 0.03 mmol, 4 mg) causing a color change to deep purple. The solution was stirred like this for another 20 minutes, before the graphite was filtered off and the purple THF solution was concentrated to dryness. The purple materials were redissolved in dichloromethane, filtered, and subjected to a vapor diffusion using pentane as the antisolvent. This resulted in the formation of large purple blocks suitable for X-ray analysis within 4 days. Yield: 25 mg (0.02 mmol, 81%). Evans Method: 2.84 μB; mass spectrometry (ESI): found 1095.5787 m/z calcd. 1095.5758 m/z for [C₆₄H₇₇N₁₄Mn₁]⁺ elemental analysis: calcd. (%) for C₆₄H₇₆N₁₄Mn₁ P₁F₆ C 61.93 H 6.17 N 15.80 found C 61.53 H 6.18 N 15.58.

3. NMR spectroscopy

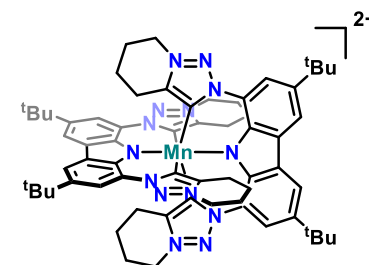
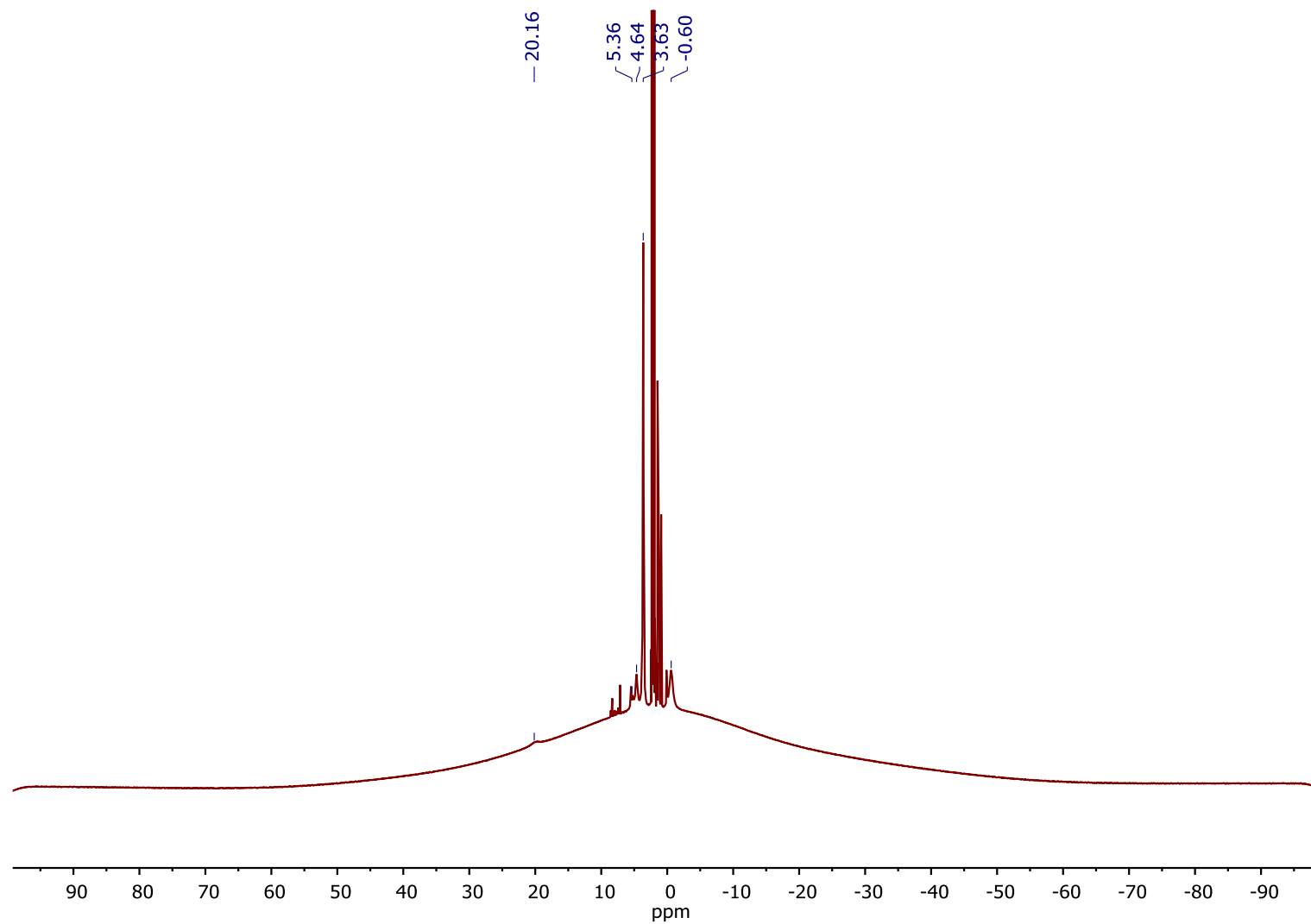


Figure S 1: ^1H NMR (700 MHz) of $2[\text{PF}_6]_2$ between -100 and 100 ppm in MeCN-d_3 at 298 K. Signals in the diamagnetic region arise from solvent impurities in the NMR solvent.

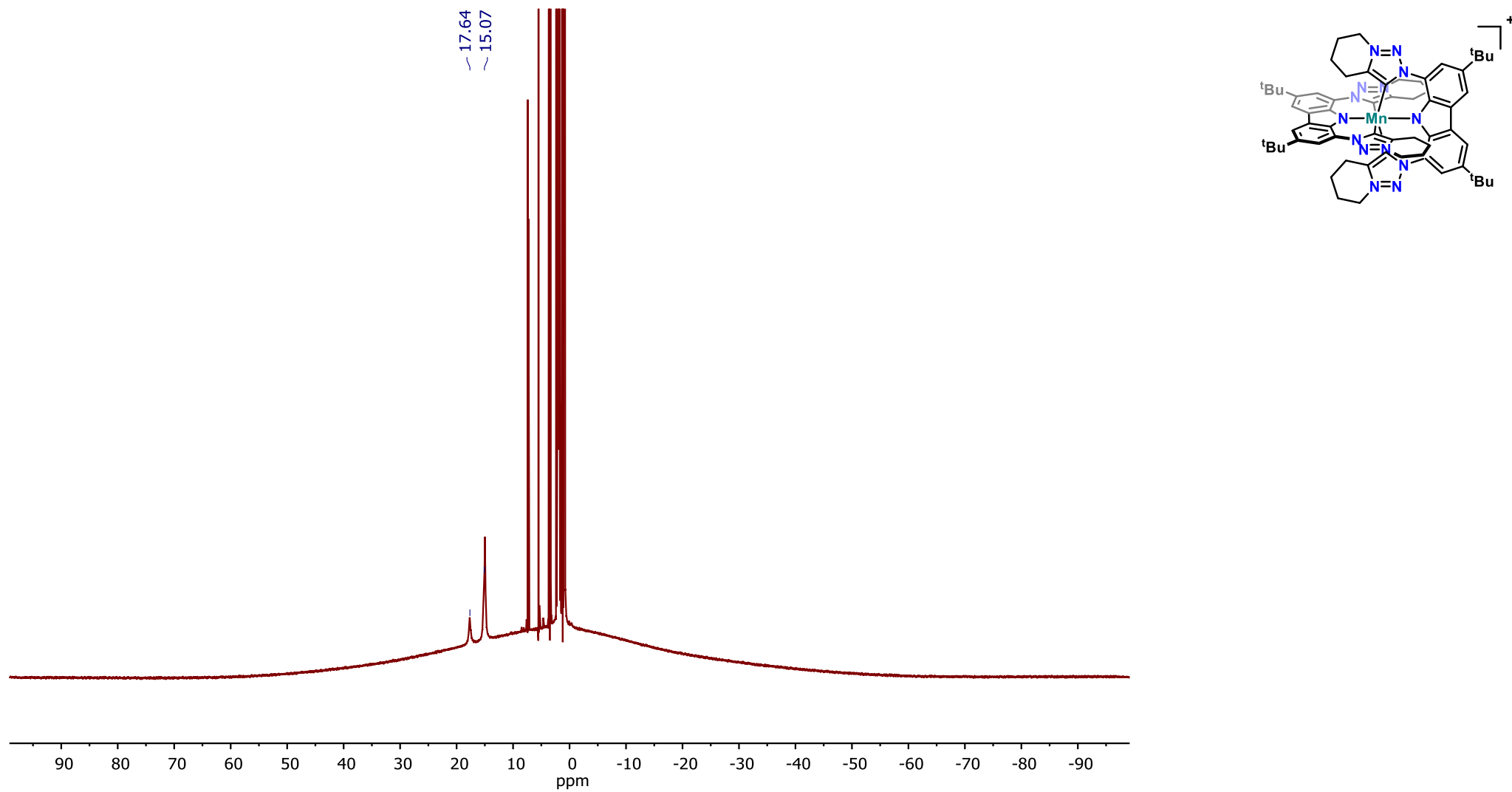


Figure S 2: ^1H NMR (700 MHz) of $2[\text{PF}_6]_2$ between -100 and 100 ppm in MeCN-d_3 at 298 K. Signals in the diamagnetic region arise from solvent impurities in the NMR solvent.

4. Mass Spectrometry

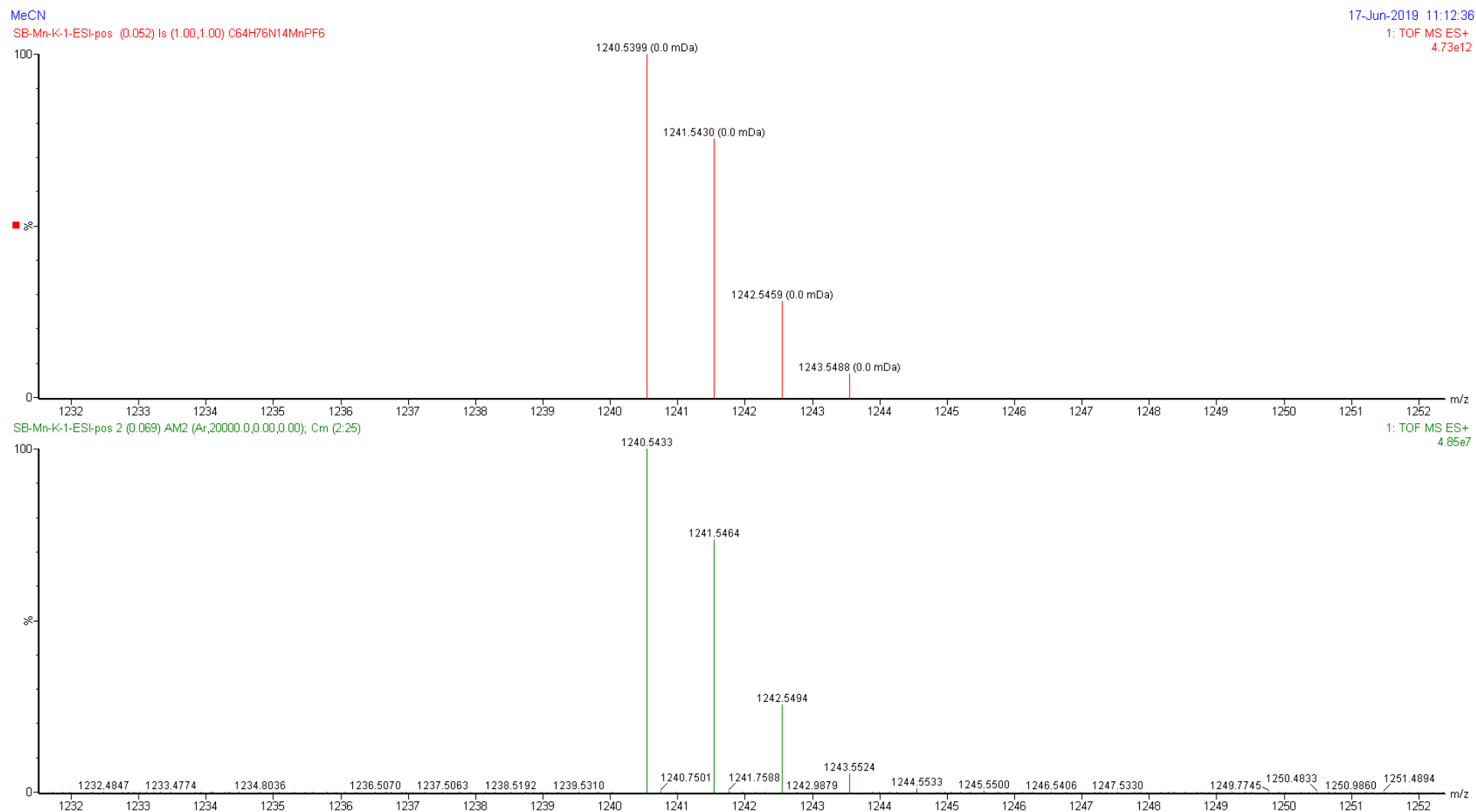


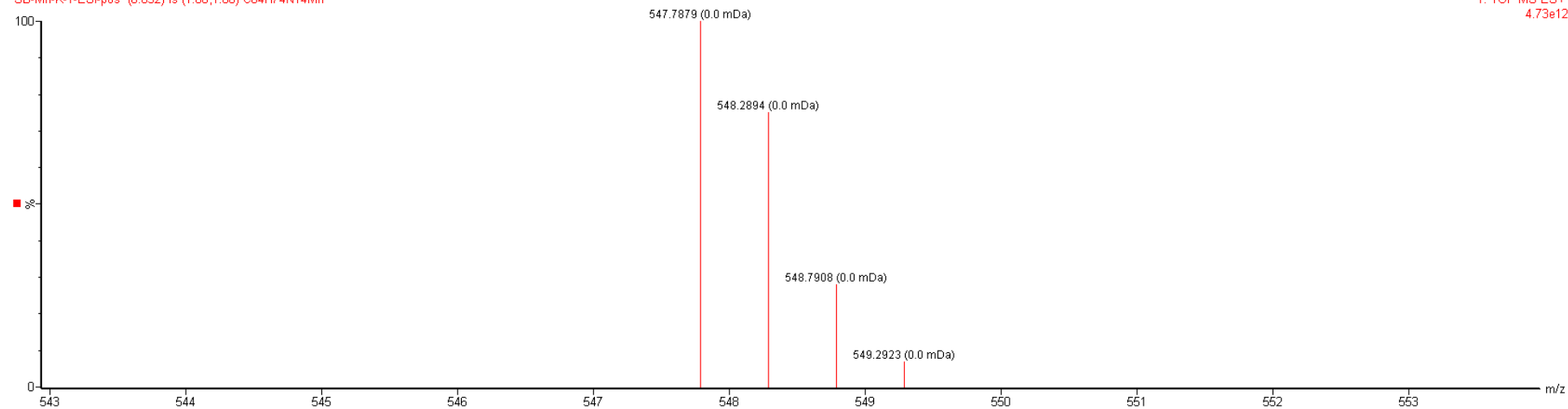
Figure S 3: Measured (bottom, green) and simulated (top, red) mass of the tentative species $[2(PF_6)]^+$

MeCN

17-Jun-2019 11:12:36

SB-Mn-K-1-ESI-pos (0.052) Is (1.00,1.00) C₆₄H₇₄N₁₄Mn

1: TOF MS ES+
4.73e12



SB-Mn-K-1-ESI-pos 2 (0.069) AM2 (Ar,20000.0,0.00,0.00); Cm (2.25)

