

**Solvents-induced aggregation based on a heteroleptic Ir(III) complex *via*
hydrogen bonds**

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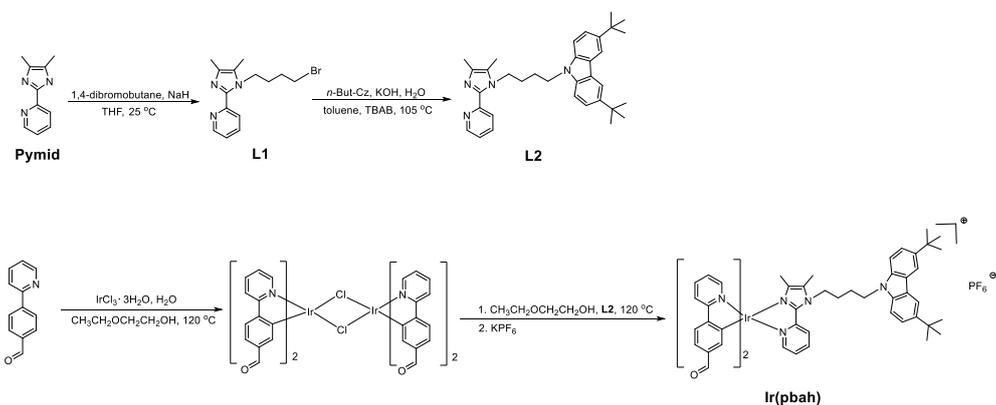
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Scheme S1. Schematic illustration of the synthetic routes and molecular structures.

Table S1. Photophysical data for complex in solution

Solvent	Absorption	Emission	Φ^b
	$\lambda_{\text{abs}}/\text{nm}$ ($\epsilon/10^4 \text{ L mol}^{-1} \text{ cm}^{-1}$) ^a	$\lambda_{\text{max}}^b/\text{nm}$	
Toluene	287(7.91), 299(9.83), 350(3.10)	534	0.006
Chloroform	241(9.93), 250(8.41), 269(9.07), 299(9.83), 350(2.86)	542	0.011
DCM	231(9.83), 240(9.26), 250(7.56), 268(8.23), 298(8.69), 319(5.37), 349(2.72)	535	0.005
THF	238(9.97), 250(7.49), 267(8.23), 286(7.08), 298(8.00), 348(2.44)	534	0.002
Ethanol	205(9.93), 231(3.29), 239(3.05), 250(2.31), 266(2.56), 297(2.63), 349(0.85)	554	—

^a Measured in solution (1.0×10^{-7} M) at 298 K under air. ^b Determined by quinine sulfate

($\Phi_{\text{PL}} = 0.54$ in 0.1M H₂SO₄) as a standard (1.0×10^{-5} M, Ir(pbah)).

Table S2. Lifetime and absolute quantum yield in DCM/Hexane (1/9) and ethanol/water (1/9) solution

Sample Solution	Quantum Yield ^a		Lifetime	
	370-480 nm	500-700 nm	430 nm	550 nm
DCM/Hexane	3.1%	29.2%	0.73 ns	1.90 μs
Ethanol/Water	1.8%	24.6%	1.16 ns	1.39 μs

^a Absolute phosphorescence quantum yield determined by calibrated integrating sphere system at 298 K.

