

Supplementary Information

Heteroleptic β -diketonate Fe^{3+} Complex: Spin-Crossover and Optical Characteristics

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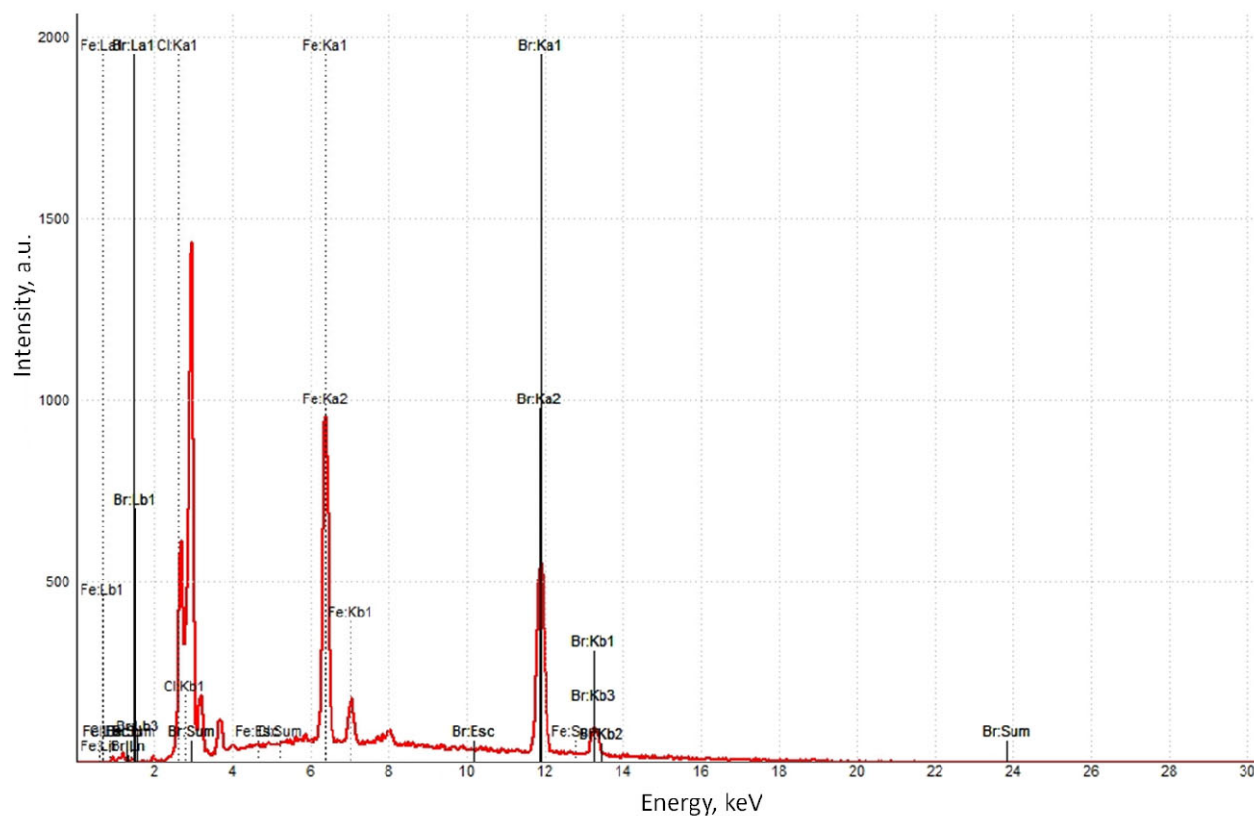


Figure S1. XRF spectrum of iron(III) bis[1-(4-fluoro-phenyl)-3-(4-bromo-phenyl)propane-1,3-dionate](2,2'-bipyridine) chloride