1: TOF MS ES+
3.88e7

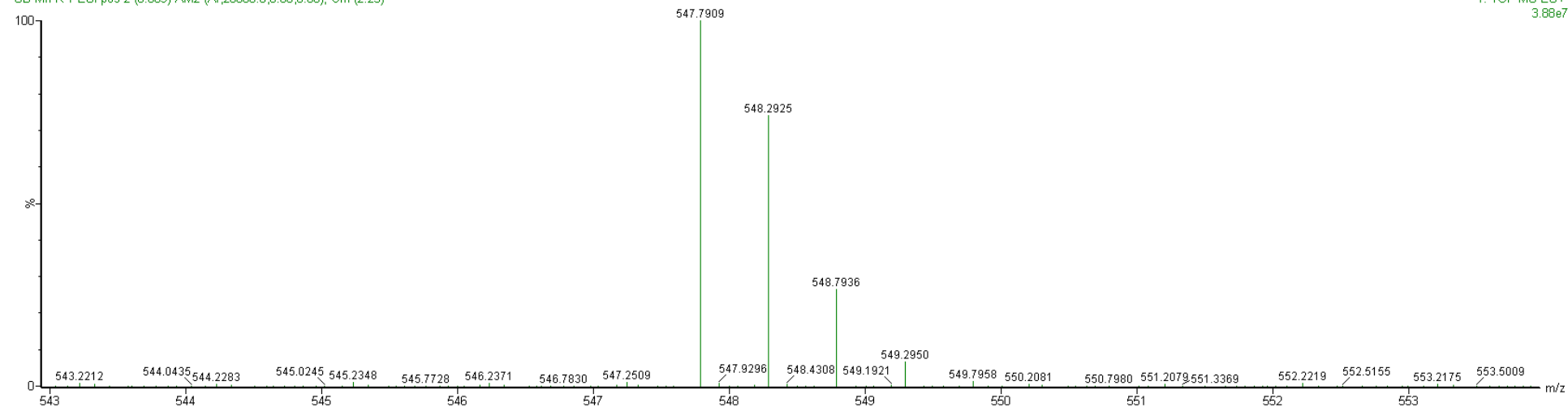


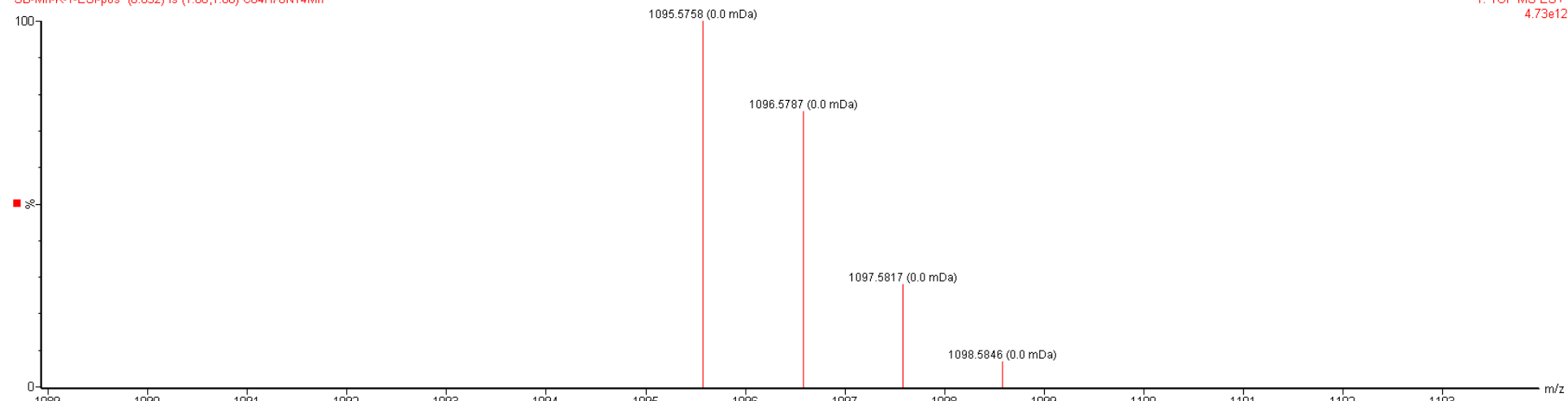
Figure S 4: Measured (bottom, green) and simulated (top, red) mass of the tentative species [2]²⁺

MeCN

17-Jun-2019 11:12:36

SB-Mn-K-1-ESI-pos (0.052) Is (1.00,1.00) C₆₄H₇₆N₁₄Mn

1: TOF MS ES+
4.73e12



SB-Mn-K-1-ESI-pos 2 (0.069) AM2 (Ar,20000.0,0.00,0.00); Cm (2:25)

1: TOF MS ES+
1.77e7

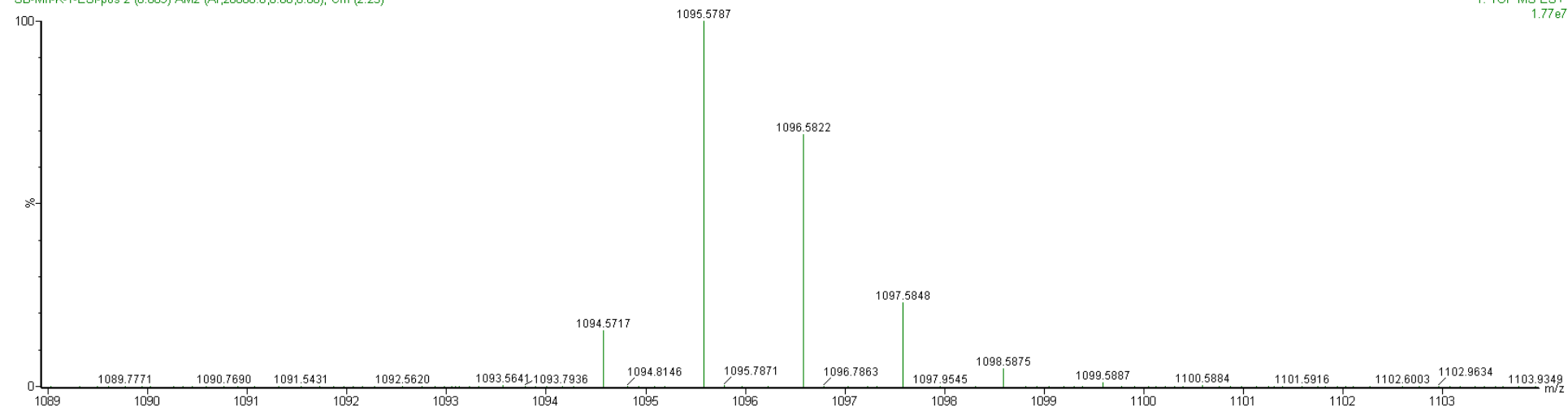


Figure S 5: Measured (bottom, green) and simulated (top, red) mass of the tentative species [2]⁺

5. Cyclic Voltammetry

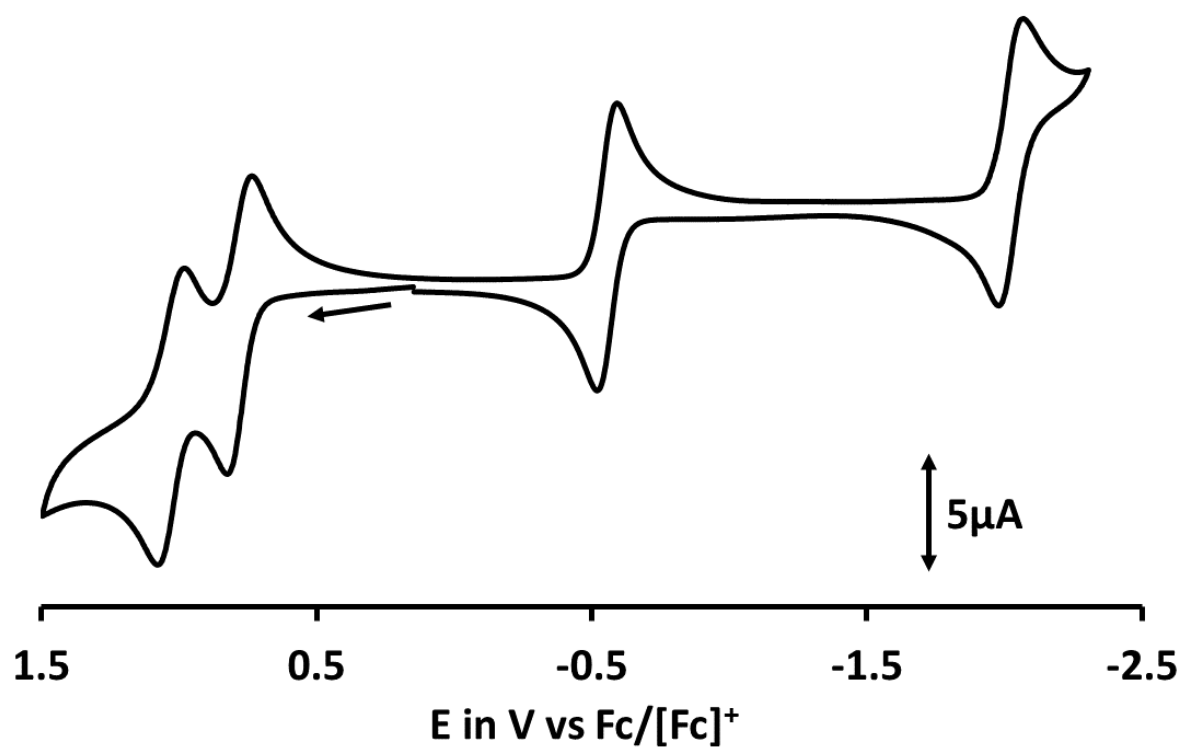


Figure S 6: Cyclic voltammogram of **2**(PF₆)₂ in 0.1M NBu₄PF₆ in MeCN at 298 K. Scan Rate: 100 mVs⁻¹

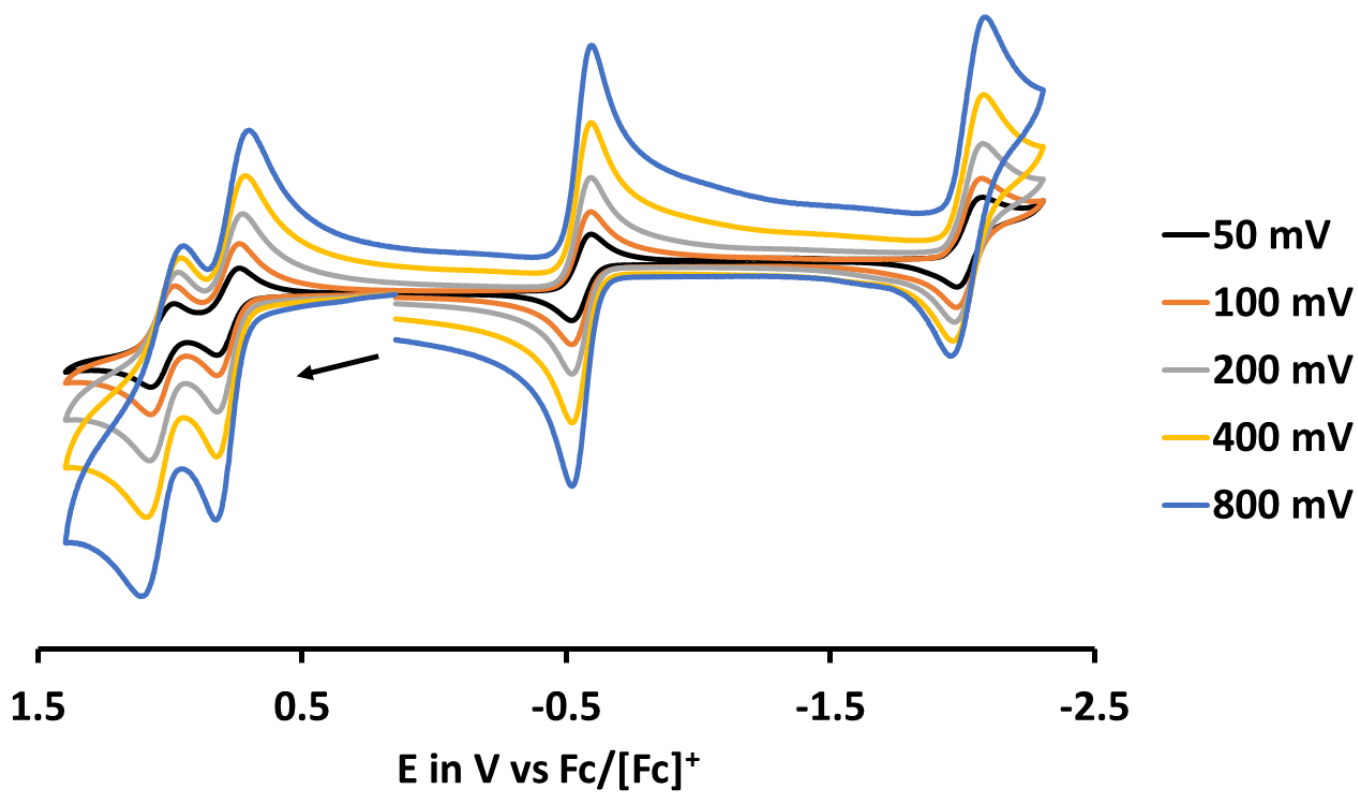


Figure S 7: Cyclic voltammograms of **2**(PF₆)₂ measured with different scan rates in 0.1M NBu₄PF₆ in MeCN at 298 K.

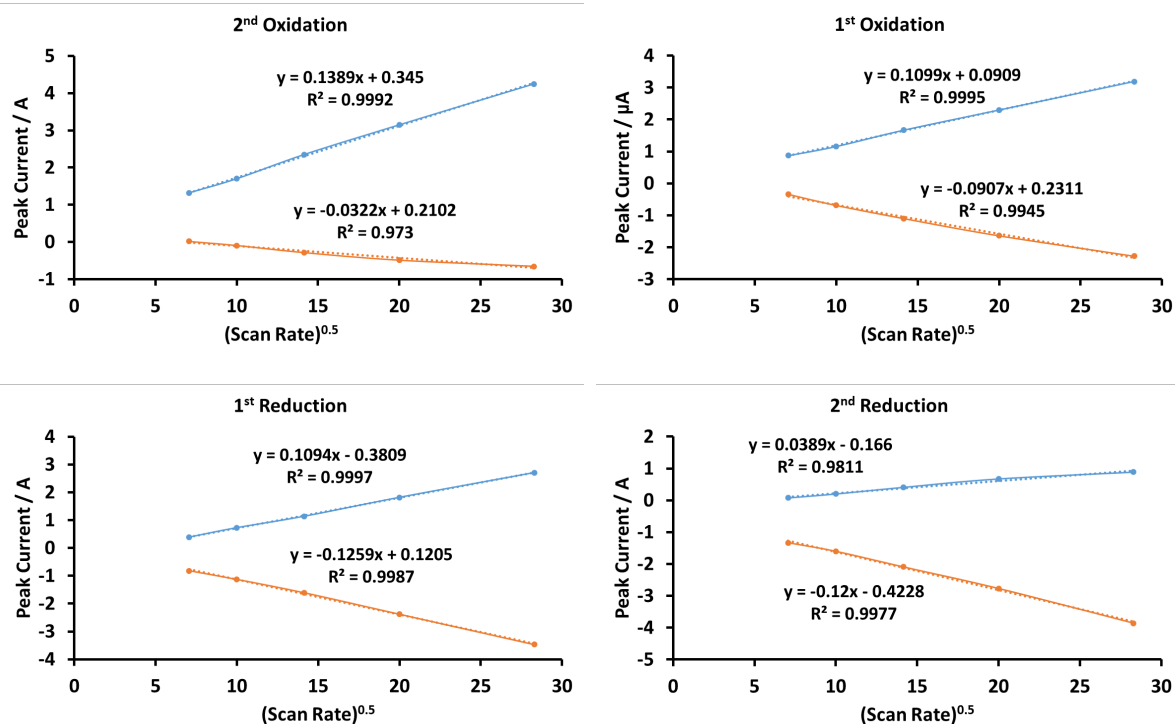


Figure S 8: Reversibility plots of the redox events in $2(\text{PF}_6)_2$

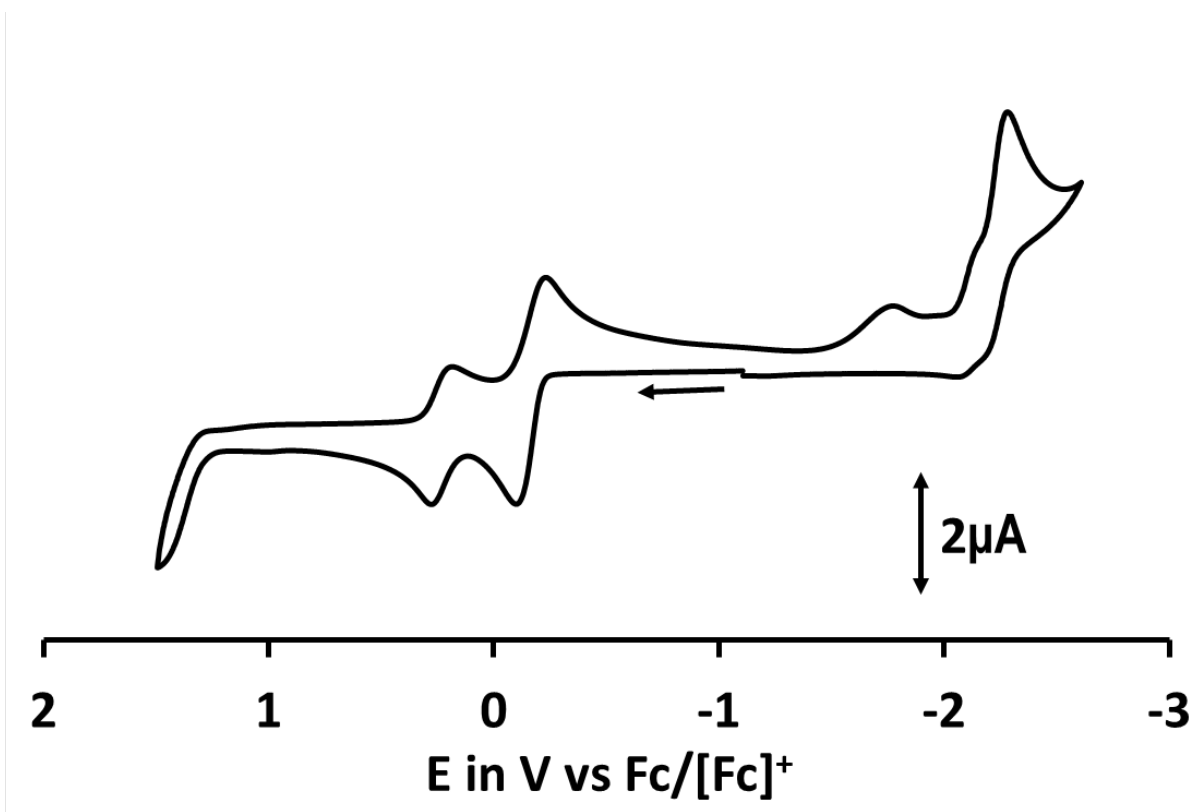


Figure S 9: Cyclic voltammogram of 1-I_2 0.1M NBu_4PF_6 in MeCN at 298 K. Scan Rate: 100 mVs^{-1}

