

## *Electronic Supplementary Information (ESI)*

### **Mechanochromic luminescent materials of bimetallic Cu(I) complexes showing thermally activated delayed fluorescence**

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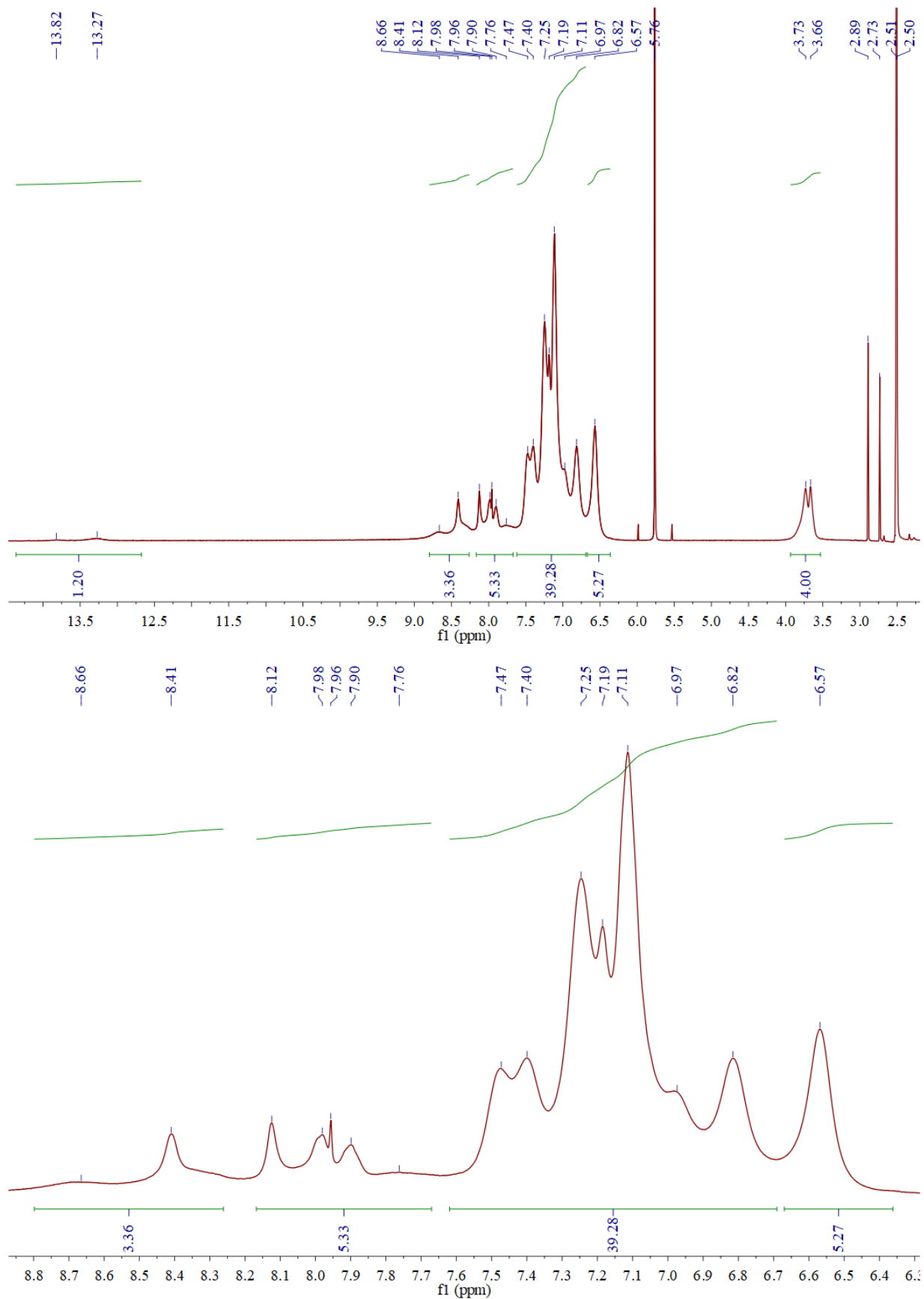