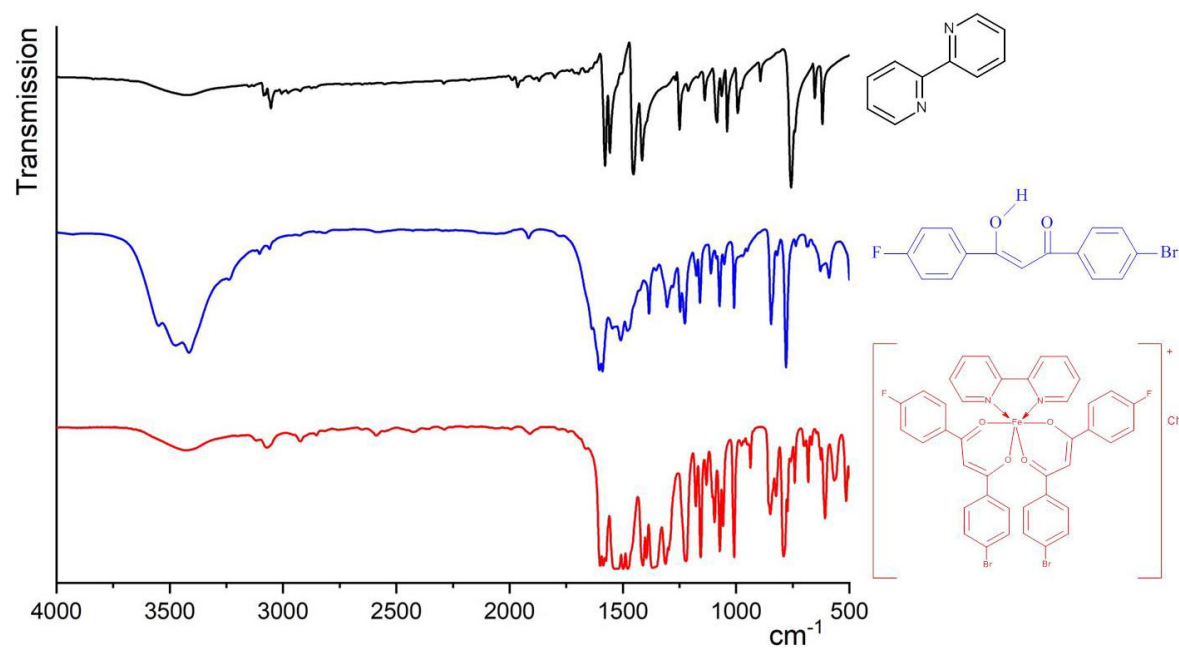


Figure S2. MIR spectrum of iron(III) bis[1-(4-fluoro-phenyl)-3-(4-bromo-phenyl)propane-1,3-dionate](2,2'-bipyridine) chloride and both ligands.

