

Electronic Supporting Information

Aggregation-Induced Emission Enhancement and Reversible Mechanochromic Luminescence of Quinoline-Based Zinc(II) Schiff Base Complexes

Di Qiao,^{a,b} Jin-Yun Wang,^a Li-Yi Zhang,^a Feng-Rong Dai,*^a and Zhong-Ning Chen*^{a,b}

^a State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, China

^b College of Chemistry and Materials Science, Fujian Normal University, Fuzhou 350007, China

*To whom correspondence should be addressed. E-mail: dfr@fjirsm.ac.cn, czn@fjirsm.ac.cn; Tel: (+86) 591-6317-3171

Table S1. Crystallographic Data for Complexes **1–3**.

	1	2	3
empirical formula	C ₃₆ H ₂₈ F ₆ N ₄ O ₈ S ₂ Zn	C ₃₈ H ₃₂ F ₆ N ₄ O ₁₀ S ₂ Zn	C ₄₀ H ₃₄ F ₆ N ₄ O ₁₀ S ₂ Zn
formula weight	888.11	948.16	974.2
crystal system	monoclinic	triclinic	monoclinic
space group	<i>P</i> 2/c	<i>P</i> -1	<i>C</i> 2/c
<i>a</i> (Å)	21.4502(17)	13.802(2)	27.506(3)
<i>b</i> (Å)	10.4993(7)	14.659(2)	10.9018(12)
<i>c</i> (Å)	18.7583(14)	19.964(4)	18.564(2)
α (°)	90	87.244(6)	90
β (°)	114.568(2)	86.516(6)	130.821(4)
γ (°)	90	89.582(6)	90
<i>V</i> (Å ³)	3842.1(5)	4027.1(12)	4212.6(8)
<i>Z</i>	4	4	4
D(calcd) (g cm ⁻³)	1.535	1.564	1.536
μ (Mo <i>K_a</i>) (mm ⁻¹)	0.833	0.804	0.771
<i>F</i> (000)	1808	1936.0	1992.0
θ range (°)	2.278 – 24.997	2.338 – 25.352	2.899 – 37.907
reflections collected / unique	48355 / 6760	86157 / 14701	66552 / 10037
	[<i>R</i> _{int} = 0.1144]	[<i>R</i> _{int} = 0.0438]	[<i>R</i> _{int} = 0.1370]
data / restraints / parameters	6760 / 502 / 515	14701 / 185 / 1180	10037 / 0 / 285
GOF	1.039	1.084	1.036
<i>R</i> ₁ (<i>I</i> >2σ(<i>I</i>))	0.0479	0.0487	0.0606
<i>wR</i> ₂ (<i>I</i> >2σ(<i>I</i>))	0.1262	0.1162	0.1796
<i>R</i> ₁ (all data)	0.0766	0.0568	0.0796
<i>wR</i> ₂ (all data)	0.1623	0.1204	0.1946
Δρ / e Å ⁻³	0.549, -0.733	0.786, -0.644	0.877, -1.225

