

Electronic Supplementary Information

Evidence for a Lowest Energy MLCT Excited State in $[\text{Fe}(\text{tpy})(\text{CN})_3]^-$

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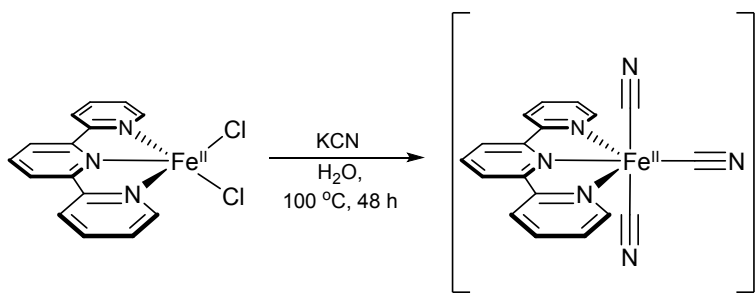
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Experimental Methods

Synthesis

All reagents and solvents were used as received. The reactions were performed using standard Schlenk techniques with dry solvents under inert gas atmosphere.



Scheme S1. Reaction scheme for the $[\text{Fe}^{\text{II}}(\text{tpy})(\text{CN})_3]^{-}$ complex.

The prepared $\text{Fe}^{\text{II}}(\text{tpy})\text{Cl}_2$ complex² in deionized water was brought to reflux under N_2 (g). To the solution, potassium cyanide (KCN) was added. The reaction mixture was magnetically stirred and refluxed for 48 hours under N_2 (g). Afterwards, the solution was cooled and filtered *in vacuo* using a fine fritted funnel. To the filtrate, cold EtOH (200) was added and cooled to promote precipitation of excess KCN from the mixture. The excess KCN was filtered off using a fine fritted funnel. This process was repeated until the white solid indicative of KCN was no longer observed. The remaining solution was concentrated, dissolved in a minimum amount of ethanol and precipitated into cold diethyl ether/ethanol mixture with equal parts of both solvents. The dark purple complex was collected on a fine fritted funnel and washed three times with 15 mL diethyl ether/ethanol and once with 15 mL of diethyl ether. Crystals suitable for X-ray crystallography were obtained by dissolving approximately 20 mg of the complex in EtOH (200) within a scintillation vial from which, the solvent evaporated over the course of several days under ambient conditions providing dark purple crystals. ¹H-NMR (300 MHz, RT, Methanol-*d*₄): δ (ppm) 8.87 (2 H, d, *J* = 5.5), 8.40 (2 H, d, *J* = 6.9), 8.24 (2 H, d, *J* = 8.0), 8.07 (1 H, t, *J* = 7.6), 7.83 (2 H, t, *J* = 7.8), 7.35 – 7.26 (2 H, m). ESI-MS: calculated *m/z* = 367.0395, observed *m/z* = 367.0401.

Other Fe(II) complexes of interest – $[\text{Fe}^{\text{II}}(\text{bpy})_2(\text{CN})_2]$ and $[\text{K}]_2[\text{Fe}^{\text{II}}(\text{bpy})(\text{CN})_4]$ were prepared according to literature methods.¹

1. *J. Am. Chem. Soc.* 1960, 82, 12, 3000–3005.
2. *U.S. Pat. Appl. Publ.* 7 pp., Chemical Indexing Equivalent to 154:109813 (WO) Patent 2011 CODEN:USXXCO

Computational methodology

All complexes were optimized in their singlet ground states at the B3LYP¹ level of theory with Grimme's D2 dispersion correction,² SDD effective core potential and the associated basis set³ on Fe and 6-311G*

basis set⁴ on all other atoms. A polarizable continuum model (PCM) was employed to account for solvation effects with water as the solvent.⁵ An ultrafine integral grid was employed for all calculations. This same level of theory was previously successfully used to describe electronic structure of Fe(II)-polypyridine complexes, and was shown to yield spin-state energetics similar to that obtained with the optimized B3LYP* functional.⁶ Time-dependent density functional theory (TD-DFT)⁷ was employed to obtain energies of the lowest-lying ^{1,3}MLCT and ³MC states, with the optimized singlet ground state utilized as the reference state for the TD-DFT calculations. The energies of ^{3,5}MC states were also obtained from single-point energy calculations at the optimized geometry of the singlet ground state. The character of the ^{3,5}MC states from the single-point energy calculations was confirmed via natural orbital analysis. All wavefunctions obtained from the DFT calculations were also tested for stability. Gaussian 09 revision D.01 was employed for all electronic structure calculations.⁸

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5. Scalmani, G.; Frisch, M. J. *J. Chem. Phys.* **2010**, 132, 114110 DOI: 10.1063/1.3359469
6. Nance, J.; Bowman, D. N.; Mukherjee, S.; Kelley, C. T.; Jakubikova, E. *Inorg. Chem.* 2015, 54, 23, 11259– 11268 DOI: 10.1021/acs.inorgchem.5b01747; Mukherjee, S.; Liu, C.; Jakubikova, E. *J. Phys. Chem. A* 2018, 122, 7, 1821–1830; DOI: 10.1021/acs.jpca.7b10932; Ashley, D. C.; Jakubikova, E. *Inorg. Chem.* 2018, 57, 9, 5585–5596 DOI: 10.1021/acs.inorgchem.8b00560
7. Bauernschmitt, R.; Ahlrichs, R. *Chem. Phys. Lett.* **1996**, 256, 454– 464 DOI: 10.1016/0009-2614(96)00440-X; Casida, M. E.; Jamorski, J.; Casida, K. J.; Salahub, D. R. *J. Chem. Phys.* **1998**, 108, 4439– 4449 DOI: 10.1063/1.475855; Stratmann, R. E.; Scuseria, G. E.; Frisch, M. J. *J. Chem. Phys.* **1998**, 109, 8218– 8224 DOI: 10.1063/1.477483
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Structural Characterization