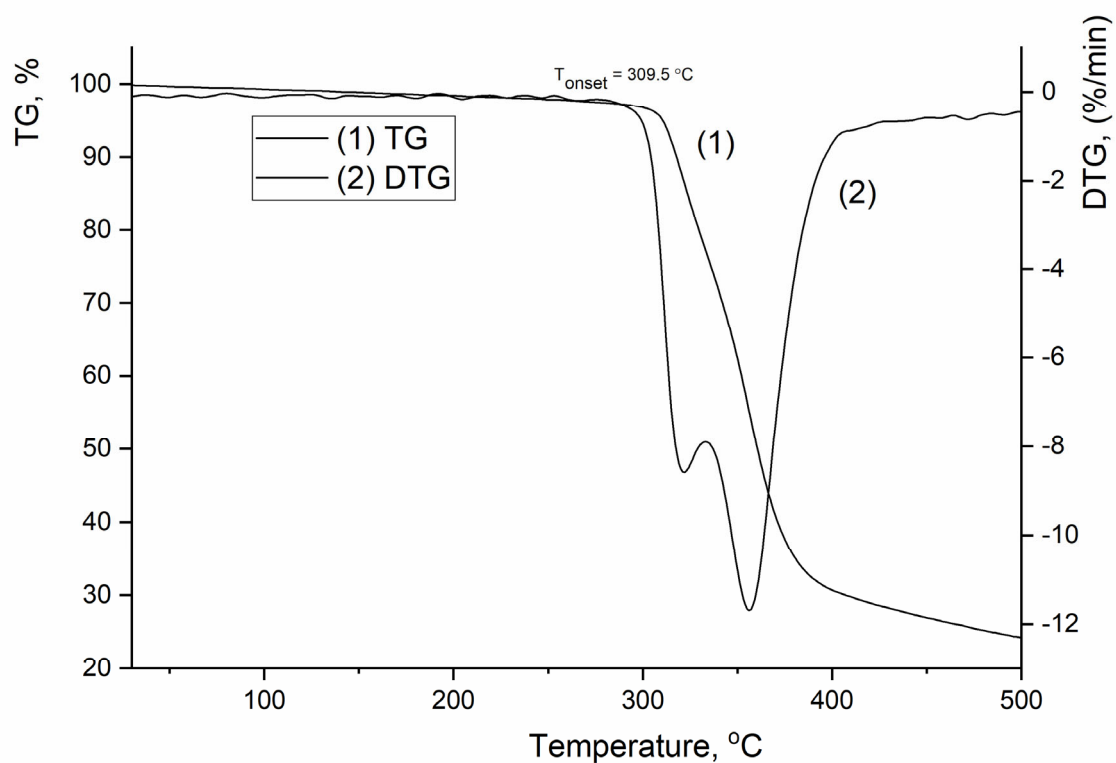


Figure S3. TG and DTG analysis data of iron(III) bis[1-(4-fluoro-phenyl)-3-(4-bromo-phenyl)propane-1,3-dionate](2,2'-bipyridine) chloride.

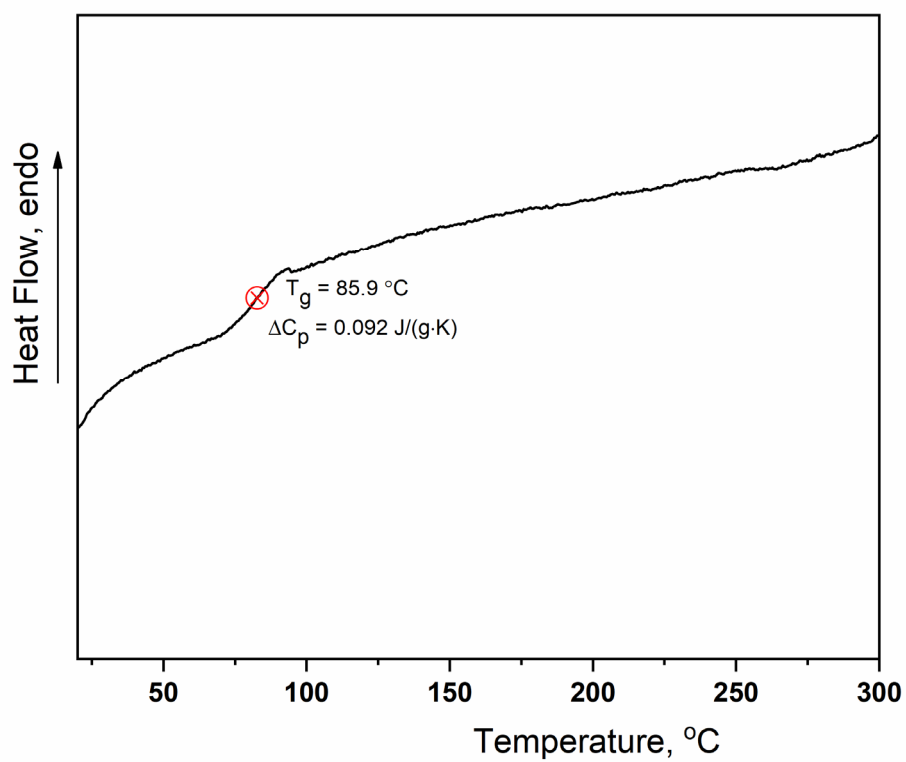


Figure S4. DSC curve of iron(III) bis[1-(4-fluoro-phenyl)-3-(4-bromo-phenyl)propane-1,3-dionate](2,2'-bipyridine) chloride, heating cycle.

