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Electronic Supplementary Information

Theoretical study on the excited state decay properties of iron (II) polypyridine complexes substituted by bromine and chlorine

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Table S1 The Electron transition configurations, excitation energies, oscillator strengths (*f*), and assignment for the main absorption band of 1 and 2.

Complexes	Excited State	Energy(nm/ eV)	*f*	Major contrib.[a]	Assignment
1	Q_6	445/2.79	0.0036	H(A)→L+2(A) (14%)	ILCT
				H-1(A)→L+3(A) (12%)	ILCT
				H-1(B)→L+3(B) (15%)	ILCT/LMCT
				H(B)→L(B) (14%)	MLCT/LLCT
	Q_{10}	407/3.05	0.0228	H(B)→L(B) (59%)	MLCT/LLCT
				H(B)→L+5(B) (13%)	MLCT/LLCT/MC
	Q_{13}	341/3.64	0.2893	H-1(A)→L(A) (10%)	ILCT/LMCT
				H(A)→L+1(A) (10%)	ILCT
				H-1(B)→L(B) (54%)	ILCT/LMCT
	Q_{14}	338/3.67	0.3986	H(A)→L(A) (29%)	ILCT/LMCT
				H-2(A)→L(A) (18%)	MLCT/LLCT
				H-2(B)→L(B) (25%)	ILCT/MC
				H-1(B)→L+1(B) (16%)	ILCT/LMCT
2	Q_5	446/2.78	0.0041	H(A)→L+3(A) (14%)	ILCT
				H-1(A)→L+2(A) (12%)	ILCT
				H(B)→L(B) (16%)	MLCT/MC
				H-1(B)→L+3(B) (14%)	ILCT
				H-2(B)→L+2(B) (10%)	ILCT/LMCT
	Q_7	420/2.95	0.0206	H(B)→L(B) (56%)	MLCT/MC
	Q_{13}	345/3.59	0.3143	H(A)→L(A) (17%)	ILCT/LMCT
				H-1(B)→L(B) (50%)	ILCT/LMCT
	Q_{14}	340/3.64	0.0634	H-2(A)→L(A) (84%)	MLCT/LLCT
	Q_{15}	339/3.66	0.3746	H(A)→L+1(A) (14%)	ILCT/LMCT
				H-1(A)→L(A) (12%)	ILCT/LMCT
				H-2(B)→L(B) (51%)	ILCT/LMCT

[a] Q is the initial letter of quintet. H means HOMO and L means LUMO. Meanwhile, A means alpha and B means beta. ILCT/LLCT are short for intraligand/ ligand-to-ligand charge transfer. LMCT/MLCT mean ligand-to-metal/ metal-to-ligand charge transfer. MC represents metal-center charge transfer.

Table S2 The list of single point energy (eV) of **1** and **2** with the same bond lengths of Fe-N_c.

	1				**2**			
Bond lengths (Å)	Singlet	Triplet	Septet	Quintet	Singlet	Triplet	Septet	Quintet
1.82	1.06	0.94	2.92	0.98	0.95	0.95	2.90	1.06
1.84	0.99	0.86		0.81	0.87	0.87		0.88
1.86	0.94	0.80	2.61	0.66	0.82	0.80	2.59	0.72
1.88	0.91	0.75		0.52	0.79	0.75		0.58
1.9	0.90	0.72	2.40	0.41	0.77	0.72	2.38	0.46
1.91	0.90	0.72	2.36	0.36	0.77	0.71	2.34	0.41
1.92	0.91	0.71	2.32	0.31	0.78	0.71	2.30	0.36
1.93	0.92	0.71	2.29	0.27	0.79	0.71	2.26	0.31
1.95	0.95	0.72		0.19	0.81	0.71		0.23
1.97	0.99	0.74	2.21	0.13	0.85	0.73	2.17	0.16
1.99	1.05	0.77		0.08	0.91	0.76		0.11
2.01	1.11	0.81	2.18	0.05	0.97	0.80	2.13	0.06
2.03	1.19	0.86	2.18	0.02	1.04	0.85	2.13	0.03
2.05	1.28	0.92	2.20	0	1.13	0.90	2.14	0.01
2.07	1.37	0.99		0	1.22	0.97		0
2.09	1.48	1.06	2.26	0	1.32	1.03	2.19	0
2.1	1.53	1.10		0	1.37	1.07		0
2.11	1.58	1.14	2.30	0	1.42	1.11	2.23	0
2.13	1.70	1.22	2.35	0.02	1.53	1.19	2.28	0
2.14	1.76	1.27		0.03	1.59	1.24		0.01

* Green, pink, purple and gray shadow separately mean the minimum point energy in singlet, triplet, septet and quintet states.