^1H NMR

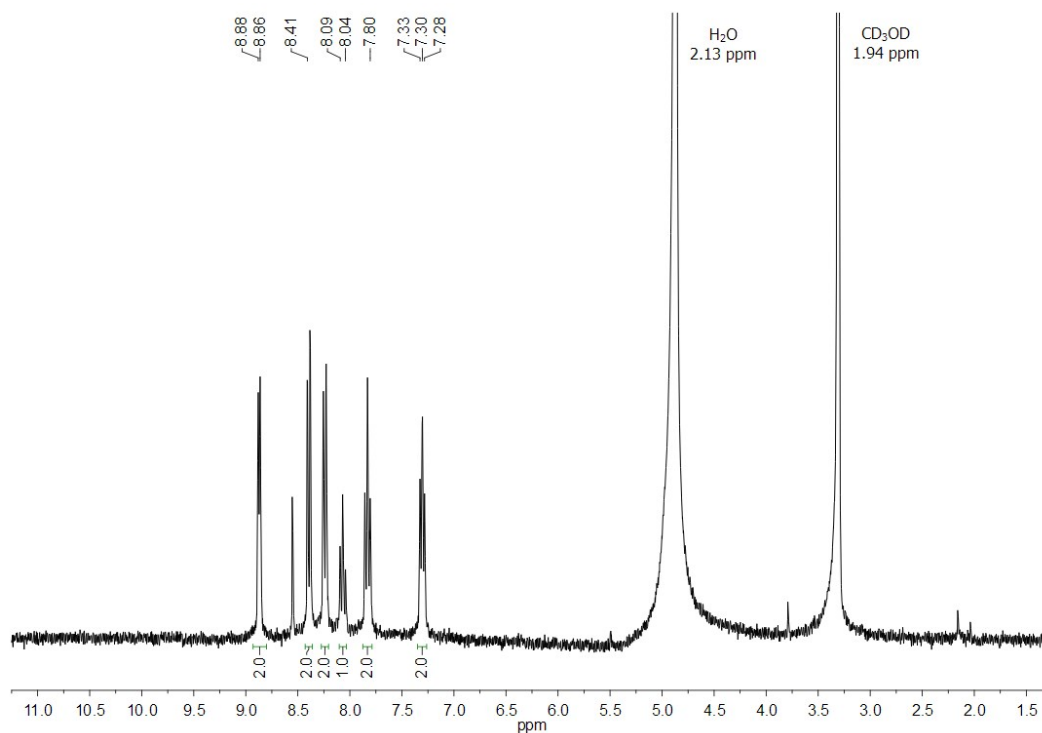


Figure S1. ^1H NMR (300 MHz, CD_3OD) of $[\text{K}][\text{Fe}^{\text{II}}(\text{tpy})(\text{CN})_3]$.

FTIR

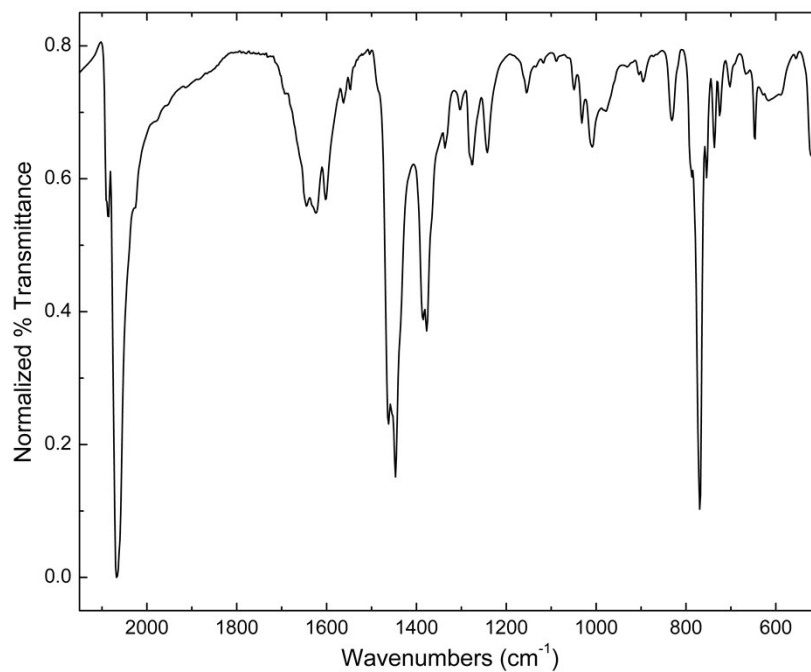


Figure S2. Infrared spectrum of $[Fe^{II}(tpy)(CN)_3]$. The complex was incorporated into Nujol and staged between potassium bromide (KBR) disks for spectroscopic analysis.

X-ray crystallography

X-ray intensity data were measured on a Bruker PHOTON II CPAD-based diffractometer with dual Cu/Mo ImuS microfocus optics (Cu $K\alpha$ radiation, $\lambda = 1.54178 \text{ \AA}$, Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$). Crystals were mounted on a cryoloop using Paratone oil and placed under a stream of nitrogen at 100 K (Oxford Cryosystems). The detector was placed at a distance of 5.00 cm from the crystal. The data were corrected for absorption with the SADABS program. The structures were refined using the Bruker SHELXTL Software Package (Version 6.1),¹ and were solved using direct methods until the final anisotropic full-matrix, least squares refinement of F^2 converged.