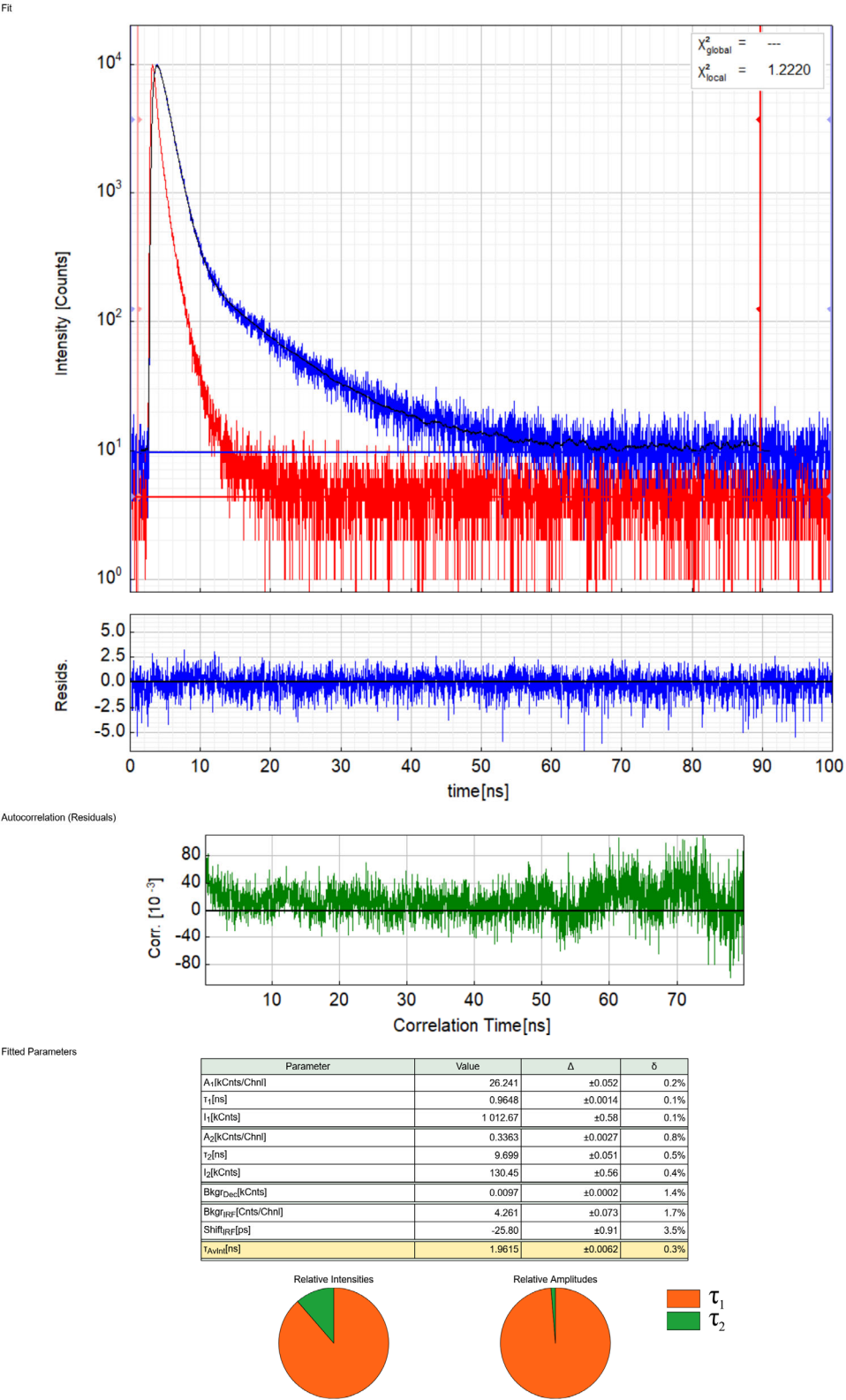


Figure S5. Fluorescence decay of [FeL2Bipy]Cl.