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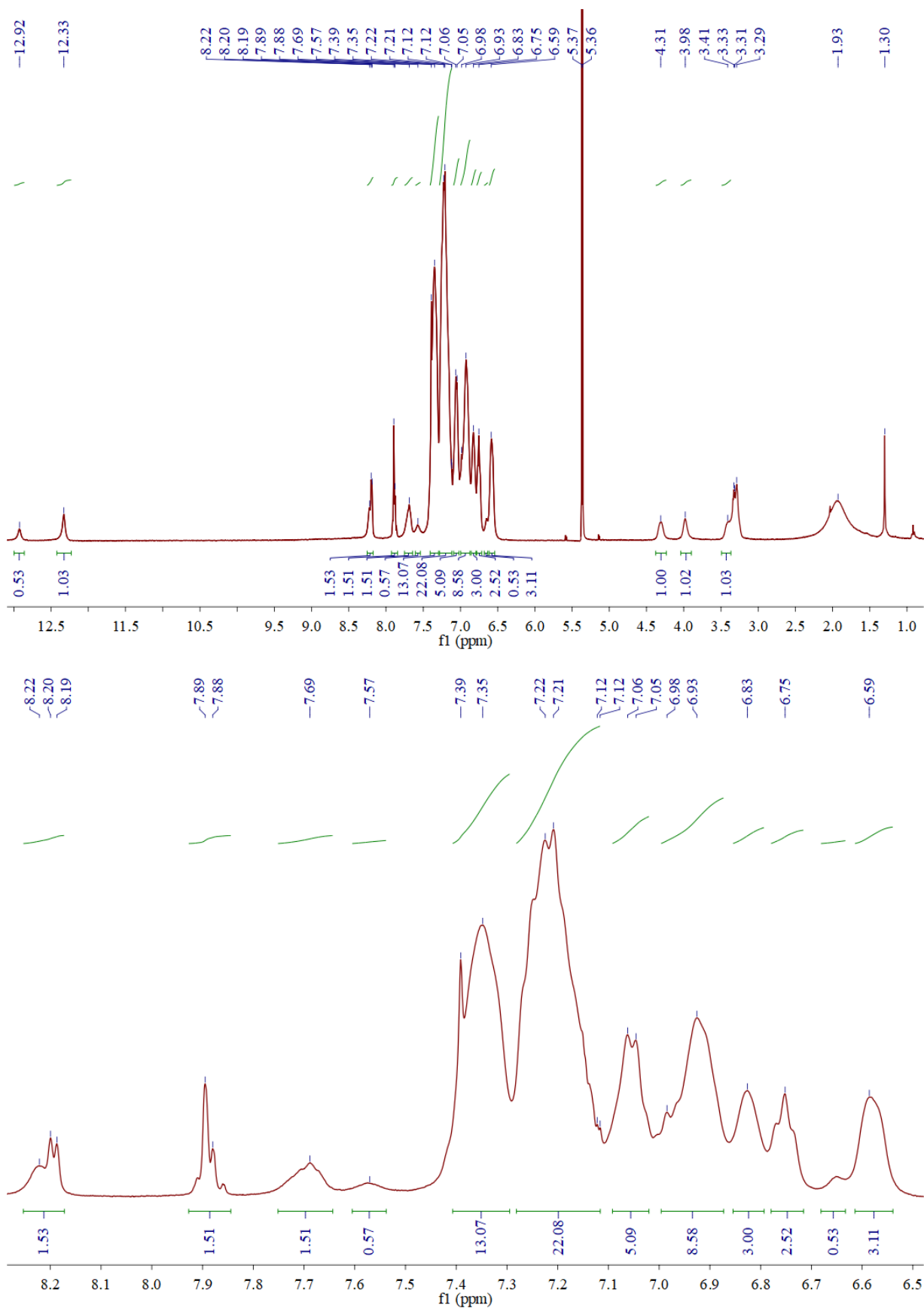
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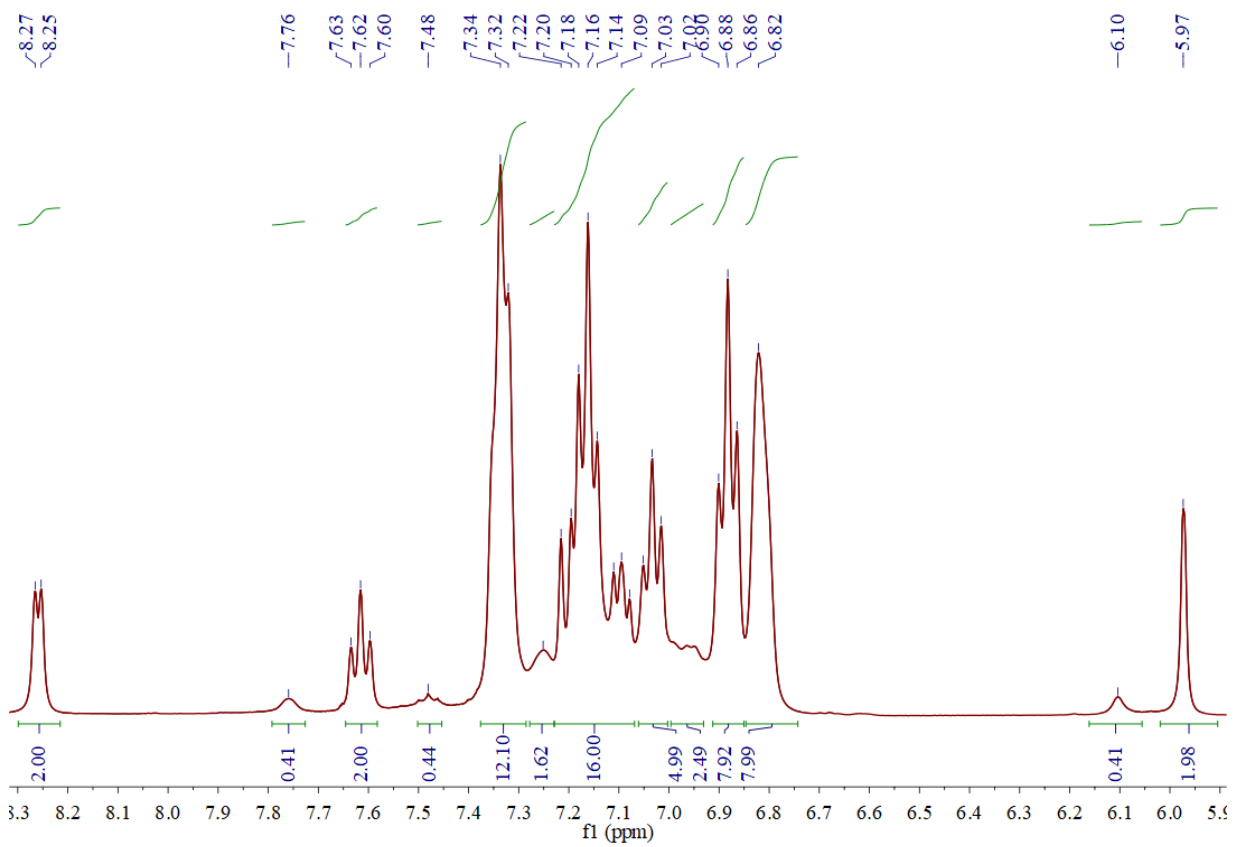
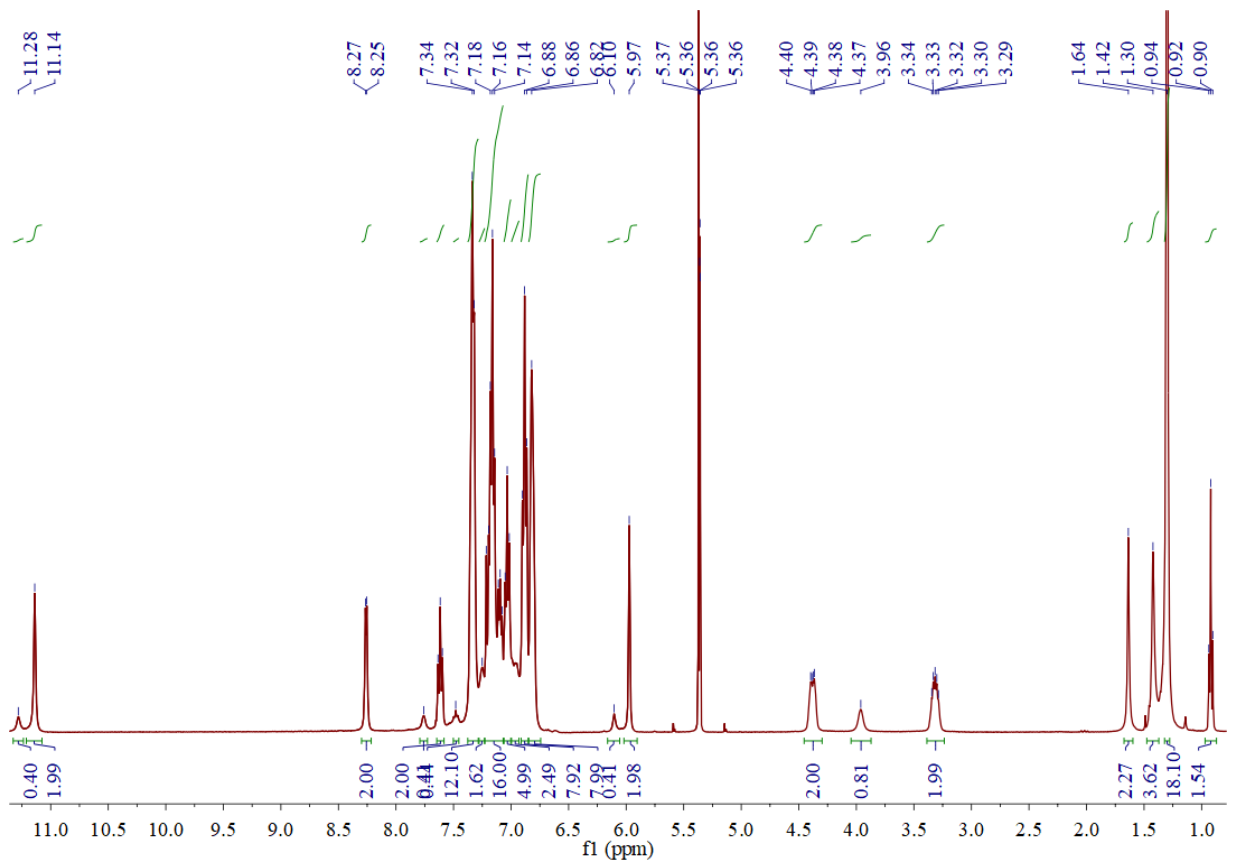
E-mail: gzchenjinglin@126.com (J.-L. Chen)



