Supplementary Information

Intense Photo- and Tribo-luminescence of Three Tetrahedral Manganese(II) Dihalides with Chelating Bidentate Phosphine Oxide Ligand

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Table S1. Selected bond lengths (Å) and angles (º) for **1**–**3**

1			
Mn(1)–O(1)	2.032(2)	Mn(1)–Cl(2)	2.3228(11)
Mn(1)–O(2)	2.050(2)	P(1)–O(1)	1.505(2)
Mn(1)–Cl(1)	2.3424(13)	P(2)–O(2)	1.496(2)
O(1)–Mn(1)–O(2)	105.51(8)	O(2)–Mn(1)–Cl(1)	106.26(7)
O(1)–Mn(1)–Cl(2)	112.84(7)	Cl(2) –Mn(1)–Cl(1)	112.60(4)
O(2)–Mn(1)–Cl(2)	111.90(7)	P(1)–O(1)–Mn(1)	157.29(14)
O(1)–Mn(1)–Cl(1)	107.23(7)	P(2)–O(2)–Mn(1)	155.24(14)
2			
Mn(1)–O(1)	2.018(2)	Mn(1)–Br(2)	2.46939(14)
Mn(1)–O(2)	2.049(2)	P(1)–O(1)	1.506(2)
Br(1)–Mn(1)	2.4869(13)	P(2)–O(2)	1.503(2)
O(1)–Mn(1)–O(2)	105.48(10)	O(2)–Mn(1)–Br(2)	111.79(7)
O(1)–Mn(1)–Br(1)	107.05(7)	Br(1)–Mn(1)–Br(2)	111.34(3)
O(2)–Mn(1)–Br(1)	108.09(7)	P(1)–O(1)–Mn(1)	158.24(17)
O(1)–Mn(1)–Br(2)	112.76(7)	P(2)–O(2)–Mn(1)	155.53(13)
3			
Mn(1)–O(1)	2.0348(18)	I(2)–Mn(1)	2.6815(10)
Mn(1)–O(2)	2.0079(18)	P(1)–O(1)	1.5030(18)
I(1)–Mn(1)	2.7108(12)	P(2)–O(2)	1.4996(18)
O(2)–Mn(1)-O(1)	104.00(7)	O(1)–Mn(1)–I(2)	106.72(6)
O(2)–Mn(1)–I(1)	102.82(6)	I(1)–Mn(1)–I(2)	115.148(18)
O(1)–Mn(1)–I(1)	116.67(6)	P(1)–O(1)–Mn(1)	157.58(11)
O(2)–Mn(1)–I(2)	110.86(6)	P(2)–O(2)–Mn(1)	163.60(12)

Table S2. Hydrogen-bond geometry for compounds **1** and **2**

D–H···A	D–H/Å	H···A/Å	D…A/Å	∠D–H···A/º
1				
O4–H4B...Cl1_$1	0.82	2.51	3.221(5)	146.4
2				
O4–H4B...Br1_$2	0.82	2.76	3.405(6)	136.8

Symmetry code $1 for **1**: x, y + 1, z; $2 for **2**: –x + 1, –y + 2, –z + 1.

