

Supporting Information

Influence of co-ligands and solvents on the packing and photoluminescence of three related Mn^{II} metal-organic frameworks

Sujing Wang, Shunshun Xiong, Lexin Song and Zhiyong Wang**

To whom correspondence should be addressed. E-mail: zwang3@ustc.edu.cn. Fax: +86-551-3603185; Tel: +86-551-3603185

Hefei National Laboratory for Physical Science at Microscale, Joint-lab of Green Synthetic Chemistry and Department of Chemistry, University of Science and Technology of China, Hefei 230026, P. R. China

1. Selected bond lengths and bond angles of compounds 1-3

Table S1. Selected Bond Lengths (Å) and Bond Angles (deg) for Compound 1 – 3

Compound 1 ^a					
Mn1-O1	2.1582(16)	O5-Mn1-O1	94.28(6)	O5-Mn2-O2	86.68(6)
Mn1-O3 ^A	2.1138(15)	O5-Mn1-O1 ^B	85.72(6)	O5-Mn2-O2 ^B	93.32(6)
Mn1-O5	2.2500(16)	O5-Mn1-O3 ^A	93.32(6)	O5-Mn2-O4 ^A	88.87(6)
Mn2-O2	2.1355(15)	O5-Mn1-O3 ^C	87.68(6)	O5-Mn2-O4 ^C	91.13(6)
Mn2-O4 ^A	2.2018(16)	O1-Mn1-O3 ^A	92.14(6)	O5 ^B -Mn2-O4 ^A	91.13(6)
Mn2-O5	2.2222(17)	O1-Mn1-O3 ^C	87.86(6)	O2-Mn2-O4 ^A	97.22(6)
		O1 ^B -Mn1-O3 ^C	92.14(6)	O2-Mn2-O4 ^C	82.78(6)

Compound 2 ^b					
Mn1-O1 ^C	2.1736(18)	O1 ^C -Mn1-O4 ^A	171.96(7)	O3 ^D -Mn1-O2	104.98(7)
Mn1-O2	2.1264(17)	O3 ^D -Mn1-N1	166.12(7)	O3 ^D -Mn1-O5	86.79(7)
Mn1-O3 ^D	2.1041(17)	O2-Mn1-O5	166.60(7)	O3 ^D -Mn1-O4 ^A	86.66(7)
Mn1-O4 ^A	2.1759(17)	N1-Mn1-O2	86.30(8)	O2-Mn1-O1 ^C	86.69(7)
Mn1-O5	2.2988(18)	N1-Mn1-O1 ^C	89.92(7)	O2-Mn1-O4 ^A	97.82(7)
Mn1-N1	2.275(2)	N1-Mn1-O5	83.04(8)	O1 ^C -Mn1-O5	85.18(7)
		N1-Mn1-O4 ^A	83.76(7)	O5-Mn1-O4 ^A	89.11(7)

Compound 3 ^c					
Mn1-O1 ^B	2.2673(16)	O1 ^B -Mn1-O3	171.80(7)	O6-Mn1-O1 ^B	91.73(8)
Mn1-O1 ^C	2.2283(17)	O1 ^C -Mn1-O4 ^A	165.19(7)	O6-Mn1-O1 ^C	95.76(8)
Mn1-O3	2.0966(17)	O5-Mn1-O6	174.28(6)	O6-Mn1-O3	89.94(8)
Mn1-O4 ^A	2.1366(18)	O5-Mn1-O1 ^B	86.42(6)	O6-Mn1-O4 ^A	87.27(8)
Mn1-O5	2.2457(14)	O5-Mn1-O1 ^C	89.24(6)	O1 ^C -Mn1-O3	92.10(7)
Mn1-O6	2.133(2)	O5-Mn1-O3	92.65(7)	O1 ^B -Mn1-O1 ^C	79.74(6)
		O5-Mn1-O4 ^A	87.19(6)	O1 ^B -Mn1-O4 ^A	85.68(7)

^a Symmetry transformations used to generate equivalent atoms: A) $-x+1/2, y+1/2, -z+1/2$; B) $-x, -y, -z$; C) $x-1/2, -y-1/2, z-1/2$. ^b Symmetry transformations used to generate equivalent atoms: A) $-x+1/2, -y, z+1/2$; B) $-x, -y, -z$; C) $-x-1/2, y-1/2, z$; D) $x, -y-1/2, z-1/2$. ^c Symmetry transformation used to generate equivalent atoms: A) $-x+1/2, y, -z$; B) $x+1/2, y+1/2, z+1/2$; C) $-x+1/2, -y+1/2, -z+1/2$.