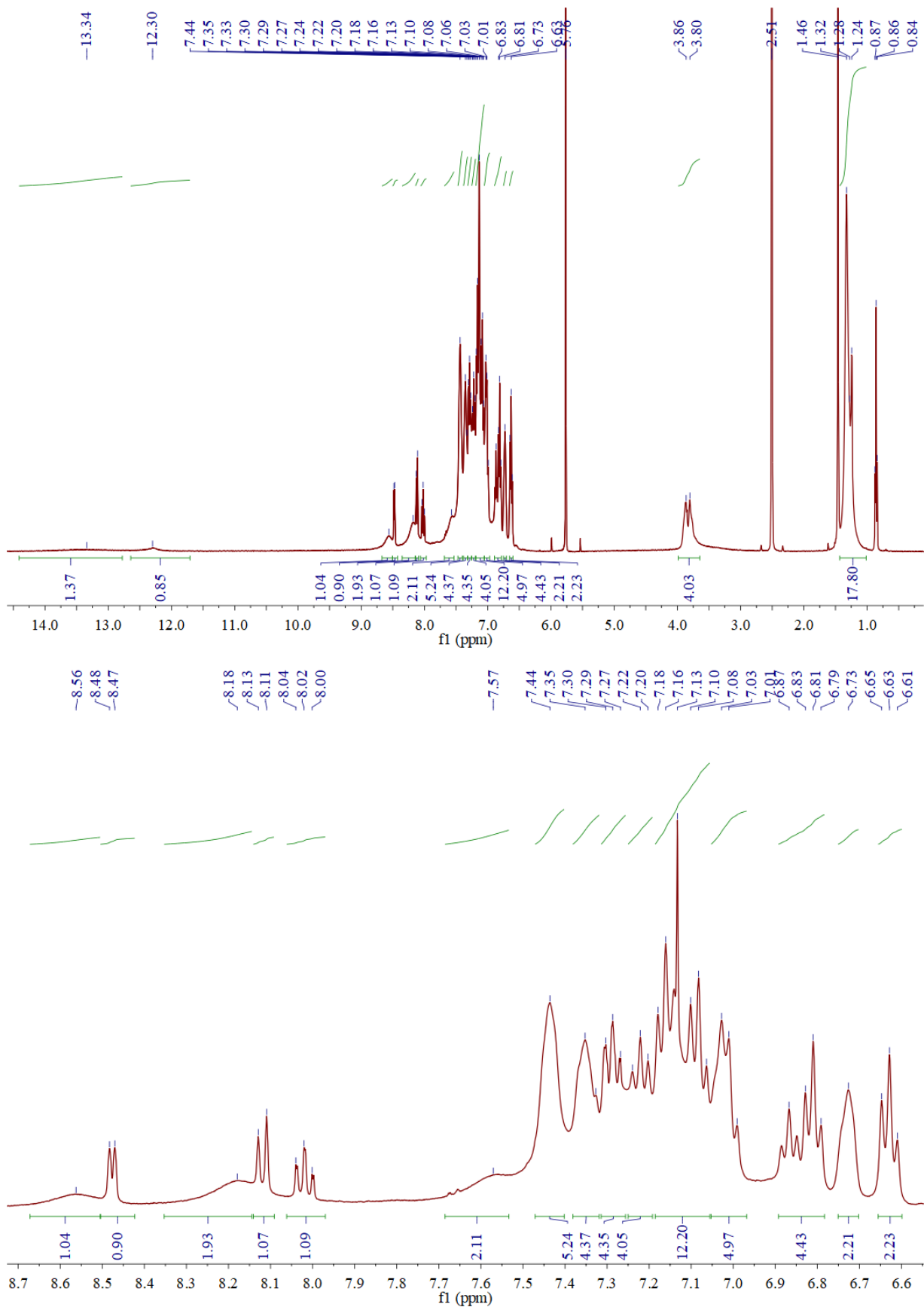
**Fig. S1**  $^1\text{H}$  NMR spectra of **1** in  $\text{DMSO-}d_6$ .