Table S 1: $E_{1/2}$ Values for Homoleptic Mn Complexes, Measured in MeCN, with 0.1 M NBu_4PF_6 as the Electrolyte (All Potentials Referenced to the Fc/Fc^+ Couple)

ligand	solvent	Mn(IV/III)	Mn(III/II)
Present case	MeCN	-0.55 V	-2.01 V
$\text{PhB}(\text{MeIM})_3^{-7}$	MeCN	-0.77 V	-2.09 V
Tp^*^8	$\text{C}_2\text{H}_4\text{Cl}_2$	0.99 V	-0.13 V
Cp^*^9	MeCN	-	-0.94 V
$\text{Tp}_{\text{Me}2}^{10}$	MeCN	0.97 V	-0.36 V
bis(2-amino-3,5-di-tert-butylphenyl)amine ¹¹	CH_2Cl_2	-1.48 V	-

6. UV-Vis Spectroscopy

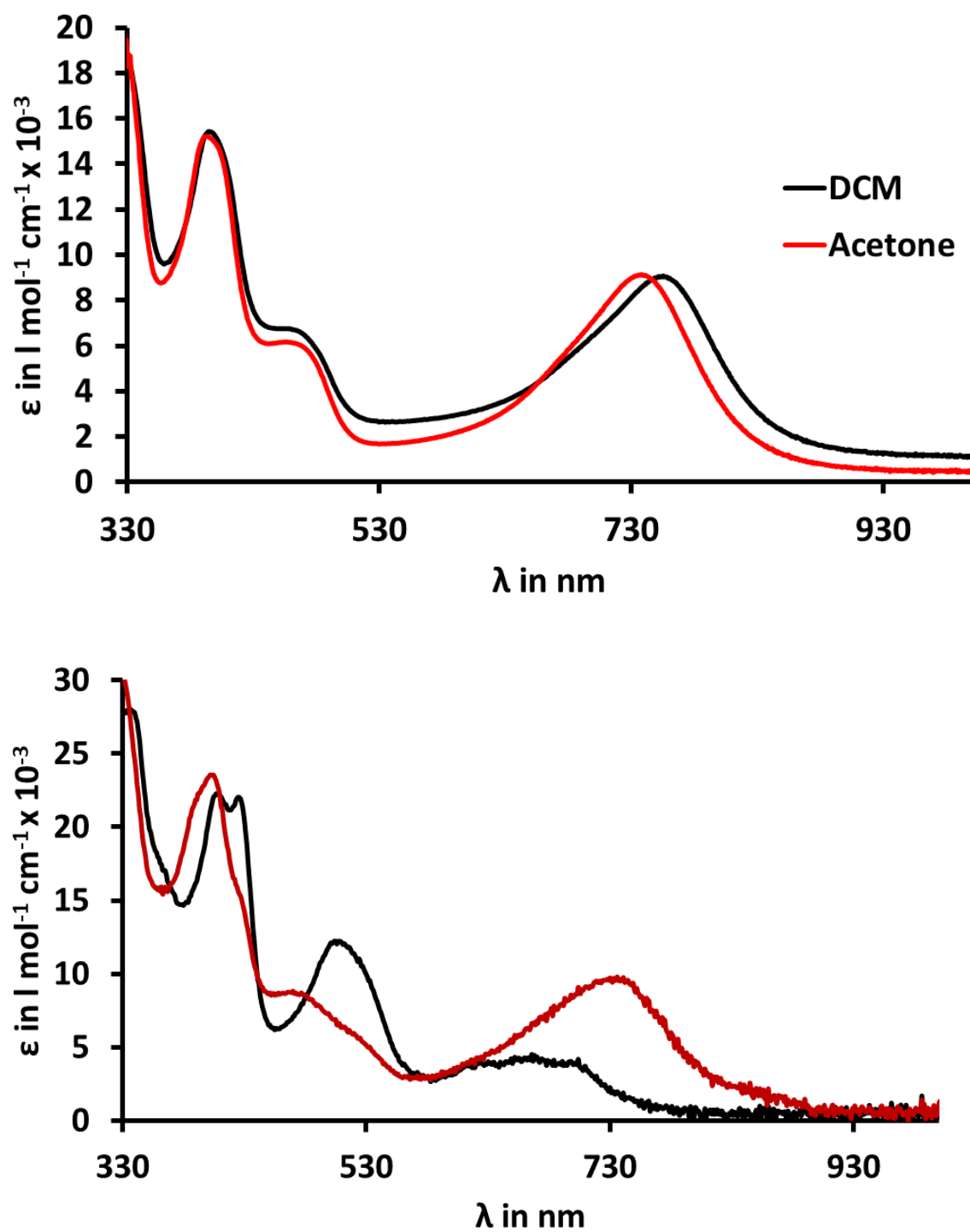


Figure S 10: UV-Vis spectra of $2(\text{PF}_6)_2$ in DCM (black trace) and acetone (red trace). (top). Comparison of the UV-Vis spectra of $2(\text{PF}_6)_2$ (red trace) and $2(\text{PF}_6)$ (black trace) in DCM. (bottom)

7. X-band EPR Spectroscopy

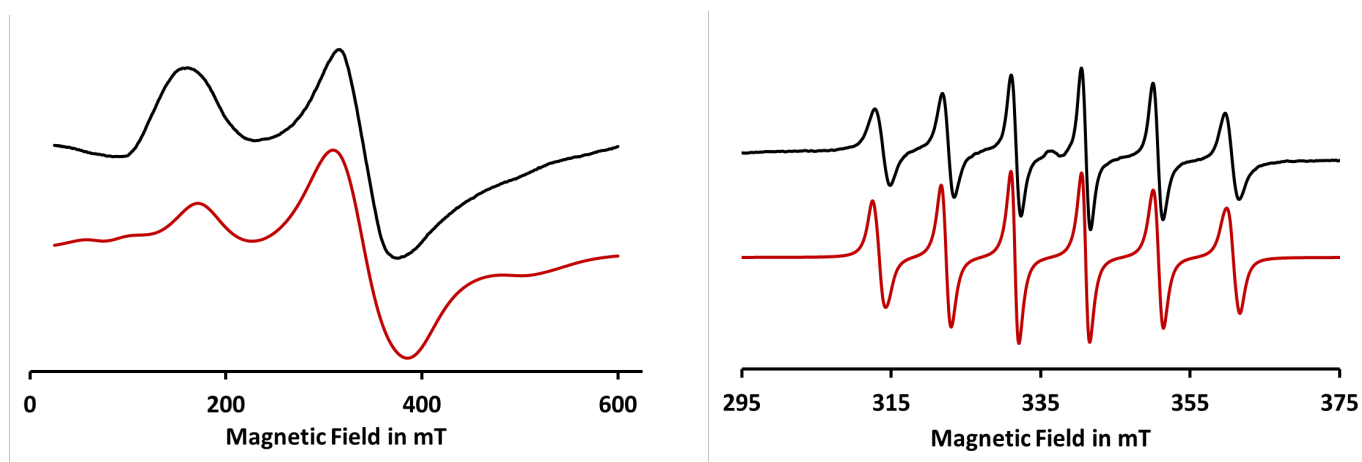


Figure S 11: Experimental (black) and simulated (red) EPR spectrum of a powdered solid sample of **2(PF₆)₂**, at 98 K and 9.466 GHz (left) and after electrolysis to the first oxidized species **[2]³⁺** (right). Simulation parameters are given in Table S1. Please not for the spectra of **[2]³⁺**: The first oxidation should produce an $S = 1$ species, and the spectrum could be simulated taking this into account (see Table S1). However, the spectrum is quite similar to that shown in Fig. 2c, and a good fit could also be obtained with an $S = 1/2$ spin Hamiltonian. Thus, we cannot fully rule out the alternative possibility that the species shown in Fig. S11, right is an $S = 1/2$ radical arising from the **[2]³⁺** ($S = 1$) species through H-atom abstraction from the solvent or supporting electrolyte. However, the calculations (see section 12, Table S9, Figure S19, right and S23) indicate a comparatively high amido-ligand–metal covalency, as well as strong multi-configurational character (lead configuration: $c = 0.38$) in mixed-valent **[2]³⁺**. Additionally, essentially degenerate triplet- and singlet ground states ($\Delta E < 0.02$ eV) are predicted.

Simulations of the EPR spectra were performed using the following $S = 3/2$ spin Hamiltonian, for **2(PF₆)₂**

$$\hat{H} = \mu_B \hat{\mathbf{S}} \cdot \mathbf{g} \cdot \mathbf{B} + D \left(\hat{S}_z^2 - \frac{S(S+1)}{3} \right) + E(\hat{S}_x^2 - \hat{S}_y^2) + \hat{\mathbf{S}} \cdot \mathbf{A}_{Mn} \cdot \hat{\mathbf{I}}_{Mn}$$

where $\mathbf{g}$ and $\mathbf{A}$ matrices were assumed to be diagonal and therefore in the same coordinate system, defined by the zero-field splitting (zfs) parameters D and E . μ_B is the Bohr magneton.

The $S = 1$ spin Hamiltonian employed for **2³⁺** was

$$\hat{H} = \mu_B \hat{\mathbf{S}} \cdot \mathbf{g} \cdot \mathbf{B} + \hat{\mathbf{S}} \cdot \mathbf{A}_{Mn} \cdot \hat{\mathbf{I}}_{Mn}$$

In this case the zfs was not included, as the shape of the spectrum in fluid solution did not seem to be affected by this effect. The spectrum was essentially isotropic; however, a very slight anisotropy in $\mathbf{A}_{Mn}$ was included to better reproduce the lineshapes. This anisotropy was a phenomenological way of accounting for an incomplete directional averaging of the real anisotropy due to a less-than fast enough molecular tumbling.

Finally, for the **2⁴⁺** $S = 1/2$ radical, the following spin Hamiltonian was used

$$\hat{H} = \mu_B \hat{\mathbf{S}} \cdot \mathbf{g} \cdot \mathbf{B} + \hat{\mathbf{S}} \cdot \mathbf{A}_{Mn} \cdot \hat{\mathbf{I}}_{Mn} + \hat{\mathbf{S}} \cdot \mathbf{A}_{N1} \cdot \hat{\mathbf{I}}_{N1} + \hat{\mathbf{S}} \cdot \mathbf{A}_{N2} \cdot \hat{\mathbf{I}}_{N2}$$

where again a small anisotropy of the $\mathbf{A}$ -matrices was found to better reproduce the intensity pattern of the hyperfine-split resonances. All simulations were performed using the Easyspin function *pepper*.

Table S 2 Simulation Parameters for **2(PF₆)₂** in the solid state, and **2⁴⁺** in 0.1 M NBu₄PF₆ MeCN solution, after electrolysis at 1.93 V

2⁴⁺			2³⁺		
S = 1/2	xy	z	S = 1	xy	z
g	2.0089	2.0089	g	2.002	2.002
A (MHz)			A (MHz)		
55Mn	292.4	288.3	55Mn	270	255
14N	15.7	17.66	14N	--	--
14N	16.0	13.9	14N	--	--
Linewidth (mT)	Gaussian	Lorentzian	Linewidth (mT)	Gaussian	Lorentzian
	0.2	0.29		0.2	0.9

2(PF₆)₂ (solid)			[2]²⁺ (MeCN solution)		
S = 3/2	xy	z	S = 3/2	xy	z
g	1.93	2.02	g	1.96	2.08
A (MHz)			A (MHz)		
55Mn	--	--	55Mn	--	--
D (MHz)	2485		D (MHz)	2361	
E (MHz)	781		E (MHz)	515	
Dstrain (MHz)	52		Dstrain (MHz)	62	
Estrain (MHz)	10		Estrain (MHz)	136	
HStrain (MHz)	382	750	HStrain (MHz)	454	1029
Linewidth (mT)	Gaussian	Lorentzian	Linewidth (mT)	Gaussian	Lorentzian
	0	35.8		0	24.9