1. Sheldrick, G. M. A Short History of SHELX. *Acta Crystallogr. Sect. A Found. Crystallogr.* **2008**, *64*, 112–122. <https://doi.org/10.1107/S0108767307043930>.

Bond precision:	C-C = 0.0020 Å	Wavelength = 0.71073	
Cell:	a = 10.1464(6) alpha = 77.100(3)	b = 13.1580(9) beta = 79.360(3)	c = 14.5400(11) gamma = 79.807(3)
Temperature:	100 K		
	Calculated	Reported	
Volume	1840.9(2)	1840.9(2)	
Space group	P -1	P -1	
Hall group	-P 1	-P 1	
Moiety formula	C36 H26 Fe2 K2 N12 O2, 2(H2 O)	?	
Sum formula	C36 H30 Fe2 K2 N12 O4	C36 H30 Fe2 K2 N12 O4	
Mr	884.62	884.62	
Dx, g cm ⁻³	1.596	1.596	
Z	2	2	
Mu (mm ⁻¹)	1.073	1.073	
F000	904.0	904.0	
F000'	906.43		
H, k, lmax	13, 17, 19	13, 17, 19	
Nref	9144	9132	
Tmin, Tmax	0.603, 0.692	0.600, 0.746	
Tmin'	0.402		

Table S1. Crystallographic data for $[Fe^{II}(tpy)(CN)_3]$.

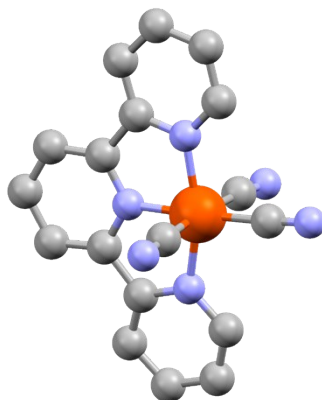


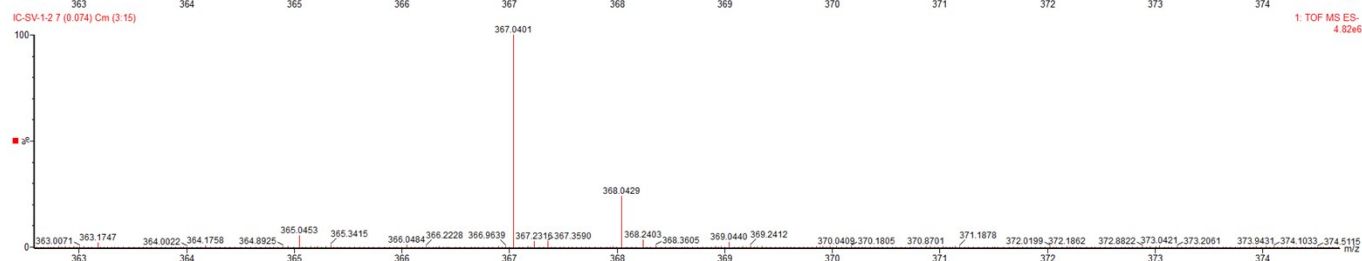
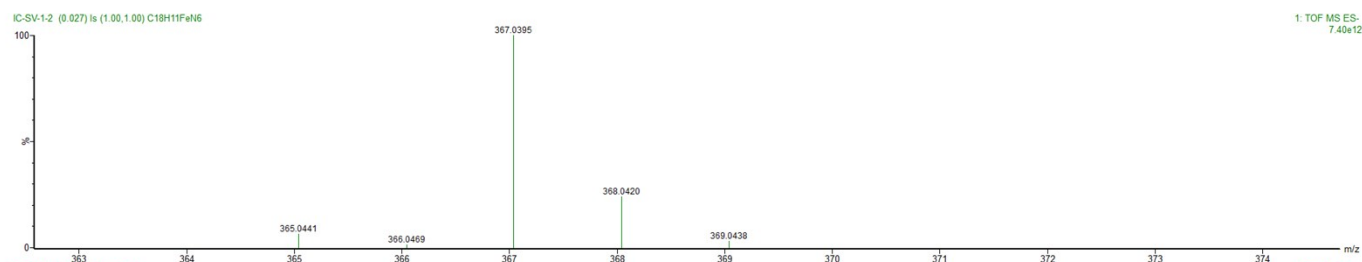
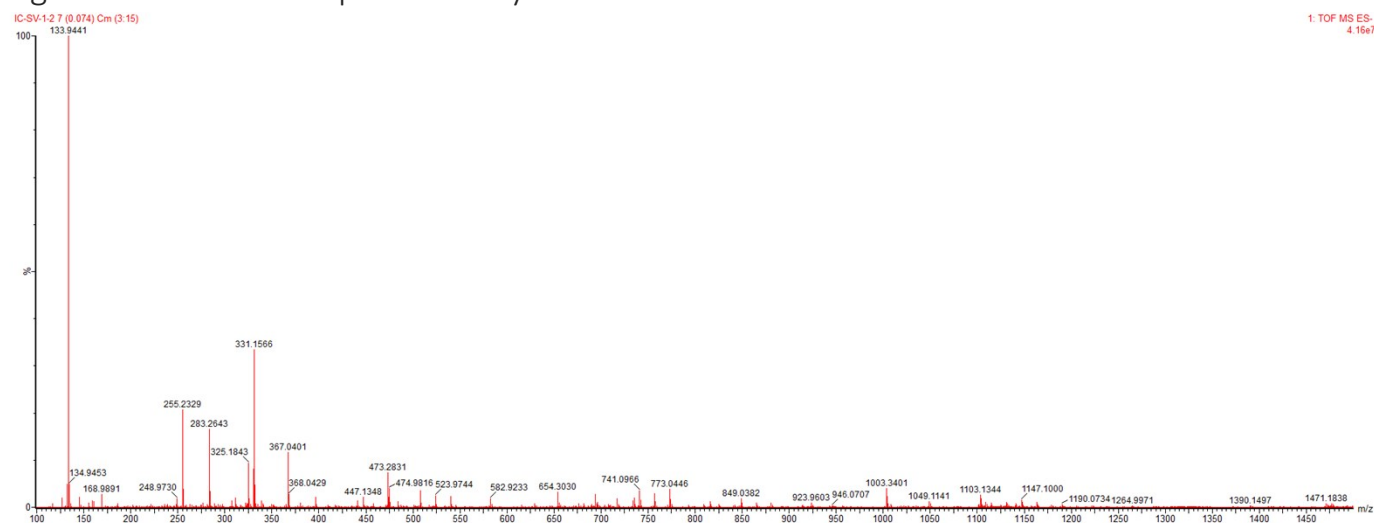
Figure S3. Crystal structure of $[\text{Fe}^{\text{II}}(\text{tpy})(\text{CN})_3]^-$.