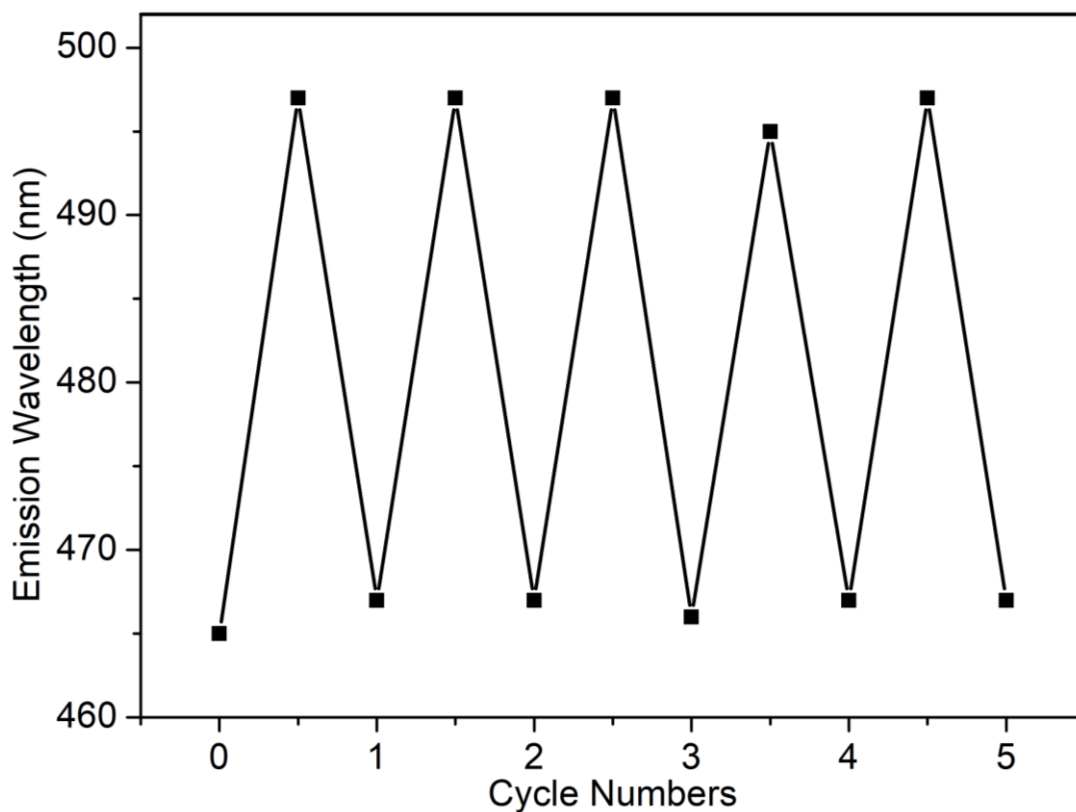
**Fig. S2**  $^1\text{H}$  NMR spectra of **2** in  $\text{CD}_2\text{Cl}_2$ .