2. PXRD patterns of compounds 1-3

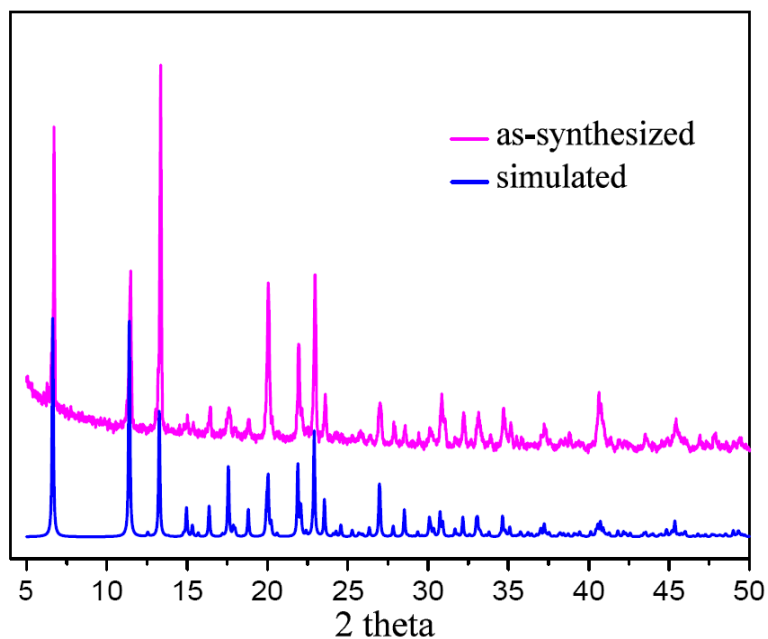


Figure S1. Powder X-ray diffraction patterns of as-synthesized (in purple) and simulated from the single-crystal diffraction data (in blue) for compound **1**.

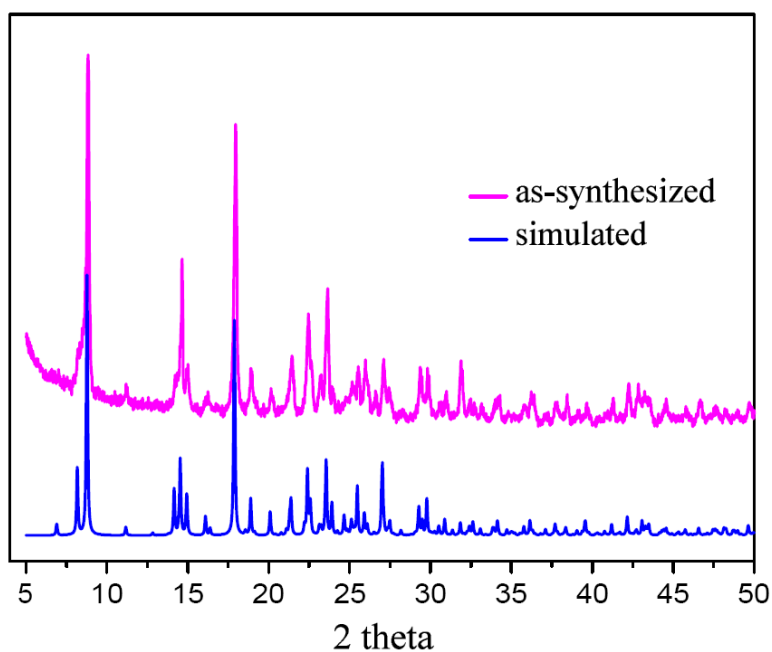


Figure S2. Powder X-ray diffraction patterns of as-synthesized (in purple) and simulated from the single-crystal diffraction data (in blue) for compound **2**.

