

Supplementary Information

Table S1 Comparison of crystal parameters of compound **2** with the already reported compound

Crystal Parametres	2	CCDC 826011
Emprical formula	C ₄₂ H ₃₆ Mn ₃ N ₆ O ₃₀	C ₄₂ H ₃₆ Mn ₃ N ₆ O ₃₀
Formula weight	1269.59	1269.59
Temperature (K)	296(2)	293(2)
Crystal system	Trigonal	Trigonal
Space group	<i>P</i> $\bar{3}$	<i>P</i> $\bar{3}$
<i>a</i> /Å	14.6618(8)	14.6673(3)
<i>b</i> /Å	14.6618(8)	14.6673(3)
<i>c</i> /Å	6.3551(4)	6.36430(1)
α °	90	90
β °	90	90
γ °	120	120
Volume (Å ³)	1183.12(1)	1185.72(4)
Z	1	1
Calculated density (g/cm ³)	1.782	1.778
Absorption coefficient (mm ⁻¹)	0.901	0.899
F(000)	645	645
Crystal size (mm ³)	0.31×0.22×0.12	0.20×0.10×0.10
Index ranges	-16≤ <i>h</i> ≤16, -16≤ <i>k</i> ≤16, -7≤ <i>l</i> ≤7	-18≤ <i>h</i> ≤19, -19≤ <i>k</i> ≤19, -8≤ <i>l</i> ≤8
Reflections collected	28974	1808
Unique data(<i>R</i> _{int})	1249	1564
Refinement method	Full-matrix least-squares on F ²	Full-matrix least-squares on F ²
Data / restraints / parameters	1249/0/123	1808 / 2 / 135
Goodness-of-fit on F ²	1.055	1.046
Final R indices[<i>I</i> >2σ (<i>I</i>)] R1/ wR2	0.0227/0.0574	0.0330/0.0840

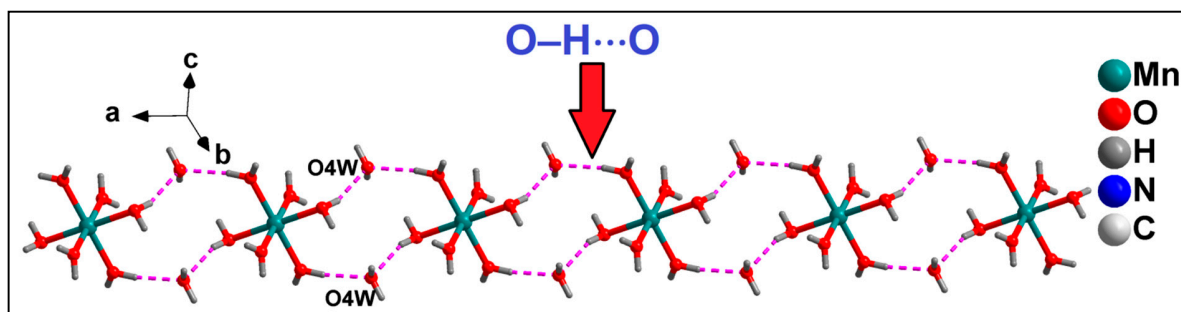


Figure S1 Supramolecular 1D Chain of compound **1** assisted by the lattice water molecule.

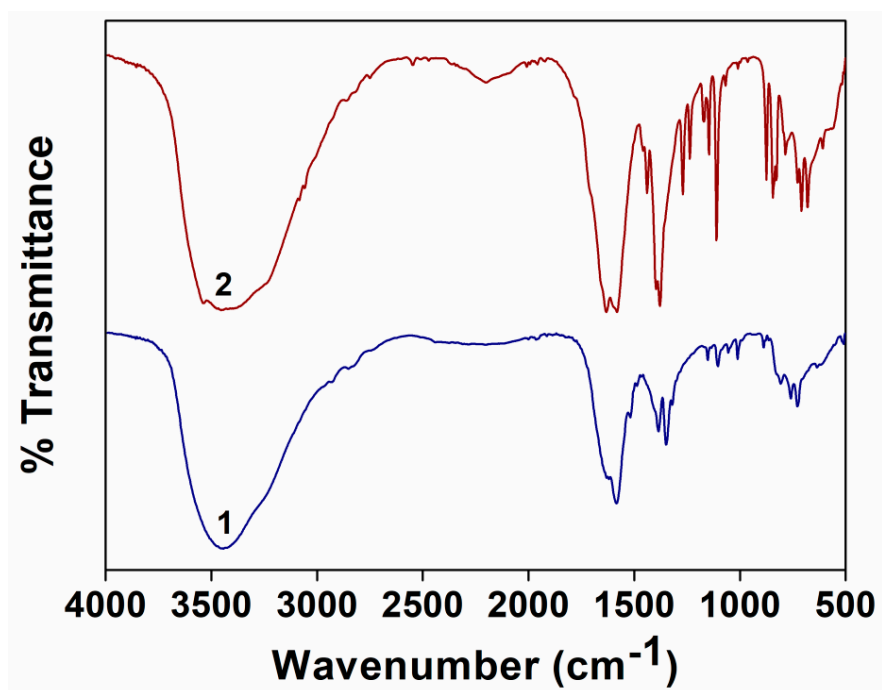


Figure S2 FT-IR spectra of the compounds **1** and **2**.