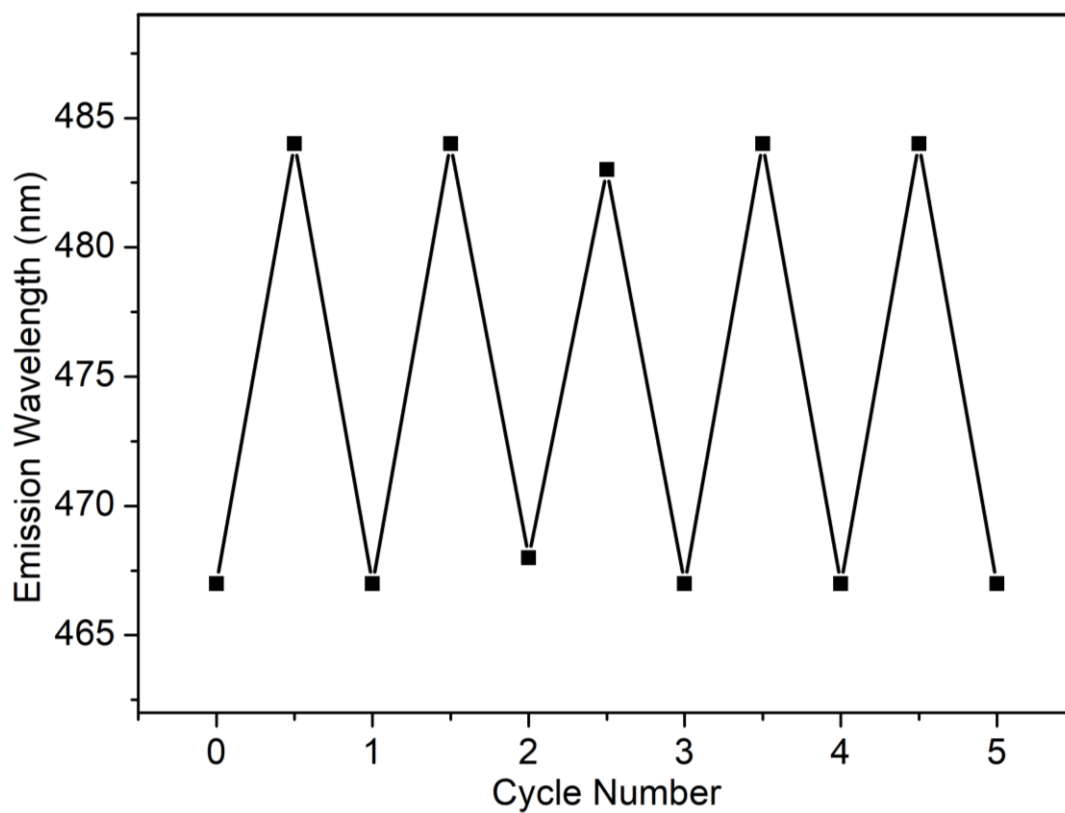
**Fig. S3**  $^1\text{H}$  NMR spectra of **3** in  $\text{CD}_2\text{Cl}_2$ .



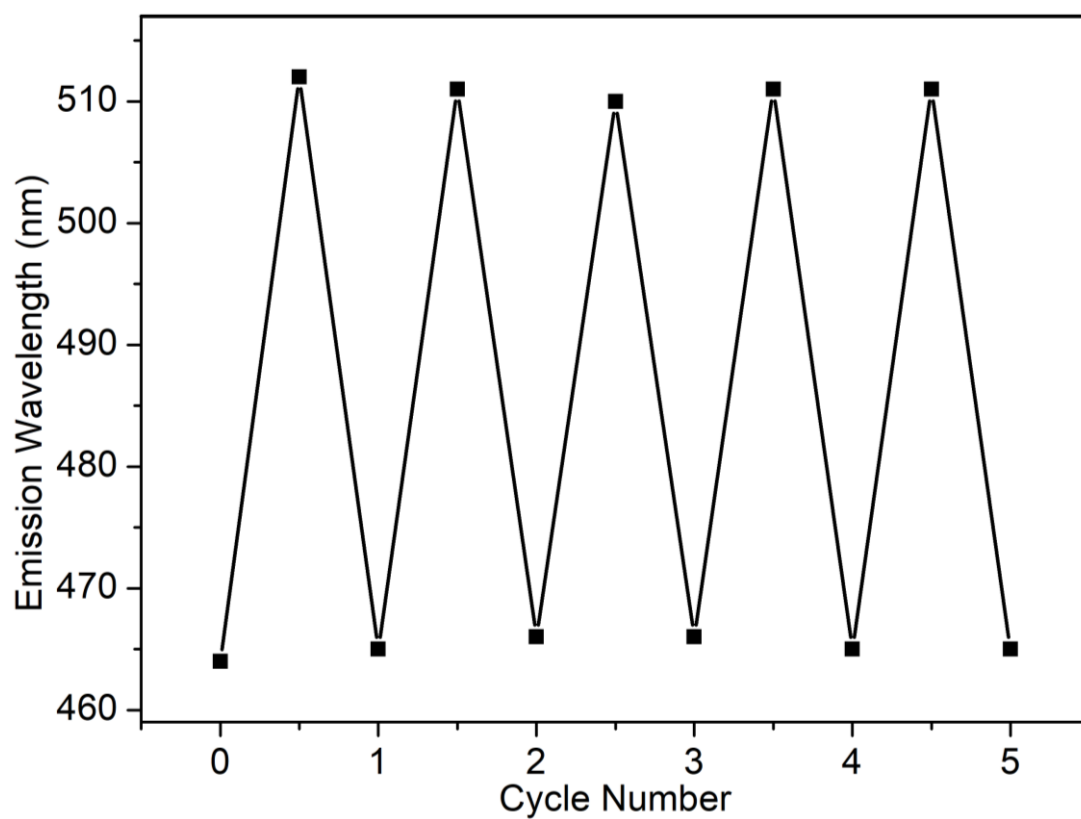
**Fig. S4**  $^1\text{H}$  NMR spectra of **3** in  $\text{DMSO-}d_6$ .