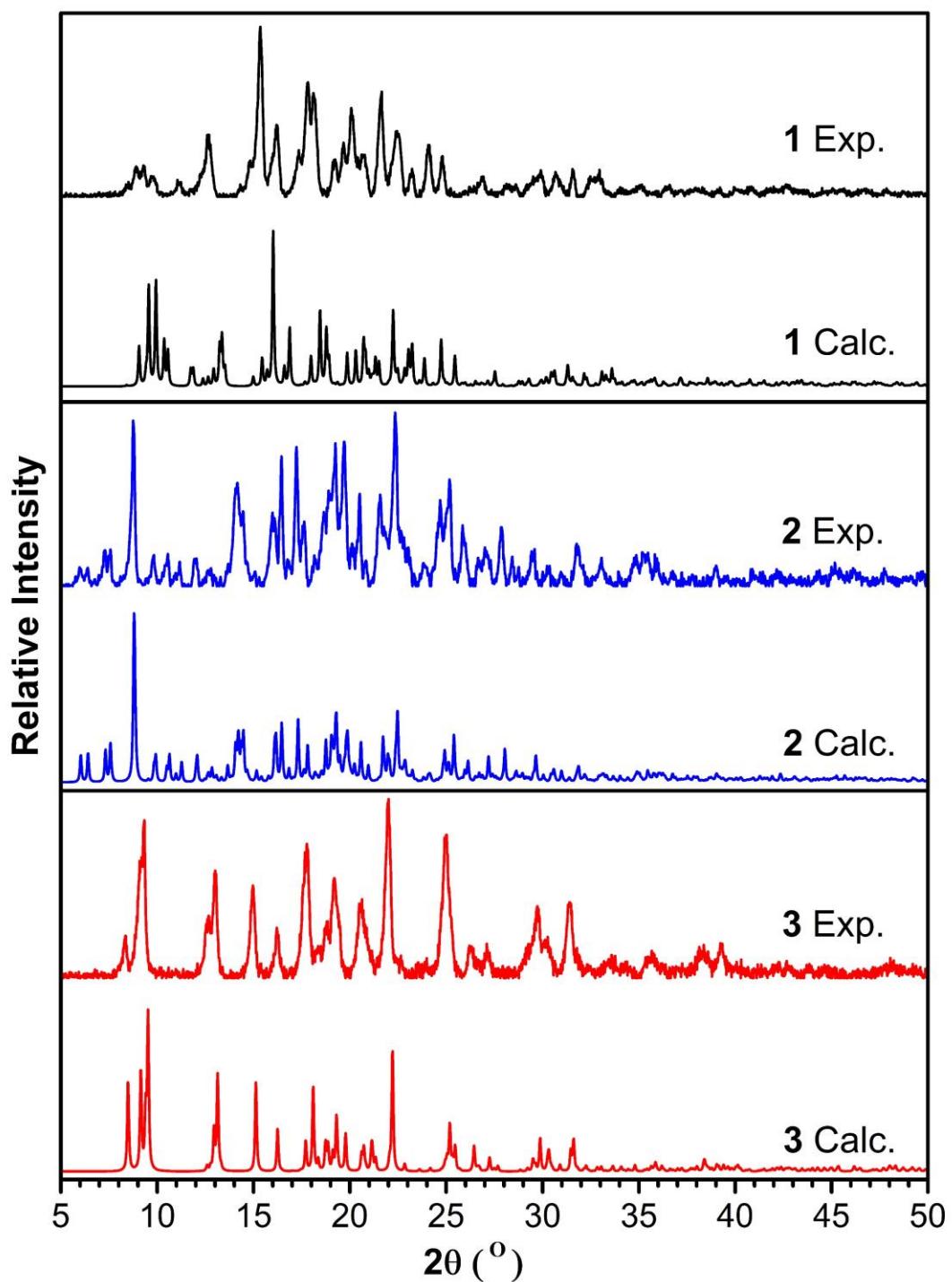


Fig. S1. Experimental PXRD patterns of complexes **1–3** in comparison with simulated patterns calculated from single-crystal structures.

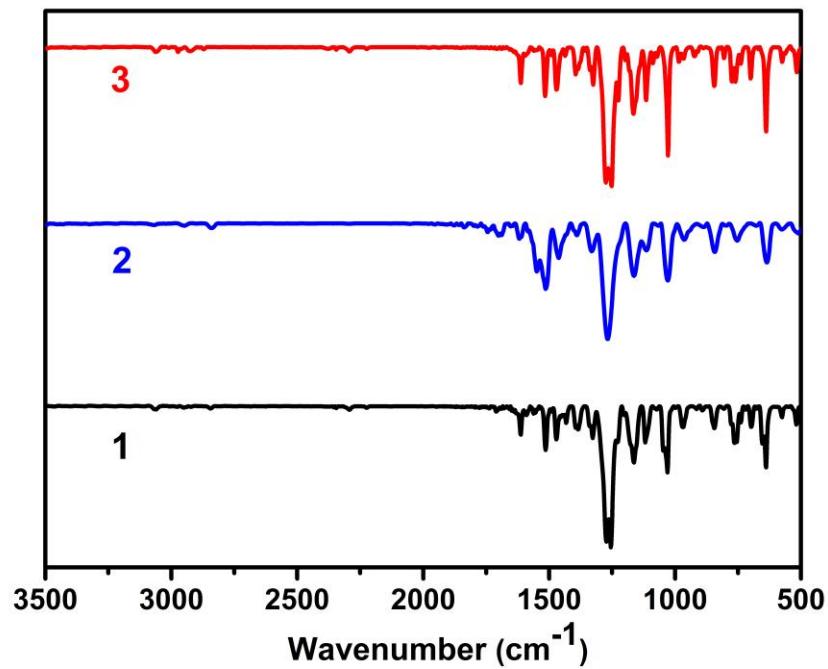


Fig. S2. FT-IR spectra of complexes **1–3**.

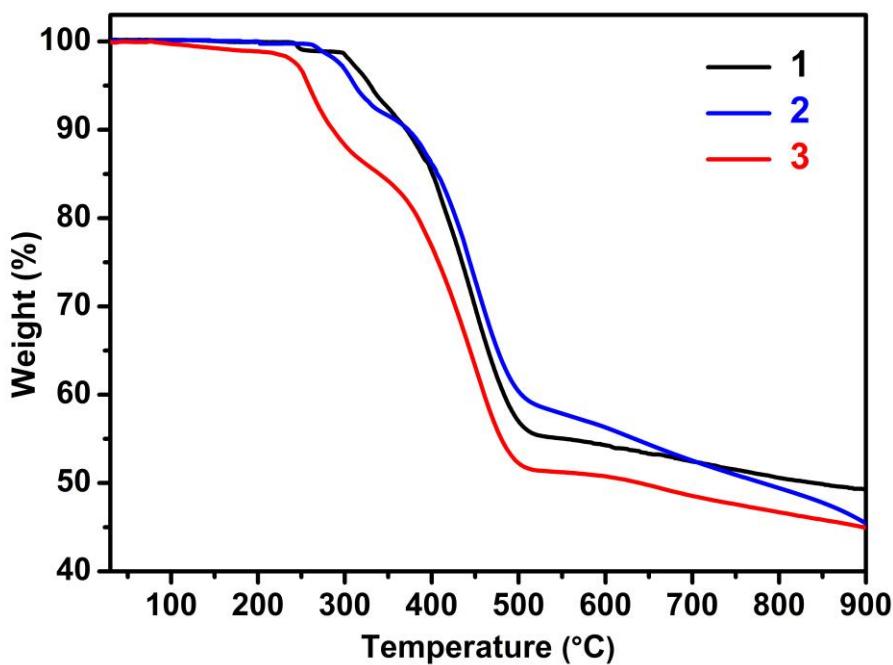


Fig. S3. TGA plots of complexes **1–3**.