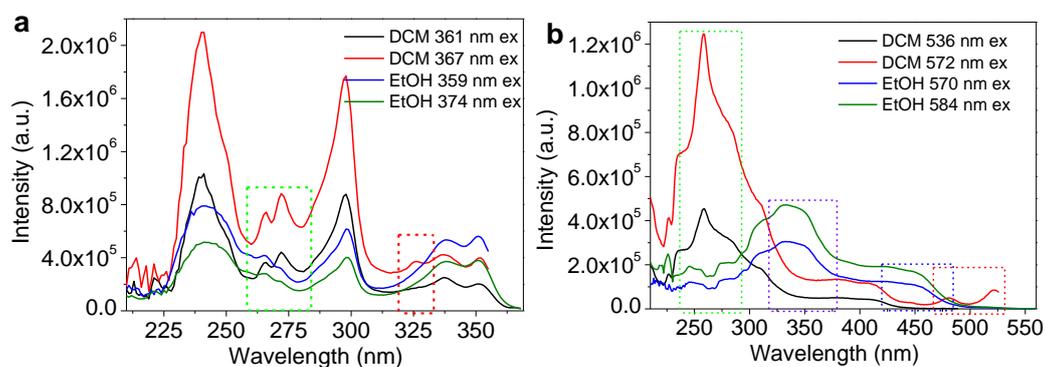
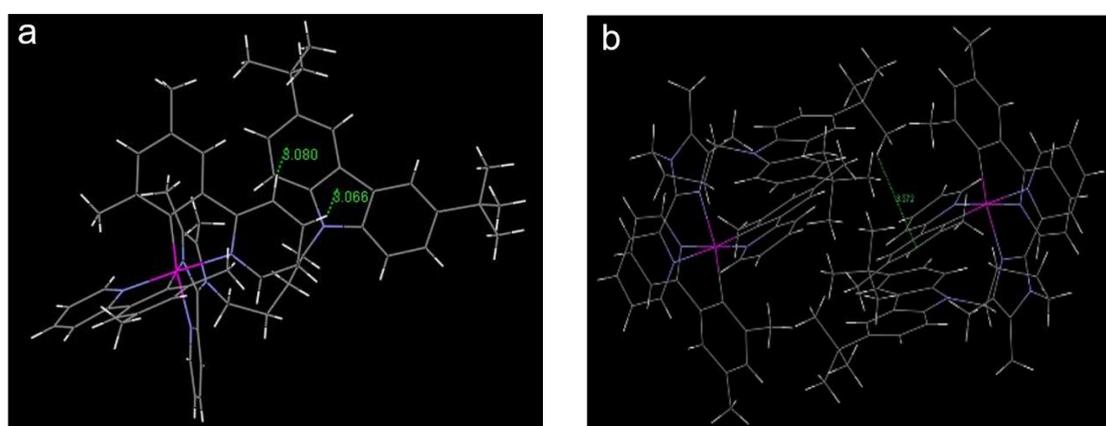


Fig. S1 Excitation spectra of the high energy emission band, the low energy emission band at two maximum peaks in DCM and EtOH, respectively ($c=1.0 \times 10^{-4}$ mol/L).



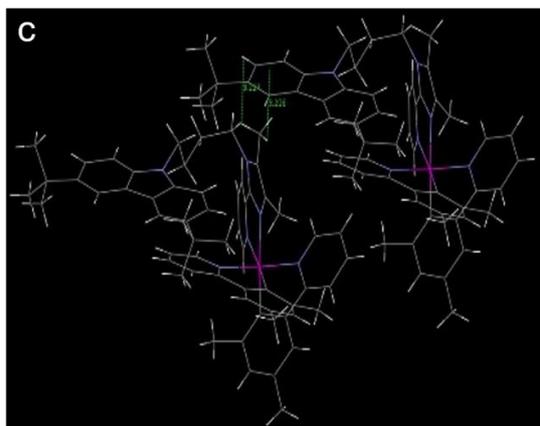
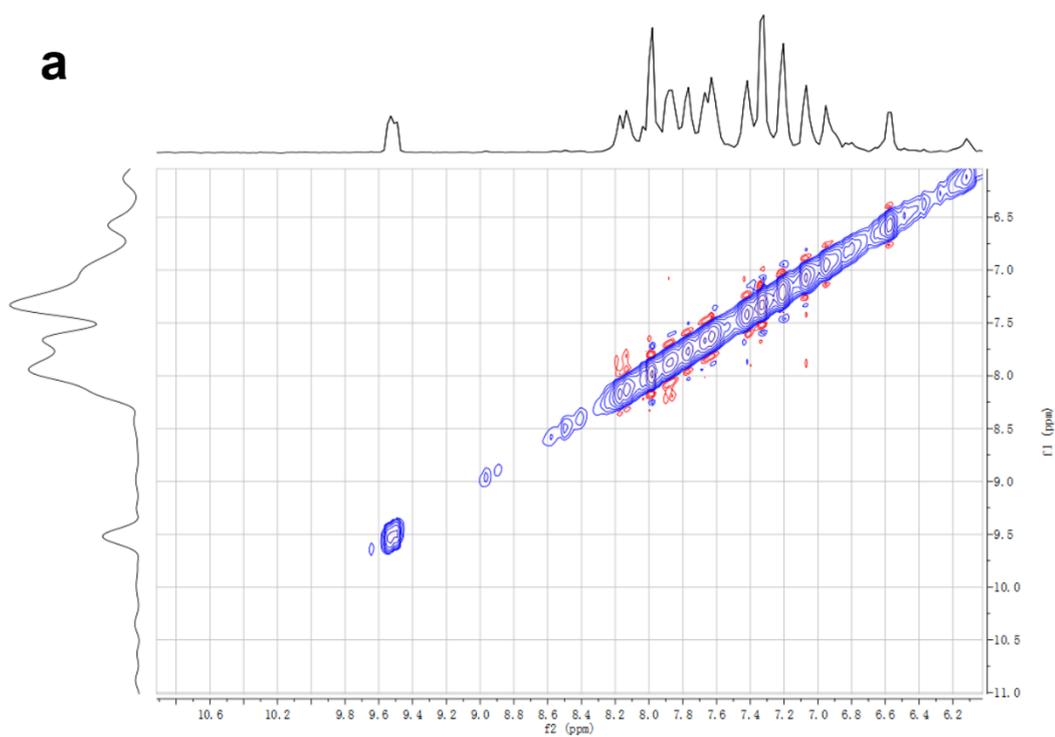