8. Magnetic Measurements

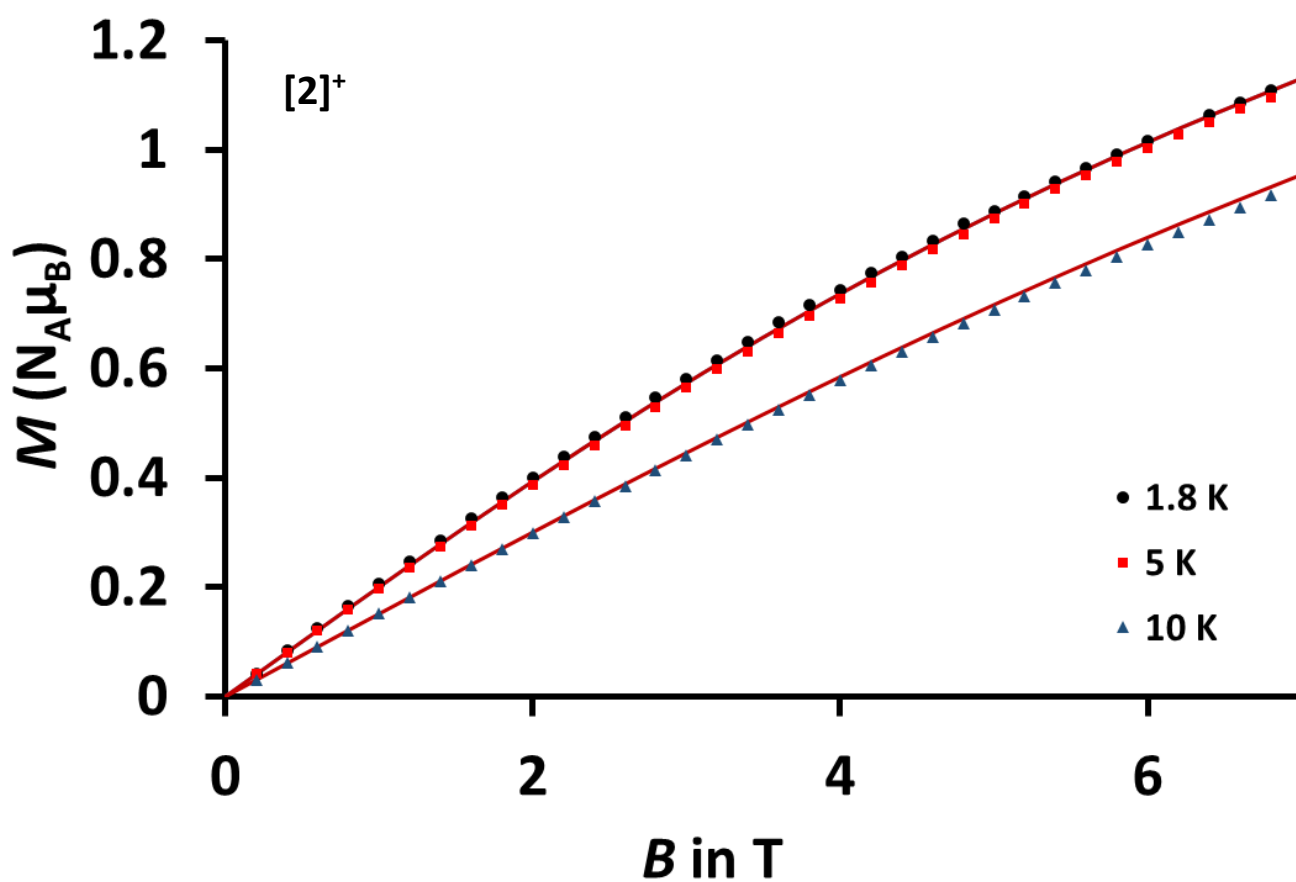
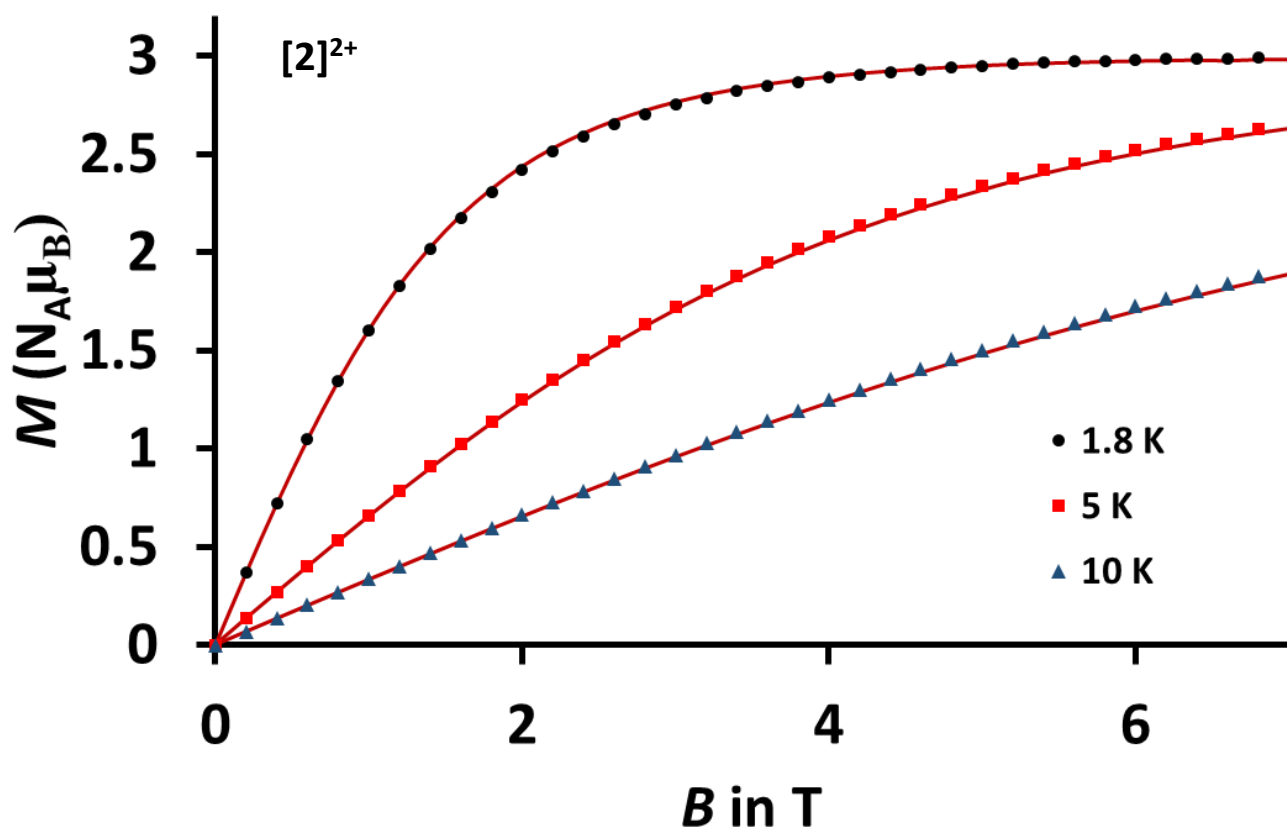


Figure S 12: Experimental (symbols) and fitted (solid lines) magnetic field dependence of the magnetization for $2(\text{PF}_6)_2$ (top) and $2(\text{PF}_6)$ (bottom) measured at 1.8, 5 and 10 K.

9. HF-EPR Measurements

The HFEPR spectra for $2(\text{PF}_6)$ were simulated considering all the spectra at different frequencies, assuming an $S = 1$ system and using the following spin Hamiltonian:

$$\hat{H} = \mu_B \hat{\mathbf{S}} \cdot \mathbf{g} \cdot \mathbf{B} + D \left(\hat{S}_z^2 - \frac{S(S+1)}{3} \right) + E(\hat{S}_x^2 - \hat{S}_y^2)$$

The parameters that best reproduce the experiments are: $g_{\perp} = 2.00(1)$ and $g_{\parallel} = 1.90(1)$ with strains of 0.12 and 0.08, respectively, and $D = 398.0(1)$ GHz with a null E contribution. A peak-to-peak Gaussian linewidth broadening of 300 mT is found. Such a large broadening prevents the observation of any hyperfine contribution to the signal, which was therefore not taken into account in the simulation.

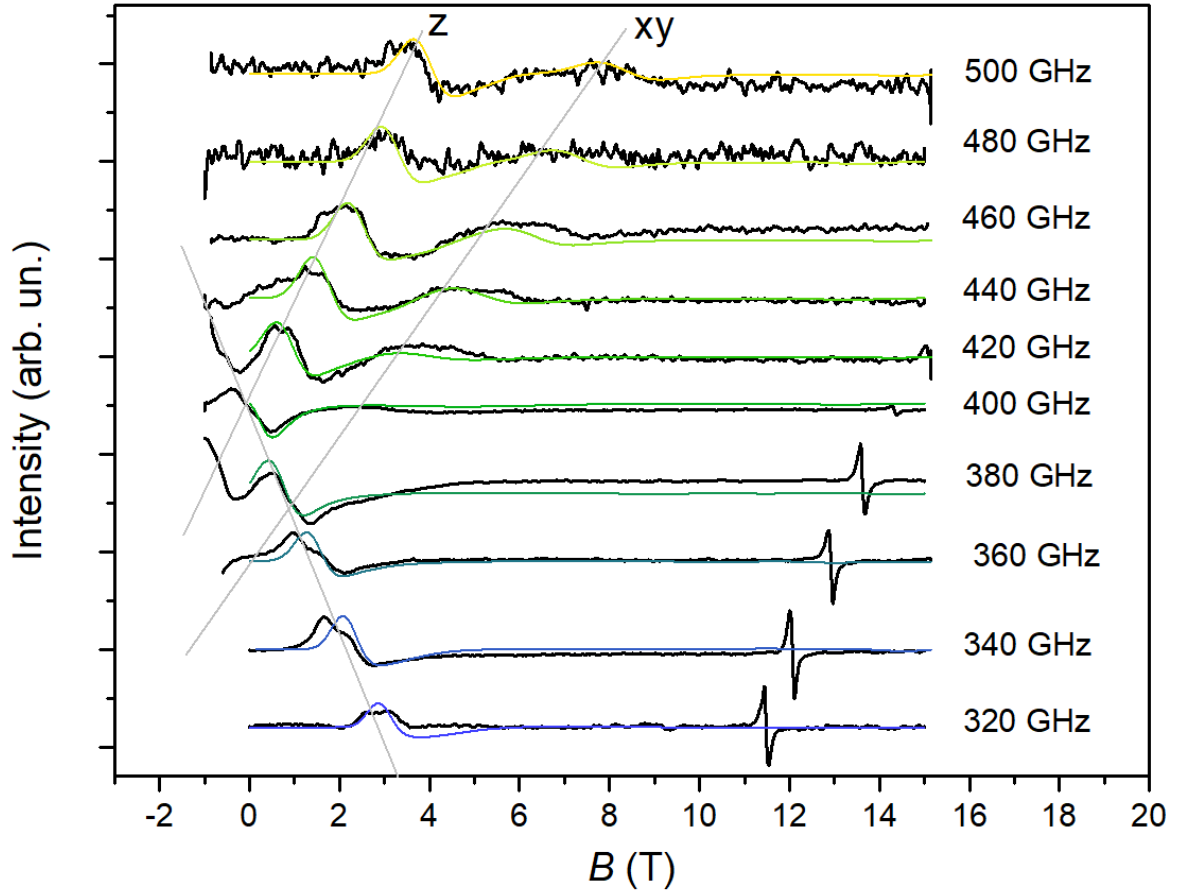


Figure S13: Experimental (black) and simulated (colored) High Field EPR spectra at various frequencies from 320 to 500 GHz of $2(\text{PF}_6)$ at the temperature of 10 K. The signal at $g=2$ is an impurity in the sample-holder. The gray lines are used to evidence the EPR z and xy transitions.

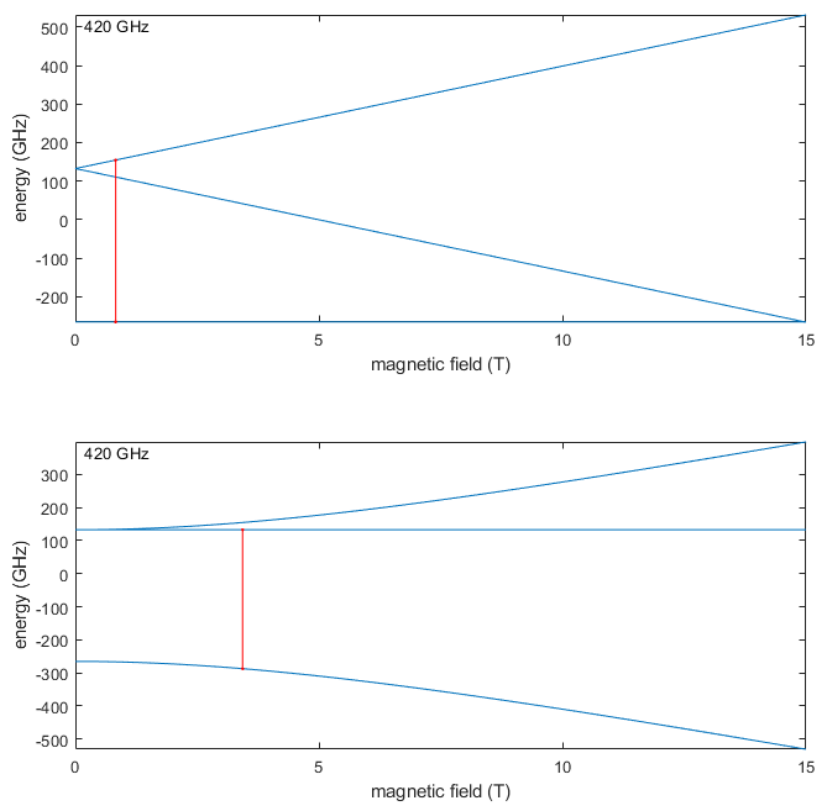


Figure S14: Simulated energy levels of $2(\text{PF}_6)$ as a function of the magnetic field for the z (top) and xy (bottom) orientations of the principal magnetic tensor. Red lines correspond to the EPR transition occurring at 420 GHz.

10. MCD Measurements

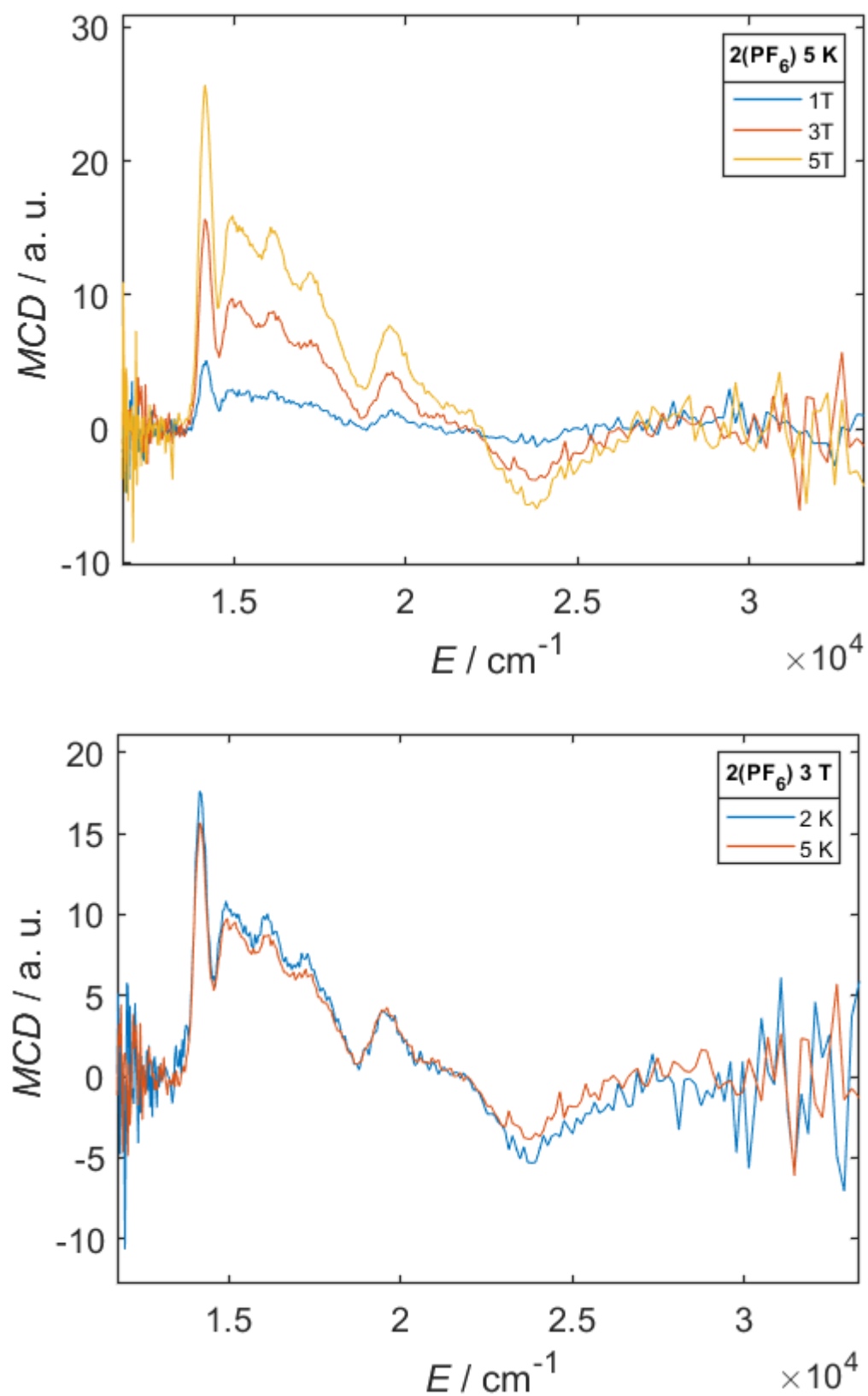


Figure S 15: Field dependence (1,3,5 T) of the MCD spectra of **2(PF₆)** in a 1:1 mixture of DCM and toluene at 5 K (top). Temperature dependence (2 and 5 K) of the MCD spectra of **2(PF₆)** in a 1:1 mixture of DCM and toluene in an applied external magnetic field of 3 T (bottom).