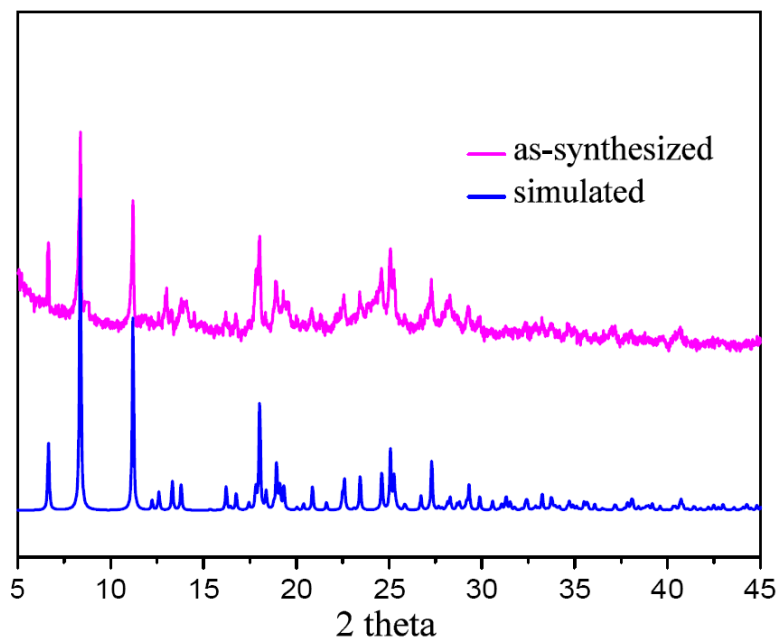


Figure S3. Powder X-ray diffraction patterns of as-synthesized (in purple) and simulated from the single-crystal diffraction data (in blue) for compound **3**.

3. TGA curves of compounds 1-3

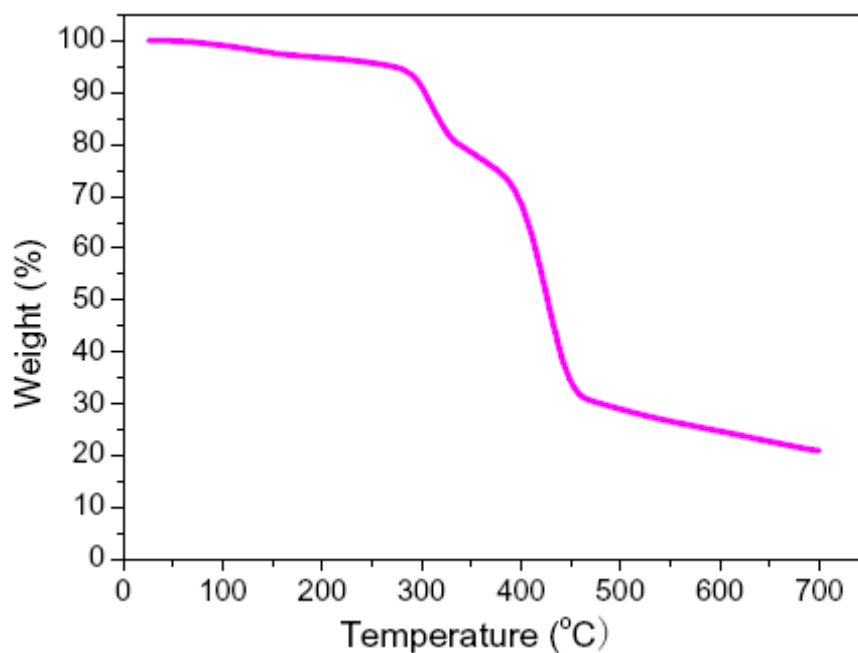


Figure S4. Thermal gravimetric analysis (TGA) for Compound **1**.