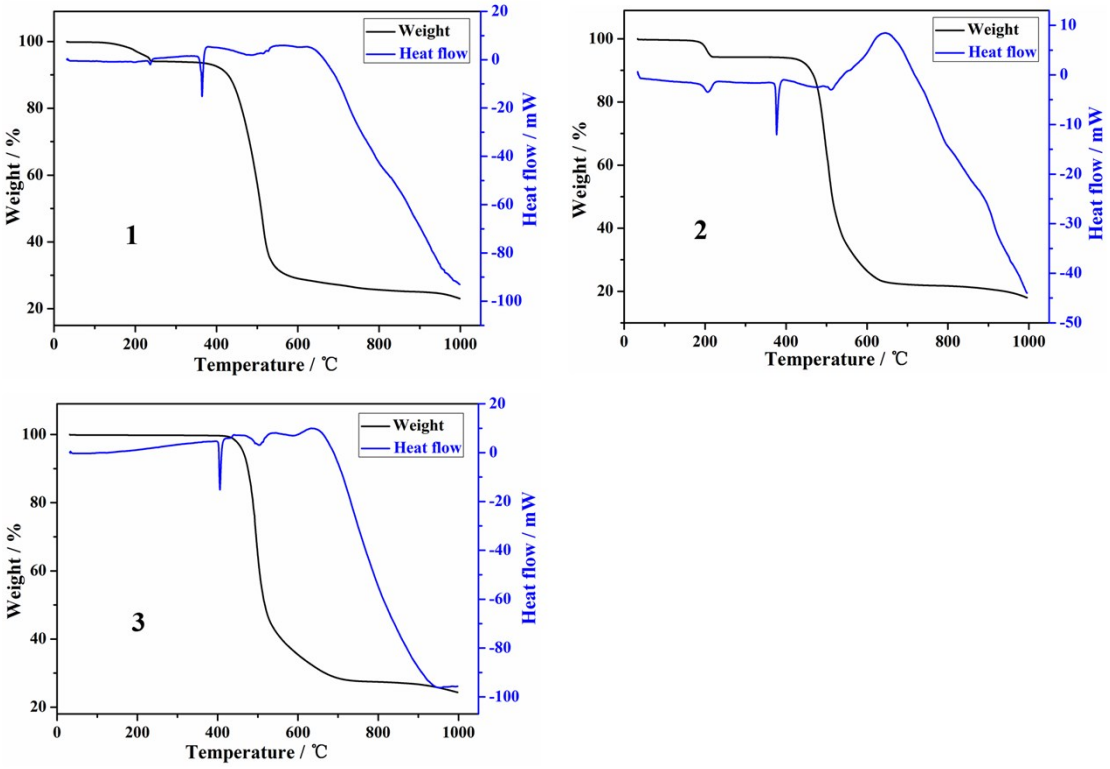

Figure S1. TGA curves for **1**–**3**.