11. Crystallographic Details

Table S 3: Crystallographic details of the complexes

	2(PF₆)₂ (2 Acetone)	2(PF₆)[*]
Chemical formula	C ₆₄ H ₇₆ N ₁₄ Mn ₁ 2(P ₁ F ₆) 2(C ₃ H ₆ O ₁)	C ₆₄ H ₇₆ N ₁₄ Mn ₁ P ₁ F ₆
<i>M_r</i>	1502.42	1241.29
Crystal system	Orthorhombic	Monoclinic
Space group	<i>Pbca</i>	<i>P2₁/c</i>
<i>a</i> (Å)	23.276(3)	13.863(5)
<i>b</i> (Å)	21.164(3)	30.786(1)
<i>c</i> (Å)	29.506(4)	17.675(6)
α (°)	90	90
β (°)	90	98.852(1)
γ (°)	90	90
<i>V</i> (Å ³)	14536(3)	7453.8(4)
<i>Z</i>	8	4
Density (g cm ⁻³)	1.373	1.106
<i>F</i> (000)	6280	2608
Radiation Type	MoK α	MoK α
μ (mm ⁻¹)	0.311	0.257
Crystal size	0.15x0.13x0.11	0.05x0.04x0.02
Meas. Refl.	115120	120957
Indep. Refl.	13805	13104
Obsvd. [<i>I</i> > 2 σ (<i>I</i>)]	8976	10290
<i>R</i> _{int}	0.0523	0.0986
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)]	0.0568	0.0844
w <i>R</i> (<i>F</i> ²)	0.1630	0.2336
<i>S</i>	1.079	1.034
$\Delta\rho_{\text{max}}$	1.157	1.352
$\Delta\rho_{\text{min}}$	-0.616	-0.642
CCDC	1953710	1993282

^{*}Please note that due to a rotational disorder and partial occupation, four molecules of THF had been removed from the asymmetric unit using the SQUEEZE algorithm.⁶

Table S 4: Selected bond lengths and angles

	1-I₂[*]	2(PF₆)₂	2(PF₆)
Mn1-N10	-	1.939(3)	1.968(3)
Mn1-N10A	-	1.938(3)	1.974(3)
Mn1-C1	-	2.080(3)	2.070(4)
Mn1-C2	-	2.073(3)	2.084(4)
Mn1-C1A	-	2.076(3)	2.075(4)
Mn1-C2A	-	2.093(3)	2.087(4)
N10-C13	1.391(6)	1.392(4)	1.387(5)
N1-N3	1.326(6)	1.330(4)	1.351(4)
N3-N5	1.311(6)	1.317(4)	1.310(5)
N5-C3	1.349(7)	1.360(4)	1.364(5)
C3-C1	1.353(8)	1.387(5)	1.416(5)
C1-N1	1.358(7)	1.371(4)	1.382(5)
N10-C24	-	1.382(4)	1.386(5)
C1-Mn1-C2	-	176.4(1)	177.48(15)
C1A-Mn1-C2A	-	177.9(1)	176.45(15)
N10-Mn1-N10A	-	178.9(1)	179.41(14)

^{*} adapted from ref. ¹

12. Computational Details

All calculations were performed with ORCA v.4.2.1.¹²

Structural parameters were obtained either (i.) from the SC-XRD structures with optimized positions of all hydrogen atoms (PBE, *optimizehydrogens true*), or optimized without constraints using the (ii.) PBE¹³ and (iii.) PBE0¹⁴ functionals at various spin states, including broken-symmetry states. The structural parameters obtained with the PBE functional gave a better fit with the experimental values found for **[2]²⁺** and **[2]⁺** in the solid state (*vide infra*). Scalar relativistic effects were considered within the Zeroth Order Regular Approximation (ZORA).¹⁵ The ZORA-def2-SVP basis set was used for all atoms except Mn, where the ZORA-def2-TZVP basis set was applied.¹⁶ The D3 dispersion correction¹⁷ with BJ damping was used. The RI (RIJCOSX, respectively)¹⁸ approximation and the related auxiliary basis set ("*SARC/J*")¹⁹ were used to speed up the calculations. Tighter than default scf ("*tightscf*") and optimization criteria ("*tightopt*") were chosen in conjunction with finer than default grid values ("*grid5*"; "*finalgrid6*"). Fully optimized ground state structures were verified as true minima by the absence ($N^{\text{imag}} = 0$) of negative eigenvalues in the harmonic vibrational frequency analysis. Localized orbitals (Figs. S16 - S20) were computed according to Knizia (IBOs) as single points using ZORA and the ZORA-def2-TZVPP basis set on all atoms; the results obtained with the PBE and PBE0 functionals were consistent.²⁰ Also the CASSCF calculations²¹ were performed using ZORA and the ZORA-def2-TZVPP basis set on all atoms using either the structural parameters from the solid state (**[2]²⁺**, **[2]⁺**) or the PBE-D3BJ optimized structures (**[2]**, **[2]³⁺**, **[2]⁴⁺**) and applying the RIJCOSX approximation. State averaging was applied (**[2]**: 1 sextet, 24 quartets, 75 doublets; **[2]⁺**: 50 singlets, 45 triplets, 5 quintets; **[2]²⁺**: 20 quartets, 40 doublets; **[2]³⁺**: 35 singlets, 25 triplets, 5 quintets; **[2]⁴⁺**: 1 sextet, 20 quartets, 40 doublets). See below for details on the choice of the active space. The spectroscopic parameters (*g*-, *D*-, *E*-values, absorption spectra) were calculated from state-averaged CASSCF/NEVPT2 calculations (*SARC/J*, *autoaux*, *nofrozencore*)²² followed by quasi-degenerate perturbation theory (QDPT; not in case of the absorption spectra shown below).²³ In case of **[2]³⁺**, only the triplets were state-averaged for the calculation of the *g*-, *D*-, and *E*-values. Absorption spectra obtained by time-dependent density functional theory (TD-DFT; PBE functional, 50 roots) calculations at the triple- ζ level of theory were performed employing the Tamm-Dancoff approximation (Figs. S21–S29).

Table S 5: Comparison of structural parameters in the solid state with PBE- and PBE0-calculated values.

[2]⁺	Mn-C	Mn-N		[2]⁺⁺	Mn-C	Mn-N
exp	2.078125	1.9702		exp	2.08025	1.93885
PBE	2.048075	1.9605		PBE	2.062275	1.94195
PBE0	2.038775	1.94945		PBE0	2.05835	1.9233

Choice of Active Space

Two strategies were followed to select the active space. In addition to the 5 *d*-orbitals, the lowest π -orbitals of each carbazolido ligand (and the antibonding combinations) were chosen. This leads overall to 9 orbitals, *i.e.* CASSCF(9,9) in case of **[2]**, CASSCF(8,9) for **[2]⁺** and CASSCF(7,9) for **[2]²⁺** as shown in Fig. S12. For **[2]³⁺** and **[2]⁴⁺**, further two π - and π orbitals of the carbazolido ligands were included (Fig. S13). A better description of the electronic structure would be obtained through additional inclusion of the MIC-based π^* orbitals (in combination with the bonding combinations), particularly for the low-valent complexes. However, active spaces derived from the 5 *d*-orbitals, 2 carbazolido π - (and π^*) orbitals as well as 4 MIC π^* orbitals, *i.e.* in case of **[2]⁴⁺** CASSCF(7,13) proved challenging to converge; additional inclusion of the bonding combinations, *i.e.* in case of **[2]⁴⁺** CASSCF(15,15) proved computationally too demanding.

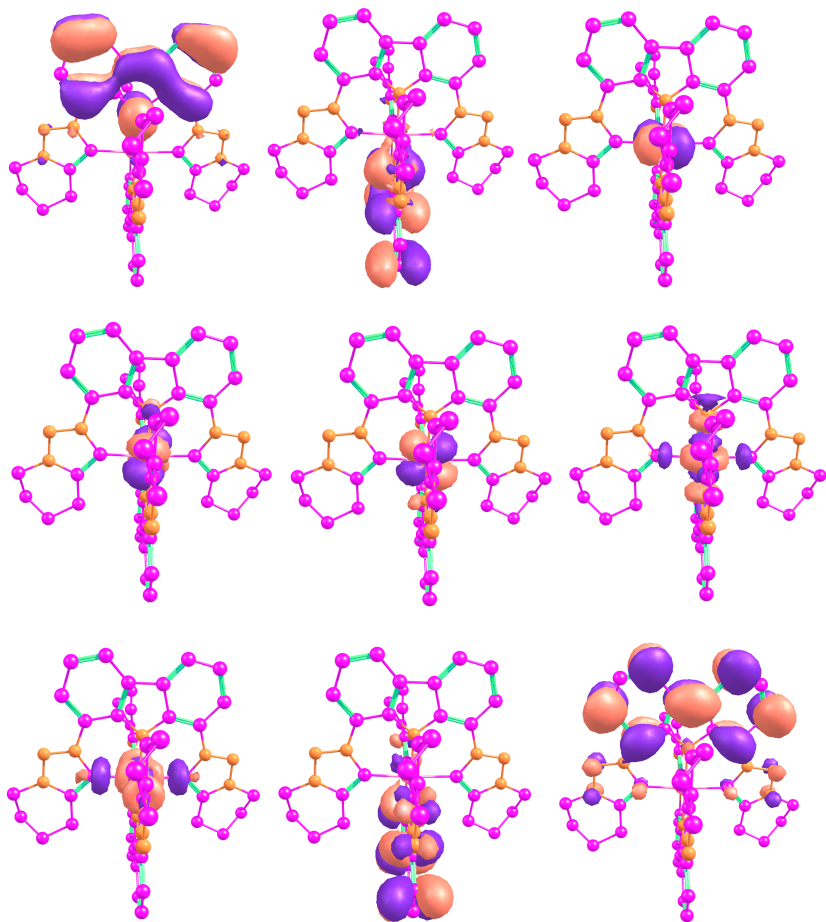


Figure S 16: Entire active space of sa-CASSCF(8,9) calculation in case of $[2]^+$. Active space for $[2]$ was chosen accordingly.

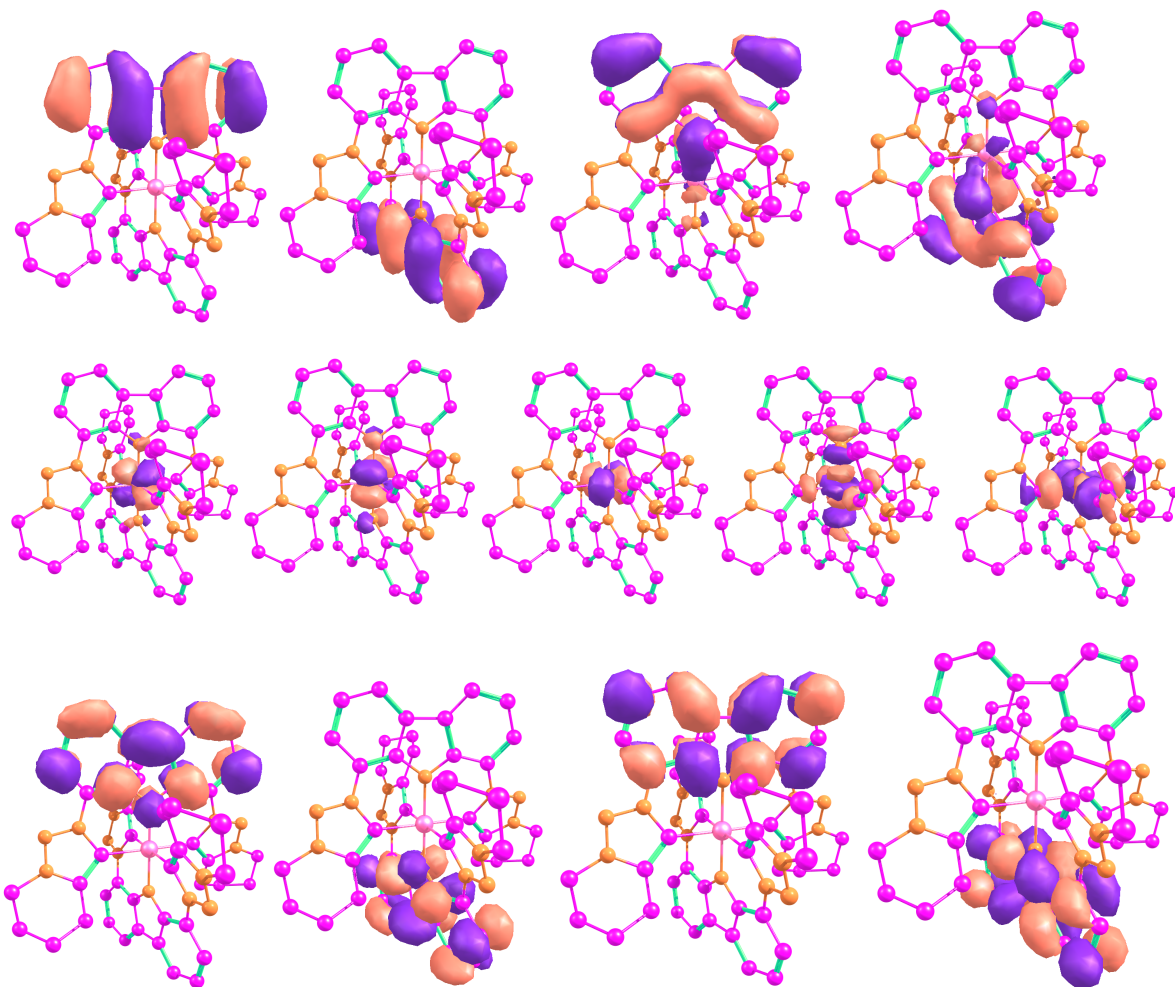


Figure S 17: Entire active space of sa-CASSCF(9,13) calculation in case of $[2]^{4+}$. Active space for $[2]^{3+}$ was chosen accordingly.

Table S 6: Configurations of sa-CASSCF(8,9) calculation for ground state of **[2]**.

0.94241 [0]: 222210000
 0.02158 [51]: 221211000
 0.00733 [66]: 221120100
 0.00508 [144]: 220212000
 0.00444 [24]: 222012000
 0.00412 [1385]: 112210011
 0.00383 [28]: 222010200
 0.00301 [1016]: 122220000

Table S 7: Configurations of sa-CASSCF(8,9) calculation for ground state of **[2]⁺**.

0.95772 [0]: 222110000
 0.01272 [79]: 220112000
 0.00352 [17]: 221200100
 0.00317 [35]: 221021000
 0.00309 [1767]: 022110002
 0.00288 [427]: 202110020
 0.00267 [83]: 220110200
 0.00260 [36]: 221020100

Table S 8: Configurations of sa-CASSCF(7,9) calculation for ground state of **[2]²⁺**.

0.35945 [50]: 211210000
 0.34995 [0]: 221110000
 0.11944 [356]: 121120000
 0.04856 [526]: 111220000
 0.03877 [357]: 121111000
 0.01561 [1]: 221101000
 0.00907 [529]: 111210010
 0.00523 [1087]: 021210001
 0.00391 [544]: 111120001
 0.00364 [78]: 211010200
 0.00328 [1094]: 021121000
 0.00324 [527]: 111211000
 0.00302 [100]: 210211000
 0.00289 [37]: 212100100
 0.00257 [207]: 201120010

Table S 9: Configurations of sa-CASSCF(10,13) calculation for **[2]³⁺** (for $S = 1$, which is predicted to be degenerate with $S = 0$).

0.37916 [0]: 2222110000000
 0.22621 [579]: 2212111000000
 0.10829 [762]: 2211121000000
 0.07332 [2057]: 2202112000000
 0.06619 [2512]: 2201122000000
 0.04735 [52]: 2221102000000
 0.01943 [227]: 2220112000000
 0.01850 [44]: 2221120000000

Table S 10: Configurations of sa-CASSCF(9,13) calculation for ground state of **[2]⁴⁺**.

0.74117 [264]: 2211111000000s
 0.08515 [11]: 2221101000000
 0.03754 [220]: 2212011000000
 0.03552 [212]: 2212101000000
 0.01387 [19]: 2221011000000
 0.01365 [1017]: 2201121000000
 0.01048 [412]: 2210211000000
 0.00891 [2]: 2222001000000
 0.00648 [447]: 2210121000000
 0.00436 [18865]: 1201111101000
 0.00436 [3616]: 2110111010100
 0.00391 [46562]: 0211111200000
 0.00386 [9212]: 2011111020000
 0.00346 [46573]: 0211111002000
 0.00341 [9221]: 2011111000200
 0.00331 [982]: 2201211000000

Electronic structure of [2], [2]²⁺, [2]³⁺ according to sa-CASSCF calculations

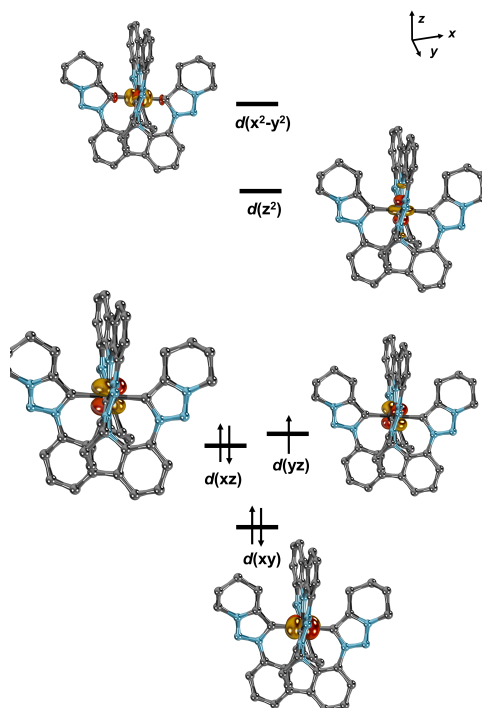


Figure S 18: Electronic Structure of **[2]** according to sa-CASSCF(7,9). Note: Placement of the unpaired electron seems more intuitive in the $d(xy)$ orbital. However, both saCASSCF as well as DFT calculations (vide infra) agree on lifted degeneracy of the $d(xz)$ and $d(yz)$ orbitals. Whereas this may be due to geometry-optimization with convergence to an “excited” Jahn-Teller state (“dynamic JT”; we did not manage convergence to the other distorted isomers), we conclude that this observation has no implications within the context of this manuscript.