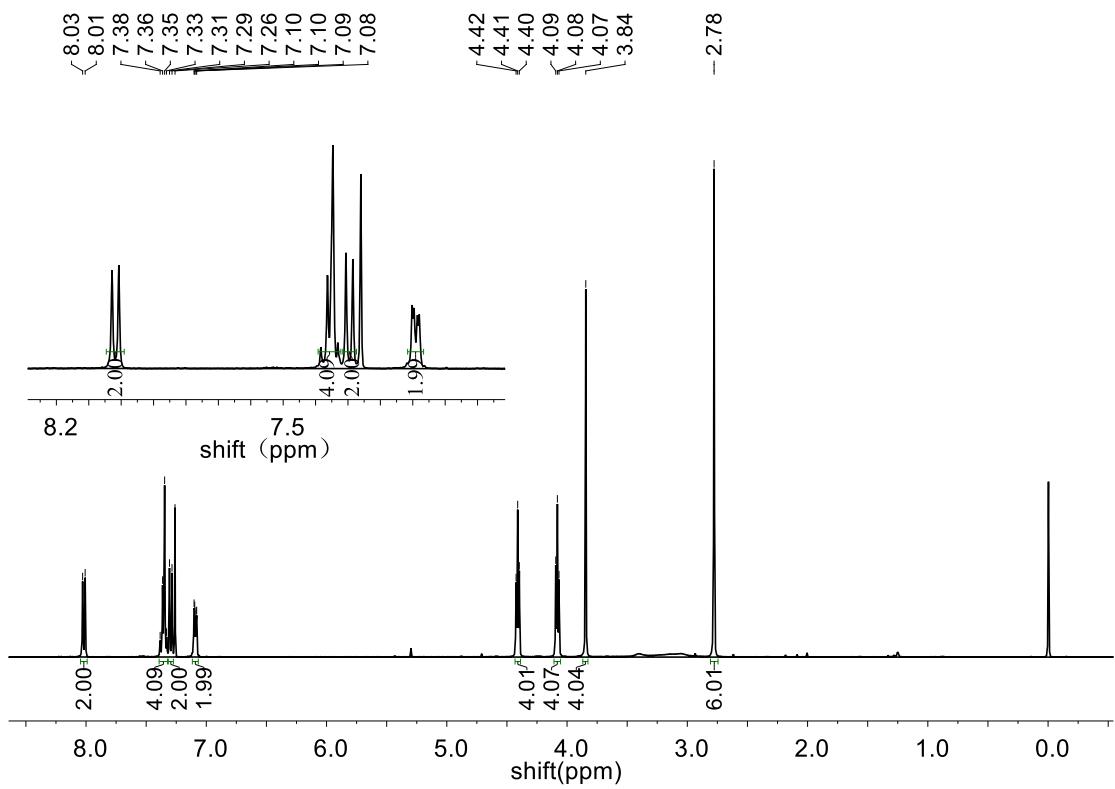


Fig. S4. ^1H NMR spectrum of 1, 2-bis(2-((2-methyl-quinolin-8-yl)oxy)ethoxy)-ethane in CDCl_3 .

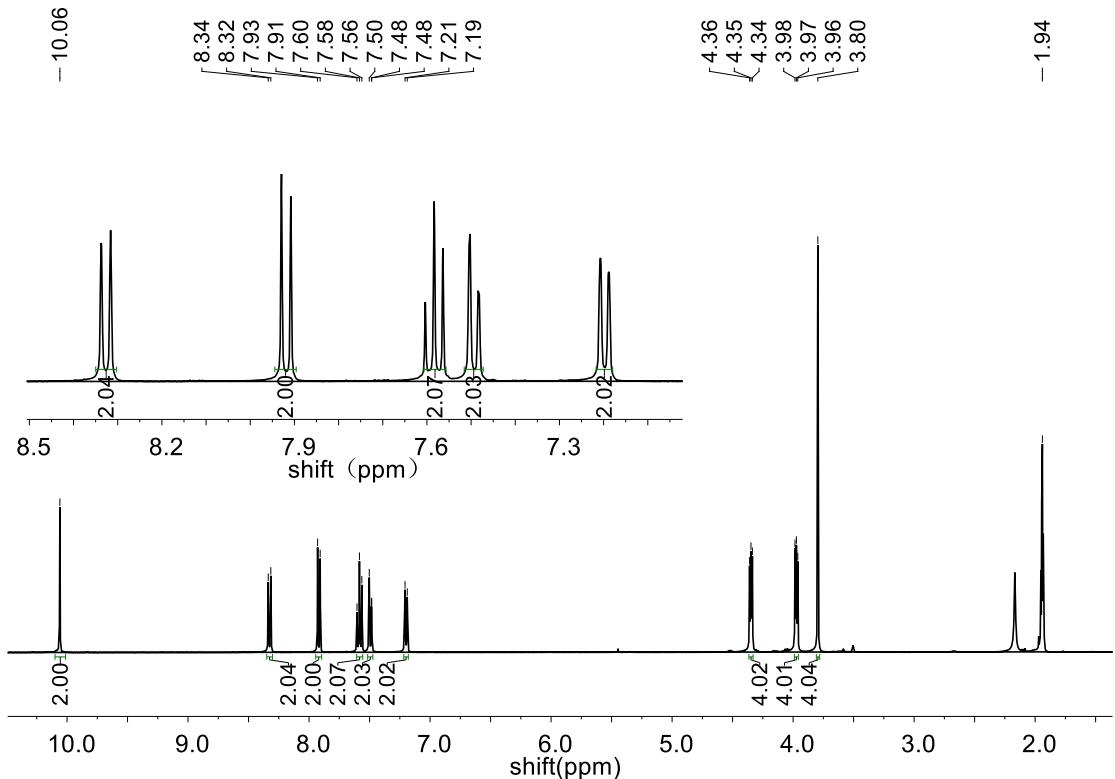


Fig. S5. ^1H NMR spectrum of **L2** in CD_3CN .