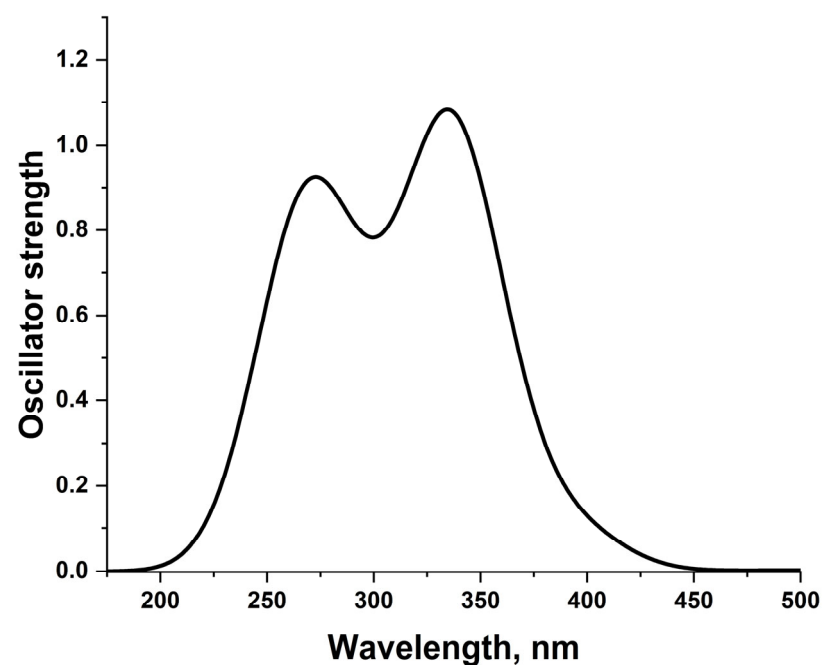


Figure S6. TDDFT spectrum of [FeL₂Bipy]Cl.

Table S1. The XYZ coordinates of optimized [FeL₂Bipy]Cl.

Br	-5.856855000000	1.920875000000	-1.999844000000
F	2.006265000000	-8.070718000000	-0.570766000000
C	1.321672000000	-4.028583000000	-0.723159000000
C	0.578248000000	-4.907473000000	-1.525252000000
C	0.807236000000	-6.276890000000	-1.480487000000
C	1.786681000000	-6.766237000000	-0.621341000000
C	2.545333000000	-5.920107000000	0.182805000000
C	2.311849000000	-4.553162000000	0.121370000000
C	1.106115000000	-2.560896000000	-0.747429000000
C	-0.108016000000	-2.015968000000	-1.197052000000
C	-0.299778000000	-0.645063000000	-1.400953000000
C	-1.644120000000	-0.085487000000	-1.697995000000
C	-2.811920000000	-0.854965000000	-1.595324000000
C	-4.065505000000	-0.266763000000	-1.702398000000
C	-4.159855000000	1.107762000000	-1.921457000000
C	-3.011079000000	1.889031000000	-2.056291000000
C	-1.763108000000	1.290356000000	-1.938013000000
O	2.078728000000	-1.858978000000	-0.310631000000
O	0.646646000000	0.214476000000	-1.289275000000
H	-0.173295000000	-4.524245000000	-2.217271000000
H	0.244973000000	-6.972121000000	-2.105012000000
H	3.303384000000	-6.345493000000	0.841692000000
H	2.895575000000	-3.869463000000	0.738681000000
H	-2.764653000000	-1.922965000000	-1.383054000000
H	-4.967477000000	-0.869534000000	-1.588929000000
H	-3.095529000000	2.961661000000	-2.236183000000
H	-0.859076000000	1.896097000000	-2.003386000000
Br	-5.856893000000	-1.920781000000	1.999869000000
F	2.006451000000	8.070676000000	0.570775000000
C	1.321759000000	4.028556000000	0.723144000000
C	0.578349000000	4.907461000000	1.525234000000
C	0.807370000000	6.276872000000	1.480477000000
C	1.786835000000	6.766200000000	0.621342000000
C	2.545474000000	5.920055000000	-0.182800000000
C	2.311956000000	4.553115000000	-0.121374000000
C	1.106166000000	2.560875000000	0.747406000000
C	-0.107984000000	2.015975000000	1.197011000000
C	-0.299781000000	0.645075000000	1.400913000000
C	-1.644138000000	0.085531000000	1.697956000000
C	-2.811931000000	0.855006000000	1.595183000000
C	-4.065523000000	0.266821000000	1.702275000000
C	-4.159887000000	-1.107684000000	1.921458000000
C	-3.011119000000	-1.888946000000	2.056398000000
C	-1.763141000000	-1.290289000000	1.938101000000
O	2.078765000000	1.858935000000	0.310613000000
O	0.646626000000	-0.214485000000	1.289251000000
Fe	2.020248000000	-0.000022000000	-0.000005000000
N	3.514436000000	0.257129000000	-1.260037000000
N	3.514415000000	-0.257198000000	1.260048000000
C	3.356493000000	0.540685000000	-2.552498000000