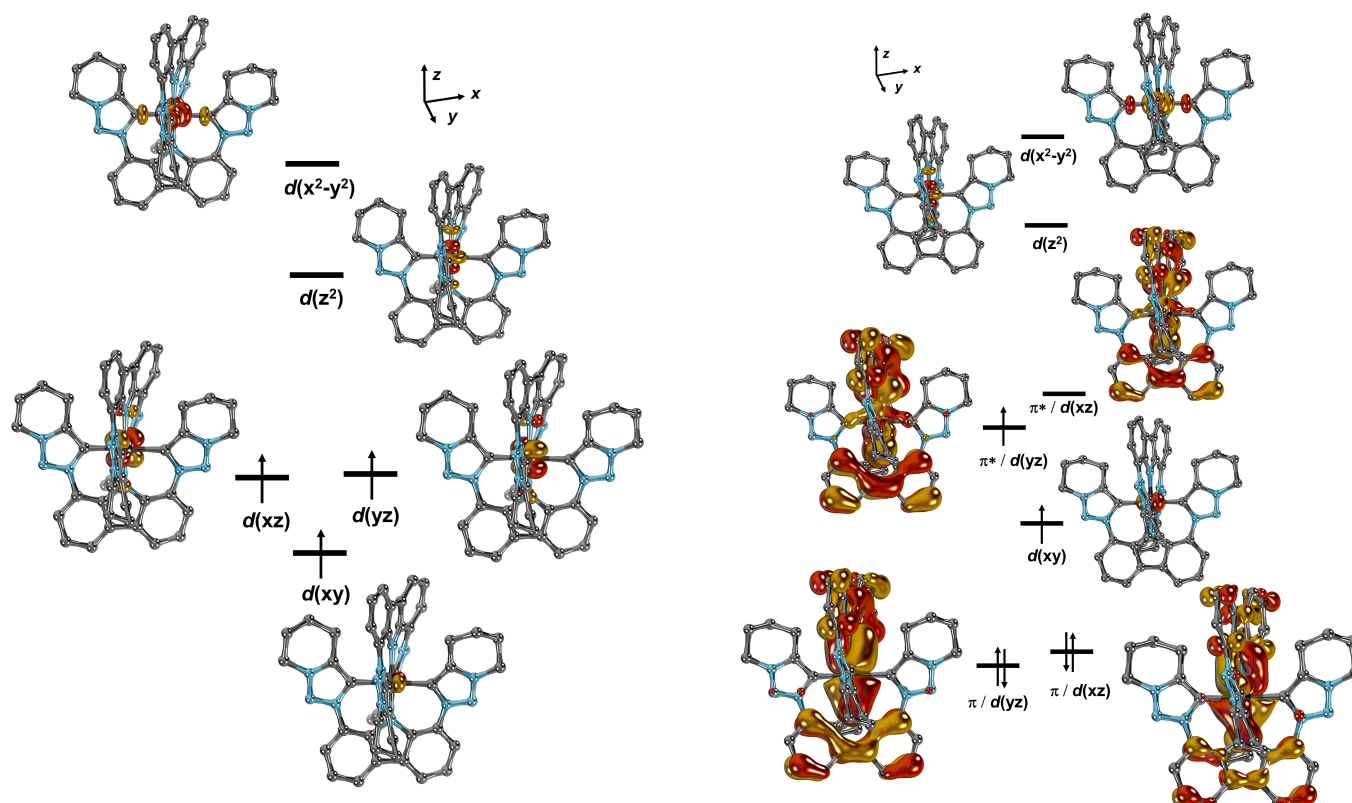


Figure S 19: Electronic Structure of **[2]²⁺** according to sa-CASSCF(9,9). (left); Electronic Structure of **[2]³⁺** according to sa-CASSCF(10,13) (right);

IBOs (PBE0)

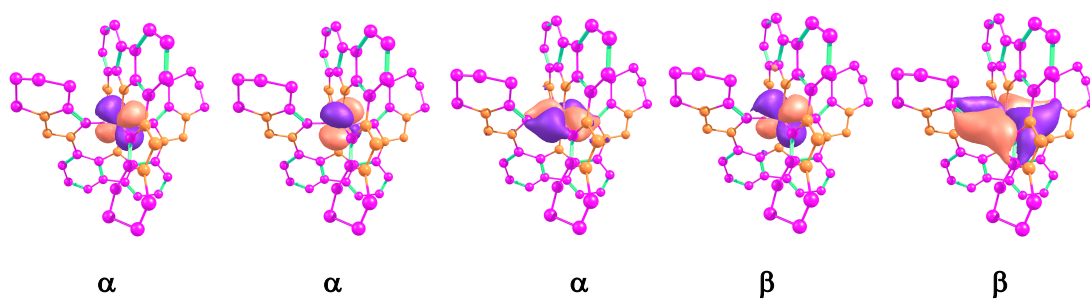


Figure S 20: Metal-centered IBOs of **[2]** ($S = 1/2$) obtained at the PBE0/def2-TZVPP//PBE0-D3BJ/def2-SVP level of theory.

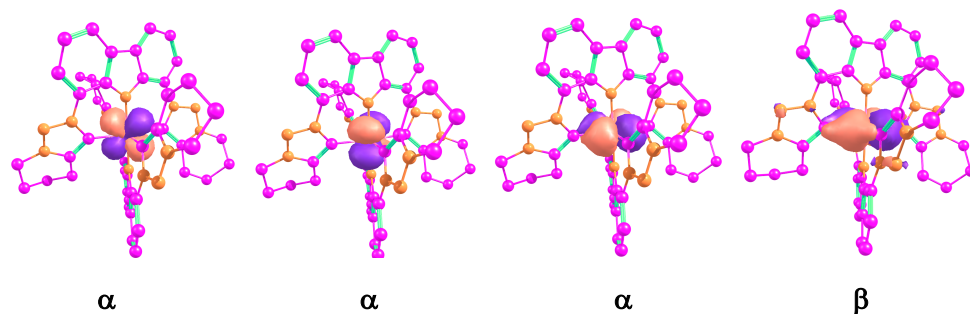


Figure S 21: Metal-centered IBOs of **[2]⁺** ($S = 1$) obtained at the PBE0/def2-TZVPP//PBE0-D3BJ/def2-SVP level of theory.

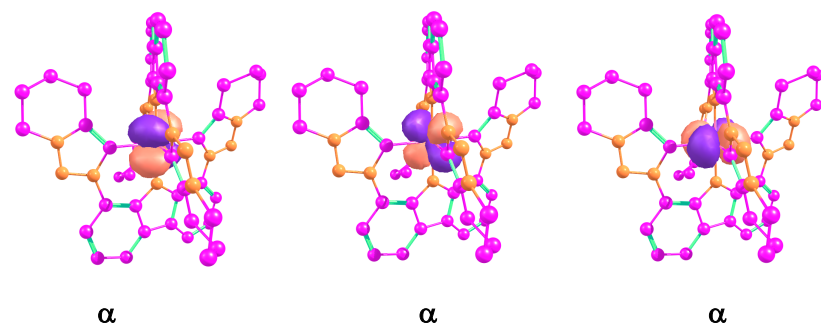


Figure S 22: Metal-centered IBOs of **[2]²⁺** ($S = 3/2$) obtained at the PBE0/def2-TZVPP//PBE0-D3BJ/def2-SVP level of theory.

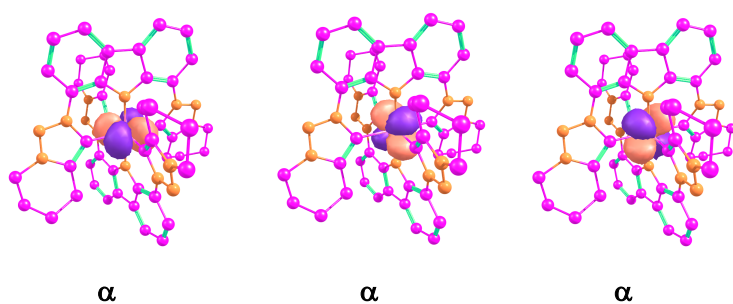


Figure S 23: Metal-centered IBOs of **[2]³⁺** ($S = 1$) obtained at the PBE0/def2-TZVPP//PBE0-D3BJ/def2-SVP level of theory.

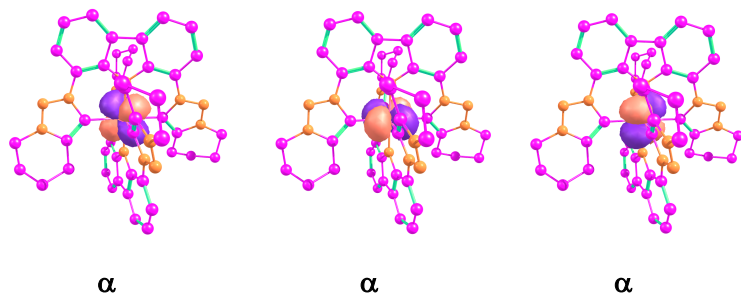


Figure S 24: Metal-centered IBOs of **[2]⁴⁺** ($S = 1/2$) obtained at the PBE0/def2-TZVPP//PBE0-D3BJ/def2-SVP level of theory.

Absorption spectra (CASSCF/NEVPT2)

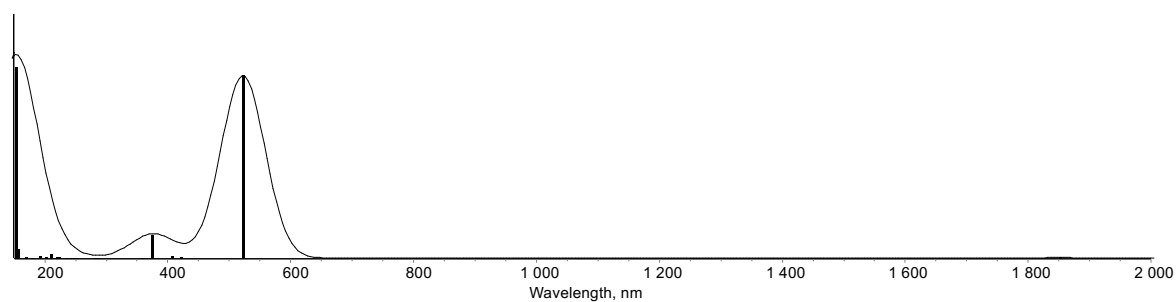


Figure S 25: Absorption spectrum of **[2]** ($S = 1/2$) as obtained at the CASSCF(9,9)/NEVPT2 level of theory. One strong transition beyond 2000 nm is omitted for clarity.

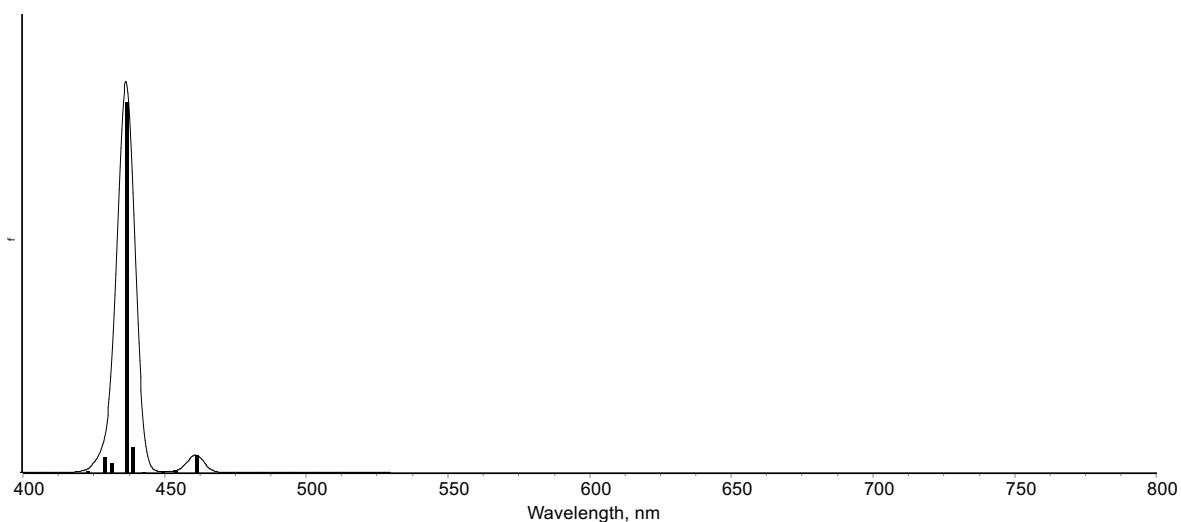


Figure S 26: Absorption spectrum of **[2]⁺** ($S = 1$) as obtained at the CASSCF(8,9)/NEVPT2 level of theory.

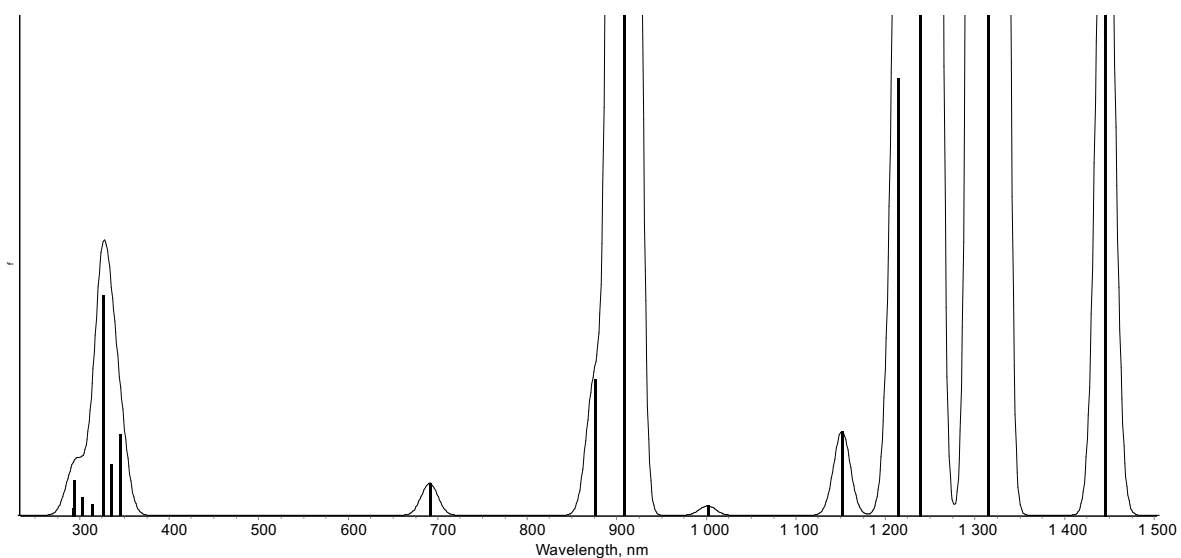


Figure S 27: Absorption spectrum of **[2]²⁺** ($S = 3/2$) as obtained at the CASSCF(7,9)/NEVPT2 level of theory.

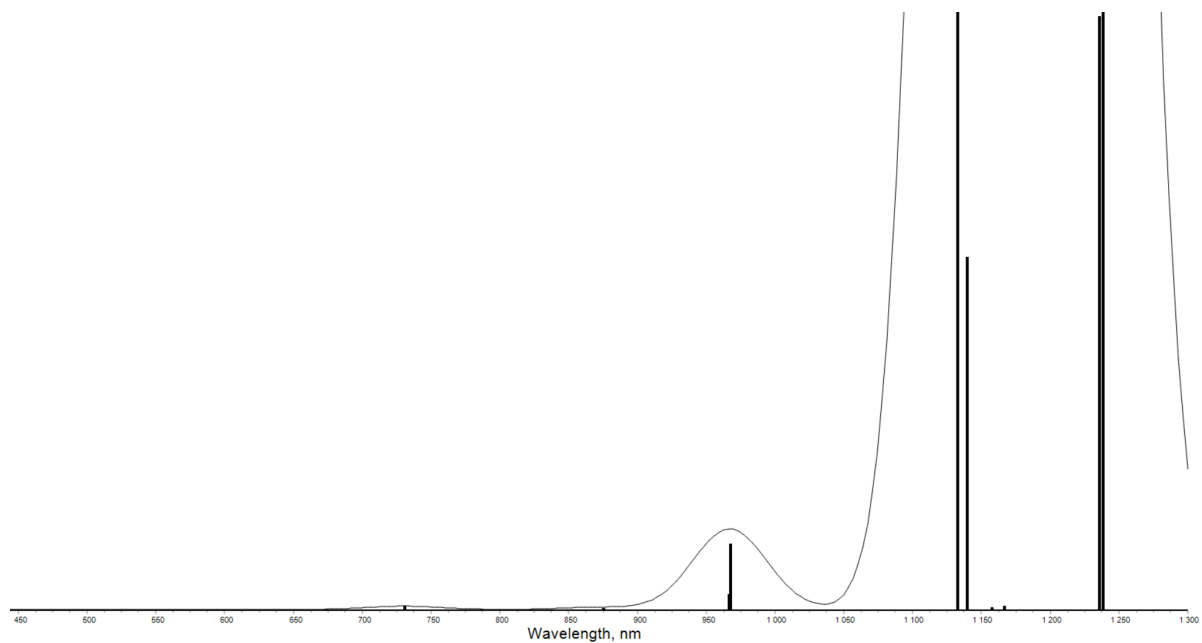


Figure S 28: Absorption spectrum of $[2]^{3+}$ ($S = 1$) as obtained at the CASSCF(7,9)/NEVPT2 level of theory (25 roots).

