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Supporting Information

A Heteroleptic Ferrous Complex with Mesoionic Bis(1,2,3-triazol-5-ylidene) Ligands: Taming the MLCT Excited State of Iron(II)

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1. Synthesis and structural identification

General

All the reactions were carried out using the standard Schlenk technique or in a glovebox. Anhydrous THF was obtained from a Braun SPS-800 system. Precoated Merck silica gel 60 F_{254} plates were used for TLC analysis. Flash column chromatography was performed on silica gel (Davisil 35-70 μm). ^{1}H, ^{13}C and 2D (COSY, HMBC, HMQC) NMR were recorded on a Bruker Avance II 400 MHz and a Bruker Avance I 500 MHz NMR spectrometers. Chemical shifts (δ) are reported to the shift-scale calibrated with the residual NMR solvent; CD_3CN (1.94 ppm for ^{1}H NMR and 1.32 and 118.26 ppm for ^{13}C NMR).[1] Electron spray ionization–high resolution mass (ESI–HRMS) spectra were recorded on a Waters Micromass Q-Tof micro mass spectrometer. Elemental analysis was performed by Mikroanalytisches Laboratorium KOLBE (Mülheim an der Ruhr, Germany). Common solvents including acetone, THF, CH_3CN, acetic acid and diethyl ether were purchased from Honeywell and used as received. Sodium ascorbate, *tert*-butanol, methyl trifluoromethansulfonate, 1,2-dichloroethane and potassium *tert*-butoxide (1 M solution in THF) were purchased from Aldrich. Triethylamine (TEA), 2,2'-bipyridine (bpy), anhydrous ferrous chloride ($FeCl_2$), tetra(*n*-butyl)ammonium bromide, ammonium hexafluorophosphate, pyridine, sodium nitrite, sodium azide and potassium carbonate were purchased from Acros. *p*-Toluidine and copper(II) sulfate pentahydrate were purchased from Fluka. 1,4-Bis(trimethylsilyl)-1,3-butadiyne was purchased from Alfa. *p*-Tolyl azide,[2] $H_2[Fe(bpy)(CN)_4]$[3] and $TBA_2[Fe(bpy)(CN)_4]$[4] (complex **2**) were synthesized using literature methods. $Fe(bpy)Cl_2$ was also synthesized according to the literature method,[5] except that the commercially available anhydrous $FeCl_2$ was directly used instead of freshly prepared from Fe powder and HCl.

1,1'-Bis(*p*-tolyl)-4,4'-bis(1,2,3-triazole). This compound was synthesized according to the literature procedure[6] with the only exception of using *p*-tolyl azide as the azide source. The crude product was purified by silica gel flash column chromatography using CH_2Cl_2/TEA (1%) and recrystallized from a mixture of CH_2Cl_2 and methanol to give light yellow brown powder (yield 70%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.53 (s, 2H, triazole), 7.70 (d, *J*=8 Hz, 4H, tolyl), 7.36 (d, *J*=8 Hz, 4H, tolyl), 2.45 ppm (s, 6H, *p*-methyl). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 140.66, 139.30, 134.79, 130.52, 120.61, 119.04, 21.29 ppm. HR−MS calc. for $[M-H]^+$ 317.1515, found 317.1511. Elemental analysis: calc. for $C_{18}H_{16}N_6$ C, 68.34; H, 5.10; N, 26.56; found C 68.29; H, 5.08; N, 26.59.

1,1'-Bis(*p*-tolyl)-4,4'-bis(1,2,3-triazolium) hexafluorophosphate. The synthesis of the titled compound was via the synthesis of its triflate salt,[7] followed by exchange of the counter-ion.

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[1] G. R. Fulmer, A. J. M. Miller, N. H. Sherden, H. E. Gottlieb, A. Nudelman, B. M. Stoltz, J. E. Bercaw, K. I. Goldberg, *Organometallics* **2010**, *29*, 2176-2179.
[2] D. G. Brown, N. Sanguantrakun, B. Schulze, U. S. Schubert, C. P. Berlinguette, *J. Am. Chem. Soc.* **2012**, *134*, 12354-12357.
[3] A. A. Schilt, *J. Am. Chem. Soc.* **1960**, *82*, 3000-3005.
[4] H. E. Toma, M. S. Takasugi, *J. Sol. Chem.* **1983**, *12*, 547-561.
[5] F. F. Charron Jr., W. M. Reiff, *Inorg. Chem.* **1986**, *25*, 2786-2790.
[6] J. T. Fletcher, B. J. Bumgarner, N. D. Engels, D. A. Skoglund, *Organometallics* **2008**, *27*, 5430-5433.
[7] G. Guisado-Barrios, J. Bouffard, B. Donnadieu, G. Bertrand, *Organometallics* **2011**, *30*, 6017-6021.

1,1'-Bis(*p*-tolyl)-4,4'-bis(1,2,3-triazole) (547 mg, 1.73 mmol) was suspended in 1,2-dichloroethane (20 mL) under nitrogen and the mixture was cooled down to −78°C. Methyl trifluoromethansulfonate (433 μL, 3.9 mmol) was then added dropwise using a syringe and the mixture was gradually warmed to room temperature. The solution was heated at 100°C for 48 hrs, cooled down, and the solvent was removed by evaporation. Diethyl ether was added to the residual and the precipitates were collected by filtration and washed with some more diethyl ether. After brief drying, the solid was dissolved in minimum amount of dry acetone and precipitated with tetra(*n*-butyl)ammonium bromide. The obtained bromide salt was then filtered, washed with acetone and dissolved in distilled water (10 mL). Excess of ammonium hexafluorophosphate was added and the precipitated was collected by filtration, washed with water and dried under vacuum to yield the product as pale powder (935 mg, 85%). ^{1}H NMR (400 MHz, CD_3CN) δ = 9.27 (s, 2H, triazolium), 7.85 (d, *J*=12 Hz, 4H, tolyl), 7.60 (d, *J*=12 Hz, 4H, tolyl), 4.42 (s, 6H, *p*-methyl), 2.51 ppm (s, 6H, 3,3'-methyl). ^{13}C NMR (100 MHz, CD_3CN) δ = 144.94, 133.28, 132.15, 132.09, 127.88, 122.86, 41.06, 21.41 ppm. HR−MS calc. for $[C_{20}H_{22}N_6{-}PF_6]^+$ 491.1542, found 491.1542. Elemental analysis: calc. for $C_{20}H_{22}F_{12}N_6P_2$ C, 37.75; H, 3.48; N, 13.21; found C 37.95; H, 3.58; N, 13.11.

Bis(1,1'-bis(*p*-tolyl)-4,4'-bis(1,2,3-triazol-5-ylidene))(2,2'-bipyridine)iron(II) hexafluorophosphate (Complex 1). 1,1'-Bis(*p*-tolyl)-4,4'-bis(1,2,3-triazolium) hexafluorophosphate (127 mg, 0.2 mmol) and $Fe(bpy)Cl_2$ (26 mg, 0.092 mmol) were dried in a 100-mL Schlenk tube under vacuum. Anhydrous THF (25 mL) was charged inside under nitrogen and the mixture was cooled down to −78°C. Potassium *tert*-butoxide (0.6 mL, 1 M in THF, 0.6 mmol) was added using a syringe, after which the mixture was warmed to room temperature and stirred overnight. The precipitates were collected and washed with THF to give analytically pure product as dark green powder (49 mg, 45% based on $Fe(bpy)Cl_2$). ^{1}H NMR (400 MHz, CD_3CN) δ = 7.92 (d, *J*=4 Hz, 2H, bpy), 7.40 (t, *J*=8 Hz, 2H, bpy), 7.23 (d, *J*=8 Hz, 4H, tolyl), 7.11 (d, *J*=8 Hz, 2H, bpy), 7.00 (d, *J*=8 Hz, 4H, tolyl), 6.83 (t, *J*=6 Hz, 2H, bpy), 6.66 (d, *J*=8 Hz, 4H, tolyl), 6.22 (d, *J*=8 Hz, 4H, tolyl), 4,42 (s, 6H, 3,3'-methyl), 4.12 (s, 6H, 3,3'-methyl), 2.35 (s, 6H, *p*-methyl), 2.20 ppm (s, 6H, *p*-methyl). ^{13}C NMR (100 MHz, CD_3CN) δ = 202.61, 199.20, 158.34, 154.67, 141.69, 141.40, 140.74, 140.64, 136.84, 135.68, 134.52, 129.92, 129.80, 126.50, 125.73, 125.51, 122.21, 40.39, 39.65, 21.06, 20.98 ppm. HR−MS calc. for $[\mathbf{1}{-}(PF_6)]^+$ 1045.3209, found 1045.3178. Elemental analysis: calc. for **1** ($C_{50}H_{48}F_{12}FeN_{14}P_2$) C, 50.43; H, 4.06; N, 16.47; found C, 49.99; H, 4.02; N, 16.30. Materials for growing X-ray-quality crystals were based on the bromide salt (**1Br**), which was prepared as below. The complex was dissolved in minimum amount of dry acetone and precipitated with tetra(*n*-butyl)ammonium bromide. The obtained bromide salt was then filtered and washed with acetone. Single crystals suitable for X-ray crystallography was grown by slow diffusion of diethyl ether to the methanol solution of **1Br**.

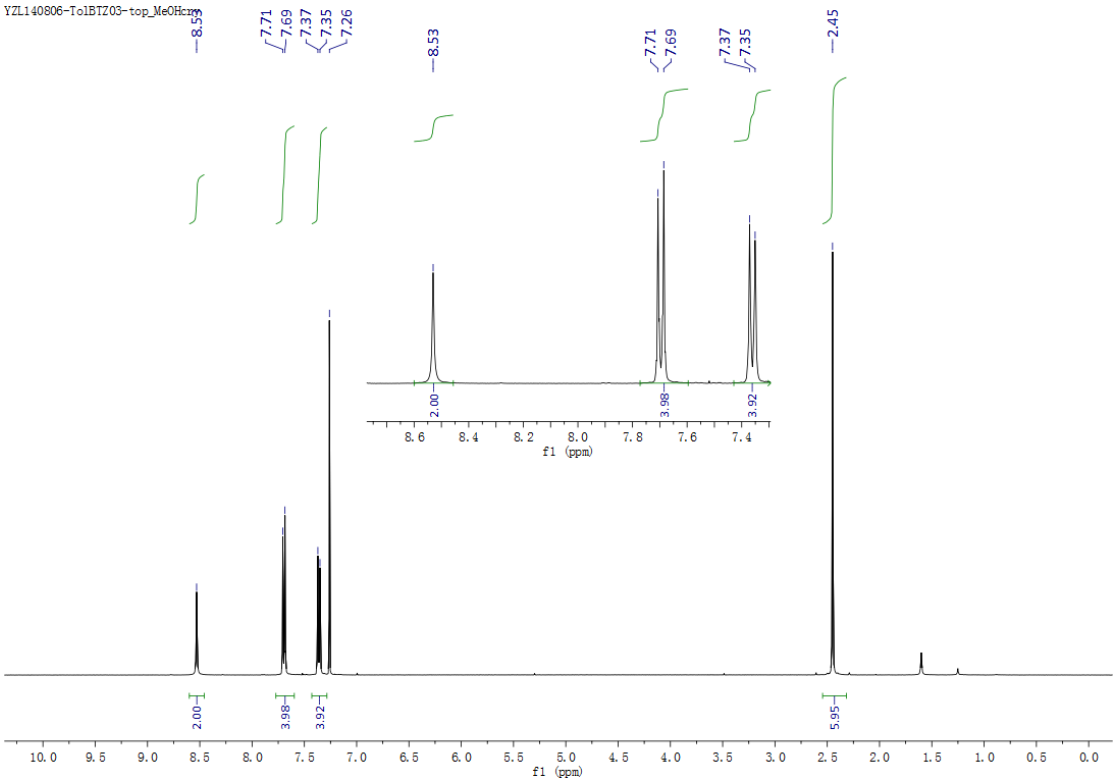


Figure S1 ^{1}H NMR of 1,1'-bis(*p*-tolyl)-4,4'-bis(1,2,3-triazole) in $CDCl_3$.

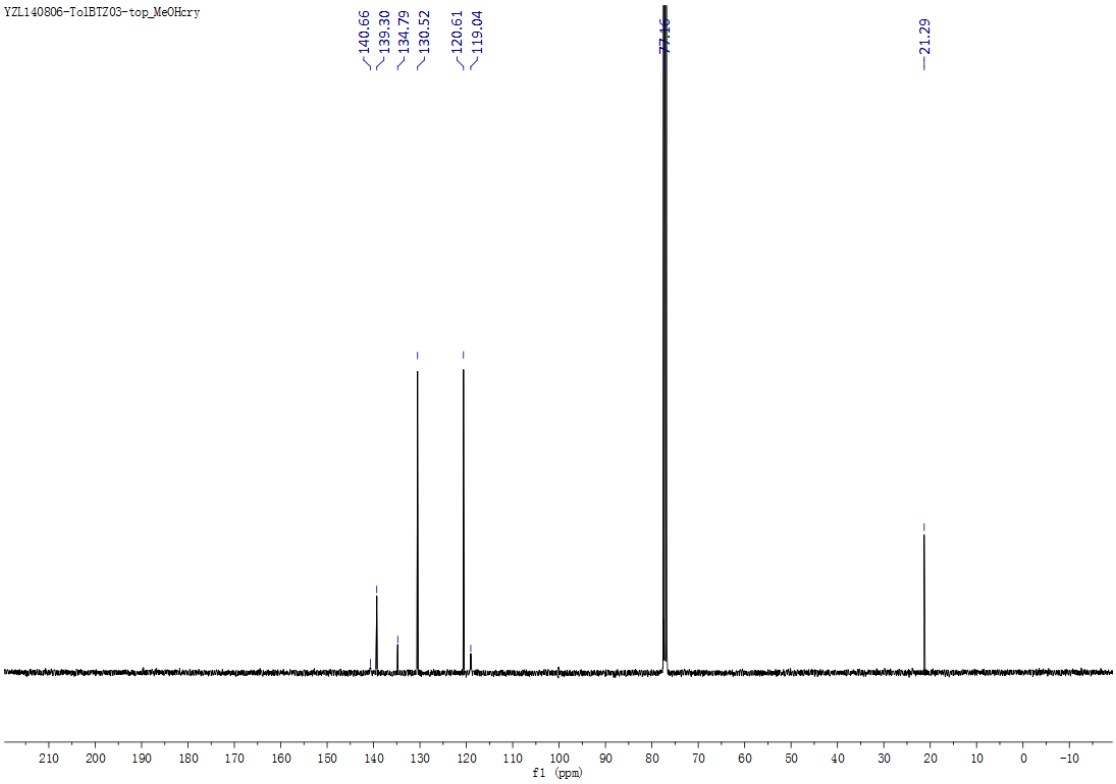


Figure S2 ^{1}H NMR of 1,1'-bis(*p*-tolyl)-4,4'-bis(1,2,3-triazole) in $CDCl_3$.