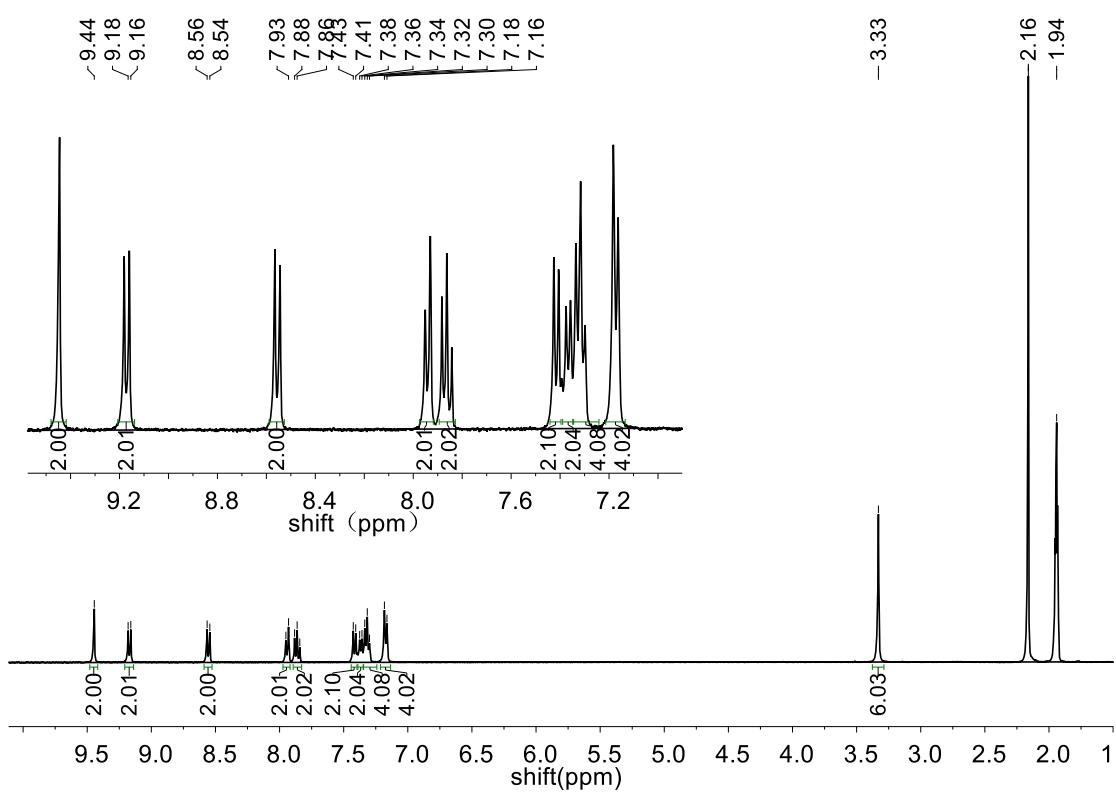


Fig. S6. ^1H NMR spectrum of complex **1** in CD_3CN .