Bonding Distances, Å

	$[\text{Fe}^{\text{II}}(\text{tpy})(\text{CN})_3]^-$ (X-ray)	$[\text{Fe}^{\text{II}}(\text{tpy})(\text{CN})_3]^-$ (DFT)
Fe-C1	1.933(1)	1.975
Fe-C2	1.917(1)	1.952
Fe-C3	1.955(1)	1.975
Fe-N1	1.981(1)	2.022
Fe-N2	1.889(1)	1.923
Fe-N3	1.988(1)	2.022

Table S2. Experimental bonding distances of $[\text{Fe}^{\text{II}}(\text{tpy})(\text{CN})_3]^-$ from X-ray structure and DFT calculations at the B3LYP+D2/SDD,6-311G* level of theory.

High-resolution mass spectrometry



Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

41 formula(e) evaluated with 1 result within limits (all results (up to 1000) for each mass)

Elements Used: C: 4-27 H: 5-14 N: 0-6 194Pt: 0-1 195Pt: 0-1 196Pt: 0-1 56Fe: 0-1

Minimum: -1.5

Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
367.0401	367.0395	0.6	1.6	16.5	926.9	n/a	n/a	C18 H11 N6 56Fe

Figure S6. Mass Spec $[\text{Fe}^{\text{II}}(\text{tpy})(\text{CN})_3]^-$.

Electronic Characterization

UV-Vis

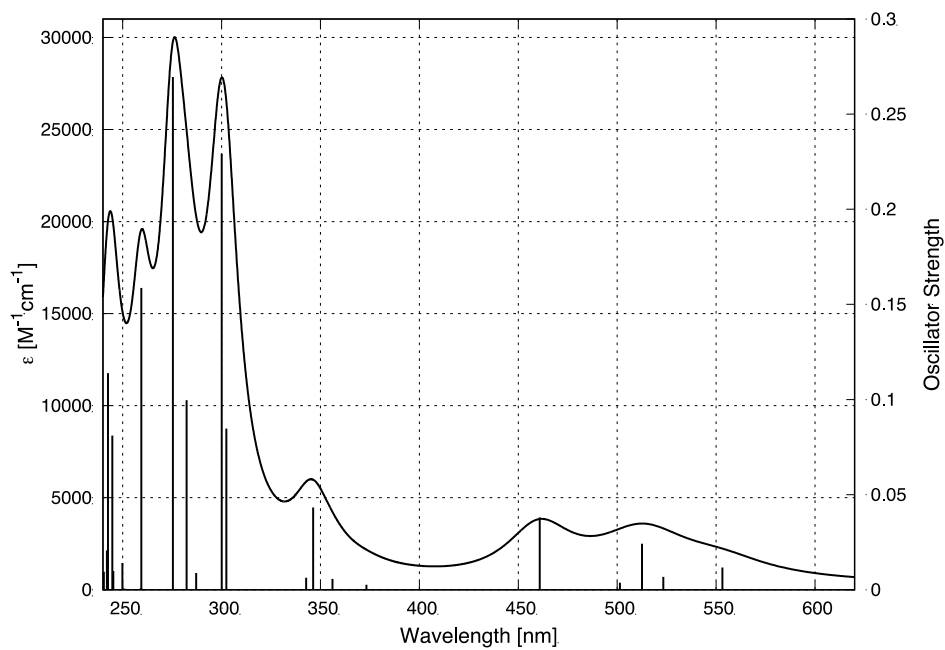


Figure S4. Calculated UV-Vis spectrum of $[\text{Fe}(\text{tpy})(\text{CN})_3]^-$ complex, 40 lowest-energy singlet excited states were obtained ($\lambda > 240$ nm). Stick spectrum was broadened using Lorentzian broadening with $hwhm=0.12$ eV.