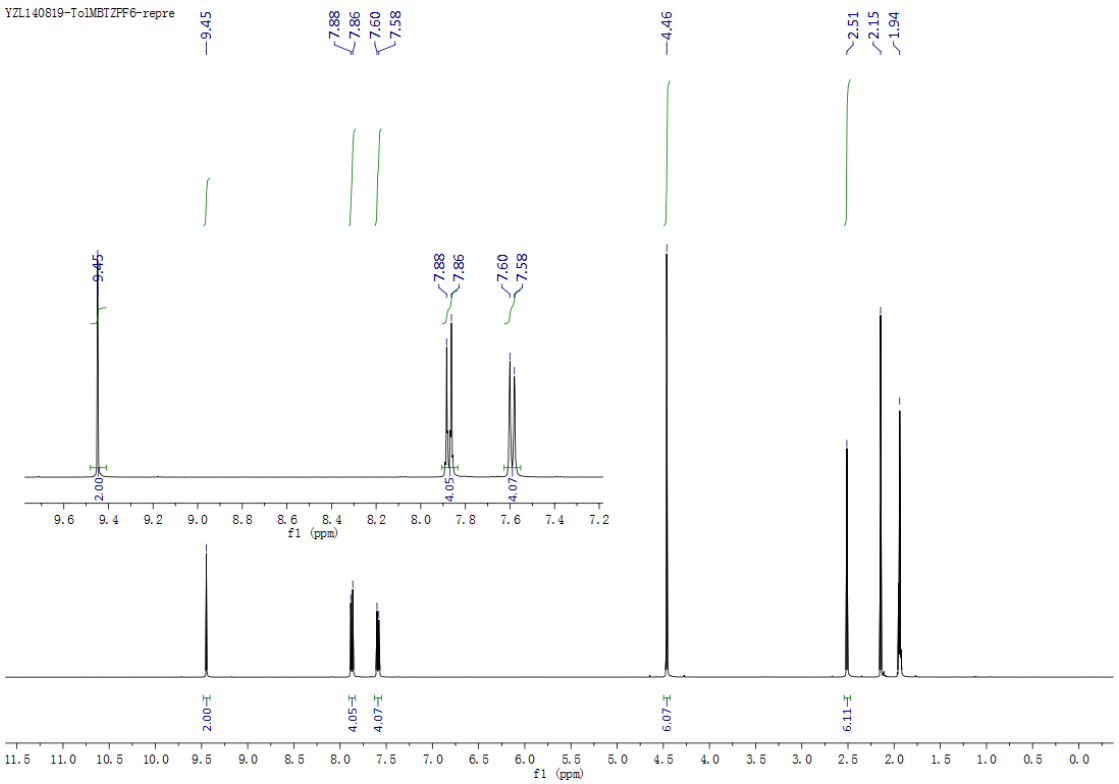


Figure S3 ^{1}H NMR of 1,1'-bis(*p*-tolyl)-4,4'-bis(1,2,3-triazolium) hexafluorophosphate in CD_3CN.

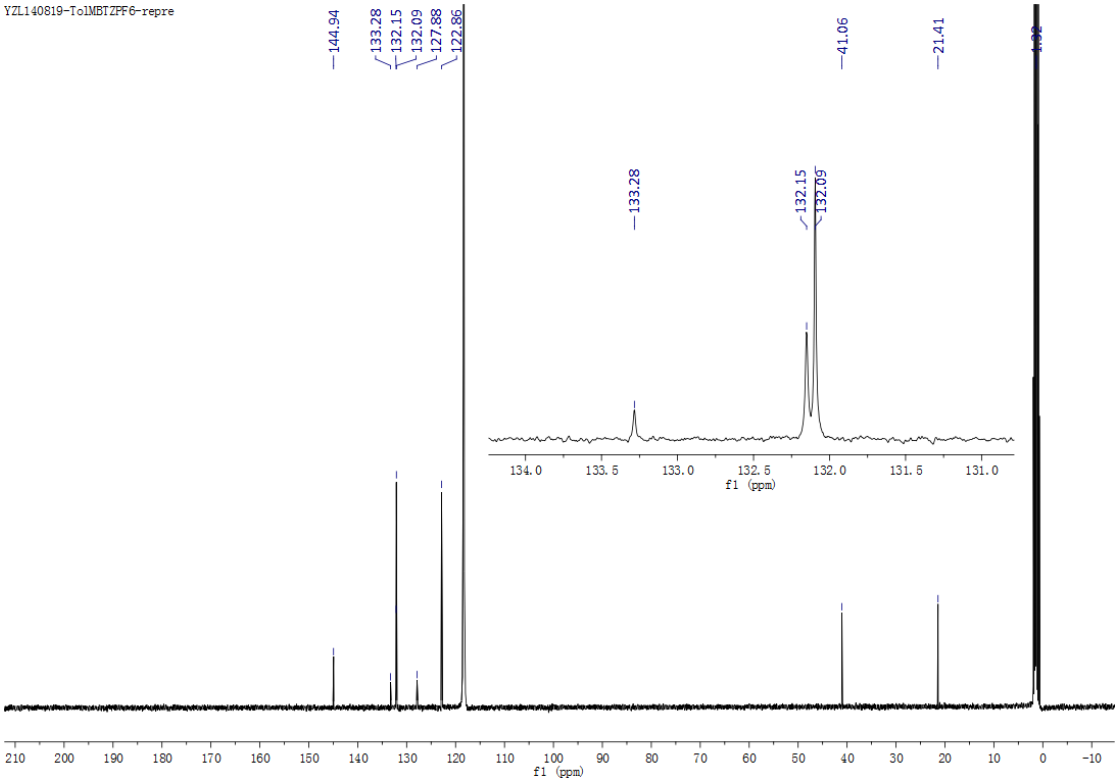


Figure S4 ^{13}C NMR of 1,1'-bis(*p*-tolyl)-4,4'-bis(1,2,3-triazolium) hexafluorophosphate in CD_3CN.

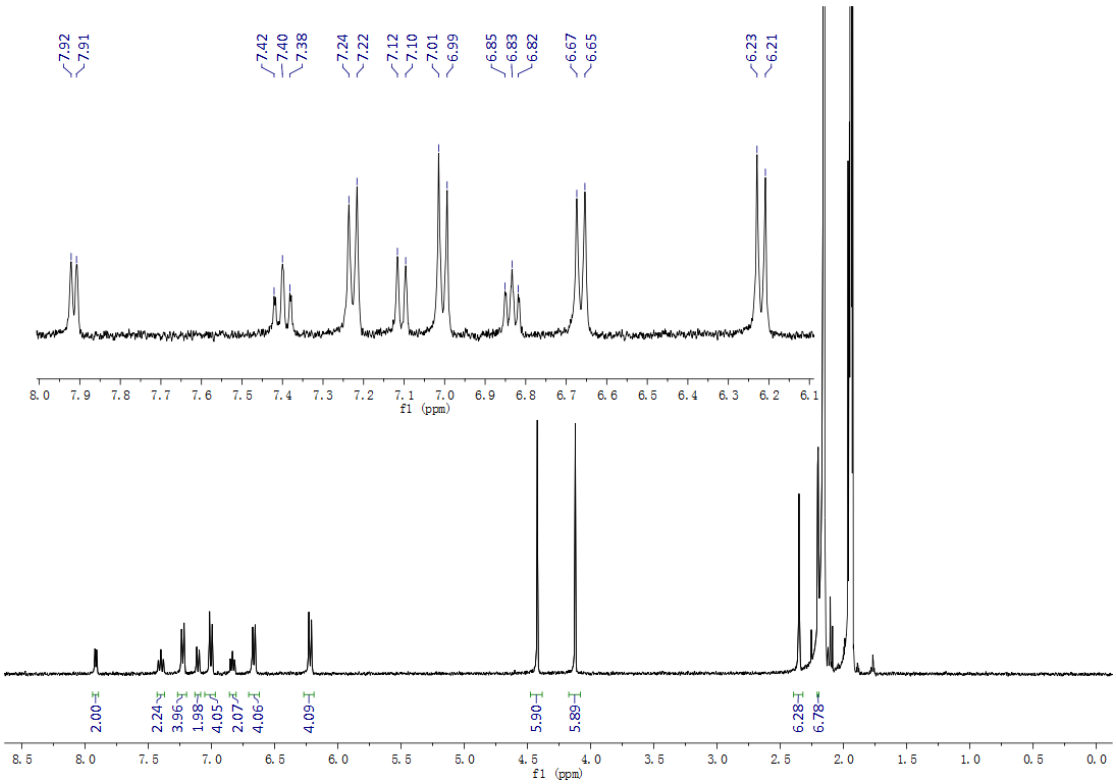


Figure S5 ^{1}H NMR of complex **1** in CD_3CN.

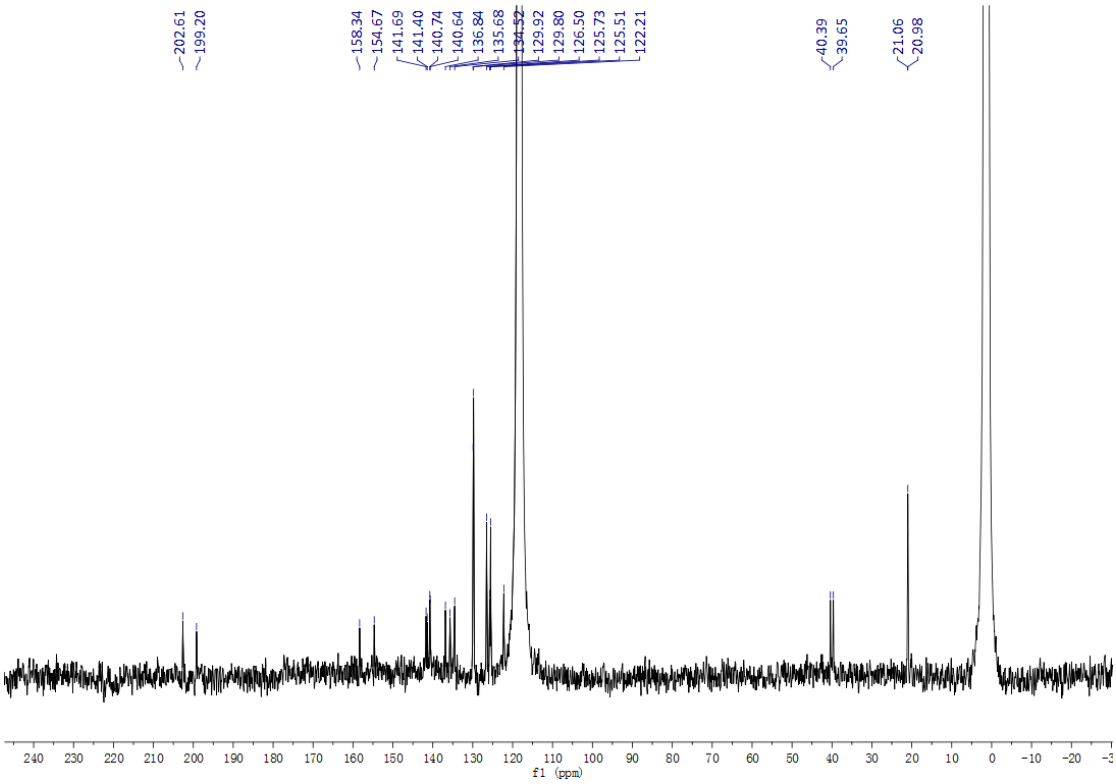


Figure S6 ^{13}C NMR of complex **1** in CD_3CN.

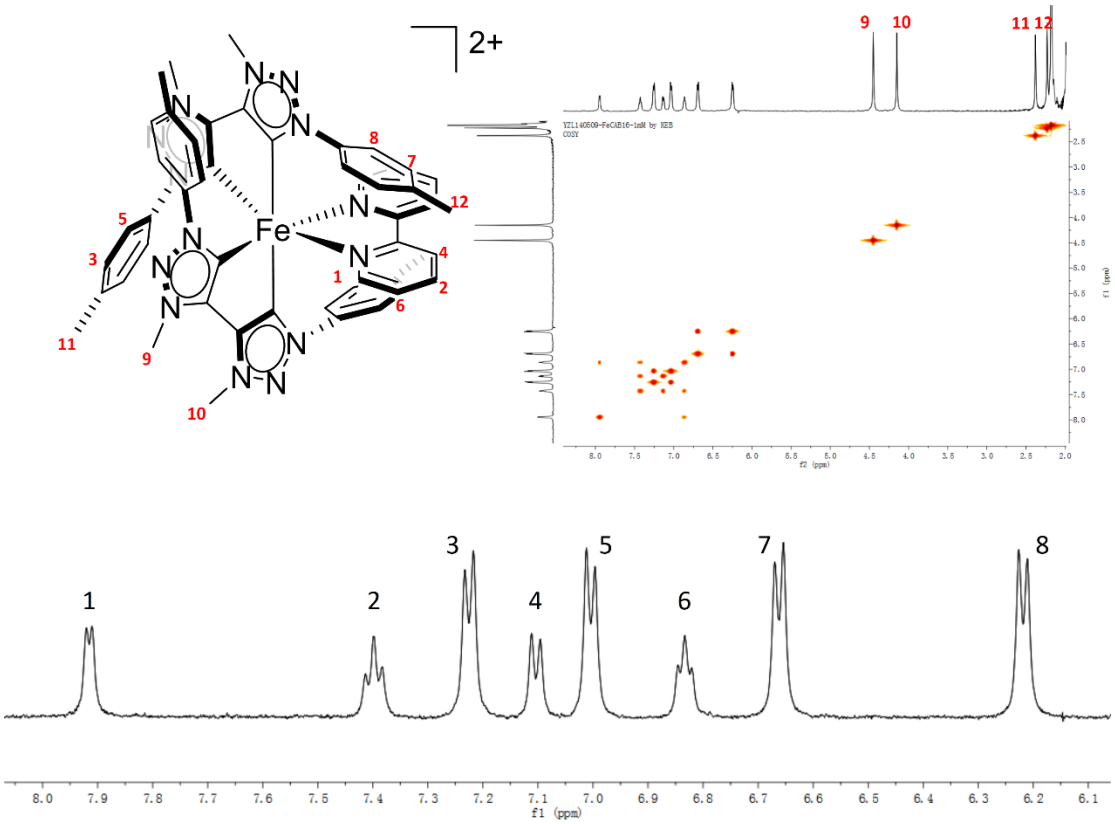


Figure S7 COSY and assignment of the ^{1}H NMR of complex **1** in CD_3CN.