Fig. S2 Single-crystal structure and their dimer of complex **2** previously reported.



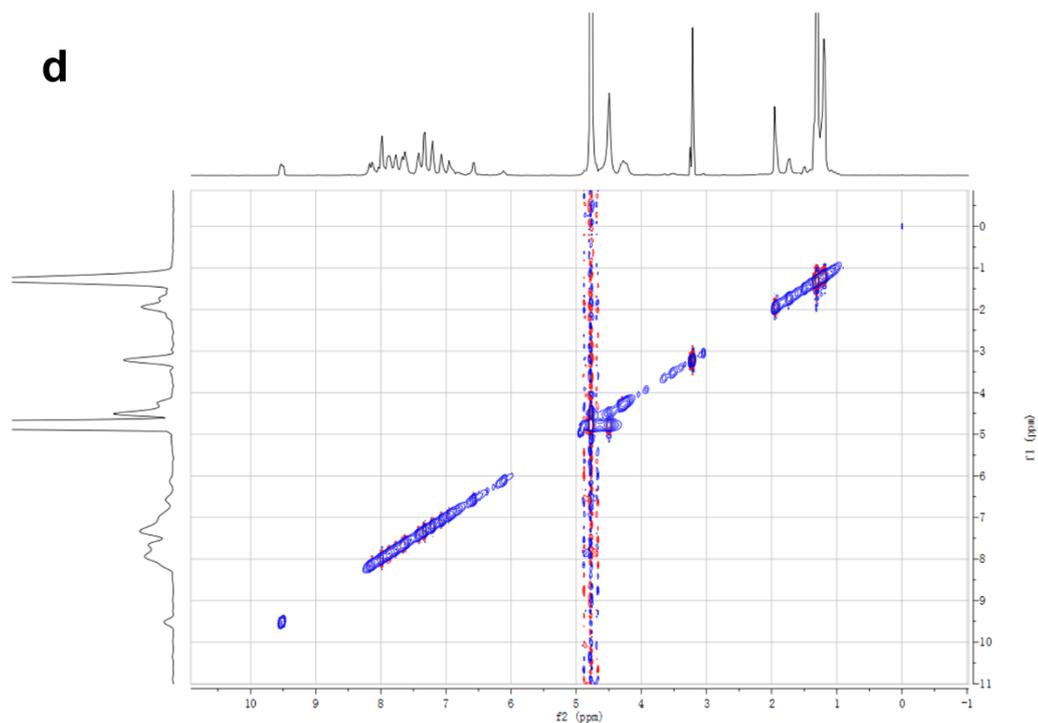


Fig. S3 ^1H - ^1H NOESY spectra of **Ir(pbah)** (0.01 mol/L, 400 MHz, 298 K) in CD_3OD , the partial chemical shift from 6.0 to 10.0 ppm a) and total chemical shift b), respectively.