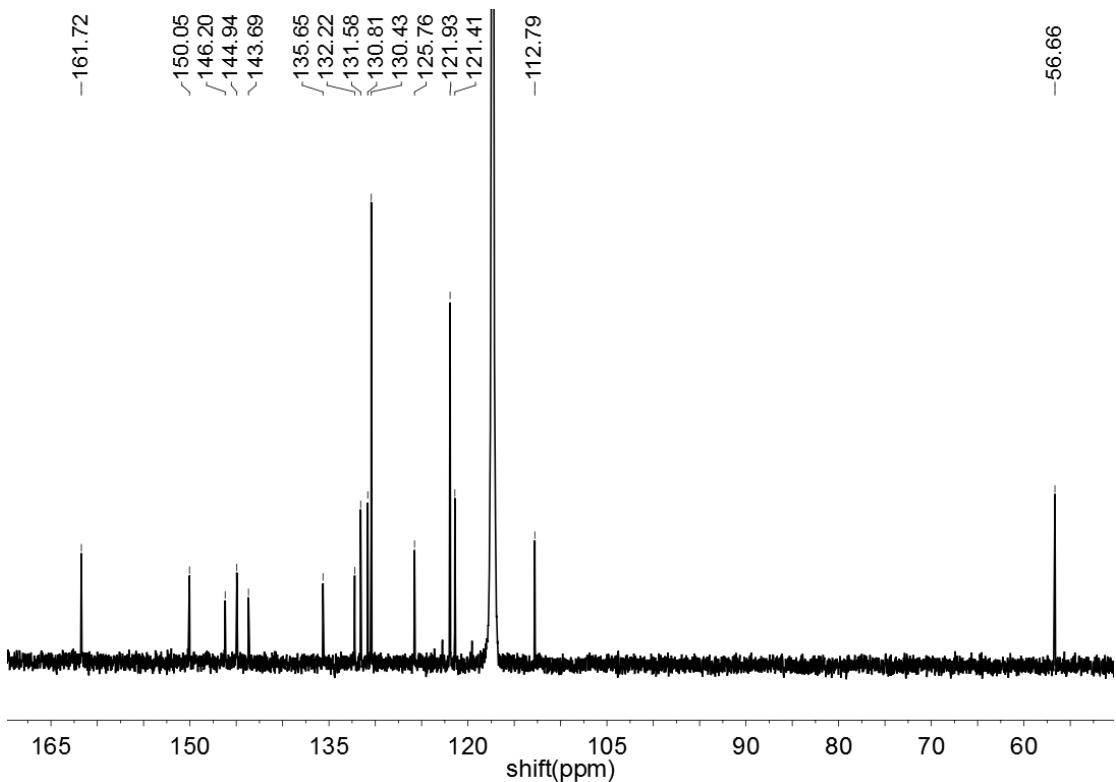
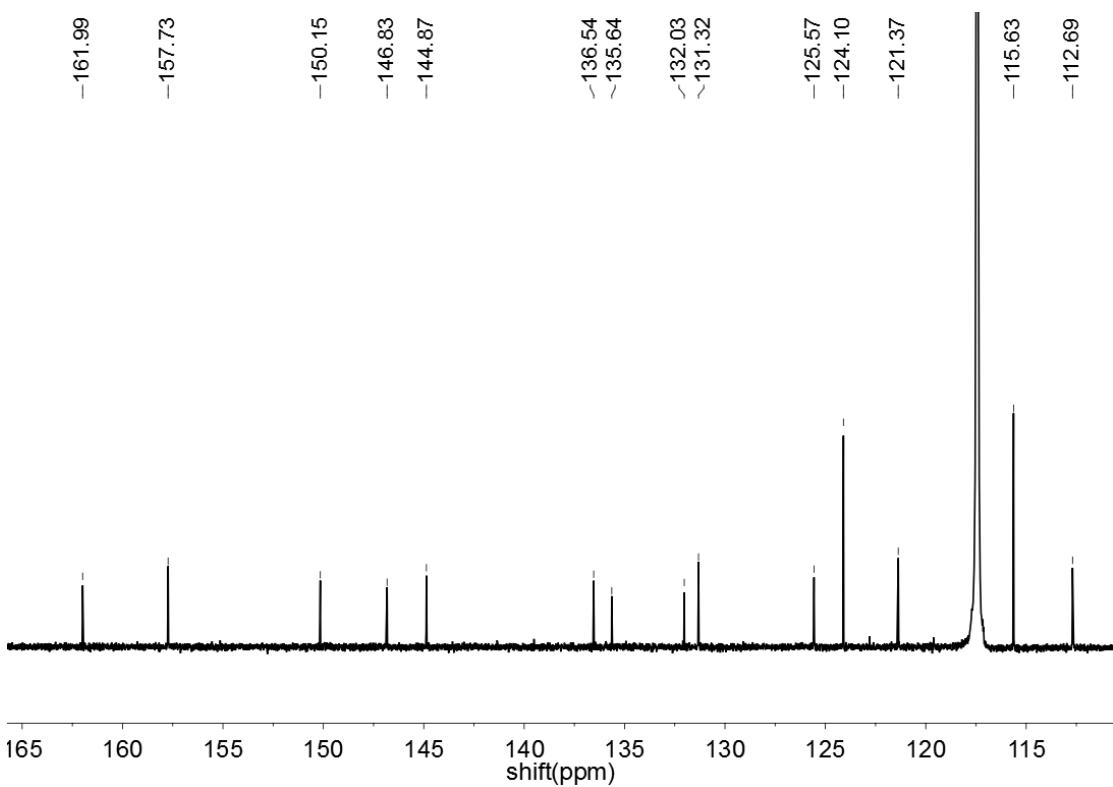
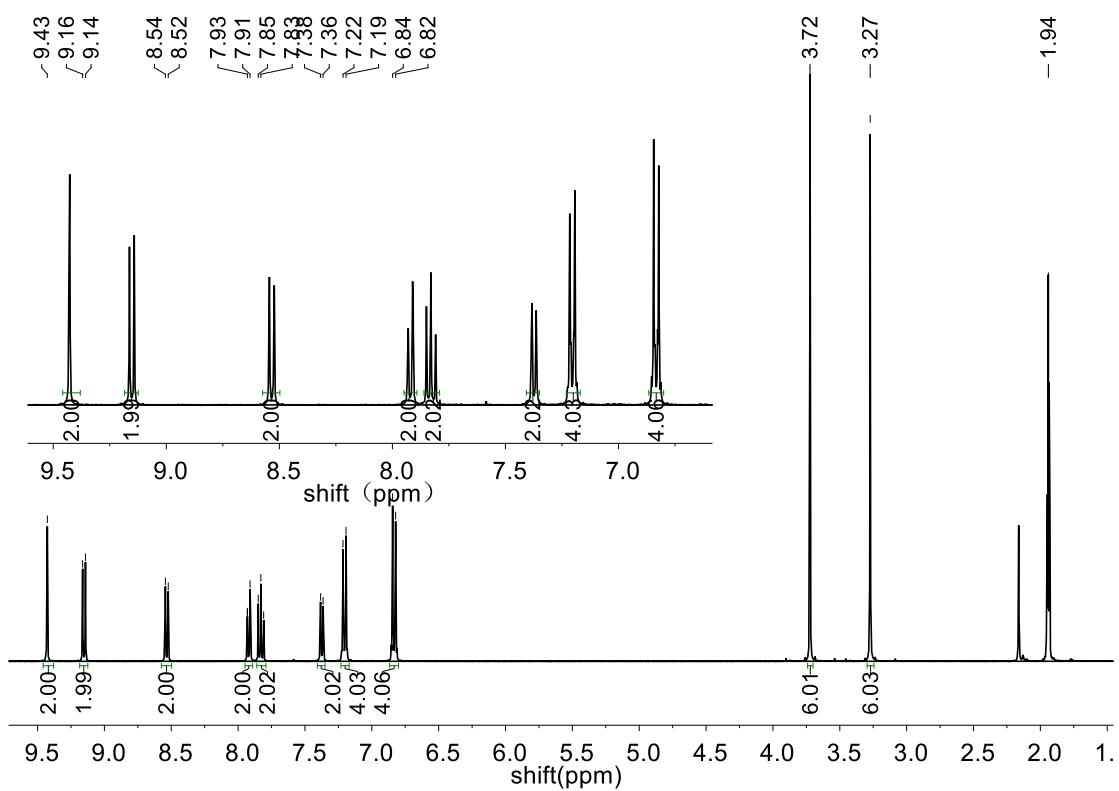