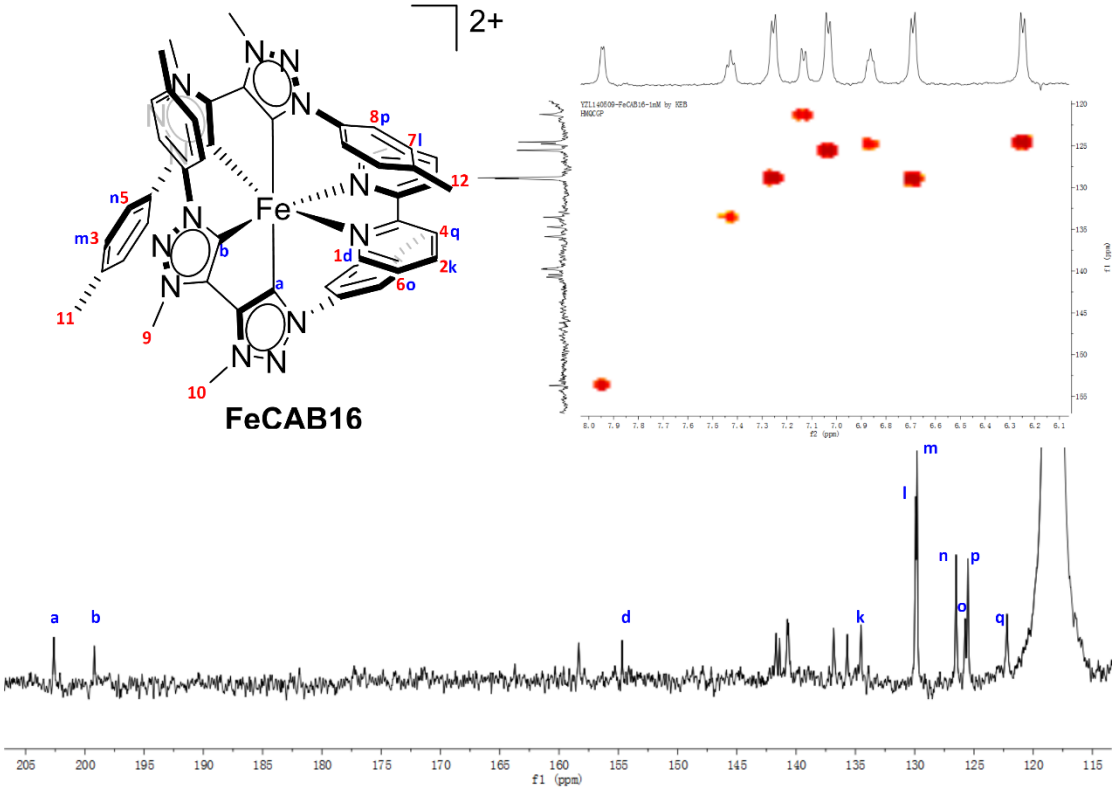


Figure S8 HMQC and assignment of the ^{13}C NMR of complex **1** in CD_3CN.

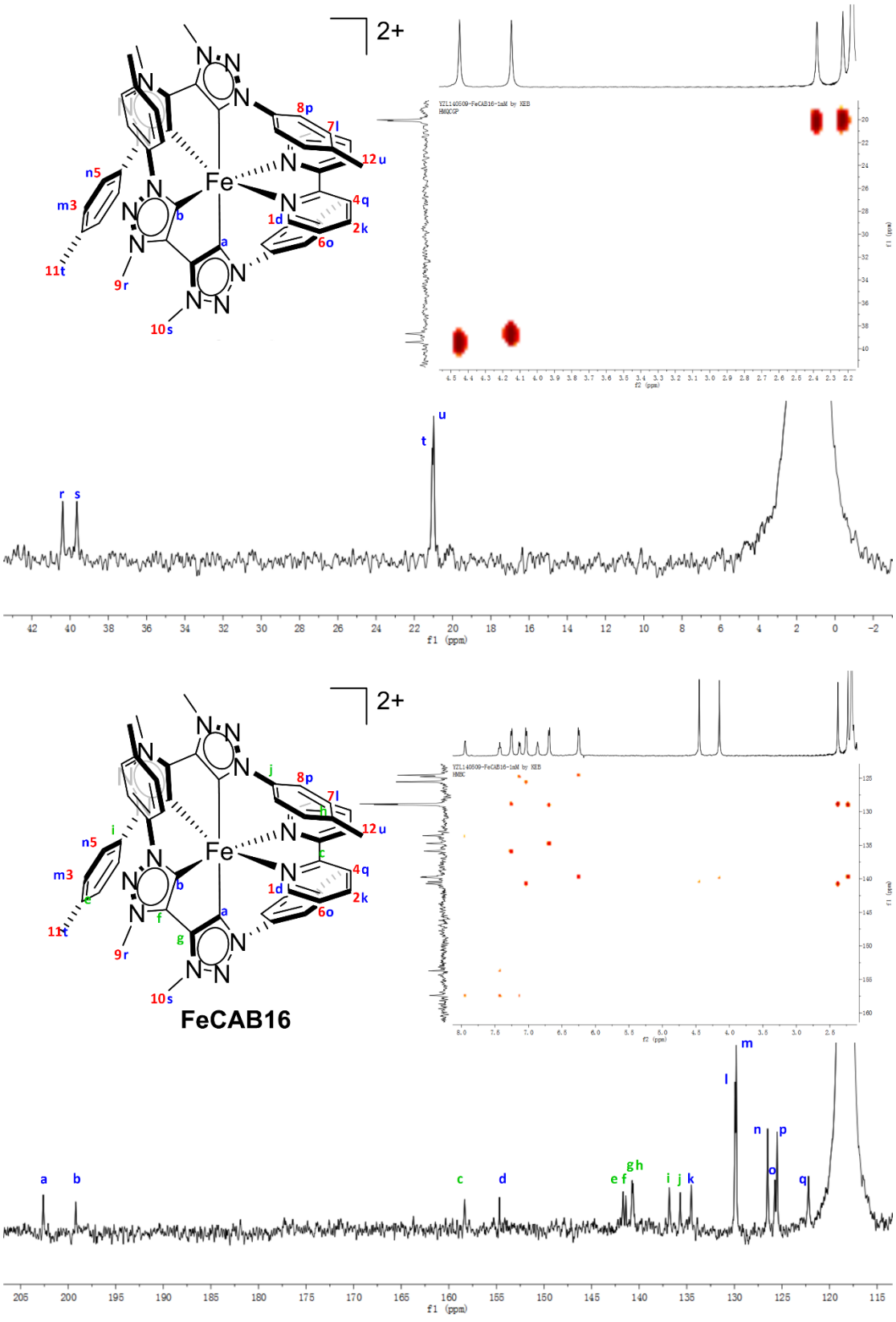


Figure S9 HMBC and assignment of the ^{13}C NMR of complex **1** in CD_3CN.

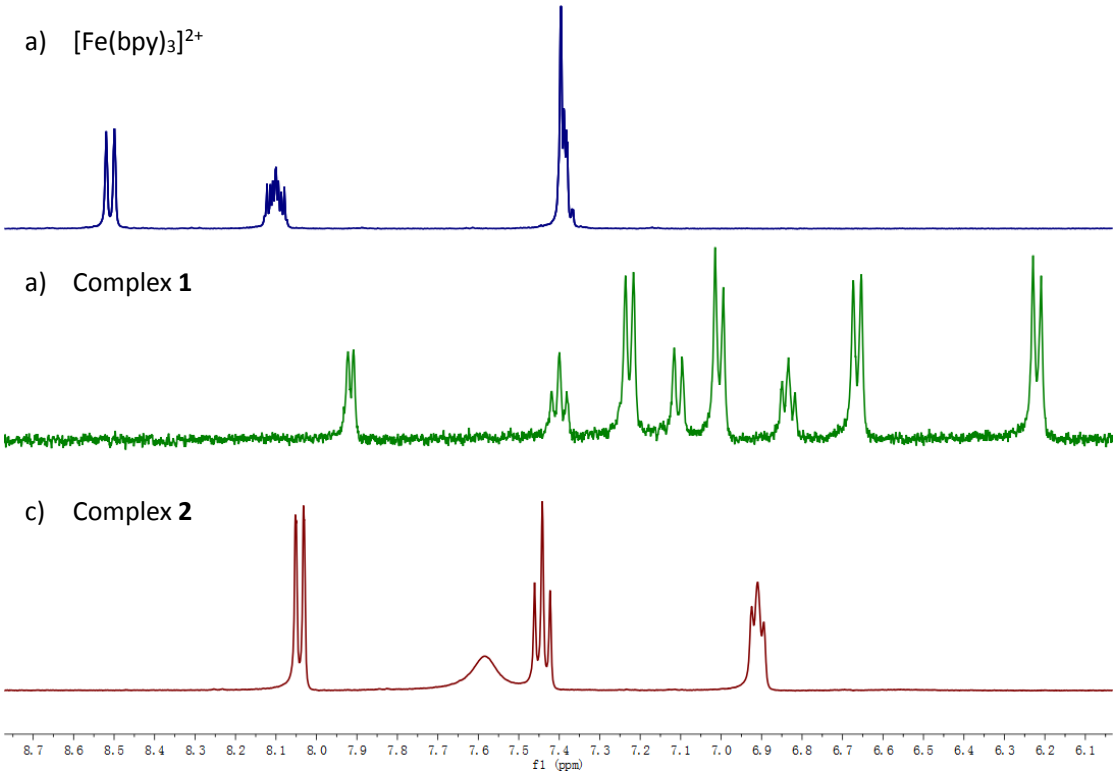


Figure S10 Comparison of the ^{1}H NMR spectra of $[Fe(bpy)_3]^{2+}$, complex **1** and **2** in CD_3CN.

2. Crystallographic data of complex 1

Intensity data for complex **1** was collected at 293 K with an Oxford Diffraction XcaliburTM 3 system using ω-scans and Mo-Kα radiation (Λ = 0.71073 Å).[8] CCD data were extracted and integrated and corrected for absorptions using a multi-scan method using Crysalis RED.[9] The structure was solved by charge flipping and refined by full-matrix least-squares calculations on F^2 using JANA2006.[10] Non-H atoms were refined with anisotropic displacement parameters. Hydrogen atoms were constrained to parent sites, using a riding model. The crystallographic data is available in CIF format, and can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif with the CCDC reference number 1018263.

The crystals were extremely thin plates that scatter only to limited resolution. To keep the ratio between data and parameters reasonable, all rings were treated as molecular fragments (four triazolylidene rings, four tolyl rings and two pyridyl rings). Hydrogen positions were fixed in a riding model. After refinement, a clearly defined residual density was identified well away from the main complex. This residual consisted of a double peak and when modelled as a pair of carbon atoms, it refined to ca 50% and 67% occupancy. The most probable explanation, given the solvent used, is a partially occupied methanol molecule. The ^{1}H NMR experiment (Figure S8) indicates the veracity of this conclusion.

Crystal data for **1Br**: $C_{50}H_{48}Br_2FeN_{14}\bullet(CH_3OH)_{0.5}$, M = 1074.69, orthorhombic, space group = Pbca (#61), *a* = 22.9329(16) Å, *b* = 19.472(3) Å, *c* = 23.180(2) Å, V = 10351.02(197) Å^3, Z = 8, density (calc.) = 1.379 g/cm^3, independent reflections = 5352 (*R*int = 0.105), GOF = 1.39. The final *R*1 factor was 0.0724 (I>2σ(I)) (w*R*2 = 0.1473).

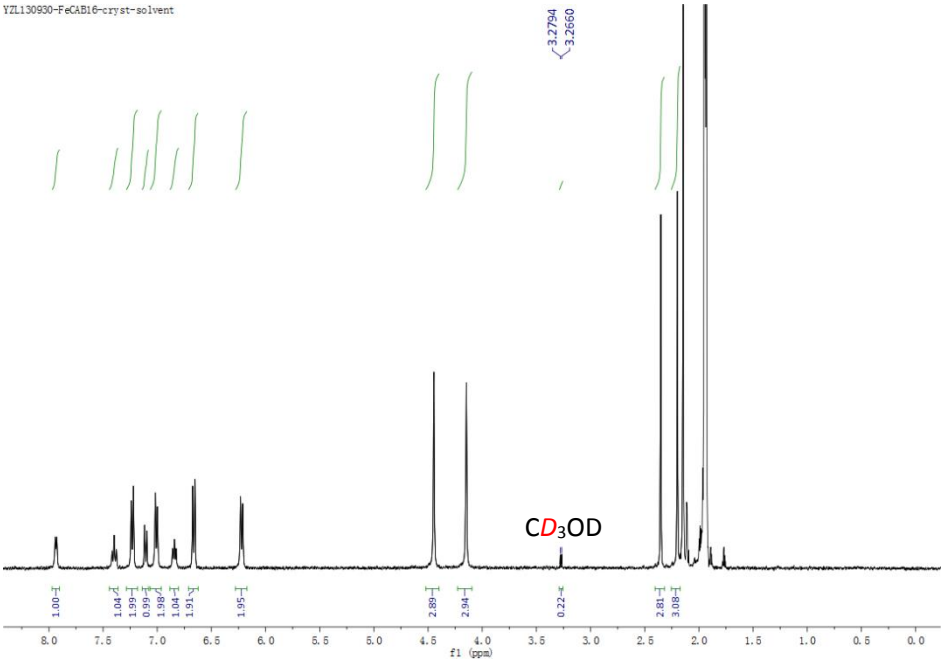


Figure S11 ^{1}H NMR of the crystals of **1Br** in CD_3CN.

[8] *Crysalis CCD*, Oxford Diffraction Ltd. Abingdon, Oxfordshire, UK, 2005.
[9] *Crysalis RED*, Oxford Diffraction Ltd. Abingdon, Oxfordshire, UK, 2005.
[10] Petricek, V., Dusek, M. & Palatinus, L. *Jana2006, Structure Determination Software Programs* (Institute of Physics, Praha, Czech Republic, 2006).

3. Cyclic voltammetry, differential pulse voltammetry and spectroelectrochemistry

All samples were dissolved in CH_3CN (Merck, spectroscopic grade, dried with 3 Å molecular sieves) with *n*-Bu_4NPF_6 (Fluka, electrochemical grade, vacuum dried at 383 K) as supporting electrolyte (0.1 M). All solutions were de-aerated by bubbling with solvent-saturated nitrogen and kept under nitrogen atmosphere during measurements.

Cyclic voltammetry (CV, scan rate 0.1 V/s) and differential pulse voltammetry (DPV, scan rate 0.05 V/s) were performed in a three-electrode, three-compartment cell controlled by an Autolab potentiostat (PGSTAT 302) with a GPES electrochemical interface (Eco Chemie). The cell was equipped with a glassy carbon disk working electrode (diam. 1 mm, CH Instruments), a glassy carbon rod auxiliary electrode, and a non-aqueous Ag^+/Ag reference electrode (CH Instruments, 0.010 M $AgNO_3$ in acetonitrile) with a potential of −0.08 V vs. the ferrocenium/ferrocene (Fc^+/Fc) couple in acetonitrile as an external standard. Potential values for reversible processes reported in this work were calculated as the average of the oxidative and reductive peak potentials in CV ($E_{1/2}=(E_{p,a} + E_{p,c})/2$), while those for the irreversible reduction processes of complex **1** were reported as the average of the oxidative and reductive peak potentials in DPV.