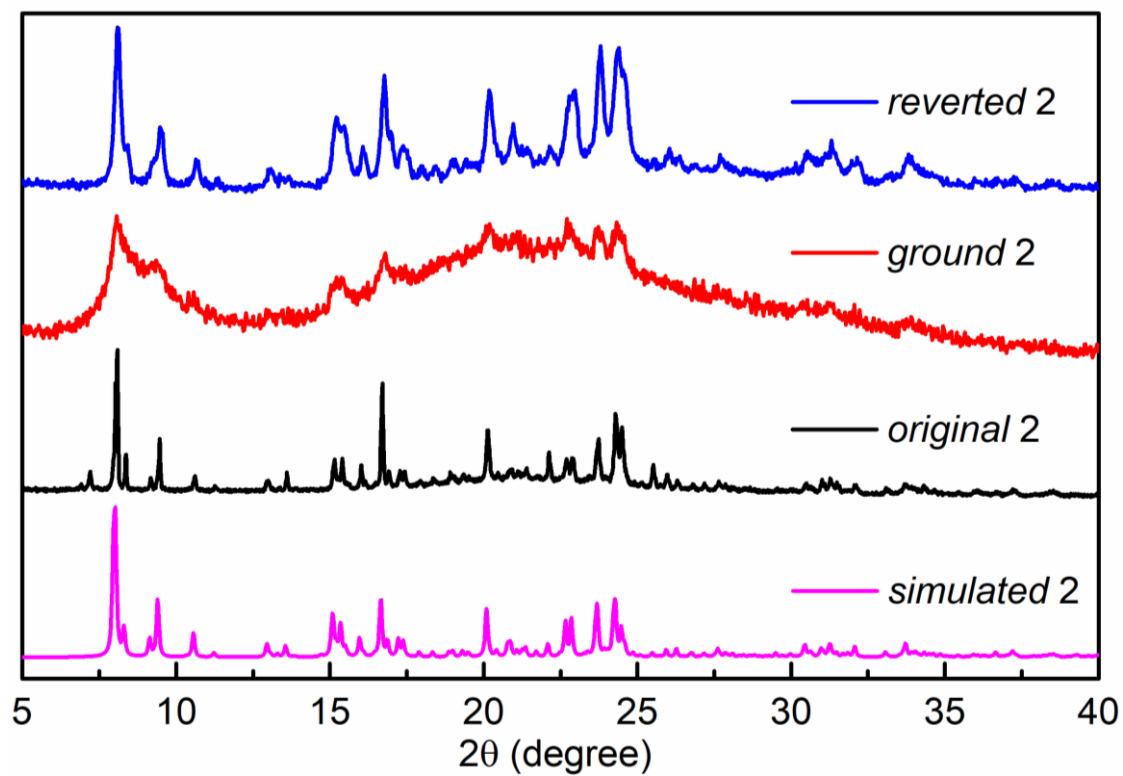
**Fig. S5** Emission maximum variation of **1** under alternate treatment of mechanical grinding and  $\text{CH}_2\text{Cl}_2$  vapor fuming.



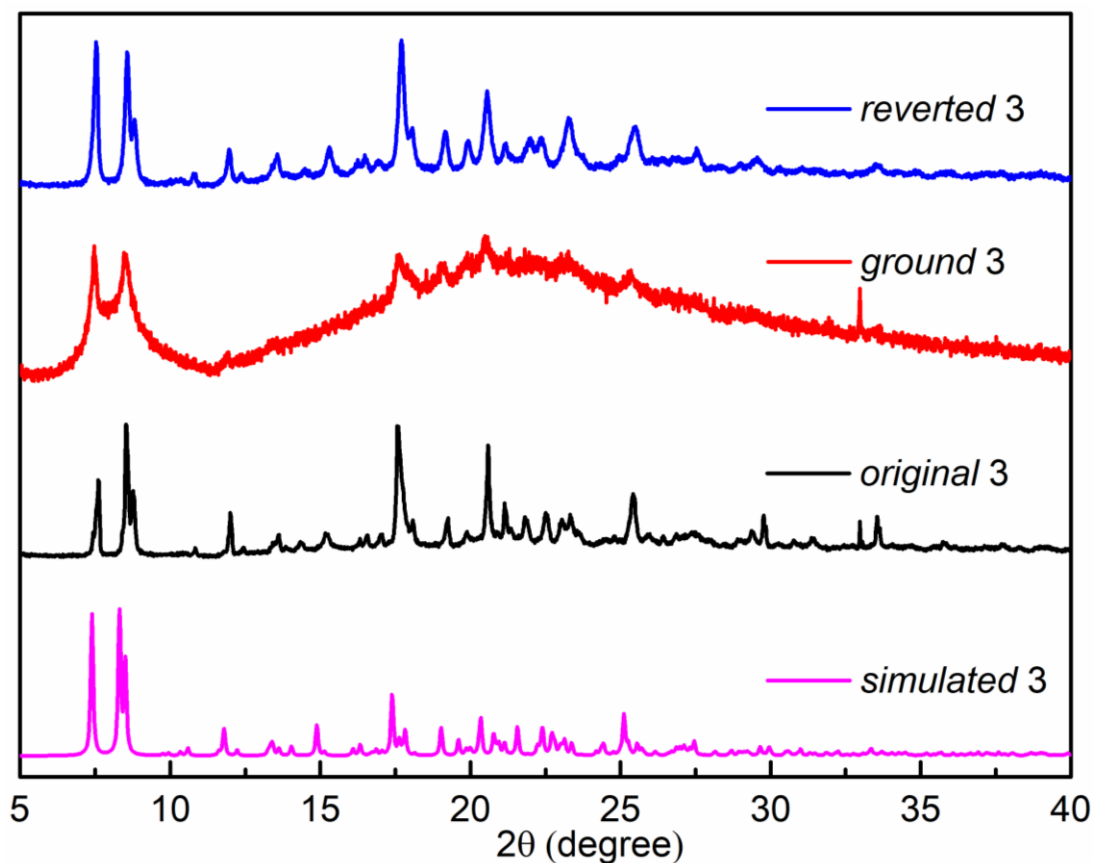
**Fig. S6** Emission maximum variation of **2** under alternate treatment of mechanical grinding and  $\text{CH}_2\text{Cl}_2$  vapor fuming.