Fig. S7. ^{13}C NMR spectrum of complex **1** in CD_3CN .



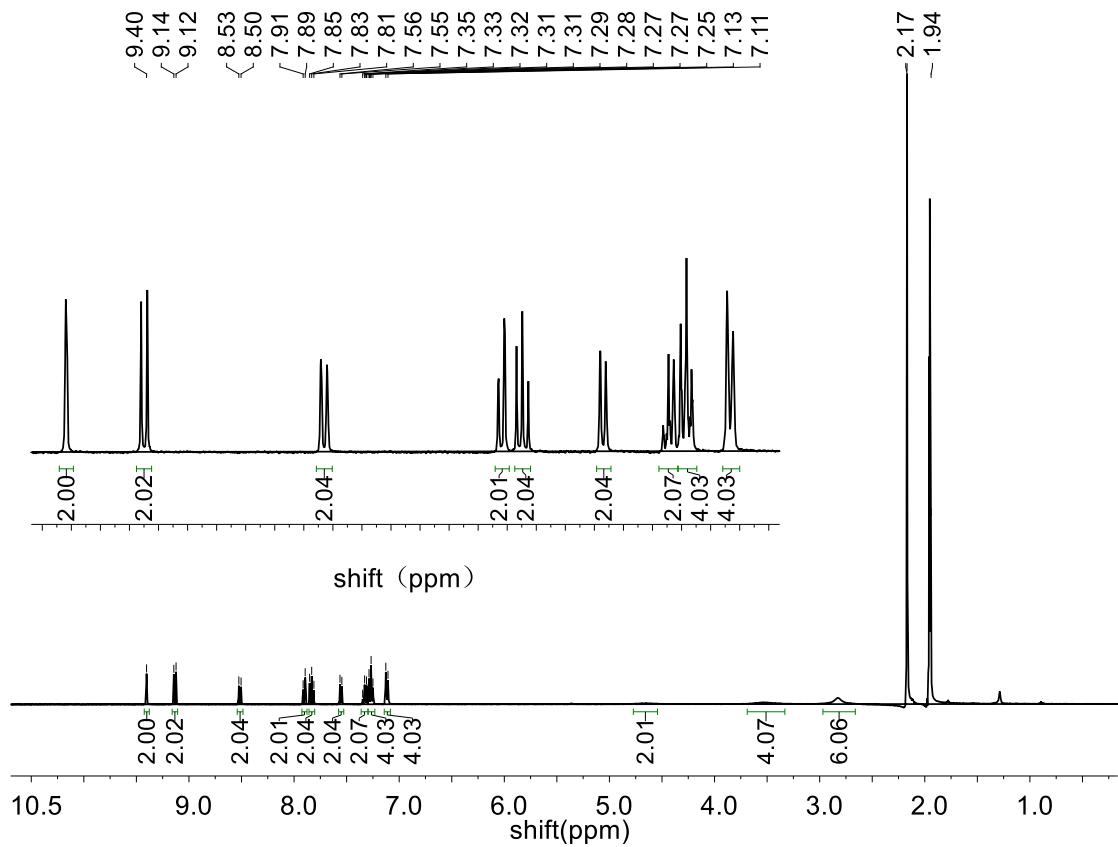


Fig. S10. ^1H NMR spectrum of complex **3** in CD_3CN .

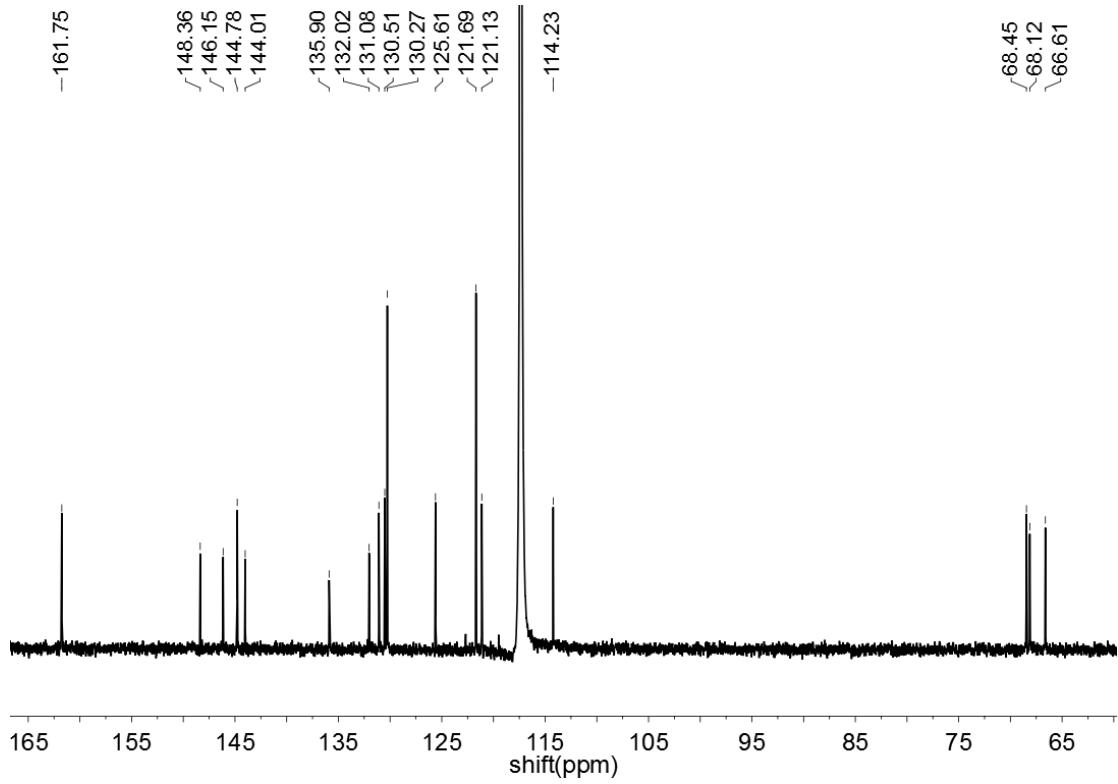


Fig. S11. ^{13}C NMR spectrum of complex **3** in CD_3CN .

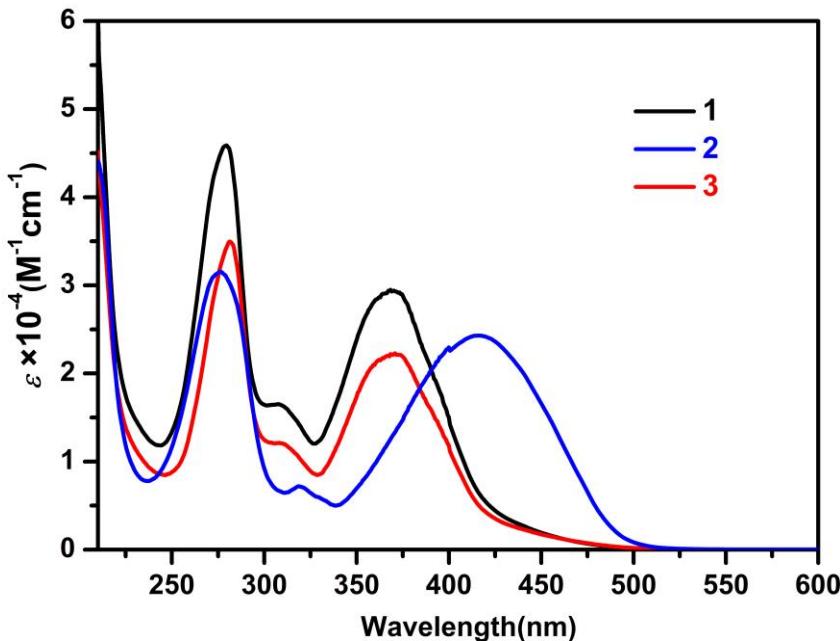


Fig. S12. UV-Vis absorption spectra of complexes **1–3** in acetonitrile solutions.