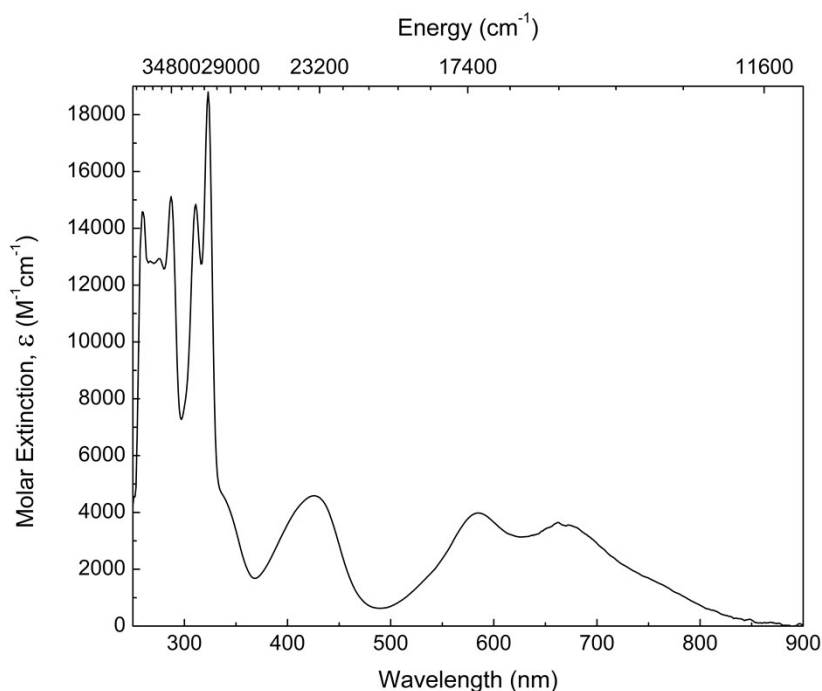


Figure S5. Molar extinction coefficient, ϵ , of $[\text{Fe}^{\text{II}}(\text{tpy})(\text{CN})_3]^-$.

Table S3. Analysis of the lowest-energy excited states for the $[\text{Fe}(\text{tpy})(\text{CN})_3]^-$ complex. Excitations 1-8 make up the lowest energy bands ($\lambda > 450 \text{ nm}$ in the calculated spectrum), excitation 13 corresponds to the most intense transition in the band centered at $\sim 350 \text{ nm}$ in the calculated spectrum.

Excited State	Energy [nm]	Oscillator Strength	Composition	Assignment
1	553.18	0.0117	89% (HOMO-1 \rightarrow LUMO) + 5%. (HOMO-2 \rightarrow LUMO+7)	MLCT
2	528.21	0.0000	84% (HOMO-2 \rightarrow LUMO) + 10% (HOMO-1 \rightarrow LUMO+7)	MLCT
3	523.35	0.0068	69% (HOMO \rightarrow LUMO) + 28% (HOMO-1 \rightarrow LUMO+1)	MLCT
4	512.56	0.0242	89% (HOMO \rightarrow LUMO+1) + 7%. (HOMO-2 \rightarrow LUMO+7)	MLCT
5	501.37	0.0037	62% (HOMO-2 \rightarrow LUMO+7) + 9% (HOMO-1 \rightarrow LUMO) + 8%. (HOMO \rightarrow LUMO+1) + 7%. (HOMO-2 \rightarrow LUMO+5) + 4% (HOMO-2 \rightarrow LUMO+10) + 3% (HOMO-2 \rightarrow LUMO+12) + 2% (HOMO-2 \rightarrow LUMO+8)	MC
6	480.36	0.0000	40% (HOMO-1 \rightarrow LUMO+7) + 23% (HOMO-1 \rightarrow LUMO+8) + 15% (HOMO-1 \rightarrow LUMO+5) + 14% (HOMO-2 \rightarrow LUMO) + 2%. (HOMO-1 \rightarrow LUMO+10)	MC

7	473.63	0.0000	94% (HOMO-2 → LUMO+1) + 2% (HOMO-2 → LUMO+1) + 2% (HOMO → LUMO+7)	MLCT
8	460.82	0.0380	70% (HOMO-1 → LUMO+1) + 26%. (HOMO → LUMO)	MLCT
13	346.24	0.0432	97% (HOMO-1 → LUMO+3) + 3%. (HOMO-3 → LUMO)	MLCT

Solvatochromism

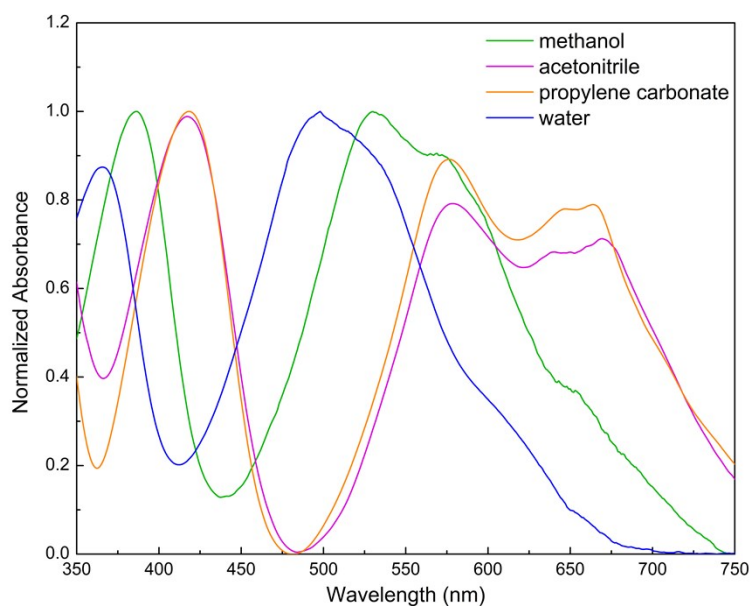


Figure S6. UV-Vis spectra of the $[Fe^{II}(tpy)(CN)_3]^-$ complex in various solvents.