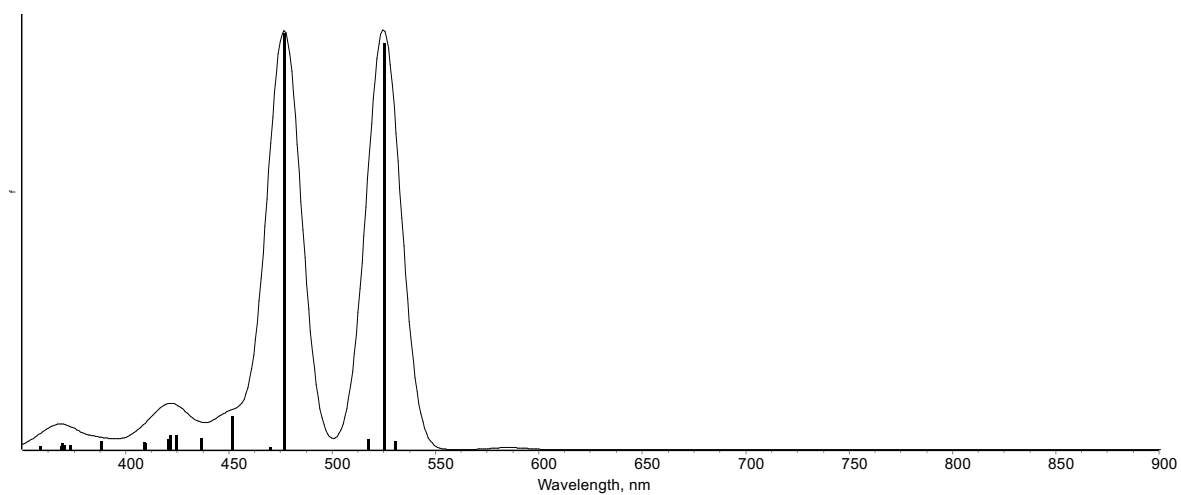


Figure S 29: Absorption spectrum of $[2]^{4+}$ ($S = \frac{1}{2}$) as obtained at the CASSCF(9,13)/NEVPT2 level of theory.

Absorption spectra (TDDFT)

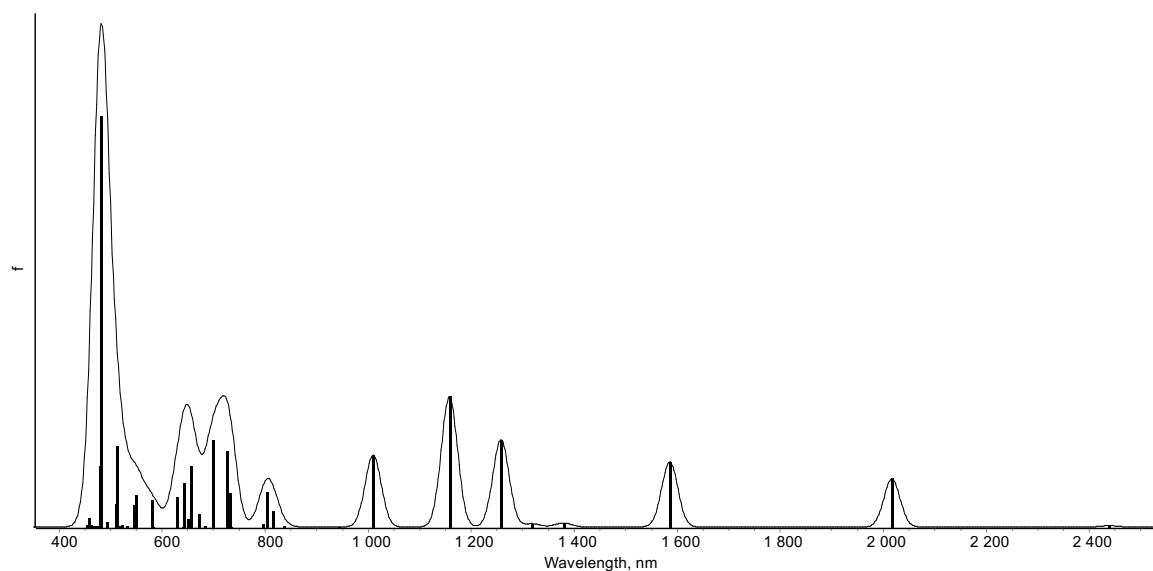


Figure S 30: Absorption spectrum of **[2]** ($S = 1/2$) as obtained at the PBE/def2-TZVPP//PBE-D3BJ/def2-SVP level of theory.

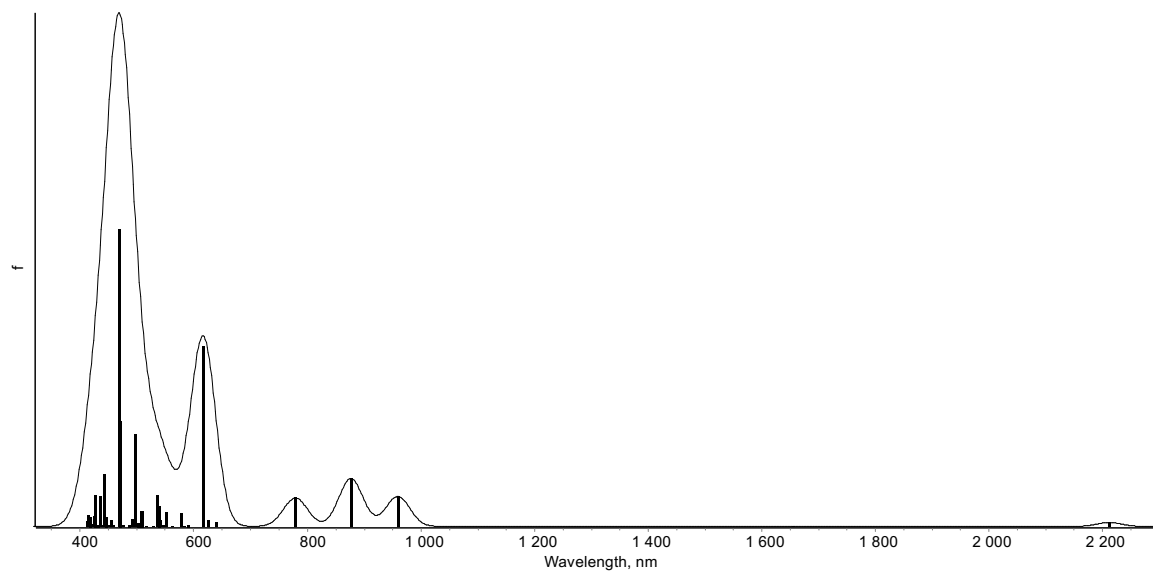


Figure S 31: Absorption spectrum of **[2]⁺** ($S = 1$) as obtained at the PBE/def2-TZVPP//PBE-D3BJ/def2-SVP level of theory.

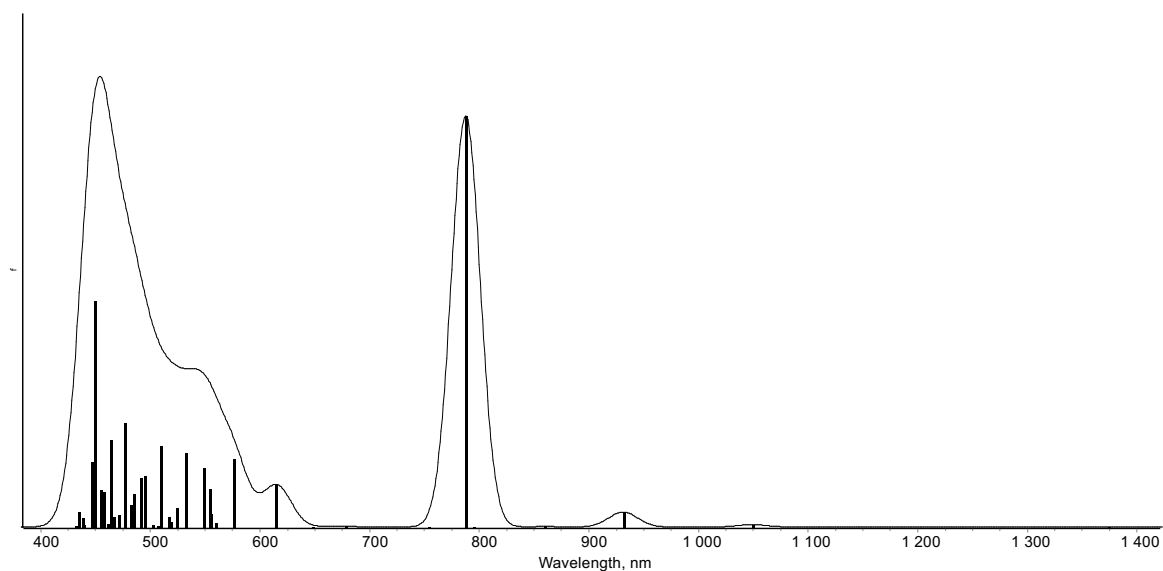


Figure S 32: Absorption spectrum of $[2]^{2+}$ ($S = 3/2$) as obtained at the PBE/def2-TZVPP//PBE-D3BJ/def2-SVP level of theory.

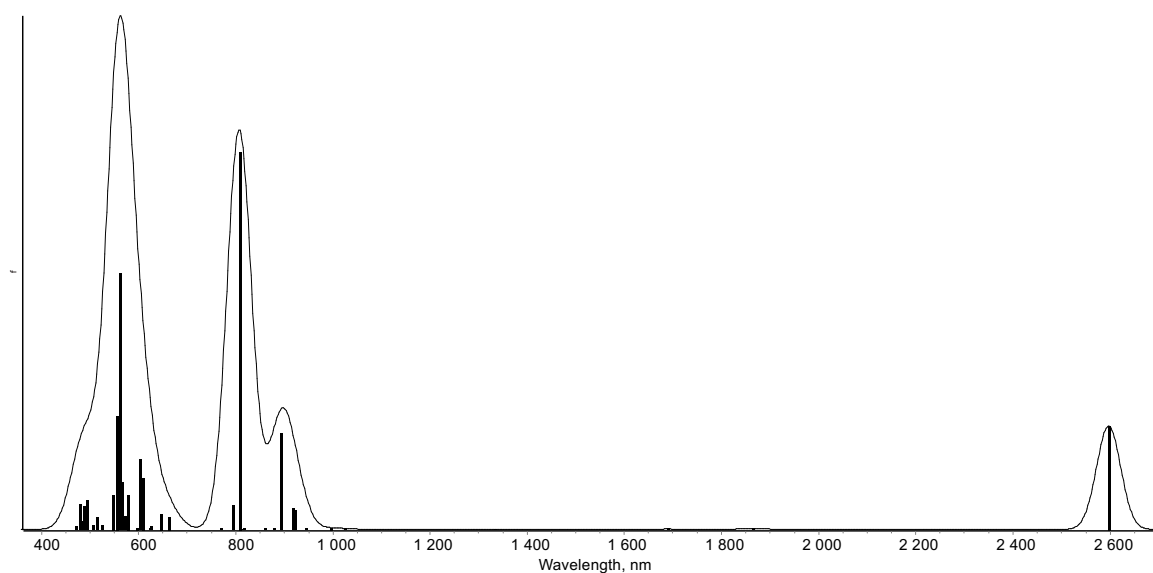


Figure S 33: Absorption spectrum of $[2]^{3+}$ ($S = 1$) as obtained at the PBE/def2-TZVPP//PBE-D3BJ/def2-SVP level of theory.

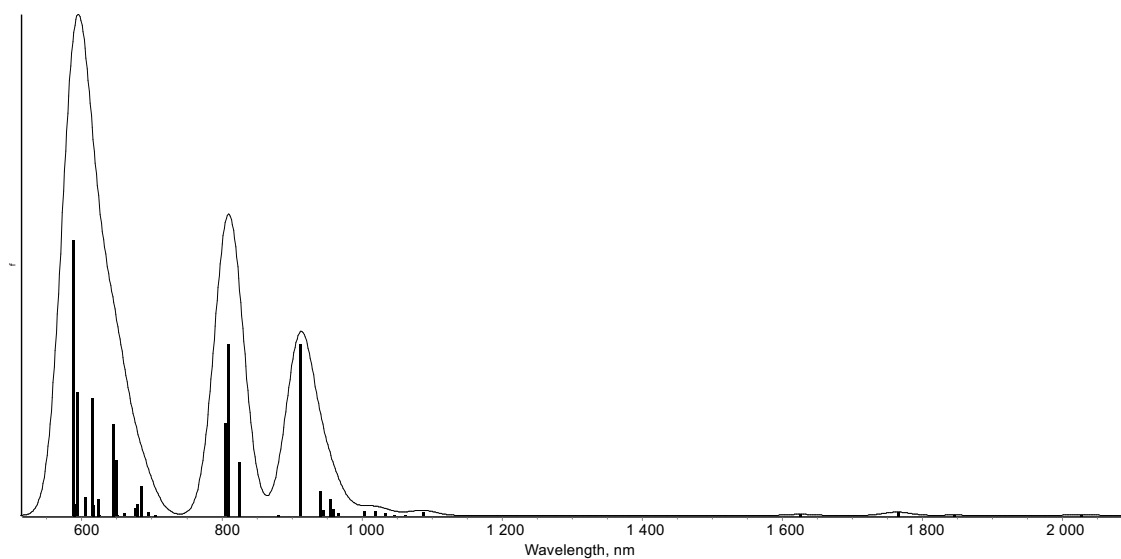


Figure S 34: Absorption spectrum of $[2]^{4+}$ ($S = 1/2$) as obtained at the PBE/def2-TZVPP//PBE-D3BJ/def2-SVP level of theory.

Table S 11: Energies of geometry-optimized structures.

