Electronic Supplementary Information

No Aggregation-induced-emission but Quenching of Phosphorescence for an Iridium Complex with a 2,2-diphenylvinyl Motif: A Joint Experimental and Theoretical Study

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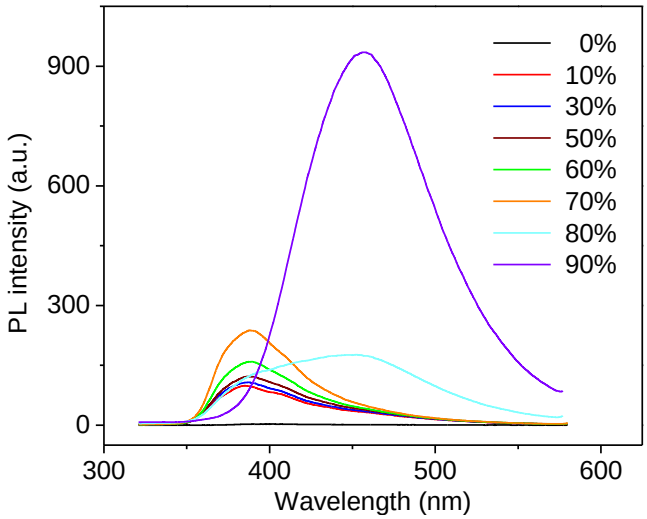


Figure S1. PL spectra of dpvppy in mixed THF/water (x%) solution (5×10^{-5} M).

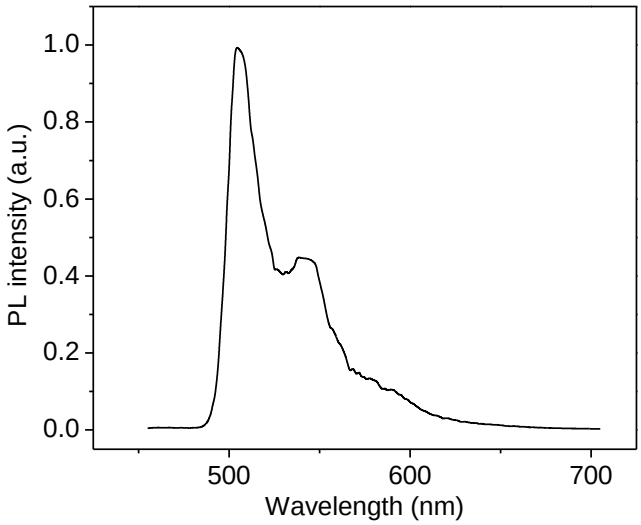


Figure S2. PL spectrum of complex 2 at 77 K in CH_2Cl_2 glass.

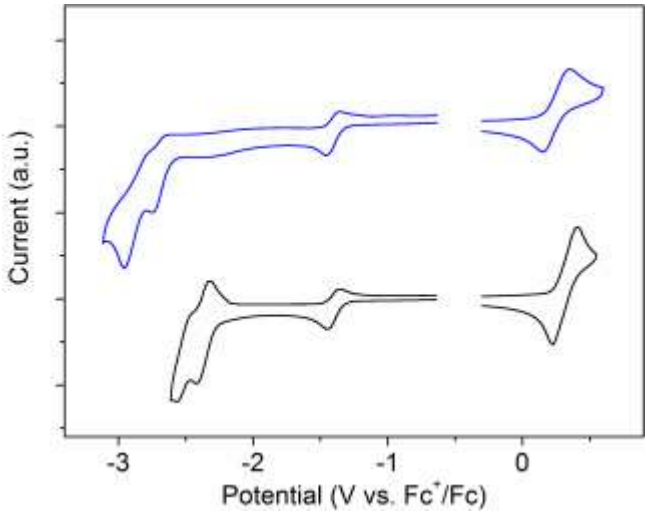


Figure S3. Cyclic voltammograms of complexes 1 and 2. The small peaks around −1.4 V arise from some unknown impurities which also appear in the blank test.

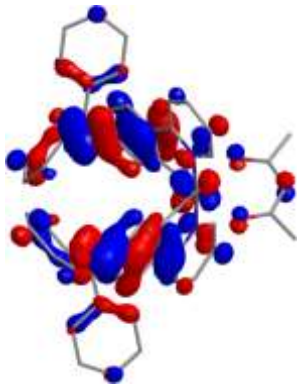
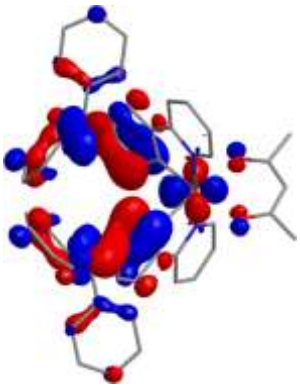
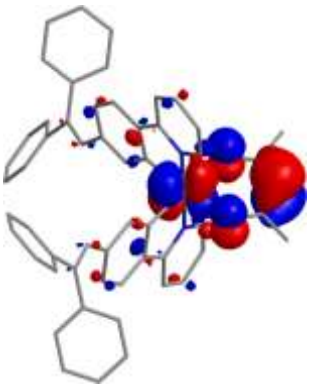
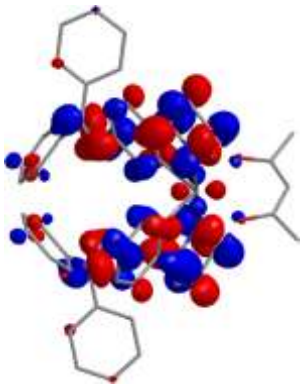
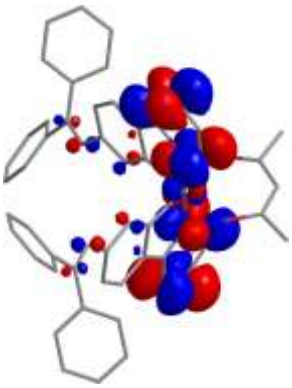
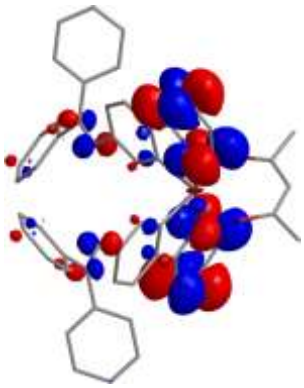
Table S1. Geometrical parameters of optimized S_0 and lowest triplet states of complexes 1 and 2. For comparison, the geometrical parameters of the single-crystal structure (Ex) for complex 1 were also shown.