C	4.448157000000	0.734417000000	-3.391820000000
C	5.728296000000	0.628268000000	-2.856347000000
C	5.881826000000	0.335283000000	-1.503218000000
C	4.743347000000	0.154133000000	-0.723498000000
C	4.743334000000	-0.154206000000	0.723529000000
C	5.881799000000	-0.335363000000	1.503267000000
C	5.728246000000	-0.628352000000	2.856393000000
C	4.448097000000	-0.734497000000	3.391844000000
C	3.356449000000	-0.540758000000	2.552505000000
H	-0.173209000000	4.524248000000	2.217243000000
H	0.245118000000	6.972114000000	2.105001000000
H	3.303541000000	6.345426000000	-0.841679000000
H	2.895671000000	3.869405000000	-0.738683000000
H	-0.927260000000	2.696949000000	1.402504000000
H	-2.764654000000	1.922987000000	1.382819000000
H	-4.967489000000	0.869586000000	1.588726000000
H	-3.095579000000	-2.961558000000	2.236391000000
H	-0.859115000000	-1.896029000000	2.003565000000
H	2.324172000000	0.609631000000	-2.901003000000
H	4.289315000000	0.962969000000	-4.445799000000
H	6.606935000000	0.773471000000	-3.487295000000
H	6.876368000000	0.252106000000	-1.066259000000
H	6.876349000000	-0.252190000000	1.066325000000
H	6.606874000000	-0.773560000000	3.487355000000
H	4.289237000000	-0.963052000000	4.445820000000
H	2.324121000000	-0.609698000000	2.900993000000
H	-0.927308000000	-2.696921000000	-1.402550000000

Table S2. Some structural parameters of [FeL₂Bipy]Cl.