Spectroelectrochemistry was recorded on an 8453 UV-Vis diode array spectrophotometer (Agilent Technologies). The custom-built three-electrode, three-compartment quartz cell with an optical path length of 1 mm was equipped with a Pt mesh working electrode and the same reference and auxiliary electrodes as described for cyclic voltammetry. Multiple spectra were recorded in the course of controlled potential electrolysis that generated the desired redox states of complex **1**. The spectra obtained after exhaustive electrolysis were used for generating simulated differential absorption spectra.

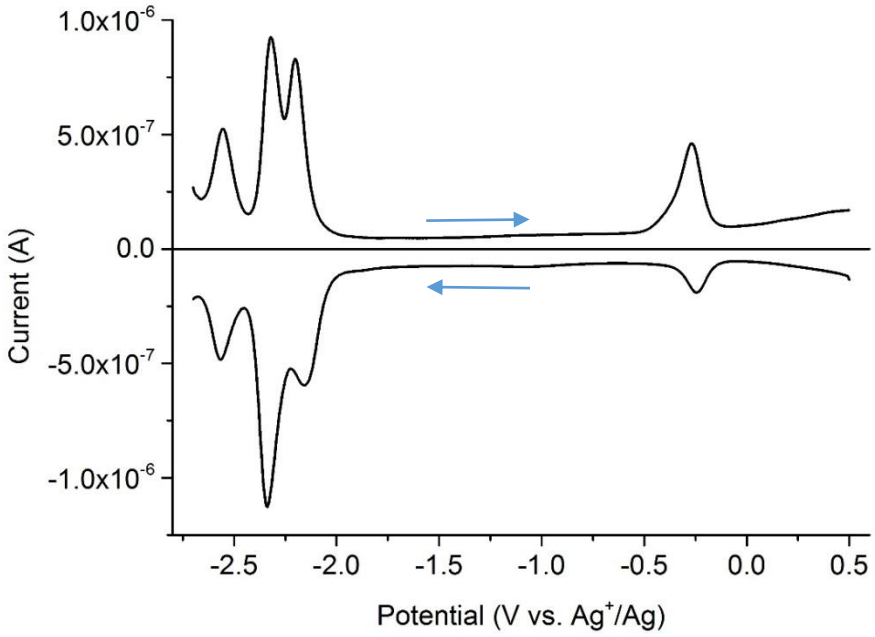


Figure S12 DPV of complex **1** in CD_3CN.

4. Solvatochromism of complex 2

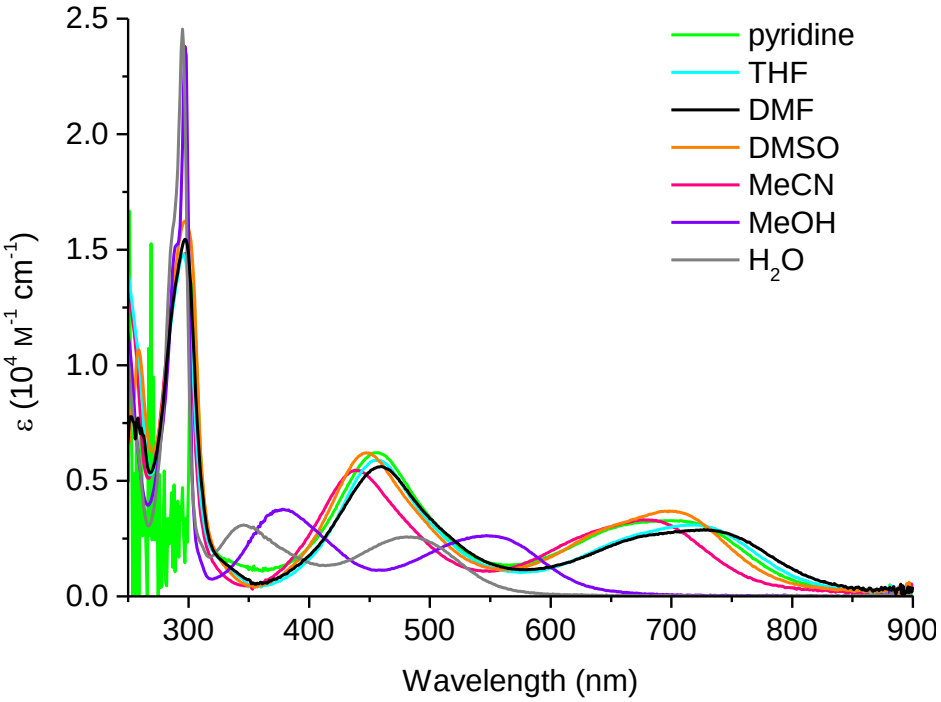


Figure S13 Solvatochromism of complex **2**.

5. Femtosecond transient absorption spectroscopy

The femtosecond laser setup is based on a MaiTai seeded Spitfire Pro XP amplifier (Spectra Physics) with central output wavelength of 795 nm and 1 kHz repetition rate delivering ~60 fs pulses. The beam was split into two parts: one for pumping a collinear optical parametric amplifier (TOPAS-C, Light Conversion) to generate the pump beam, while the second part was led through a computer-controlled delay line and used to generate the white-light continuum (WLC) probe. To generate the WLC the laser light was focused either into a 2-mm sapphire plate to probe the red part of transient spectra, or into a 3-mm CaF_2 translating optical window to probe in the blue-most tail of the transient spectra. Subsequently, the probe pulses were split into two parts: the former overlapping with the pump pulse in the sample volume and the latter serving as a reference. The probe and the reference beams were then brought to the slit of a spectrograph and dispersed onto a double photodiode array, each with 512 elements (Pascher Instruments). The intensity of excitation pulses was kept below 6.3×10^{15} photons·pulse^{-1}·cm^{-2}. Absorption spectra were measured before and after experiments to check for possible sample degradation. For complex **1**, degradation did not exceed 5% in any case (Figure S9). For complex **2**, photobleaching was observed after staying in the laser beam for 15 min and is illustrated by the comparison of the absorption spectra (Figure S10). The mutual polarization between pump and probe beams was set to the magic angle (54.7°) by placing Berek compensator in the pump beam. To correct for the Group Velocity Dispersion (GVD) of the probe light, the cross-phase modulation signal was measured for the neat solvent of each sample under identical experimental conditions, and used to correct the data.

Singular value decomposition and global analysis[11,12,13] of the transient spectra were performed according to literature procedures. To avoid any influence of the pump-probe cross-phase modulation on the analysis, the analysis was restricted to the spectra recorded at time delays greater than 0.5 ps.

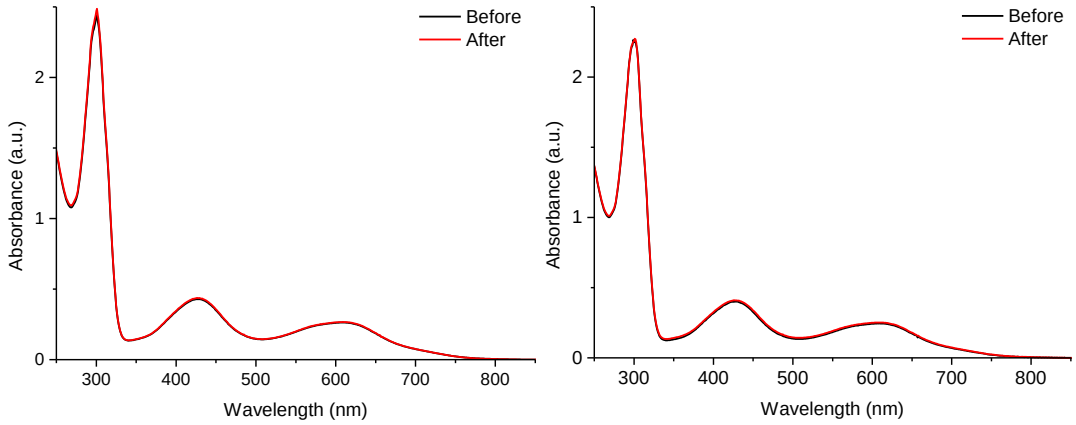


Figure S14 Steady-state UV–vis absorption spectra of complex **1** excited at 615 nm and probed in either blue (left, 340–550 nm) or red (right, 550–760 nm) window.

[11] I. H.M. van Stokkum, D. S. Larsen, R. van Grondelle, *Biochim. Biophys. Acta* **2004**, *1657*, 82-104.
[12] W. Gawelda, A. Cannizzo, V.-T. Pham, F. van Mourik, Ch. Bressler, M. Chergui, *J. Am. Chem. Soc.* **2007**, *129*, 8199-8206.
[13] C. Consani, M. Prémont-Schwarz, A. ElNahhas, Ch. Bressler, F. van Mourik, A. Cannizzo, M. Chergui, *Angew. Chem.* **2009**, *121*, 7320-7323; *Angew. Chem. Int. Ed.* **2009**, *48*, 7184-7187.

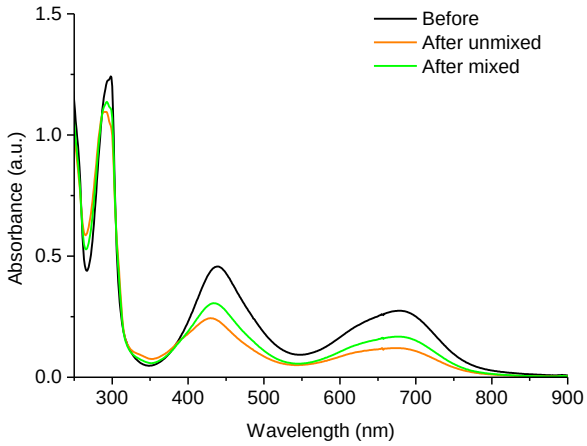


Figure S15 Steady-state UV–vis absorption spectra of complex **2** excited at 705 nm, before the TA measurement (black), right after the measurement without shaking the cuvette (orange) and after shaking the cuvette (homogenization, light green)

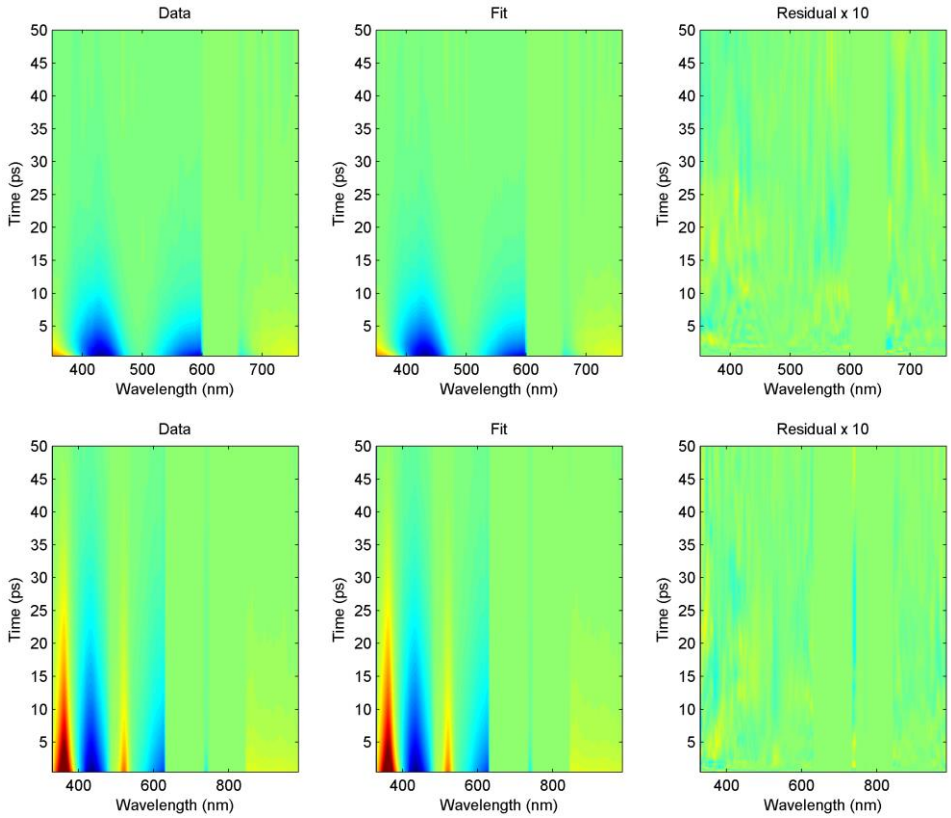


Figure S 16 2D TA plots (left: data; middle: global fit; right: residual) of complexes **1** (up) and **2** (down).

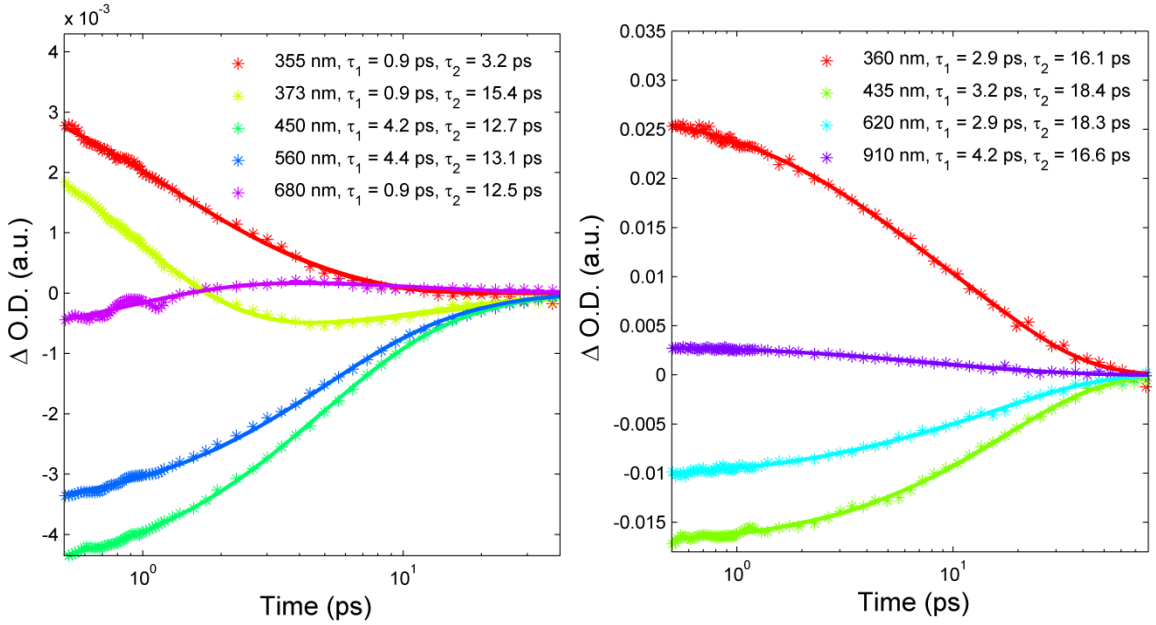


Figure S17 Kinetic fitting at single wavelengths for complexes **1** (left) and **2** (right). The star spots represent the original kinetic data points and the solid lines are the fitting curves.