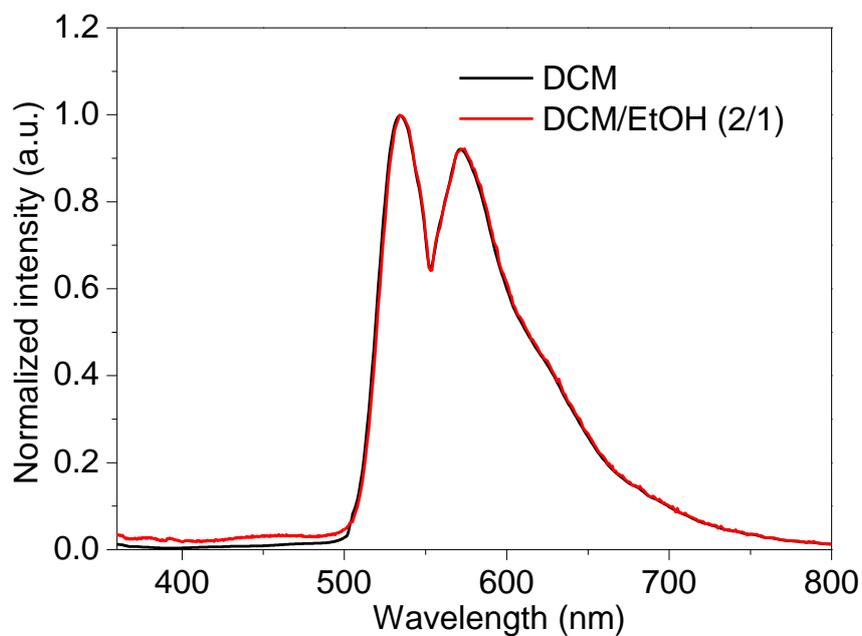


Fig. S4 Emission spectra of **Ir(pbah)** upon freezing DCM or DCM/EtOH (V/V=2/1) solution

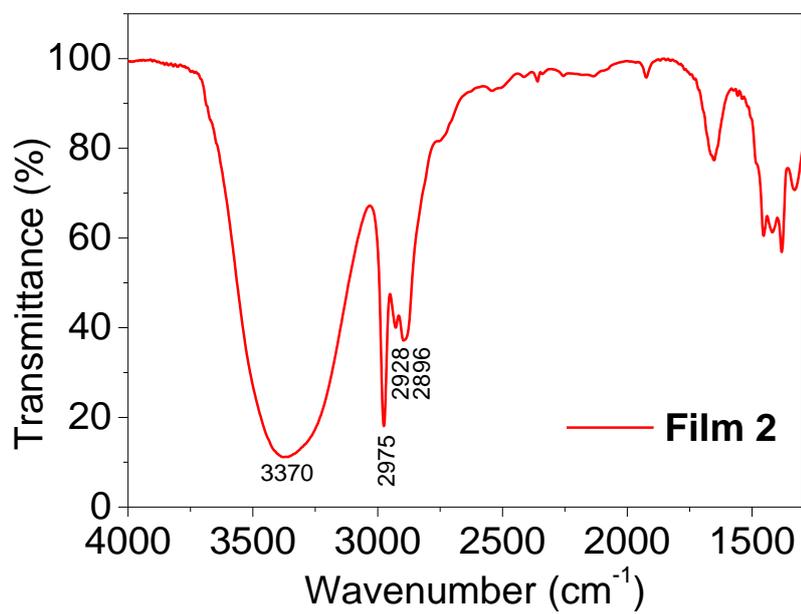


Fig. S5 FT-IR spectrum of **Film 2** made from ethanol/water solution contained **Ir(pbah)**