		PBE				PBE0			
Comp.	Spin	E	ΔE	G	$E(\text{SP, TZVPP})$	E	ΔE	G	$E(\text{SP, TZVPP})$
		[Eh]	[kJ mol ⁻¹]	[Eh]	[Eh]	[Eh]	[kJ mol ⁻¹]	[Eh]	[Eh]
[2]	0.5	-3781.9787	0.0	-3781.20036	-3784.69701	-3782.06027	0.0	-3781.24886	-3784.78758
	1.5	-3781.96537	35.0		-3784.683959	-3782.04928	28.9		-3784.77696
	2.5	-3781.91875	157.4		-3784.63776	-3782.00197	153.1		-3784.72956
[2] ⁺	0	-3781.8108	86.0		-3784.527003	-3781.88903	136.9		-3784.61522
	0 (UKS)	-3781.8275	42.2		-3784.543313	-3781.9195	56.9		-3784.61157
	1	-3781.84356	0.0	-3781.06142	-3784.55884	-3781.94116	0.0	-3781.12629	-3784.66711
	2	-3781.79794	119.8		-3784.51377	-3781.88472	148.2		-3784.61073
[2] ²⁺	0.5	-3781.55663	53.3		-3784.271257	-3781.6395	98.4		-3784.35708
	1.5	-3781.57693	0.0	-3780.79436	-3784.290847	-3781.67697	0.0	-3780.8618	-3784.40136
	2.5	-3781.49254	221.6		-3784.20738	-3781.57875	257.9		-3784.3044
[2] ³⁺	0	-3781.14335	82.6		-3783.858997	-3781.18189	199.8		-3783.90969
	0 (UKS)	-3781.15639	48.3		-3783.871741	-3781.23074	71.5		-3783.95899
	1	-3781.1748	0.0	n.a.	-3783.887039	-3781.25797	0.0	-3780.4432	-3783.98514
	2	-3781.1684	16.8		-3783.882999	-3781.25682	3.0		-3783.98371
[2] ⁴⁺	0.5	-3780.66664	0.0	-3769.71273	-3783.38101	-3780.74841	0.0	-3779.93564	-3783.47905
	1.5	-3780.65837	21.7		-3783.375205	-3780.74186	17.2		-3783.47239
	2.5	-3780.64556	33.6		-3783.36201	-3780.73469	18.8		-3783.46501

Table S 11: Absorption spectrum via transition electric dipole moments calculated by TDDFT for [2]⁺ (S=1)

Energy (cm ⁻¹)	Wavelength (nm)	f^{osc} (au ²)	T _z (au)	T _x (au)	T _y (au)	T _z (au)	Main Character
4521.4	2211.7	0.001331	0.0969	0.00349	0.14712	-0.2743	M → M
6046.4	1653.9	4.61E-05	0.00251	0.00007	0.04463	0.02275	M → M
10423.9	959.3	0.010329	0.32621	0.00542	0.26911	-0.50375	M → ML
11405.8	876.7	0.016544	0.47752	0.05832	0.60703	0.32502	M → L
12837.2	779	0.009811	0.25159	-0.50123	0.0188	0.00364	M → L
13625.8	733.9	5.32E-06	0.00013	-0.00278	0.00449	-0.01004	M → ML
14399.7	694.5	5.33E-06	0.00012	-0.01097	-0.00012	0.00116	ML → M
15681.5	637.7	0.001161	0.02438	-0.1561	0.0032	-0.00015	ML → M
16010.3	624.6	0.001983	0.04077	-0.20153	0.01169	0.00359	ML → L
16223.9	616.4	0.062356	1.26531	-1.1245	0.02827	0.0037	ML → M
16987	588.7	0.000603	0.01169	-0.00387	-0.05082	0.09536	ML → L
17147.3	583.2	8.36E-05	0.00161	-0.00249	-0.01726	0.03607	ML → L
17309.7	577.7	0.004529	0.08613	0.00265	0.13883	-0.25855	M → L
17799.6	561.8	1.37E-05	0.00025	-0.00507	-0.00619	0.01375	ML → M
18163.6	550.6	0.004747	0.08603	0.28731	0.05064	0.03031	ML → L
18324.6	545.7	0.000374	0.00672	-0.01916	-0.0699	-0.03824	L → ML
18500.4	540.5	0.002101	0.03739	-0.00815	0.17172	0.08852	M → L
18555.2	538.9	0.006997	0.12414	-0.00414	-0.16097	0.31339	ML → L
18710.1	534.5	0.010679	0.18791	-0.04386	-0.38156	-0.20099	ML → L
18985.3	526.7	5.05E-05	0.00088	-0.00033	-0.01433	0.02589	L → ML
19376.2	516.1	0.000126	0.00214	-0.00041	-0.02097	0.04119	ML → ML
19625.2	509.6	0.005319	0.08922	-0.08774	0.25047	0.13705	ML → L
19768.2	505.9	0.005373	0.08948	0.00065	0.14411	-0.26213	ML → L
19923.8	501.9	0.000979	0.01617	0.0003	0.06112	-0.11153	L → M
19949.6	501.3	0.000436	0.0072	0.07012	-0.04076	-0.02501	ML → L
20173.3	495.7	0.031786	0.51872	0.72018	-0.00685	0.004	ML → L
20367.8	491	0.002368	0.03828	0.04245	0.16839	0.09013	ML → L
20557.2	486.4	0.000628	0.01005	-0.00078	0.08841	0.04731	L → M
21063.3	474.8	0.000213	0.00333	-0.00992	0.02716	-0.04995	ML → L
21262.9	470.3	0.036643	0.56734	0.63445	-0.35799	-0.19147	ML → L

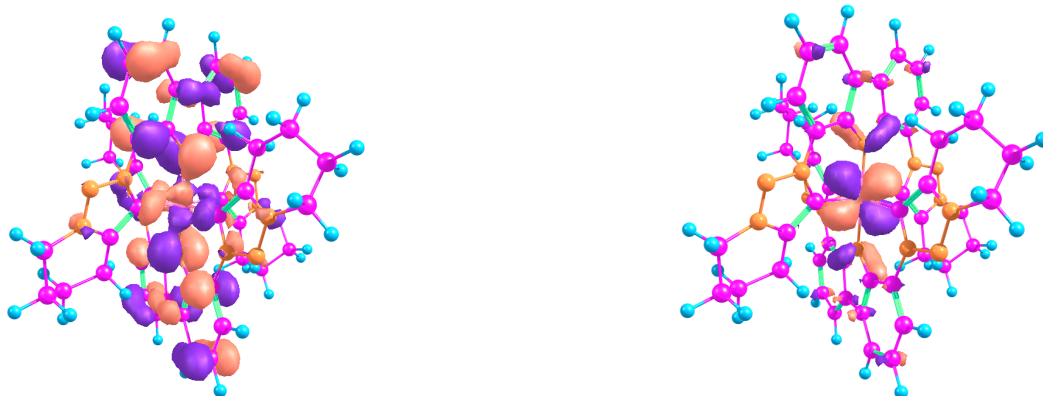


Figure S 35: Orbitals of $[2]^+(S = 1)$ obtained at the PBE/def2-TZVPP//PBE-D3BJ/def2-SVP level of theory and involved in the transition occurring at 16223.9 cm^{-1} (see Table S11).

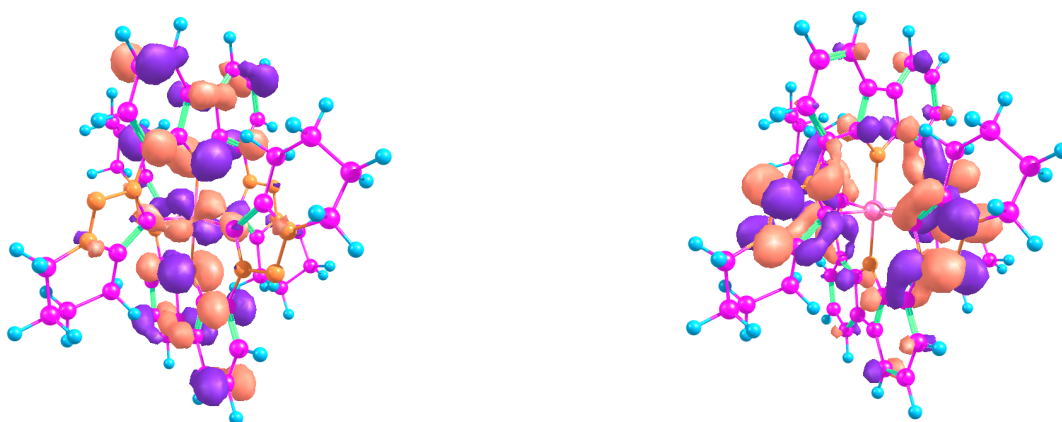


Figure S 36: Orbitals of $[2]^+(S = 1)$ obtained at the PBE/def2-TZVPP//PBE-D3BJ/def2-SVP level of theory and involved in the transition occurring at 18710.1 cm^{-1} (see Table S11).

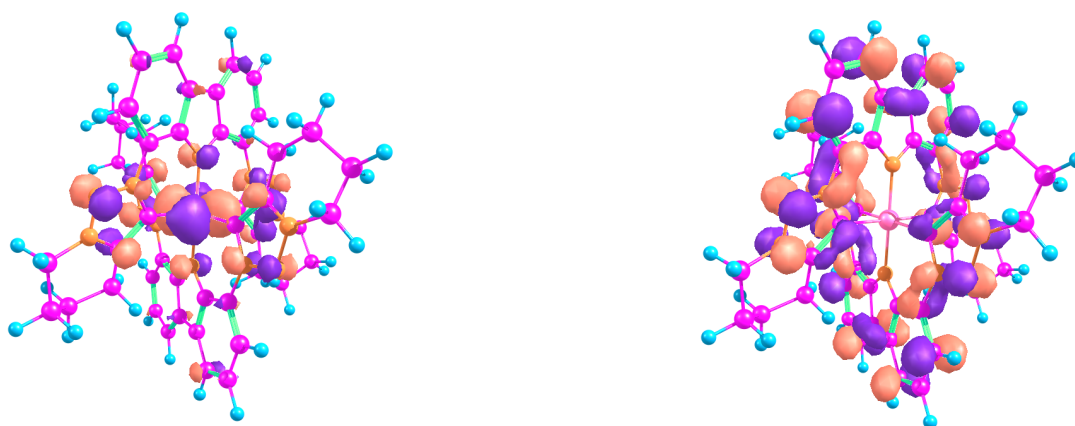


Figure S 37: Orbitals of $[2]^+(S = 1)$ obtained at the PBE/def2-TZVPP//PBE-D3BJ/def2-SVP level of theory and involved in the transition occurring at 20173.3 cm^{-1} (see Table S11).

XYZ Coordinates [PBE]

[2]_d
107

Mn	7.31172323885266	18.89894361744900	5.25508016477430
N	5.34796303324933	18.94829860881268	5.25684542063092
N	9.27610318633280	18.85443325897671	5.24310848026907
N	6.25031784510371	20.13292128177396	7.84088402150576
N	7.76649175009055	20.20710053193346	9.27217591000306
N	6.50655791279009	20.56281163345907	9.09515583062496
N	8.34547879367202	16.05371886455034	5.67321255828414
N	8.46389533648025	21.70134831397317	4.88455325810606
N	6.95443941955750	23.00102167530477	4.26276660481592
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C	12.92525867060034	7.94947204182653	23.08820819049399
H	11.82438767367698	7.88884373238280	23.12041738406912
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C	15.23066973371670	16.01031072742328	21.66332690123355
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C	13.73371902436961	16.18240758089381	21.38580518194604
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C	7.53271911811514	14.52925842180252	24.94919618033709
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H	6.49047168221315	14.46111540189024	24.59564408802537
C	7.75324509705648	13.85256973959788	26.29905683900257
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C	9.25009525520254	13.66345601420315	26.56589789189725
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H	9.76348269911885	14.64402595219747	26.53847018970042
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XYZ Coordinates [ZORA-PBE0-D3BJ/def2-SVP(def2-TZVP on Mn)]

[2]_d
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N	8.50391981962641	21.67138526197871	4.81961685062862
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C	6.44056722804167	21.73780492077100	4.22213920158183
C	4.52666324524808	18.36961381074297	4.31126367781542
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C	10.07575810325372	17.72772620199405	5.28991147676248
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C	9.69141513598779	16.38425543554975	5.46336181118017
C	12.54140862424860	20.43271580628925	5.19140590717729
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C	8.26123964269944	20.12129923492167	10.63287063987316
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H	11.21716783283473	18.60346965262380	9.71985242397232
H	10.75096705787881	20.29186225698119	9.58500974656075
C	12.21074577308544	21.78416790602362	5.14214232331970
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H	10.62537847259546	23.24802355641521	4.96300092978549
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H	13.50009751954402	17.30980869624685	5.21903007311872
C	8.25509151610175	17.40552370447419	-0.08232645950417
H	7.75824447549933	18.07630200680694	-0.79523517720414
H	8.01755204171806	16.37722960052762	-0.37549029426745
C	9.40061123623658	19.13193413315155	10.78129388515084
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C	6.21895094498148	13.75991453349418	7.20180308430723
H	7.00601684716484	13.20289095050677	7.71974121971128
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C	5.04125239695473	21.56158587098437	3.73618911974044
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C	9.62449282566218	18.80697098452287	2.18271658872266
H	10.33750766501856	18.15233119643966	2.70579721639984
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H	6.72434920414644	24.99265885696416	4.32368167753590
C	9.74963084437769	17.66912238606571	-0.04016425767616
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H	4.58985473709094	13.37140162508835	8.54057289198206
H	5.57696566582633	14.76933512952321	8.98500016580773
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N	7.68144714841549	19.93836857659590	9.34686183387034
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N	8.52542934687721	21.61292102933920	4.80626458189339
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C	2.19156507696006	19.93027154223096	6.6408733778248
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C	8.19690610162858	18.41926673310039	2.29341012172804
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C	6.28525141904722	16.13166917496308	6.48509963971797
C	11.44138588587825	17.98147103869986	5.26726703523503
C	9.83708479704634	21.21199739308291	5.10459648279635
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C	9.66554610278491	16.31687403485864	5.48329683814946
C	12.53991380474625	20.35167858596898	5.24103667402336
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C	8.27470810948378	20.07800819898987	10.66396824005767
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H	14.51857265937175	11.90385740348061	16.21698252988139
H	8.13489316609333	7.15316219372136	26.18525017548410
H	14.62147902767355	10.71380461188856	28.06229812874048

13. Literature

- 1 P. Pinter, C. M. Schüßlbauer, F. A. Watt, N. Dickmann, R. Herbst-Irmer, B. Morgenstern, A. Grünwald, T. Ullrich, M. Zimmer, S. Hohloch, D. M. Guldi and D. Munz, *Chem. Sci.*, 2021, **12**, 7401–7410.
- 2 N. F. Chilton, R. P. Anderson, L. D. Turner, A. Soncini and K. S. Murray, *J. Comput. Chem.*, 2013, **34**, 1164–1175.
- 3 P. Neugebauer, D. Bloos, R. Marx, P. Lutz, M. Kern, D. Aguilà, J. Vaverka, O. Laguta, C. Dietrich, R. Clérac and J. van Slageren, *Phys. Chem. Chem. Phys.*, 2018, **20**, 15528–15534.
- 4 S. Stoll and A. Schweiger, *J. Magn. Reson.*, 2006, **178**, 42–55.
- 5 a) O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, *J. Appl. Crystallogr. (Journal of Applied Crystallography)*, 2009, **42**, 339–341; b) G. M. Sheldrick, *Acta Cryst. A*, 2015, **71**, 3–8;
- 6 A. L. Spek, *Acta Cryst. C*, 2015, **71**, 9–18.
- 7 A. P. Forshaw, R. P. Bontchev and J. M. Smith, *Inorg. Chem.*, 2007, **46**, 3792–3794.
- 8 D. C. L. de Alwis and F. A. Schultz, *Inorg. Chem.*, 2003, **42**, 3616–3622.
- 9 T. Gennett, D. F. Milner and M. J. Weaver, *J. Phys. Chem.*, 1985, **89**, 2787–2794.
- 10 M. K. Chan and W. H. Armstrong, *Inorg. Chem.*, 1989, **28**, 3777–3779.
- 11 N. Leconte, J. Moutet, K. Herasymchuk, R. M. Clarke, C. Philouze, D. Luneau, T. Storr and F. Thomas, *Chem. Commun.*, 2017, **53**, 2764–2767.
- 12 a) F. Neese, *Wiley Interdiscip. Rev.: Comput. Mol. Sci.*, 2018, **8**, e1327; b) F. Neese, *Wiley Interdiscip. Rev.: Comput. Mol. Sci.*, 2012, **2**, 73–78;
- 13 J. P. Perdew, K. Burke and M. Ernzerhof, *Phys. Rev. Lett.*, 1996, **77**, 3865–3868.
- 14 C. Adamo and V. Barone, *J. Chem. Phys.*, 1999, **110**, 6158–6170.
- 15 a) E. v. Lenthe, E. J. Baerends and J. G. Snijders, *J. Chem. Phys.*, 1993, **99**, 4597–4610; b) C. van Wüllen, *J. Chem. Phys.*, 1998, **109**, 392–399;
- 16 a) D. A. Pantazis, X.-Y. Chen, C. R. Landis and F. Neese, *J. Chem. Theor. Comput.*, 2008, **4**, 908–919; b) F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.*, 2005, **7**, 3297–3305;
- 17 a) S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys.*, 2010, **132**, 154104; b) S. Grimme, S. Ehrlich and L. Goerigk, *J. Comput. Chem.*, 2011, **32**, 1456–1465;
- 18 a) F. Neese, F. Wennmohs, A. Hansen and U. Becker, *Chem. Phys.*, 2009, **356**, 98–109; b) R. Izsák and F. Neese, *J. Chem. Phys.*, 2011, **135**, 144105;
- 19 F. Weigend, *Phys. Chem. Chem. Phys.*, 2006, **8**, 1057–1065.
- 20 G. Knizia and J. E. M. N. Klein, *Angew. Chem. Int. Ed.*, 2015, **54**, 5518–5522.
- 21 B. O. Roos, P. R. Taylor and P. E. M. Siegbahn, *Chem. Phys.*, 1980, **48**.
- 22 C. Angeli, R. Cimiraglia, S. Evangelisti, T. Leininger and J. P. Malrieu, *J. Chem. Phys.*, 2001, **114**, 10252–10264.
- 23 B. A. Heß, C. M. Marian, U. Wahlgren and O. Gropen, *Chem. Phys.*, 1996, **251**, 365–371.

14. Author Contributions

The project was developed by SH. Synthetic work was conducted by BW, ND, SB and RG. X-band EPR measurements were conducted by NIN and LD. HF-EPR and magnetic measurements were conducted and analyzed by LT. MCD was recorded by DH and analyzed by DH and LT. Computational investigations have been performed by DM. The manuscript was written by BW, LT, JvS, DM and SH and proof-read / approved by all authors.