Femtosecond pump-probe spectroscopy

Instrumentation and Methodology

Newport Transient Absorption Spectrometer (TAS)

A Spectra Physics Solstice ACE (one-box regenerative amplifier containing a Mai Tai Short Pulses femtosecond oscillator and Accend pump laser) was used to produce 800 nm pulses at a repetition rate of 1 kHz at 7.1 W average power and a pulse width of ~ 60 fs. From this unit, the beam is split twice (80:20) and (85:15) with ~ 4.7 W directed to an optical parametric amplifier (TOPAS-Prime, Light Conversion) and the other to the TAS spectrometer to create the pump (TOPAS) and probe (TAS) sources, respectively. The 355 - 400 nm pump beam was generated by fourth harmonic generation of the signal pulse from the TOPAS. The 800 nm probe beam is split from a second beamsplitter (95:5) with the 95% dumped and 5% passed through a CaF_2 plate to generate a white light continuum (~ 330 to 750 nm). A sample solution sufficient to fill a 2 mm quartz cuvette was prepared of the metal complex in propylenecarbonate, which was magnetically stirred. Transient absorption data were corrected by subtracting spectral background features that persisted from the previous pulse and appeared prepulse

as well as applying chirp correction using Surface Xplorer Pro 4.1 software (Ultrafast Systems). All kinetics were fit using single wavelength functions in Surface Xplorer Pro 4.1 software.

Experimental Data

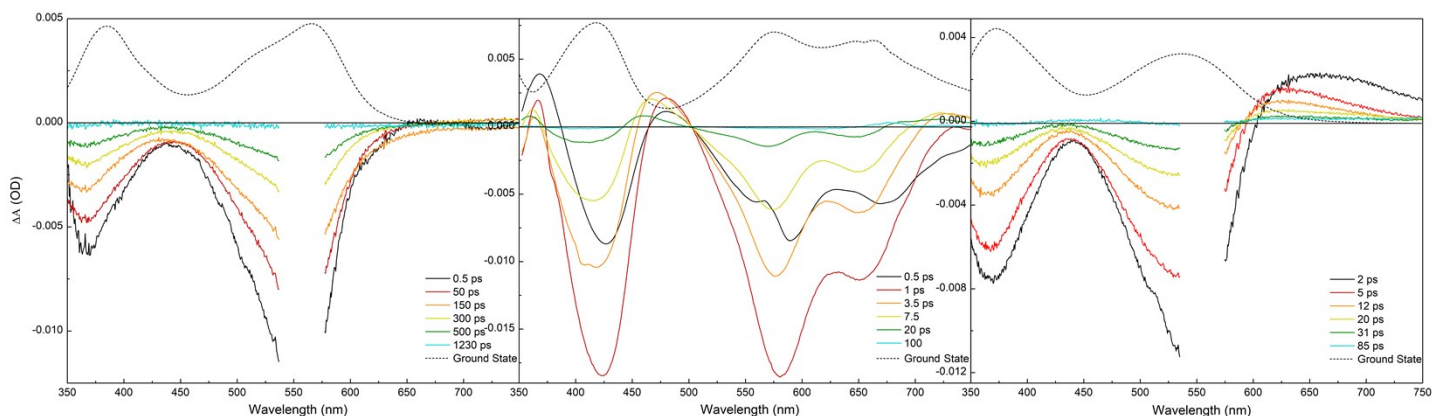


Figure S7. Transient spectra of the $[Fe^{II}(bpy)_2(CN)_2]$ (left), $[Fe^{II}(tpy)(CN)_3]$ (middle), and $[Fe^{II}(bpy)(CN)_4]^{2-}$ (right) complexes at various probe delays. The ground state spectra are overlaid as dotted traces.

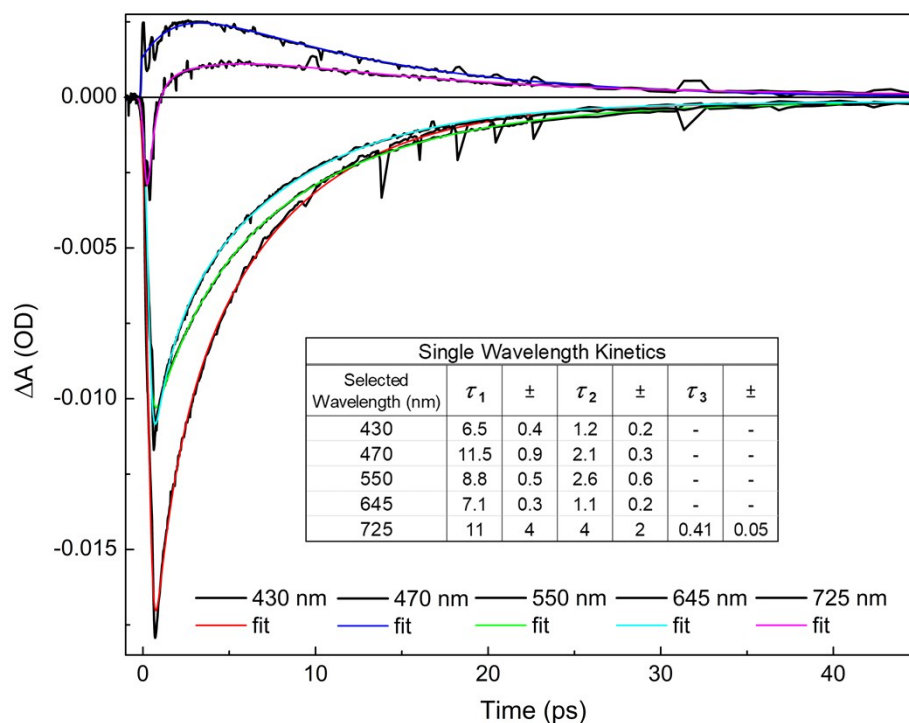


Figure S8. Single wavelength kinetic fitting of pump-probe transient absorption of the $[Fe^{II}(tpy)(CN)_3]$ complex at selected wavelengths with respective time constants (table inset).