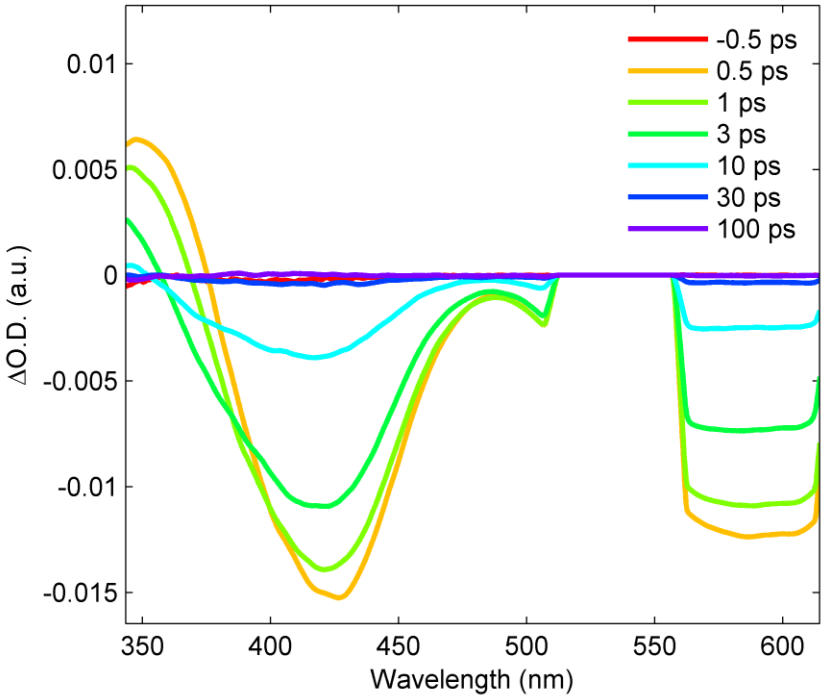


Figure S18 TA spectra of **1Br** in MeOH excited at 527 nm.

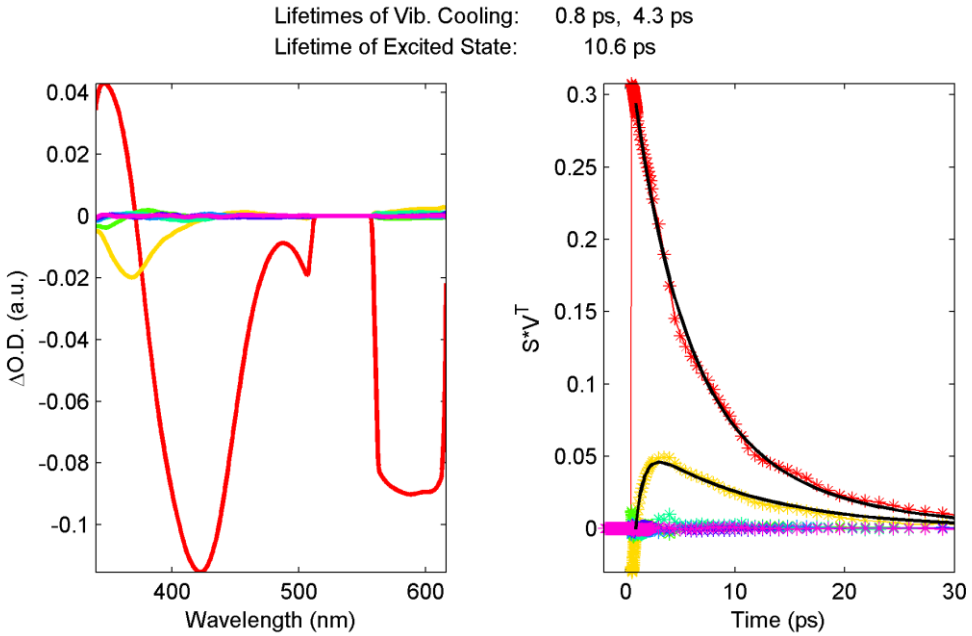


Figure S19 SVD analysis of the TA spectra of **1Br** in MeOH illustrated in Figure S18. The overall spectral evolution can be described by two major vectors. Kinetic fitting of these vectors delivered three time constants of 0.8, 4.3 and 10.6 ps. The results are similar with those for **1** in MeCN shown in Figure 5 (a) in the main text.

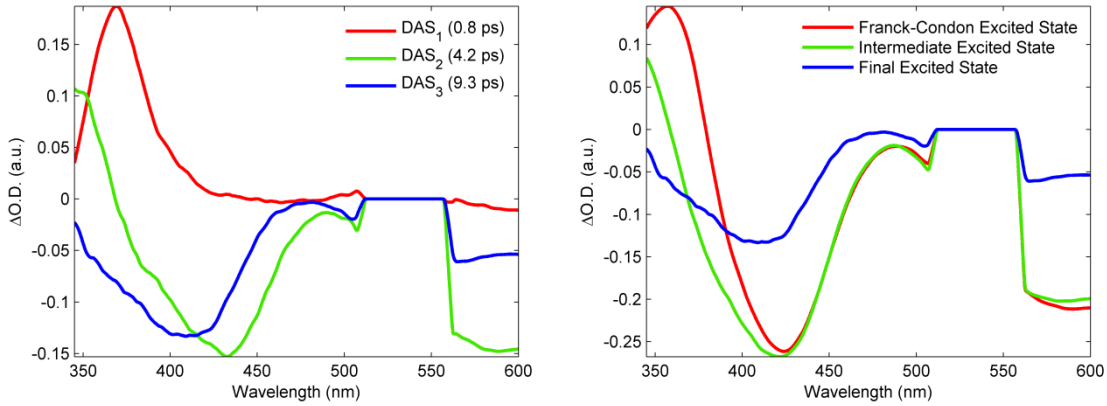
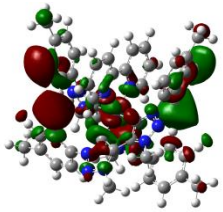
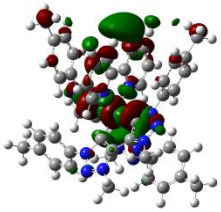
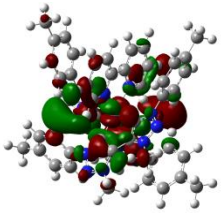
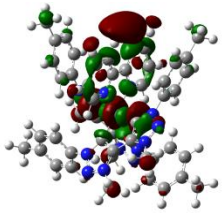
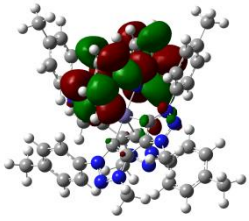
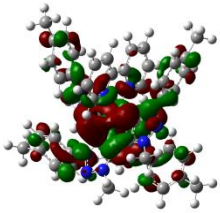


Figure S20 Global analysis of the TA spectra of **1Br** in MeOH illustrated in Figure S18. Three components are required to describe the spectral evolution, with the time constants of 0.8, 4.2 and 9.3 ps, consistent with those obtained from SVD. The results are similar with those for **1** in MeCN shown in Figure 6 (a) & (b) in the main text.

6. DFT and TD-DFT calculations

Fully optimized geometries of the ground state (GS), ^{3}MLCT, ^{3}MC and ^{5}MC were performed using the Gaussian09 program,[14] using the 6-311G(d.p) basis set, the PBE0[15][16][17] hybrid functional, and a polarizable continuum model (PCM) description of an acetonitrile solvent environment. No symmetry was imposed in the optimization of the structures and frequency calculations were empolyed to confirm all optimized geometries are local minima. Ground state properties have been calculated using the spin-restricted singlet formalism, while spin-unrestricted DFT (uDFT) calculations have been performed for the lowest triplet and quintet state calculations. The time-dependent formulation of DFT (TD-DFT) was used to probe the absorption properties of the complexes.

Table S1 Relevant PBE0|6-311G(d,p)|PCM(acetonitrile) calculated HOMOs and LUMOs of complex **1**.

	 LUMO+23	 LUMO+22	
 LUMO+21	 LUMO+20	 LUMO+17	 LUMO+16

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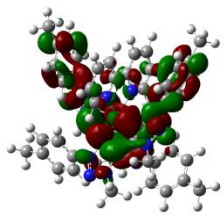
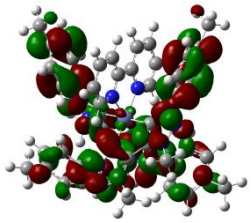
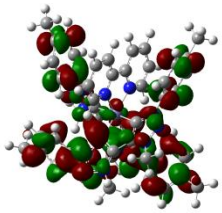
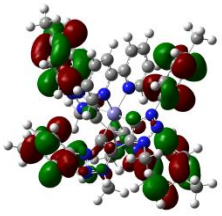
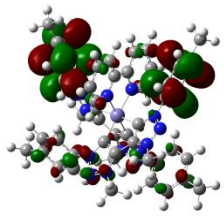
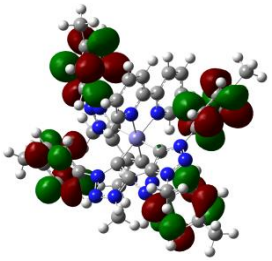
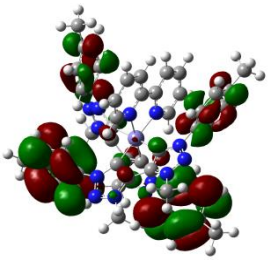
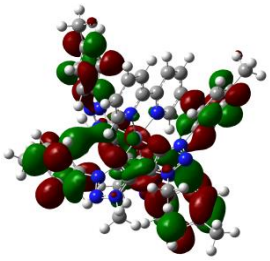
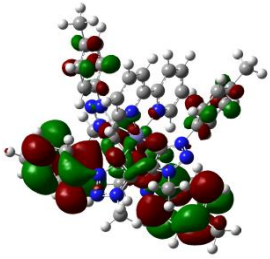
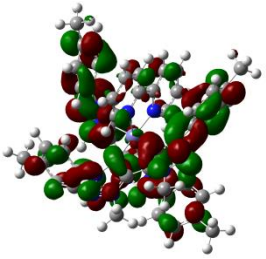
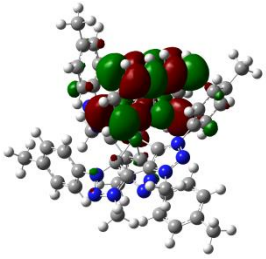
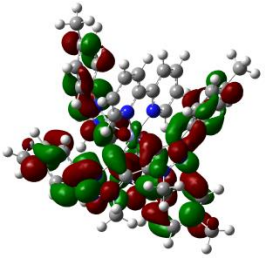
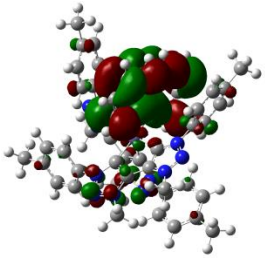
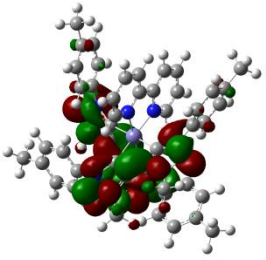
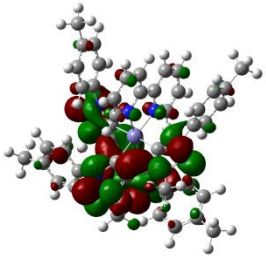
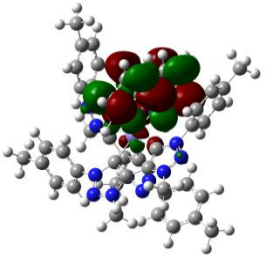
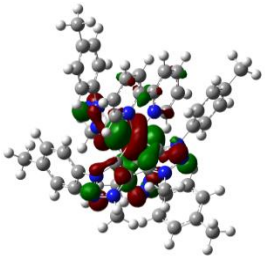
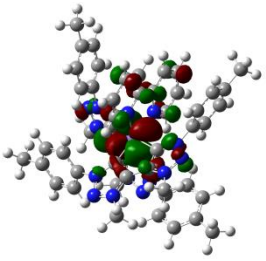
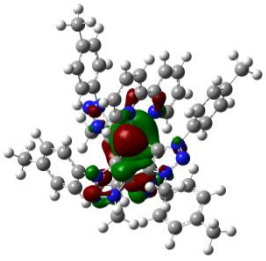
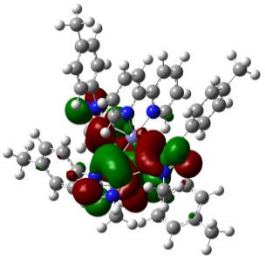
 LUMO+15	 LUMO+14	 LUMO+13	 LUMO+12
 LUMO+11	 LUMO+10	 LUMO+9	 LUMO+8
 LUMO+7	 LUMO+6	 LUMO+5	 LUMO+4
 LUMO+3	 LUMO+2	 LUMO+1	 LUMO
 HOMO	 HOMO-1	 HOMO-2	 HOMO-3

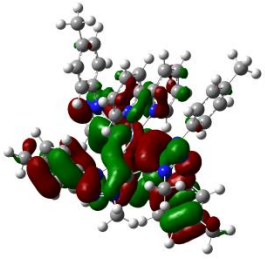
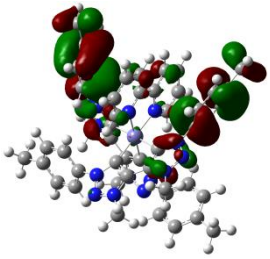
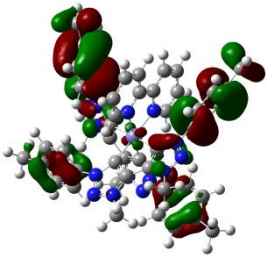
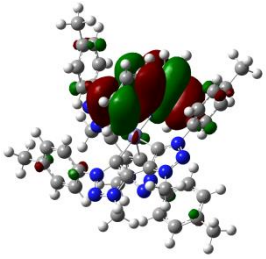
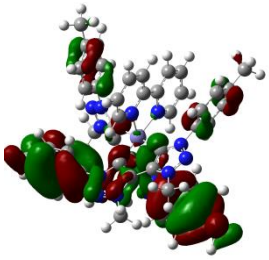
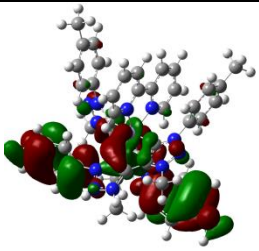
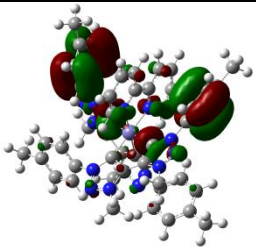
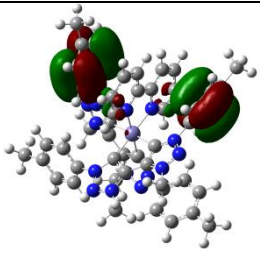
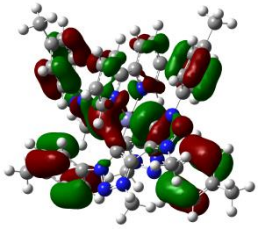
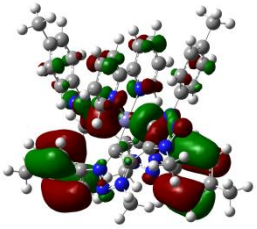
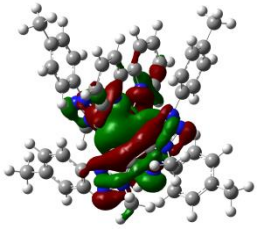
 HOMO-4	 HOMO-5	 HOMO-6	 HOMO-7
 HOMO-8	 HOMO-9	 HOMO-10	 HOMO-11
 HOMO-12	 HOMO-14	 HOMO-15	

Table S2 List of calculated transitions from GS singlet to excited states singlets of complex **1** using DFT, PBE0|6-311G(d,p)|PCM(acetonitrile).