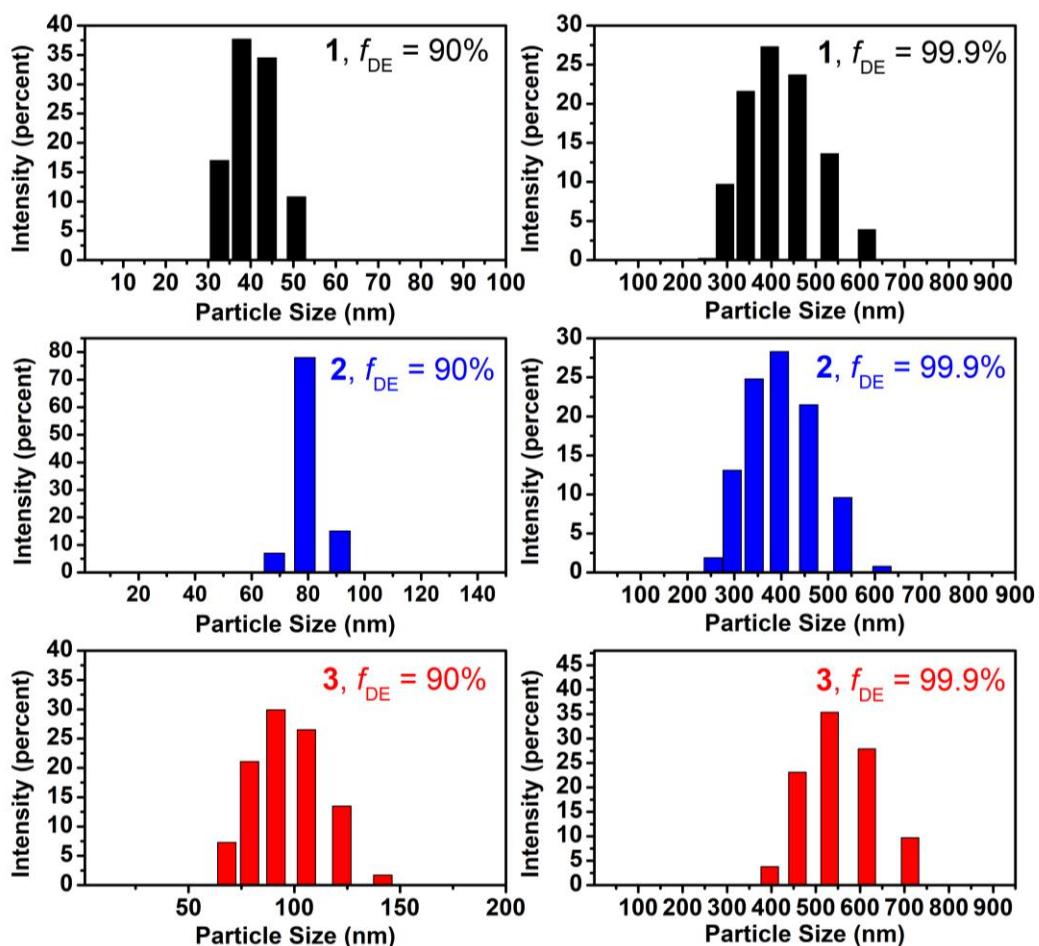


Fig. S13. Particle size distributions of complexes **1–3** ($25 \mu\text{M}$) in $\text{Et}_2\text{O}/\text{CH}_3\text{CN}$ mixture with different Et_2O fractions, indicating the formation of nano-aggregated

phases.

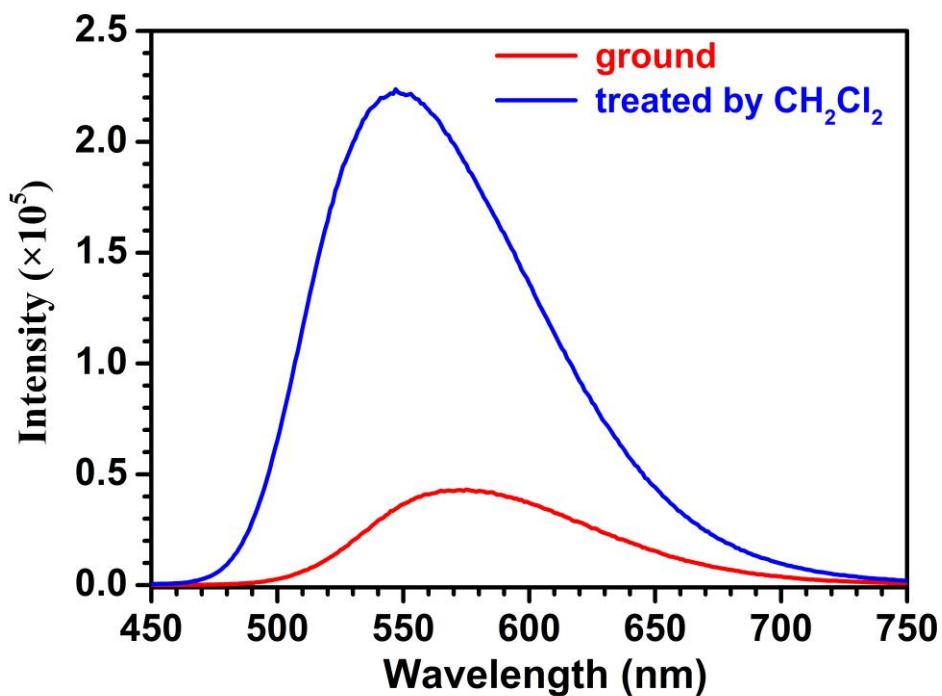


Fig. S14. Emission spectra of complex **1** during the grinding-fuming cycle.