Tables of Energies of Relevant Electronic States for Fe(II) Complexes

Table S4. Electronic energies (in hartree) for 1A (ground state) and the lowest-energy quintet (5MC) and triplet (3MC) metal-centered states obtained at the B3LYP+D2/SDD,6-311G* level of theory in water (PCM) at the 1A optimized geometries for Fe(II)-polypyridine complexes. All wavefunctions were tested for stability.

	[Fe(bpy) ₃] ²⁺	[Fe(bpy) ₂ (CN) ₂] ⁰	[Fe(tpy)(CN) ₃] ¹⁻	[Fe(bpy)(CN) ₄] ²⁻
1A	-1610.38971167	-1300.86552183	-1145.49592639	-991.327316728
5MC (DFT)	-1610.33746424	-1300.79658941	-1145.41286301	-991.228899657
3MC (DFT)	-1610.34614476	-1300.82018051	-1145.45417713	-991.278119255

Table S5. Calculated excitation energies (in eV) for the lowest-energy 1,3MLCT and 3MC states obtained from TD-DFT calculations at the the B3LYP+D2/SDD,6-311G* level of theory in water (PCM), utilizing 1A as the reference state.

	[Fe(bpy) ₃] ²⁺	[Fe(bpy) ₂ (CN) ₂] ⁰	[Fe(tpy)(CN) ₃] ¹⁻	[Fe(bpy)(CN) ₄] ²⁻
1MLCT (TD-DFT)	2.8553	2.4339	2.2413	2.0775
3MLCT (TD-DFT)	2.6811	2.1894	1.8510	1.8937
3MC (TD-DFT)	1.3585	1.4397	1.3465	1.7256

Cartesian coordinates of optimized Fe(II)-polypyridines

[Fe(tpy)(CN)₃]⁻ singlet ground state

E = -1145.49592639 hartree

```

Fe -0.00912200 0.00001100 0.00000100
N -0.35055700 -1.38478200 -1.43381400
N -1.93260400 -0.00011900 -0.00007500
N -0.35085700 1.38475900 1.43379200
C 0.56304300 -2.06432300 -2.13578400
C 0.21891100 -3.00246500 -3.10395500
C -1.12986000 -3.24609900 -3.35445600
C -2.08648500 -2.54370500 -2.62882000
C -1.66921200 -1.61830100 -1.67397000
C 0.56259500 2.06442100 2.13583500
C 0.21825900 3.00251300 3.10398300
C -1.13056500 3.24596000 3.35438100
C -2.08703700 2.54343800 2.62866800
C -1.66956400 1.61809500 1.67384600
C -2.58493100 -0.81684900 -0.84504300
C -3.97925700 -0.84017000 -0.86925900
C -4.67473400 -0.00030900 -0.00018200

```

C	-3.97944000	0.83964800	0.86895000
C	-2.58510800	0.81651900	0.84484400
H	1.59392300	-1.83360200	-1.89804800
H	0.99676800	-3.52688300	-3.64559400
H	-1.43324200	-3.97038200	-4.10162400
H	-3.14250400	-2.71061100	-2.80002500
H	1.59352600	1.83384500	1.89817800
H	0.99600100	3.52703600	3.64568500
H	-1.43410500	3.97019800	4.10152800
H	-3.14309100	2.71019900	2.79979300
H	-4.51193400	-1.49495200	-1.54690000
H	-5.75832600	-0.00038300	-0.00022400
H	-4.51226200	1.49435500	1.54654900
C	0.01414000	-1.42264700	1.36965000
C	1.94293600	0.00013600	0.00007400
C	0.01406100	1.42267900	-1.36963900
N	0.00141600	2.26703000	-2.17495300
N	3.11095000	0.00021200	0.00013500
N	0.00154800	-2.26698400	2.17498000

[Fe(bpy)₃]²⁺ singlet ground state

E = -1610.38971167

C	-4.14232000	-0.65507400	-2.28857100
C	-3.27902700	0.33182200	-2.75553300
C	-2.06661500	0.51989600	-2.10399700
N	-1.69403200	-0.21391100	-1.04564300
C	-2.53174900	-1.17551400	-0.58414400
C	-3.76402500	-1.41716700	-1.18897800
H	-5.09674500	-0.83039900	-2.77056000
H	-3.53166800	0.94941500	-3.60806100
H	-1.36371400	1.27166200	-2.43420200
H	-4.42137800	-2.18688100	-0.80838800
N	-0.82604000	-1.49227000	1.04640500
C	-0.28292800	-2.10828700	2.10617800
C	-0.90369700	-3.16802400	2.75531600
C	-2.13685600	-3.60972900	2.28481800
C	-2.70478700	-2.97733500	1.18459600
C	-2.02696300	-1.91889000	0.58215300
H	-0.42362900	-3.62966700	3.60881600
H	-2.65066400	-4.43419100	2.76466300
H	-3.66093100	-3.30655600	0.80144800
Fe	-0.00436600	-0.00072600	-0.00075400
H	1.87106000	4.82418500	-2.74035100
C	1.53255900	3.90995100	-2.26749500
C	1.93832700	2.66759200	-2.74614700
C	0.68295700	3.96450500	-1.16829400
C	1.47993600	1.52373600	-2.10482100