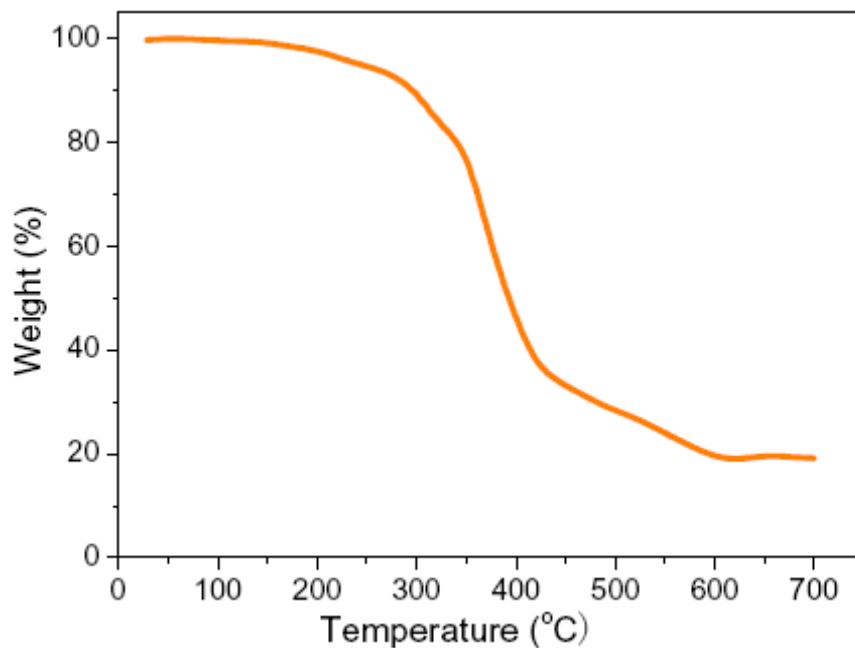


Figure S5. Thermal gravimetric analysis (TGA) for Compound 2.

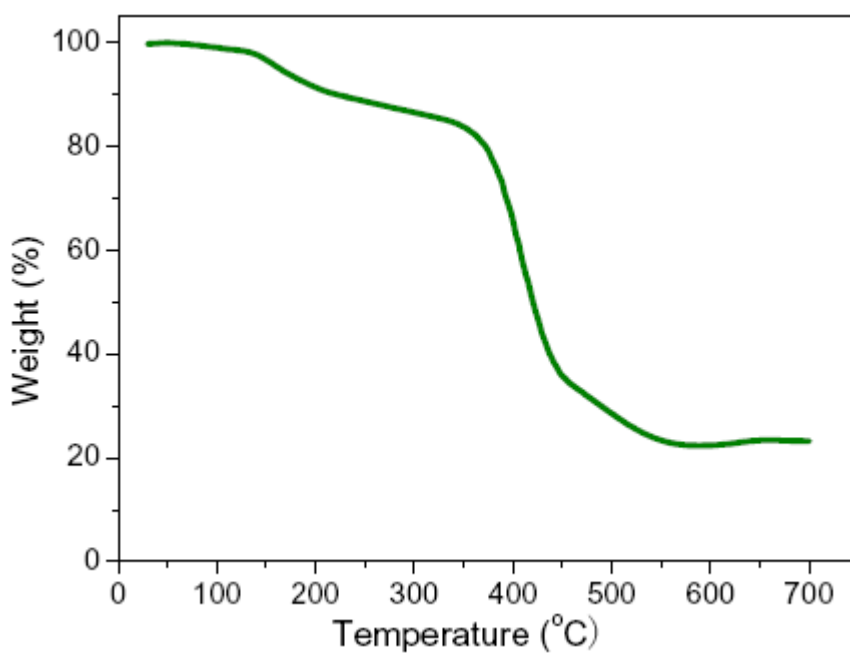


Figure S6. Thermal gravimetric analysis (TGA) for Compound 3.