Excitation	Energy (eV)	Wavelength (nm)	Oscillator Strength (f)	Transitions				Type
1	2.1839	567.73	0.0003	HOMO	→	LUMO	0.59848	MLCT
				HOMO	→	LUMO+1	0.10864	
				HOMO	→	LUMO+3	0.13793	
				HOMO	→	LUMO+16	-0.18592	
				HOMO	→	LUMO+21	0.11208	
				HOMO	→	LUMO+23	0.12806	
2	2.4426	507.59	0.0034	HOMO-2	→	LUMO	0.43103	MLCT
				HOMO-2	→	LUMO+3	0.11027	
				HOMO-2	→	LUMO+16	-0.17356	
				HOMO-2	→	LUMO+21	0.11935	
				HOMO-2	→	LUMO+23	0.13229	
				HOMO	→	LUMO	0.2762	
				HOMO	→	LUMO+7	0.10592	
				HOMO	→	LUMO+16	0.20171	
				HOMO	→	LUMO+21	-0.15547	
				HOMO	→	LUMO+23	-0.16503	
3	2.6042	476.09	0.0002	HOMO-2	→	LUMO	0.5228	MLCT
				HOMO-2	→	LUMO+16	0.11335	
				HOMO-2	→	LUMO+21	-0.10903	
				HOMO-2	→	LUMO+23	-0.11151	
				HOMO	→	LUMO	-0.17348	
				HOMO	→	LUMO+7	-0.10718	
				HOMO	→	LUMO+16	-0.1911	
				HOMO	→	LUMO+21	0.13599	
				HOMO	→	LUMO+23	0.14576	
4	2.6187	473.45	0.0197	HOMO-1	→	LUMO	0.41302	MLCT
				HOMO-1	→	LUMO+16	-0.19206	
				HOMO-1	→	LUMO+21	0.13915	
				HOMO-1	→	LUMO+23	0.15013	
				HOMO	→	LUMO+20	-0.25745	
				HOMO	→	LUMO+22	-0.28781	
5	2.7516	450.6	0.0252	HOMO-2	→	LUMO+16	-0.15796	MLCT
				HOMO-2	→	LUMO+21	0.12649	
				HOMO-2	→	LUMO+23	0.13276	
				HOMO-1	→	LUMO+22	-0.10933	

				HOMO	→	LUMO	-0.12984	
				HOMO	→	LUMO+1	0.60141	
6	2.7576	449.6	0.0271	HOMO-2	→	LUMO+20	0.1297	MLCT
				HOMO-2	→	LUMO+22	0.14934	
				HOMO-1	→	LUMO	0.53558	
				HOMO-1	→	LUMO+16	0.14125	
				HOMO-1	→	LUMO+21	-0.10463	
				HOMO-1	→	LUMO+23	-0.11226	
				HOMO	→	LUMO+20	0.17741	
				HOMO	→	LUMO+22	0.20213	
7	2.7737	447	0.0067	HOMO-2	→	LUMO+7	0.1236	MLCT/ MC
				HOMO-2	→	LUMO+16	0.24233	
				HOMO-2	→	LUMO+21	-0.19296	
				HOMO-2	→	LUMO+23	-0.20337	
				HOMO-1	→	LUMO+20	0.22567	
				HOMO-1	→	LUMO+22	0.25575	
				HOMO	→	LUMO+1	0.33626	
				HOMO	→	LUMO+16	0.13089	
				HOMO	→	LUMO+23	-0.10171	
8	2.8587	433.71	0.0154	HOMO	→	LUMO+2	0.69658	MLCT
9	2.9993	413.37	0.0024	HOMO-1	→	LUMO+1	0.69701	MLCT
10	3.012	411.64	0.0102	HOMO-2	→	LUMO	-0.11649	MLCT
				HOMO-2	→	LUMO+1	0.69317	
11	3.1053	399.27	0.0088	HOMO-1	→	LUMO+2	0.70127	MLCT
12	3.1167	397.81	0.0004	HOMO-2	→	LUMO+2	0.70283	MLCT
13	3.2338	383.4	0.0025	HOMO-1	→	LUMO+4	-0.1061	MLCT/ MC
				HOMO-1	→	LUMO+20	0.2226	
				HOMO-1	→	LUMO+22	0.25187	
				HOMO	→	LUMO	-0.11043	
				HOMO	→	LUMO+3	0.53748	
15	3.3551	369.54	0.0017	HOMO-2	→	LUMO+16	0.11484	MLCT
				HOMO-1	→	LUMO+4	0.22514	
				HOMO-1	→	LUMO+13	-0.11768	
				HOMO-1	→	LUMO+20	-0.22413	
				HOMO-1	→	LUMO+22	-0.25355	
				HOMO	→	LUMO+3	0.40476	
				HOMO	→	LUMO+7	0.16488	
				HOMO	→	LUMO+16	0.17885	
16	3.3752	367.34	0.0259	HOMO-2	→	LUMO+20	0.13731	MLCT
				HOMO-2	→	LUMO+22	0.15295	

				HOMO-1	→	LUMO	-0.10802	
				HOMO-1	→	LUMO+3	0.16832	
				HOMO	→	LUMO+5	0.54959	
				HOMO	→	LUMO+8	0.19767	
				HOMO	→	LUMO+13	0.10008	
				HOMO	→	LUMO+15	0.17669	
17	3.5052	353.71	0.0094	HOMO-2	→	LUMO+4	0.14301	MLCT
				HOMO-2	→	LUMO+5	0.23438	
				HOMO-2	→	LUMO+20	0.14805	
				HOMO-2	→	LUMO+22	0.16947	
				HOMO-1	→	LUMO+3	0.30466	
				HOMO-1	→	LUMO+6	-0.12896	
				HOMO	→	LUMO+4	0.35235	
				HOMO	→	LUMO+5	-0.20719	
				HOMO	→	LUMO+20	-0.11322	
				HOMO	→	LUMO+22	-0.12565	
18	3.5504	349.22	0.0034	HOMO-2	→	LUMO	-0.11129	MLCT
				HOMO-2	→	LUMO+3	0.66877	
				HOMO-2	→	LUMO+6	-0.11629	
19	3.5998	344.42	0.0166	HOMO-1	→	LUMO+4	-0.12297	MLCT
				HOMO-1	→	LUMO+5	-0.15679	
				HOMO	→	LUMO+3	0.10888	
				HOMO	→	LUMO+6	0.64532	
20	3.6241	342.11	0.0206	HOMO-2	→	LUMO+4	-0.16552	MLCT
				HOMO-2	→	LUMO+5	0.16001	
				HOMO-2	→	LUMO+8	0.10803	
				HOMO-1	→	LUMO+3	0.51342	
				HOMO	→	LUMO+4	-0.32711	
21	3.6656	338.24	0.0297	HOMO-1	→	LUMO+4	0.26048	MLCT
				HOMO-1	→	LUMO+5	0.59358	
				HOMO	→	LUMO+6	0.19854	
22	3.6842	336.53	0.0465	HOMO-2	→	LUMO+4	0.45107	MLCT
				HOMO-2	→	LUMO+5	0.38599	
				HOMO-2	→	LUMO+13	-0.11616	
				HOMO	→	LUMO+4	-0.15719	
				HOMO	→	LUMO+5	0.1968	
				HOMO	→	LUMO+8	-0.15651	
				HOMO	→	LUMO+15	-0.10674	
23	3.7174	333.52	0.0006	HOMO-2	→	LUMO+4	-0.19676	MC/
				HOMO-2	→	LUMO+5	0.31614	MLCT

				HOMO-2	→	LUMO+20	0.2171	
				HOMO-2	→	LUMO+22	0.24241	
				HOMO-1	→	LUMO+3	-0.23074	
				HOMO-1	→	LUMO+7	-0.17666	
				HOMO-1	→	LUMO+16	-0.16963	
				HOMO	→	LUMO+4	-0.16439	
				HOMO	→	LUMO+5	-0.18932	
				HOMO	→	LUMO+8	0.15836	
24	3.7636	329.43	0.0032	HOMO-2	→	LUMO+6	0.1274	MLCT
				HOMO-1	→	LUMO+4	0.50651	
				HOMO-1	→	LUMO+5	-0.18689	
				HOMO-1	→	LUMO+8	-0.19736	
				HOMO-1	→	LUMO+13	-0.16748	
				HOMO-1	→	LUMO+15	-0.10973	
				HOMO-1	→	LUMO+20	0.11016	
				HOMO-1	→	LUMO+22	0.11526	
				HOMO	→	LUMO+7	-0.19524	
25	3.7991	326.35	0.0014	HOMO-2	→	LUMO+4	0.31547	MLCT
				HOMO-2	→	LUMO+5	-0.14281	
				HOMO-1	→	LUMO+3	0.11726	
				HOMO-1	→	LUMO+6	0.38558	
				HOMO	→	LUMO+5	-0.15916	
				HOMO	→	LUMO+8	0.28318	
				HOMO	→	LUMO+9	-0.13999	
				HOMO	→	LUMO+15	0.15059	
				HOMO	→	LUMO+22	0.1036	
26	3.8735	320.08	0.0086	HOMO-2	→	LUMO+6	0.63792	MLCT
				HOMO	→	LUMO+7	0.17288	
27	3.9203	316.27	0.0034	HOMO-3	→	LUMO	0.14973	MLCT
				HOMO-2	→	LUMO+4	-0.22796	
				HOMO-2	→	LUMO+5	0.17164	
				HOMO-1	→	LUMO+6	0.50985	
				HOMO-1	→	LUMO+7	0.11874	
				HOMO-1	→	LUMO+16	0.10951	
				HOMO	→	LUMO+4	0.14897	
				HOMO	→	LUMO+8	-0.10789	
29	3.9937	310.45	0.0002	HOMO-2	→	LUMO+6	-0.10395	MLCT/ MC
				HOMO-1	→	LUMO+4	0.21128	
				HOMO-1	→	LUMO+5	-0.14625	
				HOMO-1	→	LUMO+8	0.17054	

				HOMO-1	→	LUMO+9	-0.1012	
				HOMO-1	→	LUMO+15	0.12694	
				HOMO-1	→	LUMO+22	0.1057	
				HOMO	→	LUMO+7	0.49801	
				HOMO	→	LUMO+21	0.14702	
				HOMO	→	LUMO+23	0.12772	
30	4.0005	309.92	0.0103	HOMO-3	→	LUMO	0.68016	MLCT
31	4.0523	305.96	0.0118	HOMO-1	→	LUMO+4	0.10959	MLCT/ MC
				HOMO-1	→	LUMO+5	-0.15664	
				HOMO-1	→	LUMO+8	0.45392	
				HOMO-1	→	LUMO+9	-0.19559	
				HOMO-1	→	LUMO+13	0.14481	
				HOMO-1	→	LUMO+15	0.25059	
				HOMO	→	LUMO+7	-0.26809	
32	4.1272	300.41	0.0002	HOMO	→	LUMO+8	0.28125	MLCT
				HOMO	→	LUMO+9	0.63	
33	4.1819	296.48	0.0042	HOMO-3	→	LUMO+1	0.13369	MLCT/ MC
				HOMO-2	→	LUMO+8	0.36607	
				HOMO-2	→	LUMO+9	-0.16351	
				HOMO-2	→	LUMO+15	0.1534	
				HOMO-1	→	LUMO+6	0.12006	
				HOMO-1	→	LUMO+7	-0.32904	
				HOMO-1	→	LUMO+21	-0.10704	
				HOMO	→	LUMO+4	0.13439	
				HOMO	→	LUMO+8	-0.13183	
				HOMO	→	LUMO+11	-0.18844	
				HOMO	→	LUMO+13	0.20261	
34	4.203	294.99	0.001	HOMO	→	LUMO+7	0.10316	MLCT
				HOMO	→	LUMO+10	0.67129	
				HOMO	→	LUMO+12	0.13569	
35	4.2216	293.69	0.1293	HOMO-3	→	LUMO+1	0.61867	MLCT
				HOMO-1	→	LUMO+6	-0.10286	
				HOMO-1	→	LUMO+7	0.13807	
				HOMO	→	LUMO+11	-0.1454	
36	4.2474	291.91	0.0037	HOMO-2	→	LUMO+7	0.62651	MLCT
				HOMO-2	→	LUMO+21	0.1733	
				HOMO-2	→	LUMO+23	0.14203	
37	4.2558	291.33	0.0265	HOMO-3	→	LUMO+1	0.21545	MLCT
				HOMO-1	→	LUMO+7	-0.14481	
				HOMO	→	LUMO+11	0.61197	

				HOMO	→	LUMO+13	-0.11553	
38	4.3172	287.19	0.0144	HOMO	→	LUMO+10	-0.15252	MLCT
				HOMO	→	LUMO+12	0.66779	
39	4.3314	286.24	0.0035	HOMO-1	→	LUMO+7	0.29422	MLCT/ MC
				HOMO-1	→	LUMO+21	0.10119	
				HOMO	→	LUMO+8	-0.26353	
				HOMO	→	LUMO+9	0.11358	
				HOMO	→	LUMO+11	0.22367	
				HOMO	→	LUMO+13	0.40488	
				HOMO	→	LUMO+15	0.20426	
40	4.3421	285.54	0.1915	HOMO-4	→	LUMO	-0.33802	MLCT
				HOMO-3	→	LUMO+2	0.57725	
41	4.3498	285.04	0.0961	HOMO-9	→	LUMO	-0.10845	LC
				HOMO-5	→	LUMO	0.1413	
				HOMO-4	→	LUMO	0.56823	
				HOMO-3	→	LUMO+2	0.33772	
42	4.3796	283.1	0.0007	HOMO-2	→	LUMO+8	0.36619	MLCT/ MC
				HOMO-2	→	LUMO+9	-0.16763	
				HOMO-1	→	LUMO+7	0.361	
				HOMO-1	→	LUMO+16	-0.11387	
				HOMO	→	LUMO+8	0.17999	
				HOMO	→	LUMO+13	-0.18866	
				HOMO	→	LUMO+15	-0.21174	
44	4.4286	279.97	0.0008	HOMO-1	→	LUMO+8	0.25195	MLCT
				HOMO-1	→	LUMO+9	0.63496	
45	4.4477	278.76	0.0432	HOMO-5	→	LUMO	0.67384	LC
				HOMO-4	→	LUMO	-0.15055	
46	4.4645	277.71	0.0001	HOMO-8	→	LUMO	-0.23023	LC
				HOMO-6	→	LUMO	0.65533	
47	4.4784	276.85	0.0071	HOMO	→	LUMO+14	0.66756	MLCT
49	4.511	274.85	0.0011	HOMO-2	→	LUMO+10	0.59522	MLCT
				HOMO-2	→	LUMO+12	0.14482	
				HOMO-1	→	LUMO+11	0.28169	
50	4.5154	274.58	0.0145	HOMO-7	→	LUMO	-0.17735	MLCT
				HOMO-2	→	LUMO+10	-0.30291	
				HOMO-1	→	LUMO+9	0.10019	
				HOMO-1	→	LUMO+11	0.54736	
				HOMO-1	→	LUMO+13	-0.15783	
51	4.5448	272.8	0.0003	HOMO-4	→	LUMO+2	-0.12733	MLCT
				HOMO-2	→	LUMO+4	-0.11191	