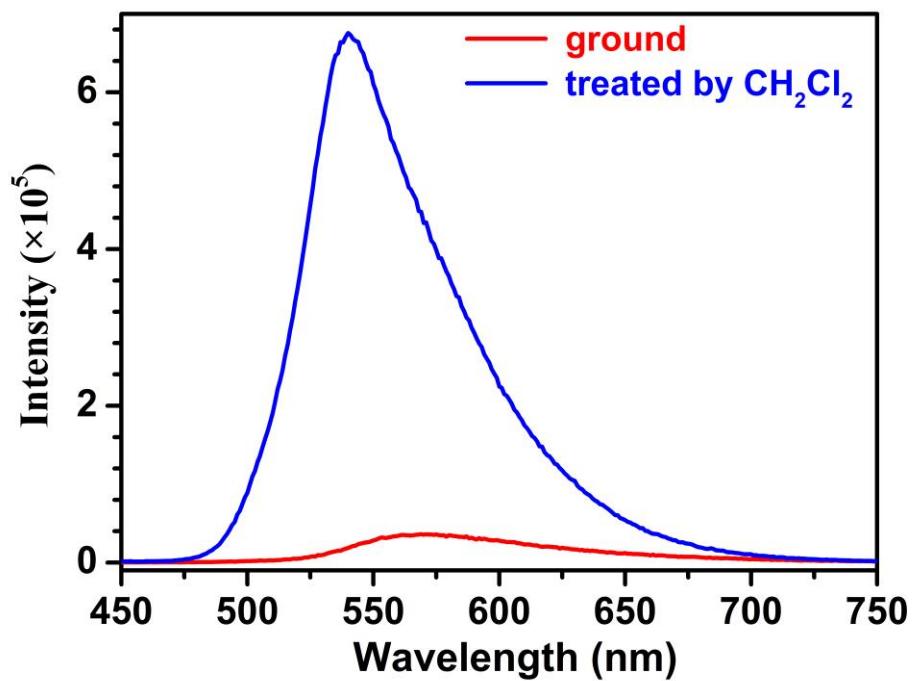


Fig. S15. Emission spectra of complex **2** during the grinding-fuming cycle.

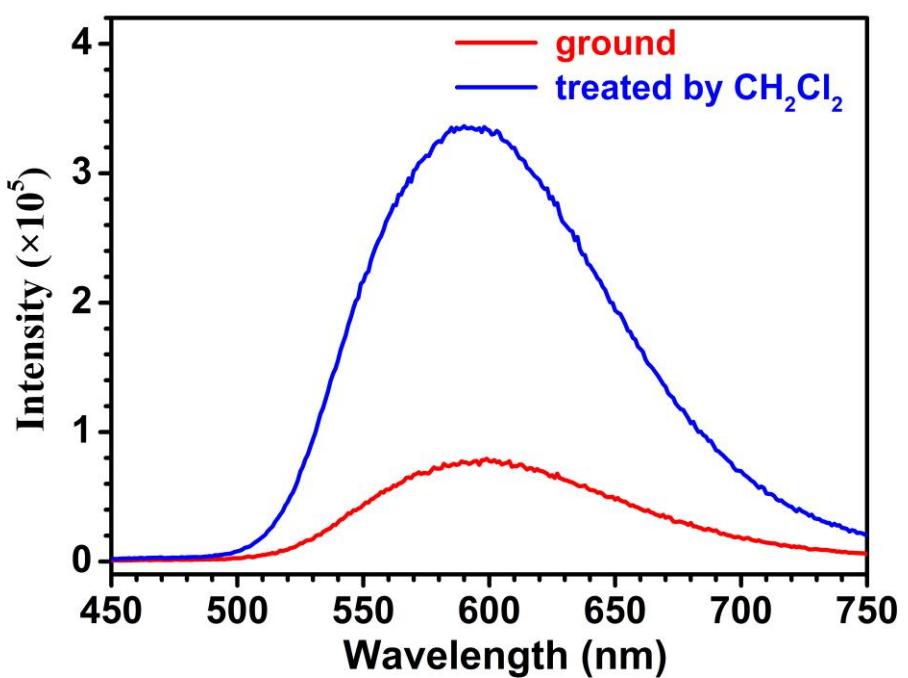


Fig. S16. Emission spectra of complex 3 during the grinding-fuming cycle.

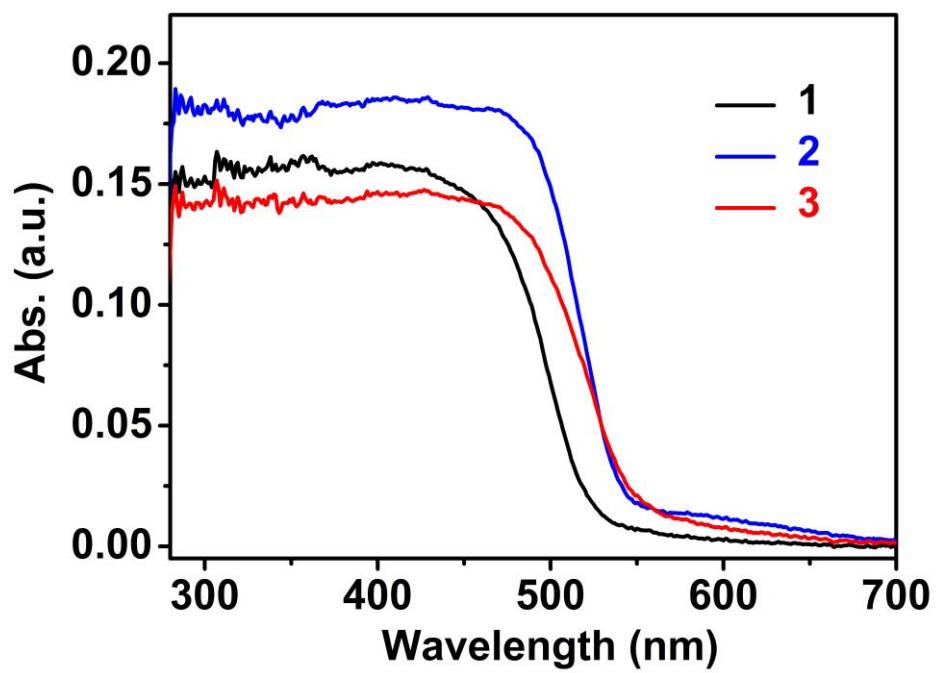


Fig. S17. UV-Vis spectra of complexes 1–3 in solid state.