H	2.59815400	2.57620000	-3.59956900
C	0.25972000	2.77654200	-0.57468200
H	0.35741300	4.91954500	-0.77937600
N	0.65971400	1.56904800	-1.04534000
C	-0.64131700	2.71228500	0.58794600
N	-0.88468200	1.45845000	1.04434700
C	-1.21478800	3.82976200	1.19211300
C	-1.69950400	1.29675800	2.09666900
C	-2.05585200	3.65488300	2.28528300
H	-1.01160700	4.82291700	0.81572800
C	-2.30395200	2.36540000	2.74670000
H	-1.86082700	0.27912300	2.42317800
H	-2.50976000	4.51316300	2.76624000
H	-2.95232900	2.18085700	3.59382000
H	0.67267300	-1.72964600	2.44044400
C	2.62859800	-3.26449100	-2.28400200
C	1.34214300	-3.01054300	-2.75060100
C	0.57452600	-2.05173300	-2.10147800
N	1.02474700	-1.35912000	-1.04558800
C	2.27699800	-1.60300000	-0.58516300
C	3.10095200	-2.55211700	-1.18743300
H	3.25647300	-4.00582300	-2.76375900
H	0.93191500	-3.54038000	-3.60093000
H	-0.42800100	-1.81991600	-2.43209600
H	4.09610500	-2.73601400	-0.80650500
N	1.70029800	0.03506100	1.04329100
C	1.96427300	0.81710300	2.09976500
C	3.19444500	0.81351400	2.74516400
C	4.19362400	-0.03314700	2.27392100
C	3.92799400	-0.84456900	1.17663200
C	2.67036000	-0.79108600	0.57828900
H	3.35577400	1.46296400	3.59619800
H	5.16623700	-0.06265400	2.75053100
H	4.69161600	-1.50676500	0.79230400
H	1.15837300	1.45509700	2.43394000
H	1.76660300	0.53850100	-2.44432800

[Fe(bpy)₂(CN)₂]⁰ singlet ground state

E = -1300.86552183 hartree

C	-4.06309200	-0.63109300	-2.31689700
C	-3.15964300	0.30767800	-2.80782900
C	-1.94420200	0.46785600	-2.15365200
N	-1.60375400	-0.24251900	-1.07060300
C	-2.47510400	-1.16209400	-0.59232100
C	-3.71510100	-1.37575300	-1.19621400

H	-5.02212100	-0.78417200	-2.79794200
H	-3.38427300	0.90844700	-3.68046700
H	-1.21231800	1.18309700	-2.50301200
H	-4.40094300	-2.11206800	-0.79963800
N	-0.77046400	-1.53621600	1.03025600
C	-0.25204400	-2.16706000	2.09494200
C	-0.92619900	-3.17653300	2.77097300
C	-2.19076800	-3.55278700	2.32594900
C	-2.73181800	-2.90816600	1.22012300
C	-1.99915800	-1.90234000	0.58837400
H	-0.46256100	-3.65105300	3.62701100
H	-2.74733800	-4.33522100	2.82856600
H	-3.71107300	-3.18645900	0.85480100
Fe	0.11123300	-0.05381200	-0.00112900
H	1.70296100	4.84556700	-2.82507800
C	1.43311800	3.92326100	-2.32393000
C	1.92048700	2.69779600	-2.77061900
C	0.59173500	3.94735400	-1.21823700
C	1.54471000	1.54246100	-2.09636900
H	2.58029900	2.62858900	-3.62665800
C	0.25564700	2.74849500	-0.58792600
H	0.20370000	4.88796400	-0.85158300
N	0.72872600	1.55748200	-1.03139200
C	-0.62036500	2.66269200	0.59263400
N	-0.80218200	1.40868900	1.07014500
C	-1.22173000	3.76789500	1.19664800
C	-1.57122100	1.23508600	2.15269700
C	-2.02293600	3.57884900	2.31641800
H	-1.06857100	4.76270800	0.80073900
C	-2.19978800	2.28776300	2.80668400
H	-1.67901100	0.21729600	2.50151400
H	-2.49803000	4.42601600	2.79724500
H	-2.81137200	2.09102300	3.67854700
H	0.72995500	-1.83344000	2.40102900
H	1.89030900	0.56515800	-2.40410300
C	1.67893400	0.05753200	1.15014300
C	0.99123000	-1.35509900	-1.15409600
N	2.60398400	0.12710600	1.85804800
N	1.50241800	-2.12868800	-1.86260900

[Fe(bpy)(CN)₄]²⁻ singlet ground state

E = -991.327316728 hartree

C	-4.04341300	-0.71502500	-2.35766200
C	-3.18379900	0.27639100	-2.82616900
C	-1.99238300	0.50338100	-2.14796800
N	-1.63051800	-0.19003500	-1.05881400

C	-2.46175900	-1.15519000	-0.59869200
C	-3.67596400	-1.43857800	-1.23028800
H	-4.98176300	-0.92217900	-2.85955700
H	-3.42546900	0.86738800	-3.70156000
H	-1.28875200	1.26010400	-2.46935000
H	-4.32664500	-2.21406400	-0.84863000
N	-0.77534200	-1.44874100	1.05707100
C	-0.26303100	-2.04274000	2.14465400
C	-0.91360400	-3.06605100	2.82327900
C	-2.15382500	-3.49705400	2.35703900
C	-2.69193900	-2.88720100	1.23097400
C	-1.98026500	-1.86388000	0.59862000
H	-0.45222200	-3.51006700	3.69733000
H	-2.69278500	-4.29230000	2.85945600
H	-3.65390000	-3.20441200	0.85082200
Fe	0.09573800	0.06532100	-0.00007900
H	0.70103600	-1.66968400	2.46469100
C	1.67574400	0.14795600	1.13256800
C	0.97239100	-1.26881100	-1.16120800
N	2.61189100	0.16548300	1.83309500
N	1.46203800	-2.07418800	-1.85182600
C	-0.82834900	1.37031000	1.15660300
C	0.75212700	1.50631600	-1.13008200
N	-1.40114800	2.12503800	1.84047100
N	1.11545300	2.36958200	-1.83016600