4. Semilogarithmic emission decay plots of the free H₂DTDC ligand and compounds 1-3

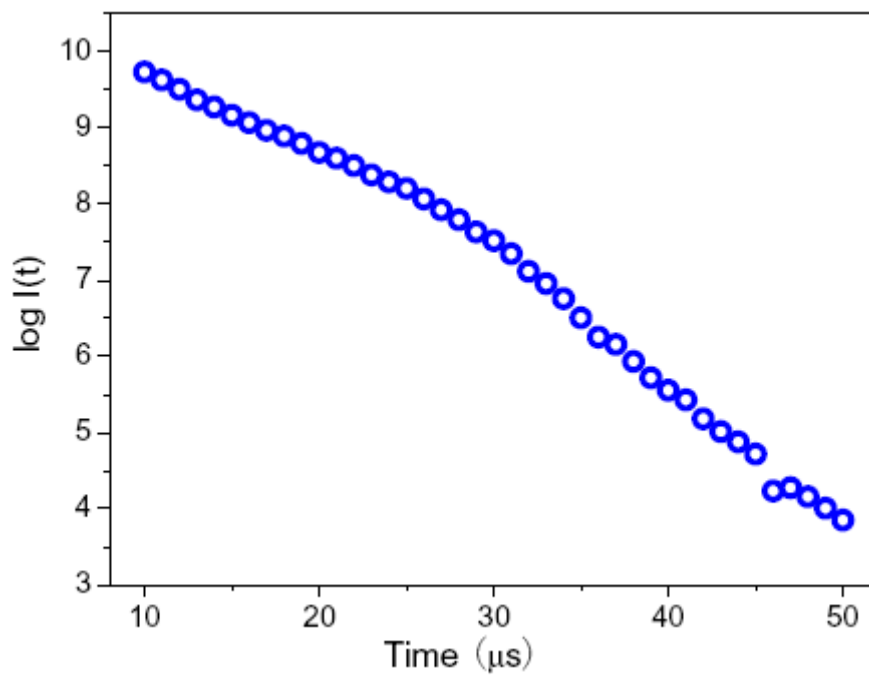


Figure S7. Semilogarithmic emission decay plots of the free H₂DTDC ligand.

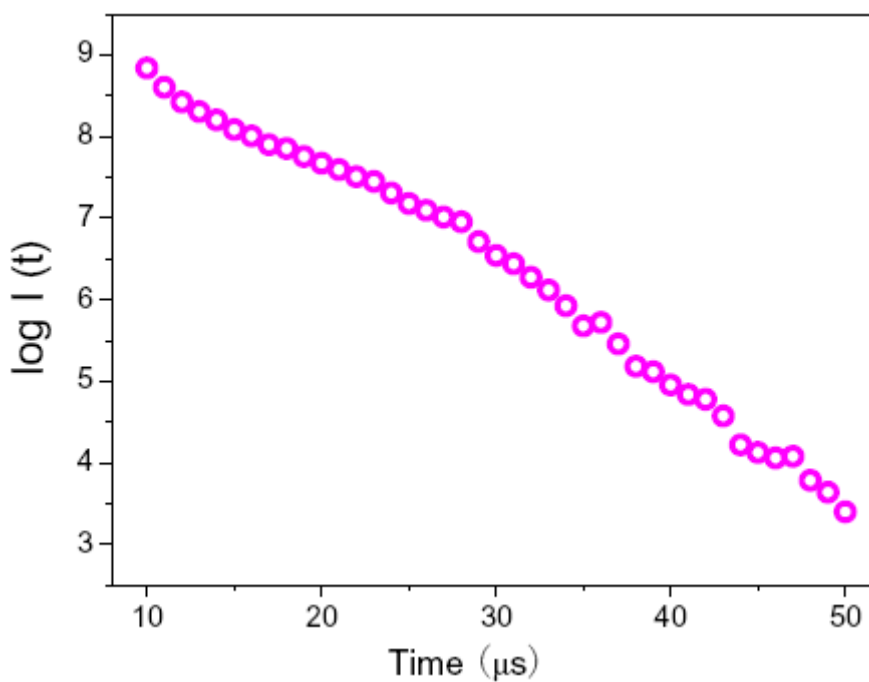


Figure S8. Semilogarithmic emission decay plots of compound 1.