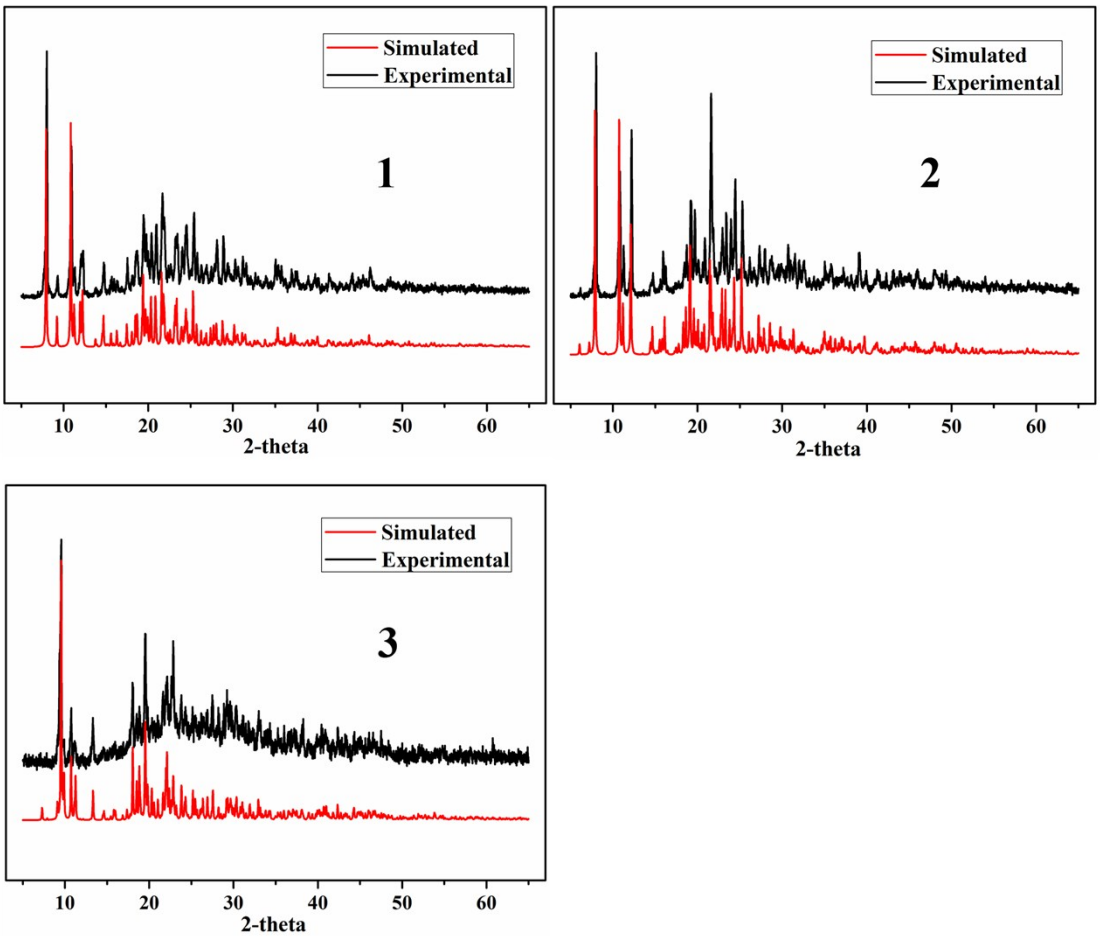

Figure S2. Powdered X-ray diffraction (PXRD) patterns of **1**–**3**.

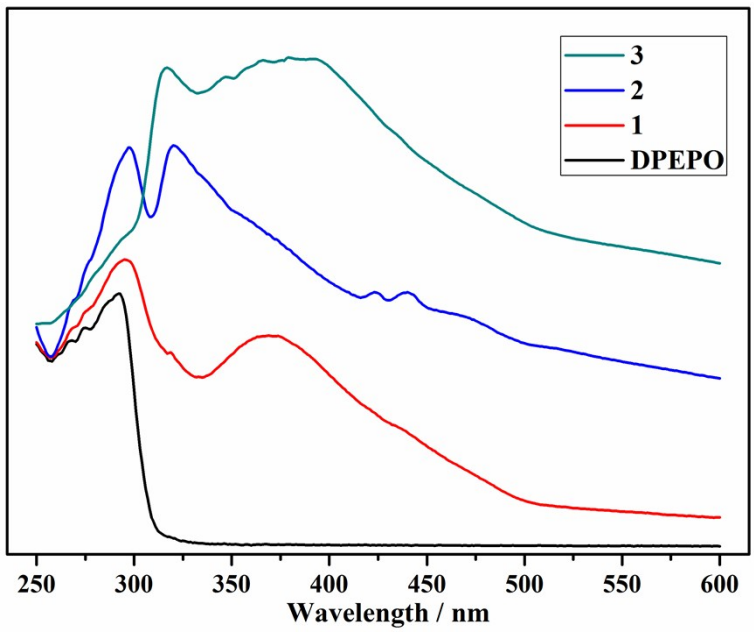

Figure S3. Solid-state UV/Vis absorbance spectra of DPEPO and **1**–**3** measured at 298K.

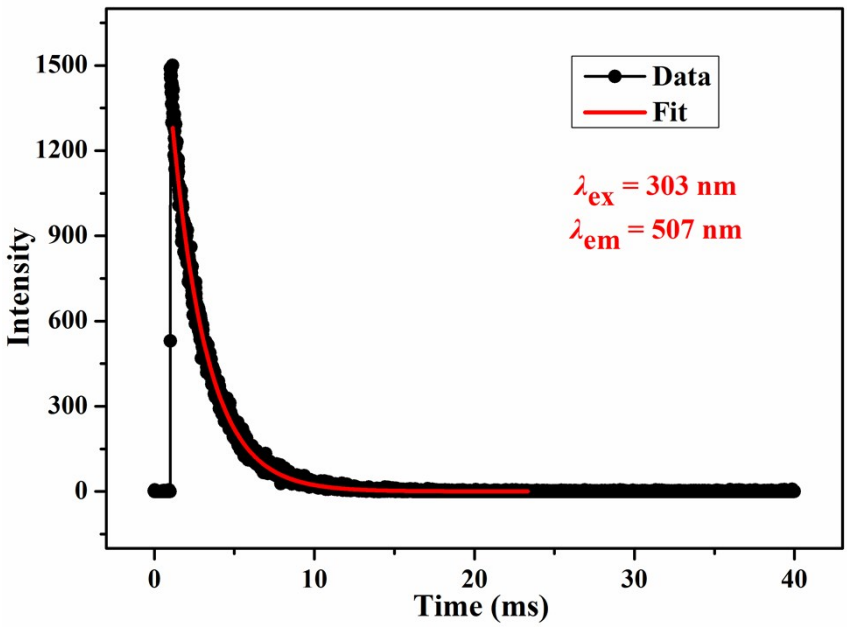

Figure S4. Photoluminescence lifetime of **1** in the solid state measured at 298K, and using an excitation of 303 nm and an emission of 507 nm.