	State	Bond lengths (Å)			Bite angles (°)		Dihedral angles (°)		
		Ir−C	Ir−N	Ir−O	C−Ir-N	O-Ir-O	Φ_1 [a]	Φ_2 [b]	Φ_3 [b]
1	S_0	2.005 /2.005	2.063 /2.063	2.205 /2.205	80.5 /80.5	86.2	27/ 27	58/ 40	58/ 40
	T_1	2.009 /2.006	2.062 /2.063	2.205 /2.203	80.6 /80.5	86.3	26/ **2**	59/ 40	**82**/ **84**
	Ex [c]	2.011/ 1.973	2.046/ 2.058	2.152/ 2.151	80.5/ 80.2	87.9	20/ 37	65/ 32	74/ 30
2	S_0	2.006 /2.006	2.064 /2.064	2.204 /2.204	80.5 /80.5	86.2	–	–	–
	T_1	1.979 /1.979	2.067 /2.067	2.217 /2.217	80.6 /80.5	86.3	–	–	–

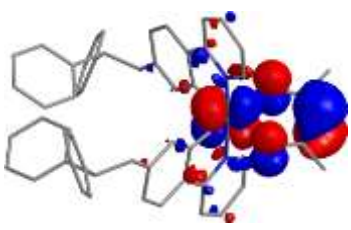
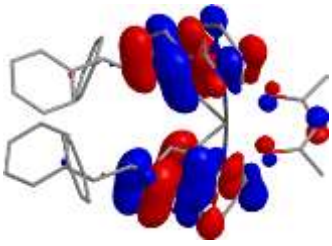
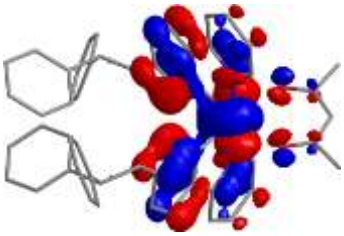
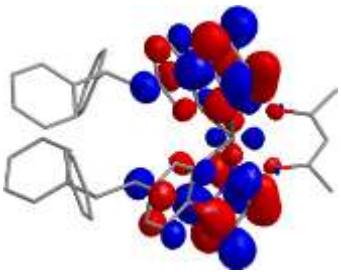
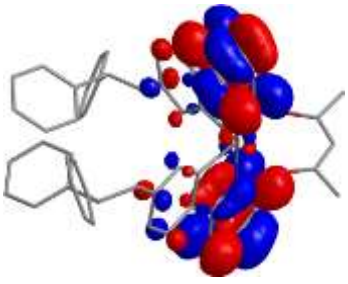
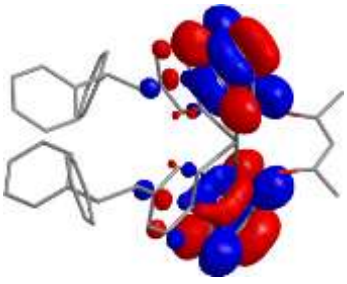
[a] Dihedral angle between the cyclometalated phenyl ring and the vinyl group. [b] Dihedral angle between the terminal phenyl ring and the vinyl group. [c] Single-crystal experimental data.

Table S2. Surface distributions of HOMO-3 to HOMO-1 and LUMO+1 to LUMO+3 for complexes 1 and 2.

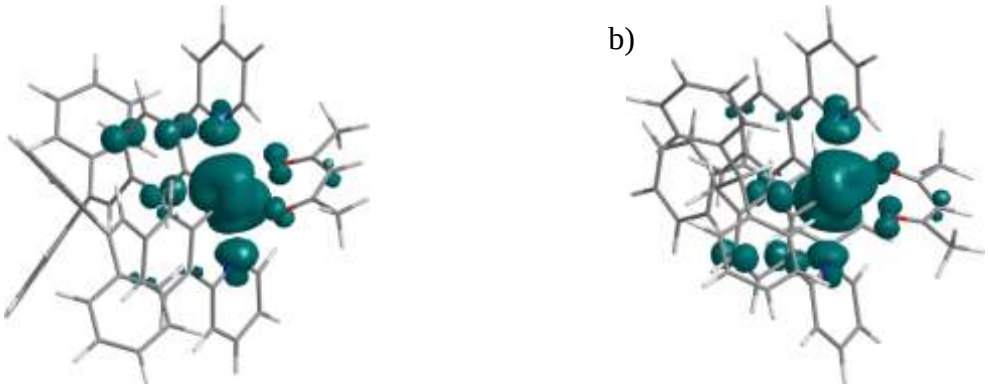
Complex 1

H-1	H-2	H-3
		
L+1	**L+2**	**L+3**
		

Complex 2

H-1	H-2	H-3
		
L+1	**L+2**	**L+3**
		

a) b)



E_T = 2.85 eV E_T = 2.79 eV

Figure S4. Spin-density distribution of the ^{3}MC state for a) complex 1 and b) complex 2.