				HOMO-2	→	LUMO+11	0.56892	
				HOMO-2	→	LUMO+13	-0.29101	
				HOMO	→	LUMO+15	0.15315	
52	4.546	272.73	0.0636	HOMO-6	→	LUMO+2	-0.11627	MLCT
				HOMO-4	→	LUMO+1	0.6525	
				HOMO-1	→	LUMO+11	-0.10381	
53	4.5717	271.2	0.1794	HOMO-7	→	LUMO	0.57536	LC
				HOMO-7	→	LUMO+1	0.11241	
				HOMO-1	→	LUMO+8	0.14212	
				HOMO-1	→	LUMO+11	0.13743	
				HOMO-1	→	LUMO+13	-0.19737	
54	4.594	269.88	0.0072	HOMO-4	→	LUMO+2	-0.21934	MLCT
				HOMO-2	→	LUMO+8	0.12582	
				HOMO-2	→	LUMO+11	-0.26928	
				HOMO-2	→	LUMO+13	-0.13434	
				HOMO-1	→	LUMO+12	0.28391	
				HOMO	→	LUMO+13	-0.26393	
				HOMO	→	LUMO+15	0.38241	
55	4.6069	269.13	0.0044	HOMO-4	→	LUMO+2	0.11453	MLCT
				HOMO-2	→	LUMO+8	-0.12068	
				HOMO-2	→	LUMO+11	0.16641	
				HOMO-1	→	LUMO+12	0.61722	
				HOMO	→	LUMO+13	0.1022	
				HOMO	→	LUMO+15	-0.10859	
56	4.6185	268.45	0.0115	HOMO-7	→	LUMO	-0.13257	MLCT
				HOMO-2	→	LUMO+12	0.40433	
				HOMO-1	→	LUMO+8	0.22398	
				HOMO-1	→	LUMO+11	-0.2073	
				HOMO-1	→	LUMO+13	-0.38471	
				HOMO-1	→	LUMO+15	-0.16317	
57	4.6265	267.98	0.011	HOMO-7	→	LUMO	0.12771	MLCT
				HOMO-2	→	LUMO+10	-0.14562	
				HOMO-2	→	LUMO+12	0.53107	
				HOMO-1	→	LUMO+8	-0.18031	
				HOMO-1	→	LUMO+11	0.14981	
				HOMO-1	→	LUMO+13	0.28132	
				HOMO-1	→	LUMO+15	0.12734	
58	4.6488	266.7	0.1171	HOMO-8	→	LUMO+1	-0.20287	MLCT
				HOMO-6	→	LUMO+1	-0.33653	
				HOMO-5	→	LUMO+2	0.14343	

				HOMO-4	→	LUMO+2	0.48723	
				HOMO	→	LUMO+13	-0.12694	
				HOMO	→	LUMO+15	0.20333	
59	4.6679	265.61	0.0142	HOMO-14	→	LUMO	-0.18962	LC
				HOMO-12	→	LUMO	-0.28313	
				HOMO-10	→	LUMO	0.25807	
				HOMO-8	→	LUMO	-0.2849	
				HOMO-8	→	LUMO+1	0.12119	
				HOMO-6	→	LUMO	-0.14465	
				HOMO-2	→	LUMO+11	0.14802	
				HOMO-2	→	LUMO+13	0.29945	
				HOMO	→	LUMO+13	-0.13013	
				HOMO	→	LUMO+15	0.12619	
61	4.729	262.18	0.1021	HOMO-12	→	LUMO+1	0.13278	LC
				HOMO-8	→	LUMO+1	0.57806	
				HOMO-5	→	LUMO+2	0.21125	
				HOMO-4	→	LUMO+2	0.10254	
				HOMO-3	→	LUMO+3	-0.11399	
62	4.7345	261.87	0.0457	HOMO-8	→	LUMO+2	0.14773	LC
				HOMO-6	→	LUMO+2	-0.27769	
				HOMO-5	→	LUMO+1	0.53255	
				HOMO-2	→	LUMO+14	0.14409	
				HOMO-1	→	LUMO+13	0.10004	
				HOMO	→	LUMO+16	-0.11836	
63	4.7518	260.92	0.0014	HOMO-6	→	LUMO+1	0.23117	MLCT
				HOMO-5	→	LUMO+2	-0.14958	
				HOMO-4	→	LUMO+2	0.14673	
				HOMO-2	→	LUMO+13	0.11882	
				HOMO-1	→	LUMO+14	0.55946	
64	4.7584	260.56	0.0004	HOMO-9	→	LUMO+1	0.18007	MLCT
				HOMO-8	→	LUMO+2	-0.31339	
				HOMO-2	→	LUMO+14	0.53832	
65	4.78	259.38	0.0001	HOMO-12	→	LUMO	-0.12234	LC/ MLCT
				HOMO-10	→	LUMO	-0.30269	
				HOMO-6	→	LUMO+1	-0.27486	
				HOMO-5	→	LUMO+2	0.17499	
				HOMO-4	→	LUMO+2	-0.20977	
				HOMO-3	→	LUMO+3	0.34768	
				HOMO-1	→	LUMO+14	0.28785	
66	4.7876	258.97	0.0079	HOMO-11	→	LUMO	0.61842	LC

				HOMO-9	→	LUMO	-0.12287	
				HOMO-9	→	LUMO+1	-0.11548	
				HOMO-7	→	LUMO+1	-0.20225	
				HOMO-2	→	LUMO+14	0.13435	
67	4.7908	258.8	0.0005	HOMO-12	→	LUMO	0.21639	LC
				HOMO-10	→	LUMO	0.4955	
				HOMO-8	→	LUMO	0.2196	
				HOMO-6	→	LUMO+1	-0.20376	
				HOMO-5	→	LUMO+2	0.10811	
				HOMO-4	→	LUMO+2	-0.17496	
				HOMO-3	→	LUMO+3	0.10523	
				HOMO-1	→	LUMO+14	0.12442	
				HOMO	→	LUMO+17	-0.13007	
68	4.7947	258.59	0.0037	HOMO-11	→	LUMO	-0.23767	LC/ MLCT
				HOMO-9	→	LUMO+1	-0.24918	
				HOMO-8	→	LUMO+2	0.25765	
				HOMO-6	→	LUMO+2	0.11239	
				HOMO-2	→	LUMO+14	0.33101	
				HOMO	→	LUMO+16	0.26782	
				HOMO	→	LUMO+21	0.17001	
				HOMO	→	LUMO+23	0.11992	
69	4.8224	257.1	0.0264	HOMO-15	→	LUMO	-0.12558	LC
				HOMO-14	→	LUMO	-0.18225	
				HOMO-12	→	LUMO	-0.33907	
				HOMO-8	→	LUMO	0.42036	
				HOMO-6	→	LUMO	0.13256	
				HOMO-4	→	LUMO+2	-0.12009	
				HOMO-3	→	LUMO+3	-0.29674	
70	4.8244	256.99	0.0487	HOMO-11	→	LUMO	0.1384	LC/ MLCT
				HOMO-9	→	LUMO+1	0.13736	
				HOMO-7	→	LUMO	-0.11825	
				HOMO-7	→	LUMO+1	0.45845	
				HOMO-5	→	LUMO+1	0.13471	
				HOMO-1	→	LUMO+15	-0.18168	
				HOMO	→	LUMO+16	0.28397	
				HOMO	→	LUMO+21	0.184	
				HOMO	→	LUMO+23	0.13085	
71	4.8389	256.22	0.0083	HOMO-8	→	LUMO+2	0.18393	LC/ MLCT
				HOMO-7	→	LUMO+1	0.35017	
				HOMO-6	→	LUMO+2	0.12588	

				HOMO-1	→	LUMO+8	-0.12651	
				HOMO-1	→	LUMO+13	-0.20185	
				HOMO-1	→	LUMO+15	0.39992	
				HOMO	→	LUMO+16	-0.16891	
				HOMO	→	LUMO+21	-0.11419	
72	4.8441	255.95	0.0038	HOMO-14	→	LUMO	-0.10094	MLCT/ LC
				HOMO-12	→	LUMO	-0.18406	
				HOMO-12	→	LUMO+1	0.15223	
				HOMO-8	→	LUMO	0.17411	
				HOMO-6	→	LUMO+1	0.18421	
				HOMO-5	→	LUMO+2	-0.10482	
				HOMO-4	→	LUMO+2	0.16582	
				HOMO-3	→	LUMO+3	0.36728	
				HOMO-2	→	LUMO+13	-0.13609	
				HOMO	→	LUMO+17	-0.34022	
73	4.8552	255.36	0.006	HOMO-12	→	LUMO+1	0.21193	MLCT
				HOMO-10	→	LUMO	0.13419	
				HOMO-10	→	LUMO+1	-0.12894	
				HOMO-3	→	LUMO+3	0.22929	
				HOMO	→	LUMO+17	0.54609	
74	4.8582	255.2	0.0003	HOMO-9	→	LUMO+1	0.20639	LC/ MLCT
				HOMO-8	→	LUMO+2	0.35663	
				HOMO-6	→	LUMO+2	0.22262	
				HOMO-3	→	LUMO+2	-0.11857	
				HOMO-1	→	LUMO+13	0.20448	
				HOMO-1	→	LUMO+15	-0.29968	
				HOMO	→	LUMO+16	-0.18509	
				HOMO	→	LUMO+21	-0.11493	
75	4.8663	254.78	0.0034	HOMO-14	→	LUMO+1	0.17607	LC
				HOMO-12	→	LUMO+1	0.43526	
				HOMO-10	→	LUMO+1	-0.26686	
				HOMO-8	→	LUMO	-0.11246	
				HOMO-8	→	LUMO+1	-0.17893	
				HOMO-6	→	LUMO+1	-0.12879	
				HOMO-4	→	LUMO+2	-0.10526	
				HOMO-3	→	LUMO+3	-0.20098	
				HOMO	→	LUMO+17	-0.14468	
76	4.8814	253.99	0.1363	HOMO-9	→	LUMO	0.10772	LC
				HOMO-9	→	LUMO+1	0.50696	
				HOMO-8	→	LUMO+2	0.11186	

				HOMO-7	→	LUMO+1	-0.23523	
				HOMO-5	→	LUMO+1	0.1419	
				HOMO-1	→	LUMO+13	-0.11869	
				HOMO-1	→	LUMO+15	0.18605	
				HOMO	→	LUMO+16	0.13201	
77	4.9086	252.58	0.0128	HOMO-11	→	LUMO	0.16304	LC
				HOMO-9	→	LUMO	0.63793	
				HOMO-7	→	LUMO+1	0.11332	
				HOMO-4	→	LUMO	0.14142	
78	4.9181	252.1	0.0073	HOMO-9	→	LUMO+2	0.24713	LC
				HOMO-7	→	LUMO+2	0.42669	
				HOMO-5	→	LUMO+2	0.16533	
				HOMO-2	→	LUMO+13	-0.12068	
				HOMO-2	→	LUMO+15	0.36008	
				HOMO-1	→	LUMO+16	-0.13481	
79	4.928	251.59	0.0016	HOMO-14	→	LUMO+2	0.2175	LC
				HOMO-12	→	LUMO+2	0.45492	
				HOMO-10	→	LUMO+2	-0.27399	
				HOMO-9	→	LUMO+1	0.14369	
				HOMO-6	→	LUMO+2	-0.22927	
				HOMO-5	→	LUMO+1	-0.13062	
				HOMO-3	→	LUMO+4	-0.14411	
80	4.9284	251.57	0.0038	HOMO-9	→	LUMO+2	-0.13204	MLCT/ LC
				HOMO-7	→	LUMO+2	-0.37792	
				HOMO-5	→	LUMO+2	-0.13272	
				HOMO-2	→	LUMO+13	-0.13167	
				HOMO-2	→	LUMO+15	0.42569	
				HOMO-1	→	LUMO+16	-0.1763	
				HOMO	→	LUMO+17	0.1274	

Table S3 PBE0|6-311G(d,p)|PCM(acetonitrile) spin density on Fe transitioning from MLCT triplets and quintets on the left to MC states on the right. The geometries used for these values are named across the top and calculated values of spin on Fe center.

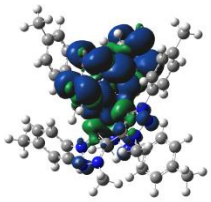
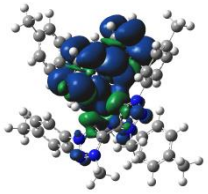
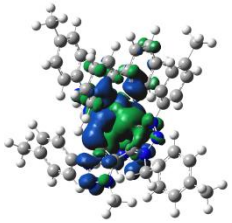
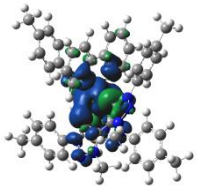
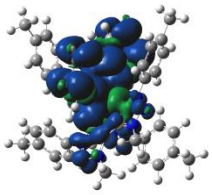
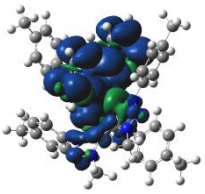
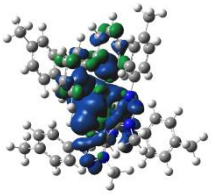
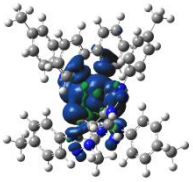
	GS	^{3}MLCT	^{3}MC	^{5}MC
T1				
	1.16	1.14	2.09	1.99
Q1				
	2.88	2.18	3.73	3.79

Table S4 Optimized coordinates for each stationary point geometry (GS (ground state), ^{3}MLCT, ^{3}MC, and ^{5}MC states) of complex **1**.