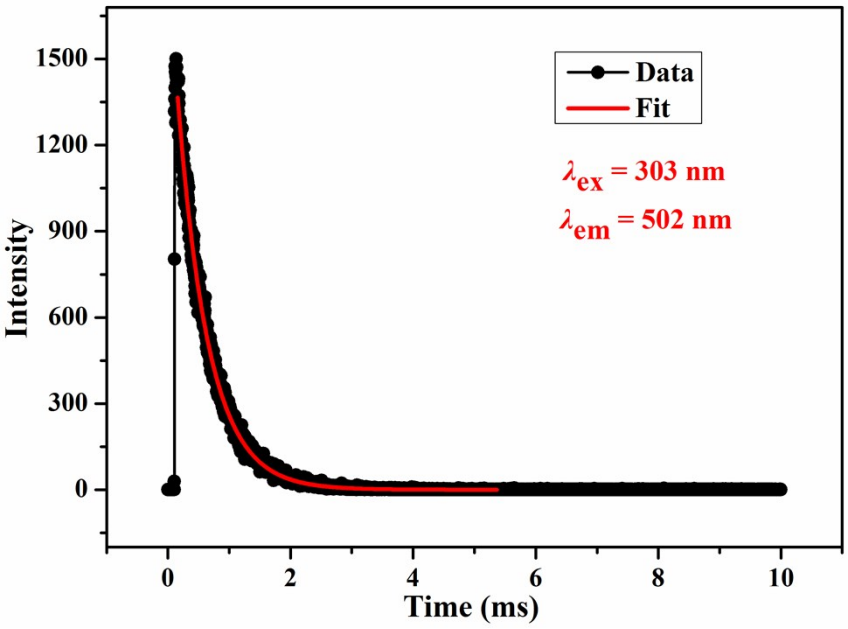

Figure S5. Photoluminescence lifetime of **2** in the solid state measured at 298K, and using an excitation of 303 nm and an emission of 502 nm.

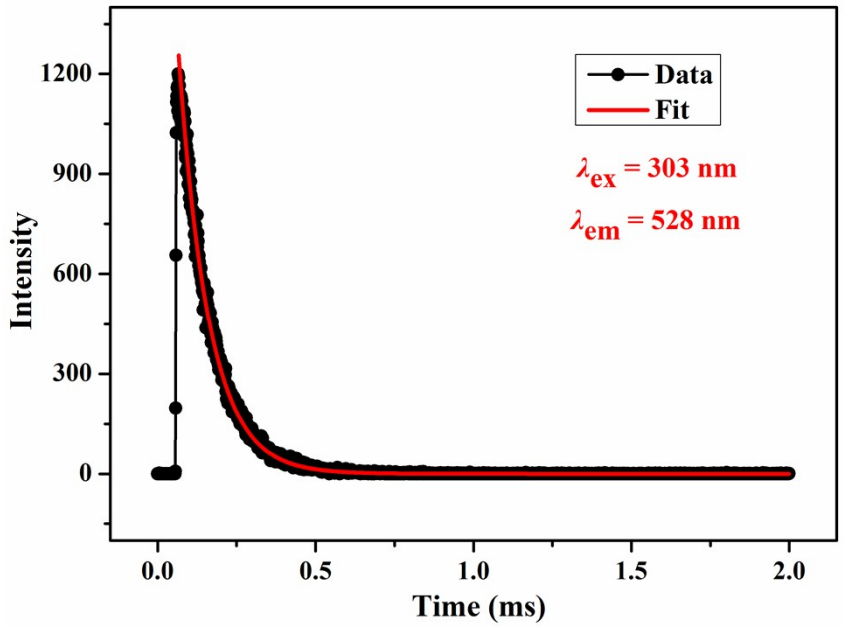

Figure S6. Photoluminescence lifetime of **3** in the solid state measured at 298K, and using an excitation of 303 nm and an emission of 528 nm.