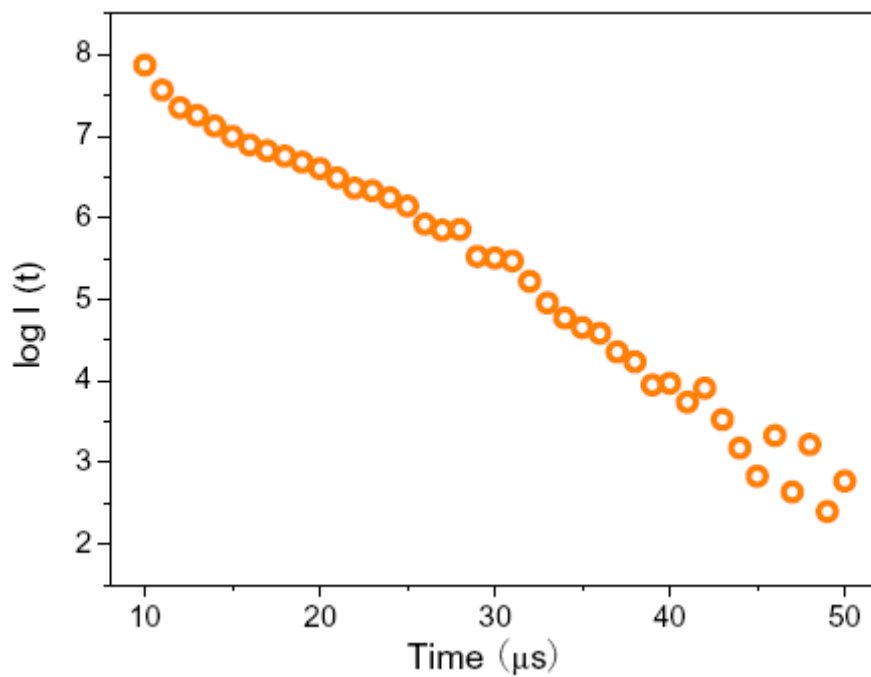


Figure S9. Semilogarithmic emission decay plots of compound 2.

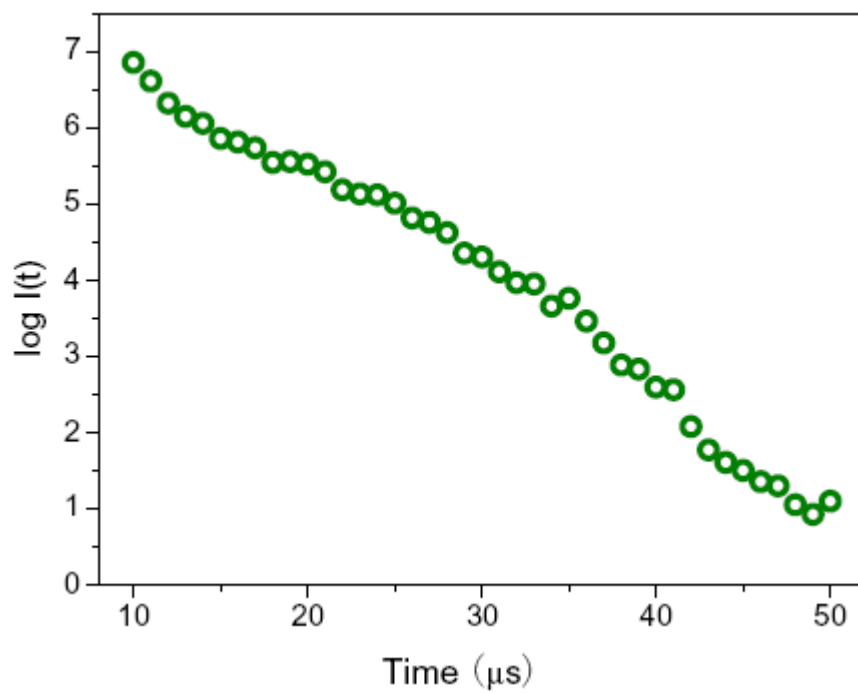


Figure S10. Semilogarithmic emission decay plots of compound 3.