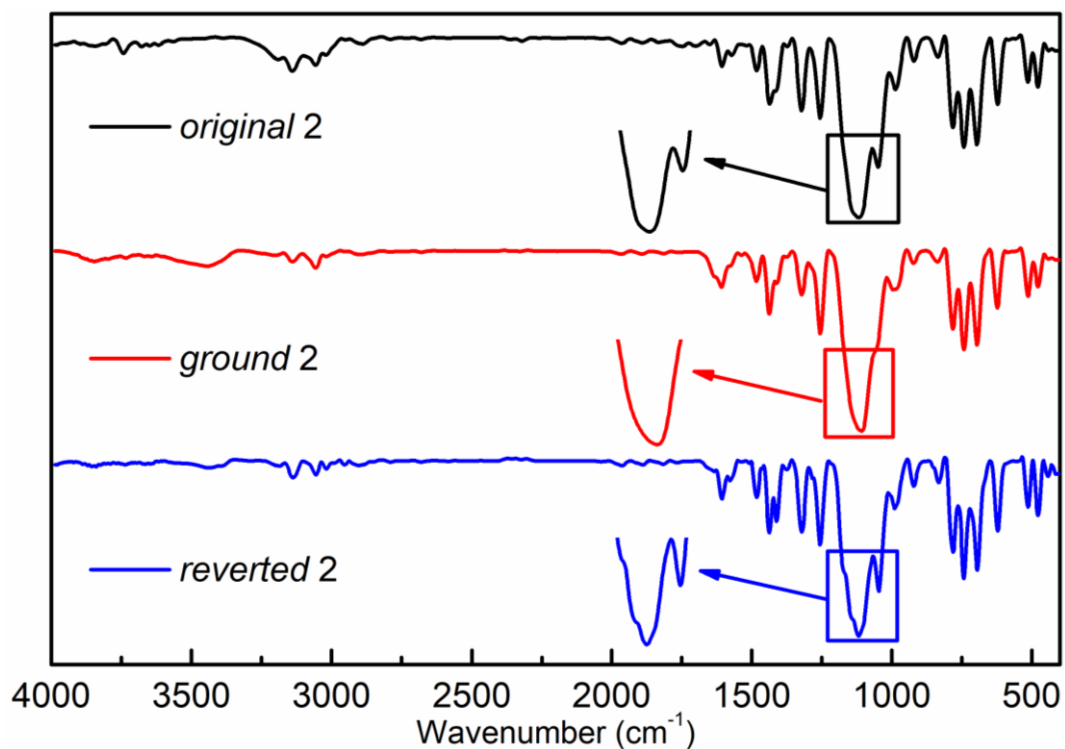
**Fig. S7** Emission maximum variation of **3** under alternate treatment of mechanical grinding and  $\text{CH}_2\text{Cl}_2$  vapor fuming.



**Fig. S8** PXRD patterns of the *original*, *ground* and *reverted* samples of **2** and that calculated from its single-crystal data of **2**.

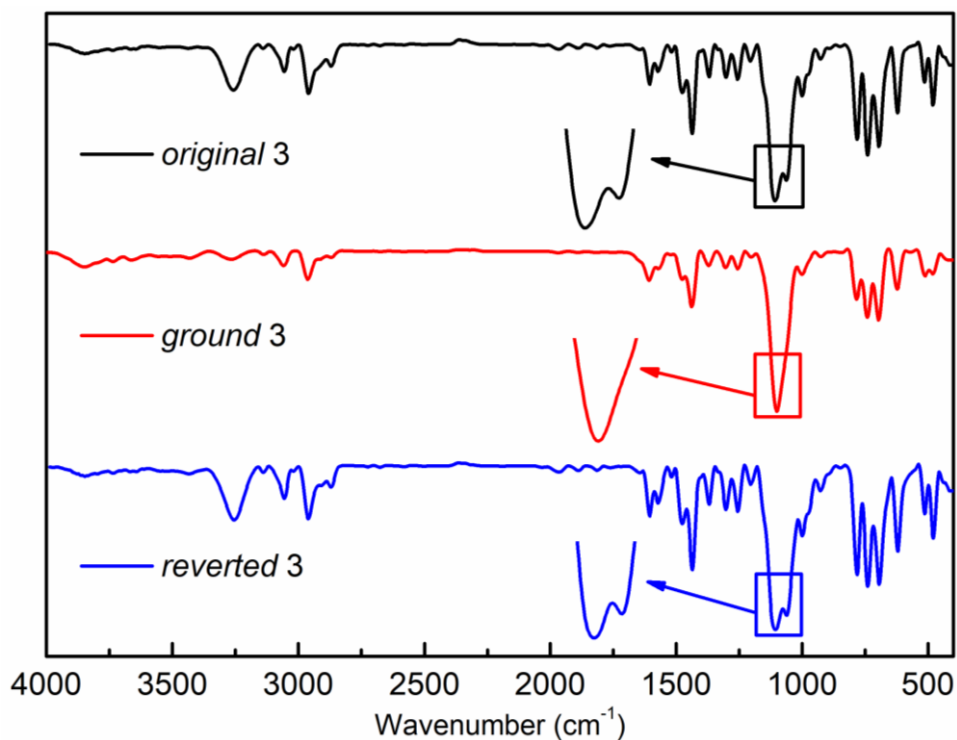


**Fig. S9** PXRD patterns of the *original*, *ground* and *reverted* samples of **3** and that calculated from its single-crystal data of **3**.