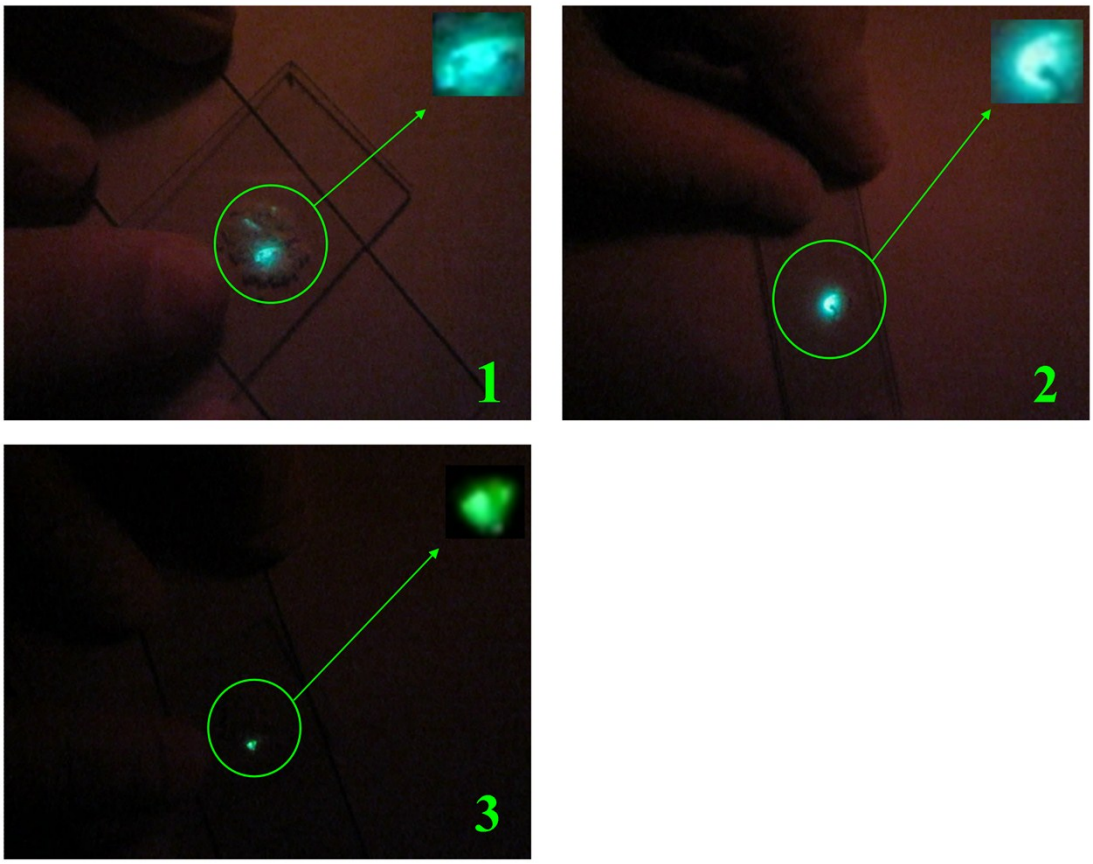

Figure S7. Photographs of the TL light captured from crystals of **1**–**3**.

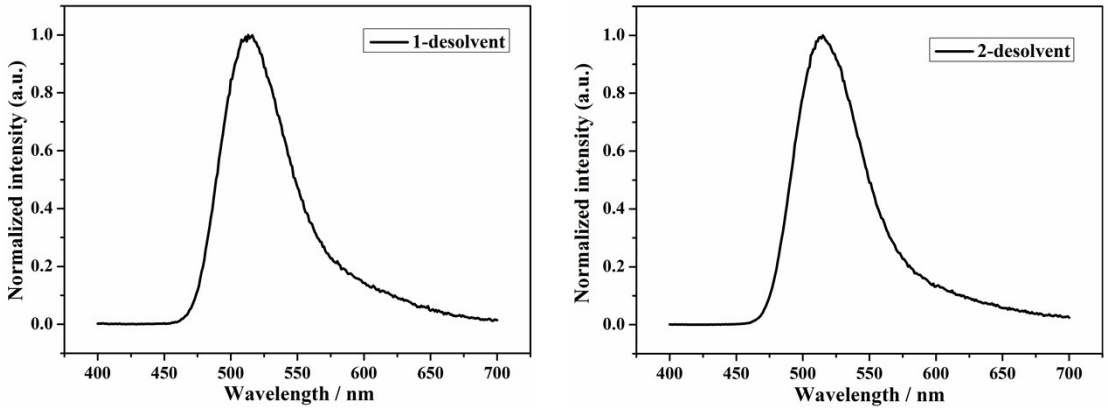

Figure S8. Solid-state emission spectra of desolvated samples for **1** and **2** measured at 298 K (λ_{ex} = 303 nm).