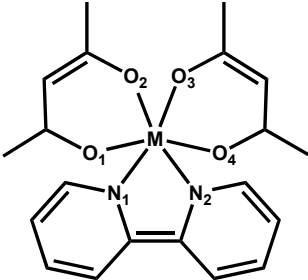
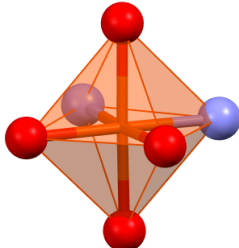
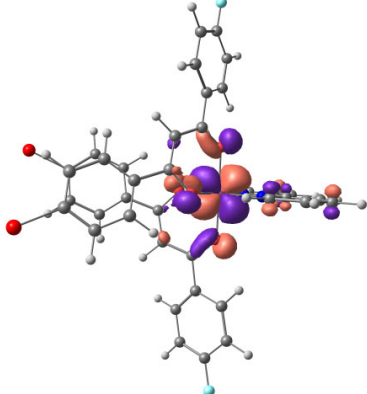
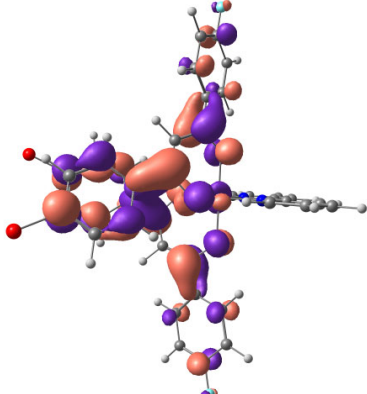
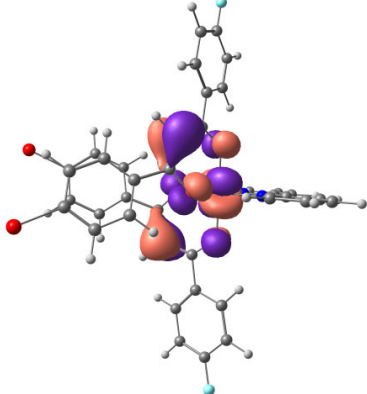
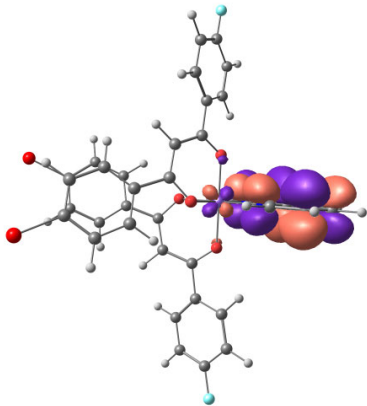
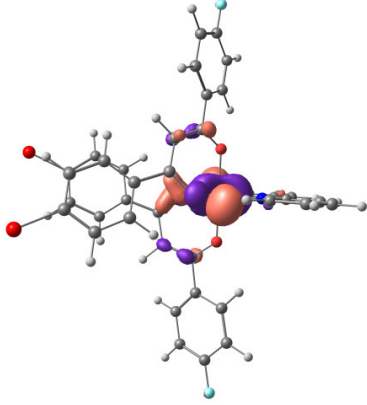
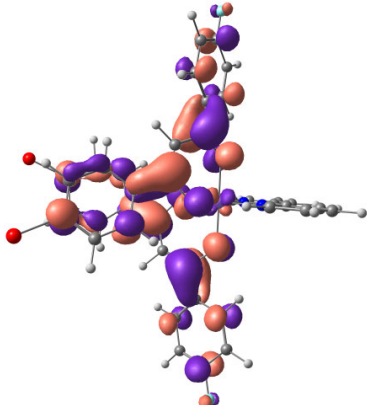
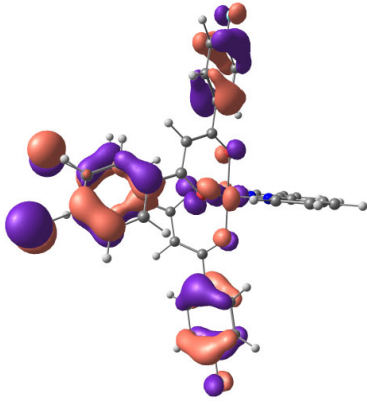
	
M – O1, Å	1.886
M – O2, Å	1.896
M – O3, Å	1.896
M – O4, Å	1.886
M – N1, Å	1.971
M – N2, Å	1.971
O1 – M – O2, deg.	91.3
O3 – M – O4, deg.	91.3
N1 – M – N2, deg.	81.4
O1 – M – O4, deg.	176.4
O2 – M – N2, deg.	176.8
O3 – M – N3, deg.	176.8
Coordination polyhedron	

Table S3. Results of TDDFT analysis of [FeL₂Bipy]Cl.

Electronic transition (%)	Energy, eV (nm)	Oscillator strength	FMO type
HOMO-1 – LUMO+2 (25)	3.69 (336)	0.29	 HOMO-1  LUMO+2
HOMO – LUMO (18)	3.70 (335)	0.69	 HOMO

			 LUMO
HOMO-2 – LUMO+1 (9)	4.60 (270)	0.24	 HOMO-2  LUMO+1
HOMO-5 – LUMO+1 (24)	4.62 (268)	0.21	 HOMO-5