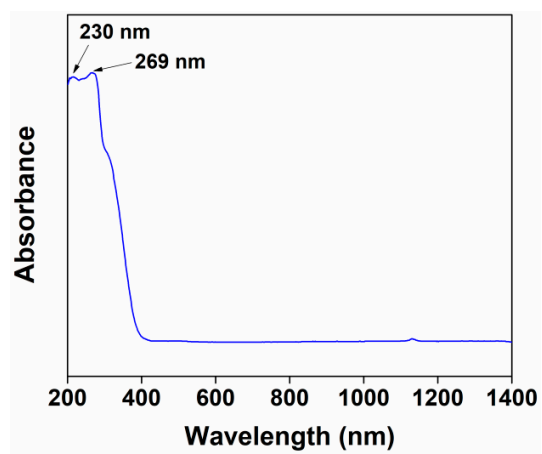
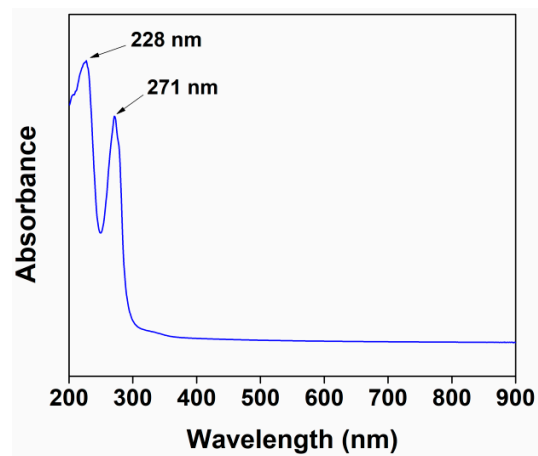


Figure S3(a) UV-Vis-NIR spectrum of **1**



(b) UV-Vis spectrum of **1**.

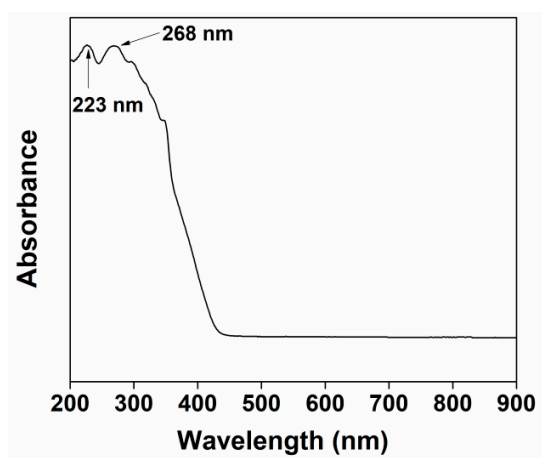
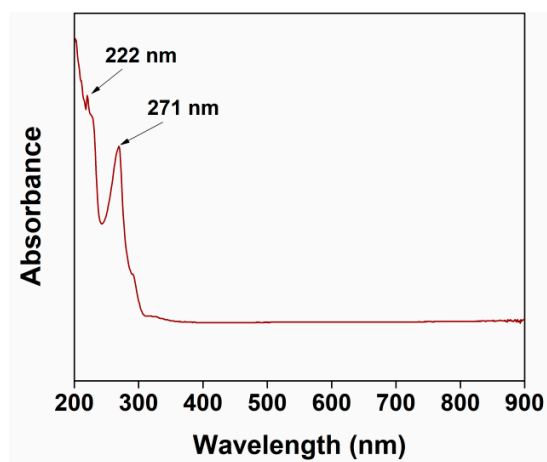


Figure S4(a) UV-Vis-NIR spectrum of **2**



(b) UV-Vis spectrum of **2**.

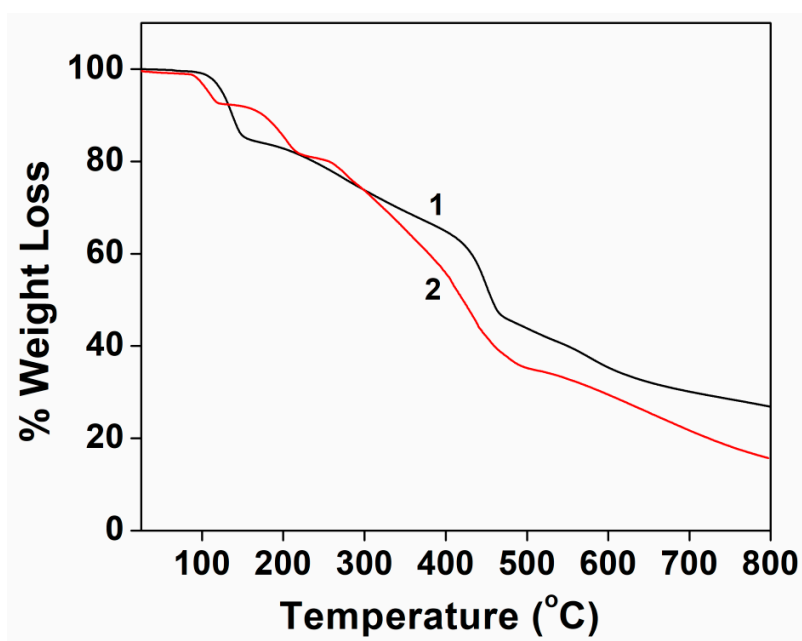


Figure S5 Thermogravimetric curves of the compounds **1** and **2**.