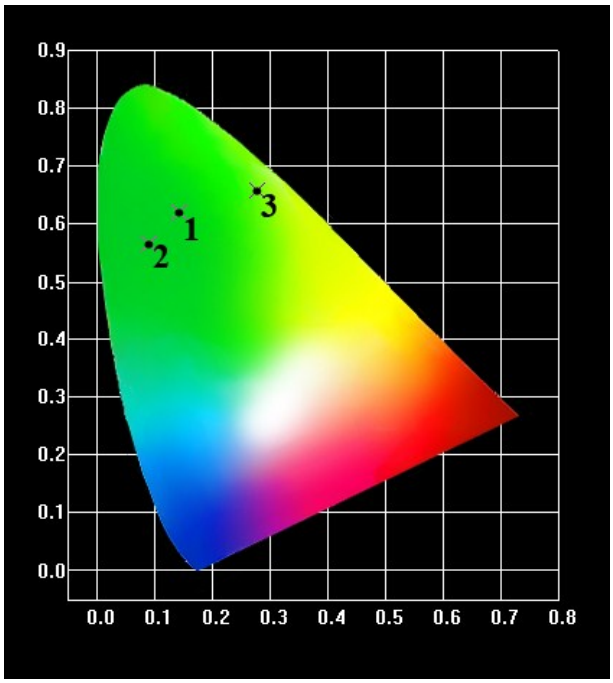

Figure S9. CIE chromaticity diagram for **1**–**3** in the solid state at 298K.

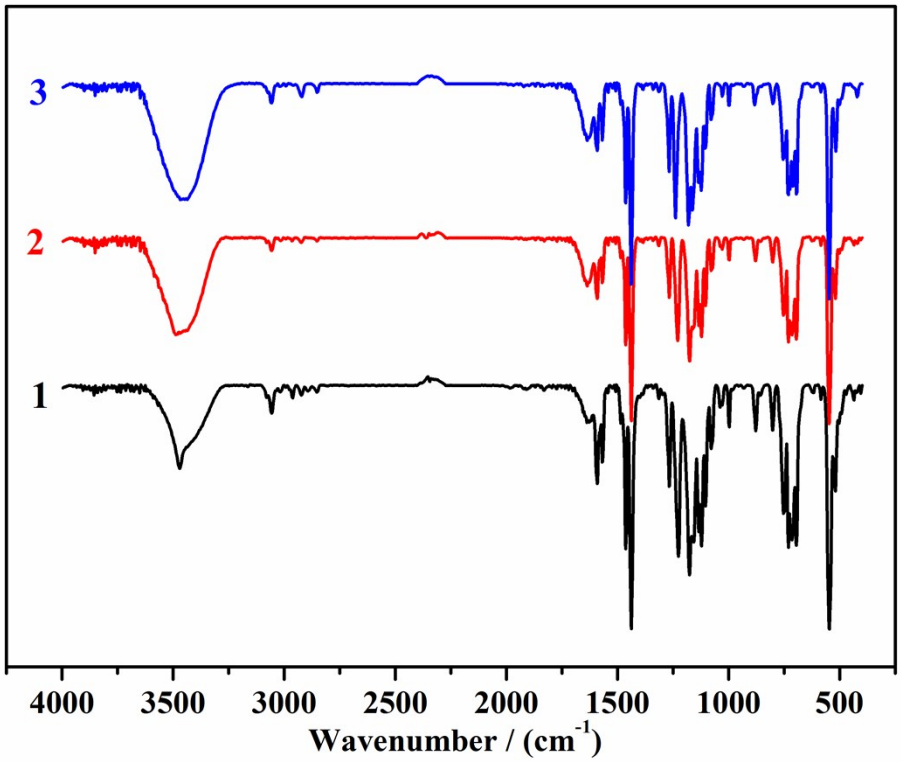

Figure S10. The FT-IR spectra of **1**–**3**.