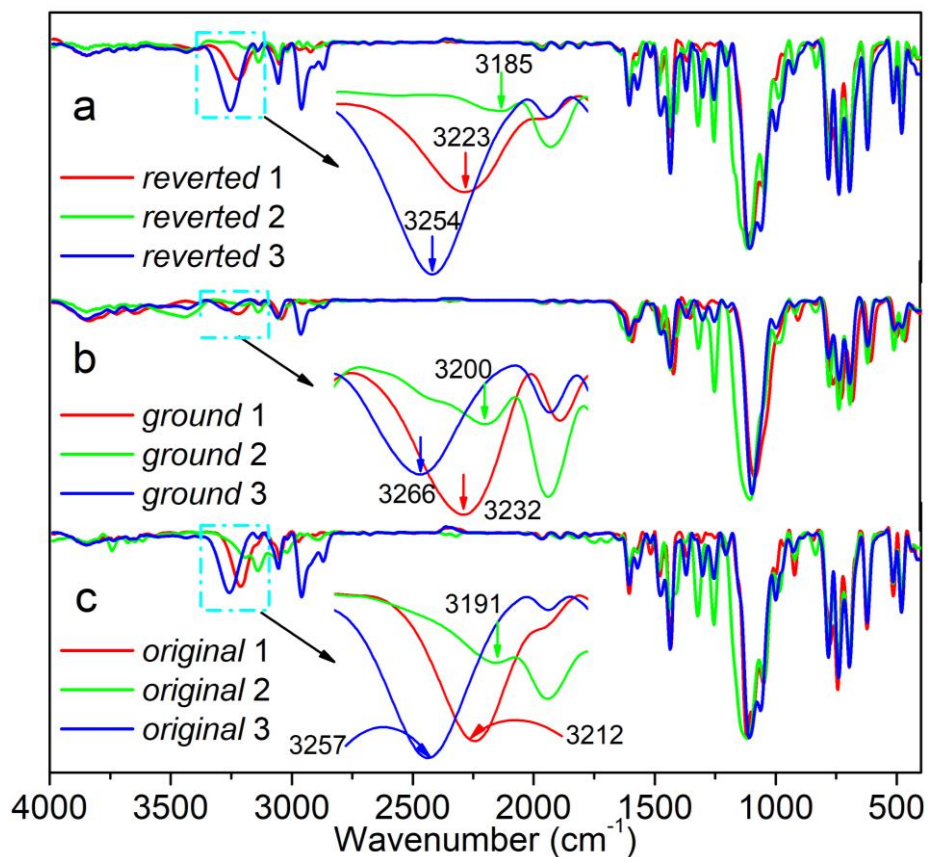


**Fig. S10** FT-IR spectra of the *original*, *ground* and *reverted* samples of **2**. Inset: the zoom of the Cl-O stretching vibration peaks of the *original*, *ground* and *reverted* samples of **2**.





**Fig. S11** FT-IR spectra of the *original*, *ground* and *reverted* samples of **3**. Inset: the zoom of the Cl-O stretching vibration peaks of the *original*, *ground* and *reverted* samples of **3**.



**Fig. S12** FT-IR spectra of the *original*, *ground* and *reverted* samples of **1-3** (a-c). Inset: the zoom of FT-IR spectra of **1-3** at 3350-3100  $\text{cm}^{-1}$ .

**Table S1** Crystal data and structure refinement parameters of **1–3**.

compound	<b>1</b>	<b>2</b>	<b>3</b>
formula	C <sub>68</sub> H <sub>62</sub> Cl <sub>6</sub> Cu <sub>2</sub> N <sub>6</sub> O <sub>8</sub> P <sub>4</sub>	C <sub>68</sub> H <sub>56</sub> Cl <sub>2</sub> Cu <sub>2</sub> F <sub>6</sub> N <sub>6</sub> O <sub>8</sub> P <sub>4</sub>	C <sub>80</sub> H <sub>88</sub> Cl <sub>2</sub> Cu <sub>2</sub> N <sub>6</sub> O <sub>8</sub> P <sub>4</sub>
fw	1554.89	1521.04	1583.42
<i>T</i> (K)	304.90(10)	293(2)	298.15
crystal system	Monoclinic	Monoclinic	Monoclinic
space group	<i>P</i> 2 <sub>1</sub> / <i>c</i>	<i>P</i> 2 <sub>1</sub> / <i>c</i>	<i>P</i> 2 <sub>1</sub> / <i>c</i>
<i>a</i> (Å)	14.1916(4)	13.0616(5)	13.5675(9)
<i>b</i> (Å)	13.5140(3)	13.5475(5)	17.0941(11)
<i>c</i> (Å)	19.5634(6)	19.3487(7)	16.6948(11)
<i>α</i> (deg)	90	90	90
<i>β</i> (deg)	108.384(3)	92.0960(10)	91.593(2)
<i>γ</i> (deg)	90	90	90
<i>V</i> (Å <sup>3</sup> )	3560.49(19)	3421.5(2)	3870.4(4)
<i>Z</i>	2	2	2
$\rho_{\text{calcd}}$ (g cm <sup>-3</sup> )	1.450	1.476	1.359
$\mu$ (mm <sup>-1</sup> )	0.970	0.869	0.760
no. reflections collected	36101	51467	58224
no. unique reflections	9804	7846	8884
<i>R</i> <sub>int</sub>	0.0365	0.0390	0.0537
no. observed reflections	9804	7846	8884
no. parameters	428	433	492
GOF on <i>F</i> <sup>2</sup>	1.068	1.057	1.048
<i>R</i> 1 [ <i>I</i> > 2σ( <i>I</i> )]	0.0540	0.0535	0.0554
<i>wR</i> 2	0.1538	0.1366	0.1376

**Table S2** Selected bond lengths (Å) and angles (deg) of **1–3**.

compound	<b>1</b>	<b>2</b>	<b>3</b>
Cu1–N1	2.158(2)	2.167(3)	2.171(3)
Cu1–N2	2.086(2)	2.111(3)	2.092(3)
Cu1–P1	2.2694(7)	2.2547(9)	2.2419(9)
Cu1–P2	2.2294(7)	2.2305(8)	2.2485(9)
N1–Cu1–N2	77.74(9)	77.37(12)	77.73(11)
N1–Cu1–P1	102.62(6)	98.53(8)	102.76(8)
N1–Cu1–P2	104.59(6)	104.47(8)	99.58(8)
N2–Cu1–P1	100.62(6)	101.47(8)	112.67(8)
N2–Cu1–P2	120.10(7)	117.28(8)	105.83(8)
P1–Cu1–P2	134.68(3)	138.17(3)	138.62(3)