	GS			^{3}MLCT			^{3}MC			^{5}MC		
	x	y	z	x	y	z	x	y	z	x	y	z
C	2.175	-0.981	1.637	2.173	-0.948	1.663	2.048	-1.241	1.621	2.356	-0.870	1.692
C	1.905	-0.020	0.653	1.914	0.001	0.675	1.840	-0.168	0.745	2.158	0.093	0.702
N	3.410	-0.751	2.140	3.401	-0.702	2.176	3.312	-1.160	2.103	3.497	-0.561	2.368
N	3.971	0.279	1.564	3.954	0.324	1.589	3.946	-0.136	1.603	4.065	0.504	1.874
C	-0.127	-1.464	1.296	-0.112	-1.481	1.292	-0.321	-1.549	1.428	0.018	-1.560	1.507
C	1.064	-1.837	1.936	1.069	-1.817	1.952	0.895	-2.058	1.889	1.317	-1.846	1.931
C	4.154	-1.427	3.190	4.143	-1.359	3.241	4.032	-1.998	3.048	4.113	-1.181	3.531
H	3.602	-1.363	4.127	3.591	-1.269	4.176	3.468	-2.065	3.977	3.341	-1.399	4.268
H	4.327	-2.465	2.914	4.309	-2.403	2.986	4.197	-2.986	2.620	4.641	-2.089	3.243
H	5.106	-0.912	3.292	5.097	-0.847	3.329	4.989	-1.519	3.237	4.818	-0.465	3.945
C	1.756	-3.828	3.379	1.746	-3.771	3.455	1.609	-4.304	2.896	2.455	-3.951	2.838
H	2.611	-4.118	2.769	2.602	-4.081	2.857	2.419	-4.467	2.186	3.314	-3.789	2.187
H	2.079	-3.284	4.265	2.064	-3.199	4.325	1.995	-3.974	3.859	2.700	-3.707	3.871
H	1.202	-4.715	3.675	1.186	-4.645	3.775	1.051	-5.228	3.026	2.143	-4.990	2.773
N	0.856	-3.004	2.589	0.853	-2.968	2.633	0.688	-3.318	2.355	1.347	-3.134	2.371
N	-0.944	-2.498	1.670	-0.933	-2.502	1.667	-1.147	-2.606	1.692	-0.603	-2.744	1.782
N	3.062	0.710	0.695	3.057	0.744	0.711	3.060	0.448	0.806	3.255	0.881	0.897

C	3.400	1.914	0.000	3.411	1.925	-0.019	3.483	1.672	0.198	3.596	2.071	0.188
C	3.420	1.949	-1.386	3.369	1.933	-1.403	3.541	1.786	-1.182	3.420	2.120	-1.187
C	3.742	3.038	0.742	3.842	3.039	0.690	3.866	2.728	1.014	4.102	3.165	0.879
C	3.777	3.124	-2.031	3.759	3.077	-2.084	3.975	2.976	-1.748	3.746	3.281	-1.872
H	3.165	1.065	-1.954	3.039	1.058	-1.944	3.258	0.950	-1.809	3.036	1.254	-1.710
C	4.101	4.205	0.082	4.231	4.174	-0.007	4.301	3.911	0.434	4.429	4.316	0.177
H	3.728	2.994	1.825	3.870	3.014	1.773	3.822	2.619	2.092	4.235	3.113	1.953
C	4.120	4.271	-1.312	4.193	4.215	-1.402	4.358	4.058	-0.953	4.253	4.399	-1.205
H	3.794	3.146	-3.116	3.725	3.081	-3.169	4.024	3.060	-2.829	3.611	3.315	-2.949
H	4.368	5.082	0.664	4.566	5.045	0.547	4.600	4.736	1.073	4.824	5.170	0.718
C	-2.297	-2.748	1.282	-2.284	-2.756	1.264	-2.538	-2.704	1.405	-1.974	-3.063	1.553
C	-3.301	-1.875	1.671	-3.294	-1.894	1.661	-3.357	-1.610	1.646	-2.940	-2.094	1.791
C	-2.587	-3.877	0.531	-2.557	-3.876	0.494	-3.058	-3.880	0.882	-2.329	-4.326	1.101
C	-4.608	-2.123	1.277	-4.595	-2.144	1.252	-4.705	-1.689	1.336	-4.273	-2.396	1.565
H	-3.059	-1.025	2.296	-3.063	-1.054	2.305	-2.930	-0.715	2.082	-2.637	-1.122	2.159
C	-3.902	-4.116	0.148	-3.867	-4.116	0.096	-4.414	-3.947	0.587	-3.670	-4.613	0.883
H	-1.793	-4.560	0.250	-1.756	-4.550	0.211	-2.409	-4.730	0.706	-1.565	-5.073	0.921
C	-4.929	-3.240	0.502	-4.902	-3.251	0.455	-5.256	-2.854	0.795	-4.663	-3.657	1.105
H	-5.393	-1.440	1.585	-5.388	-1.472	1.565	-5.345	-0.833	1.528	-5.027	-1.639	1.759
H	-4.131	-5.003	-0.435	-4.087	-4.994	-0.502	-4.822	-4.867	0.179	-3.948	-5.601	0.530

C	-6.341	-3.481	0.058	-6.309	-3.492	-0.006	-6.712	-2.916	0.438	-6.108	-3.965	0.845
H	-6.484	-4.511	-0.276	-6.445	-4.519	-0.349	-7.049	-3.946	0.316	-6.274	-5.038	0.740
H	-7.050	-3.277	0.864	-7.026	-3.295	0.795	-7.327	-2.438	1.205	-6.742	-3.595	1.655
H	-6.600	-2.820	-0.777	-6.559	-2.825	-0.837	-6.900	-2.388	-0.503	-6.447	-3.481	-0.077
C	4.477	5.543	-2.023	4.577	5.457	-2.149	4.798	5.350	-1.575	4.574	5.659	-1.952
H	5.017	6.229	-1.368	5.268	6.073	-1.571	5.445	5.917	-0.902	5.315	6.260	-1.420
H	5.095	5.346	-2.903	5.044	5.216	-3.107	5.336	5.178	-2.511	4.958	5.442	-2.952
H	3.573	6.056	-2.370	3.691	6.064	-2.361	3.932	5.979	-1.807	3.676	6.274	-2.074
Fe	0.000	0.031	0.000	0.000	0.041	0.000	0.001	0.074	0.008	-0.005	0.073	0.006
C	-1.085	-1.825	-1.936	-1.089	-1.805	-1.952	-1.227	-1.887	-1.867	-1.260	-1.875	-1.939
C	-1.904	0.002	-0.653	-1.914	0.022	-0.676	-1.853	0.133	-0.727	-2.166	0.036	-0.712
C	-2.186	-0.956	-1.637	-2.184	-0.923	-1.663	-2.235	-0.895	-1.598	-2.330	-0.930	-1.704
C	0.111	-1.465	-1.297	0.095	-1.482	-1.292	0.056	-1.574	-1.413	0.032	-1.547	-1.522
N	-3.418	-0.712	-2.140	-3.408	-0.663	-2.176	-3.470	-0.610	-2.079	-3.475	-0.652	-2.386
N	-3.967	0.324	-1.564	-3.949	0.369	-1.589	-3.926	0.507	-1.585	-4.075	0.396	-1.894
N	-3.053	0.745	-0.696	-3.048	0.779	-0.711	-2.955	0.942	-0.792	-3.282	0.794	-0.911
N	-0.890	-2.994	-2.589	-0.887	-2.958	-2.633	-1.220	-3.163	-2.334	-1.256	-3.167	-2.367
N	0.336	-3.422	-2.441	0.334	-3.392	-2.471	-0.031	-3.695	-2.239	-0.060	-3.685	-2.299
N	0.915	-2.509	-1.670	0.905	-2.512	-1.667	0.708	-2.746	-1.685	0.684	-2.717	-1.790
C	-4.169	-1.379	-3.190	-4.158	-1.311	-3.241	-4.320	-1.321	-3.021	-4.066	-1.288	-3.553

H	-3.617	-1.322	-4.127	-3.605	-1.228	-4.176	-3.774	-1.489	-3.948	-3.283	-1.488	-4.284
H	-4.355	-2.416	-2.914	-4.336	-2.354	-2.986	-4.653	-2.263	-2.588	-4.572	-2.210	-3.268
H	-5.115	-0.853	-3.292	-5.107	-0.789	-3.329	-5.181	-0.687	-3.215	-4.786	-0.591	-3.973
C	-1.799	-3.808	-3.379	-1.788	-3.750	-3.455	-2.286	-3.993	-2.873	-2.342	-4.019	-2.824
H	-2.657	-4.088	-2.769	-2.648	-4.051	-2.857	-3.110	-4.029	-2.161	-3.205	-3.870	-2.177
H	-2.116	-3.261	-4.265	-2.100	-3.175	-4.325	-2.619	-3.604	-3.834	-2.591	-3.796	-3.861
H	-1.255	-4.701	-3.675	-1.238	-4.632	-3.775	-1.880	-4.992	-3.007	-2.004	-5.050	-2.744
C	-3.377	1.953	-0.001	-3.388	1.964	0.018	-3.167	2.224	-0.196	-3.659	1.972	-0.201
C	-3.396	1.988	1.385	-3.346	1.972	1.403	-3.204	2.360	1.184	-3.479	2.026	1.173
C	-3.707	3.080	-0.742	-3.806	3.083	-0.691	-3.370	3.322	-1.022	-4.203	3.049	-0.889
C	-3.740	3.167	2.031	-3.723	3.120	2.084	-3.430	3.611	1.737	-3.841	3.174	1.861
H	-3.152	1.101	1.953	-3.027	1.093	1.944	-3.063	1.495	1.819	-3.063	1.173	1.694
C	-4.052	4.252	-0.082	-4.181	4.222	0.006	-3.598	4.567	-0.454	-4.566	4.189	-0.185
H	-3.693	3.036	-1.825	-3.834	3.058	-1.774	-3.345	3.197	-2.099	-4.337	2.994	-1.963
C	-4.071	4.318	1.312	-4.144	4.263	1.401	-3.627	4.735	0.932	-4.388	4.275	1.197
H	-3.757	3.189	3.116	-3.689	3.124	3.168	-3.462	3.714	2.817	-3.703	3.211	2.937
H	-4.309	5.131	-0.664	-4.507	5.098	-0.548	-3.755	5.424	-1.101	-4.991	5.030	-0.723
C	2.265	-2.775	-1.282	2.253	-2.782	-1.264	2.073	-3.051	-1.415	2.063	-2.994	-1.561
C	3.280	-1.913	-1.671	3.273	-1.931	-1.662	3.042	-2.093	-1.681	3.001	-2.000	-1.804
C	2.543	-3.907	-0.531	2.513	-3.905	-0.494	2.421	-4.286	-0.886	2.455	-4.245	-1.103

C	4.584	-2.176	-1.277	4.571	-2.196	-1.252	4.369	-2.370	-1.391	4.343	-2.261	-1.577
H	3.047	-1.061	-2.297	3.052	-1.089	-2.306	2.747	-1.149	-2.121	2.669	-1.038	-2.175
C	3.855	-4.161	-0.148	3.820	-4.159	-0.096	3.757	-4.551	-0.610	3.804	-4.491	-0.884
H	1.741	-4.580	-0.250	1.705	-4.570	-0.211	1.655	-5.027	-0.690	1.713	-5.013	-0.919
C	4.892	-3.297	-0.502	4.865	-3.306	-0.456	4.750	-3.599	-0.846	4.769	-3.508	-1.110
H	5.377	-1.502	-1.585	5.371	-1.533	-1.566	5.125	-1.621	-1.604	5.074	-1.484	-1.774
H	4.074	-5.050	0.435	4.030	-5.040	0.502	4.029	-5.517	-0.197	4.111	-5.469	-0.526
C	-0.329	1.457	2.597	-0.295	1.443	2.615	-0.195	1.755	2.630	-0.252	1.778	2.661
C	-0.062	2.783	0.729	-0.061	2.788	0.702	0.177	3.025	0.745	-0.083	3.070	0.758
C	-0.323	2.556	3.438	-0.309	2.530	3.456	-0.085	2.855	3.463	-0.265	2.891	3.487
H	-0.435	0.453	2.989	-0.382	0.437	3.011	-0.392	0.761	3.022	-0.313	0.772	3.065
C	-0.044	3.934	1.512	-0.067	3.941	1.527	0.317	4.179	1.513	-0.073	4.237	1.519
H	-0.428	2.414	4.507	-0.408	2.387	4.525	-0.196	2.741	4.534	-0.340	2.773	4.561
H	0.087	4.906	1.054	0.044	4.919	1.074	0.543	5.130	1.050	0.016	5.208	1.050
C	0.094	2.782	-0.729	0.094	2.787	-0.702	0.306	3.015	-0.728	0.005	3.077	-0.723
C	0.089	3.933	-1.512	0.113	3.940	-1.527	0.356	4.176	-1.496	-0.040	4.248	-1.477
C	0.220	3.819	-2.886	0.233	3.816	-2.883	0.479	4.068	-2.872	0.049	4.167	-2.858
H	-0.031	4.907	-1.055	0.014	4.919	-1.074	0.287	5.152	-1.033	-0.154	5.213	-1.001
C	0.346	1.453	-2.597	0.311	1.439	-2.615	0.469	1.701	-2.612	0.204	1.802	-2.637
H	0.213	4.703	-3.514	0.239	4.700	-3.513	0.520	4.959	-3.488	0.015	5.068	-3.459

H	0.441	0.447	-2.989	0.387	0.433	-3.012	0.503	0.688	-3.004	0.294	0.801	-3.047
C	0.352	2.552	-3.439	0.338	2.526	-3.457	0.539	2.805	-3.445	0.176	2.920	-3.456
H	0.456	2.408	-4.507	0.435	2.382	-4.525	0.631	2.674	-4.516	0.247	2.811	-4.531
C	-0.176	3.821	2.885	-0.189	3.819	2.883	0.179	4.092	2.889	-0.169	4.144	2.899
H	-0.159	4.705	3.513	-0.185	4.702	3.513	0.283	4.978	3.506	-0.164	5.043	3.506
N	-0.202	1.554	1.268	-0.189	1.538	1.280	-0.075	1.833	1.304	-0.166	1.862	1.334
N	0.220	1.551	-1.269	0.207	1.535	-1.280	0.362	1.798	-1.287	0.124	1.876	-1.309
N	-0.375	-3.418	2.440	-0.373	-3.388	2.470	-0.568	-3.658	2.253	0.168	-3.687	2.301
C	6.302	-3.554	-0.058	6.269	-3.564	0.005	6.185	-3.875	-0.510	6.222	-3.772	-0.848
H	6.567	-2.896	0.777	6.526	-2.899	0.837	6.466	-3.372	0.422	6.546	-3.279	0.074
H	6.433	-4.585	0.276	6.394	-4.592	0.349	6.367	-4.943	-0.380	6.420	-4.840	-0.742
H	7.013	-3.358	-0.864	6.988	-3.375	-0.795	6.852	-3.502	-1.292	6.846	-3.384	-1.658
C	-4.412	5.593	2.023	-4.513	5.510	2.148	-3.841	6.089	1.541	-4.749	5.523	1.947
H	-5.033	5.403	2.902	-4.984	5.275	3.105	-4.399	6.020	2.478	-5.131	5.291	2.944
H	-3.503	6.096	2.371	-3.619	6.106	2.362	-2.880	6.564	1.767	-3.869	6.163	2.076
H	-4.944	6.286	1.367	-5.196	6.135	1.569	-4.383	6.750	0.862	-5.504	6.104	1.413