Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Synthesis, structure analysis and catalytic activity of two Ln-coordination polymers containing benzophenone-4,4´-dicarboxylate linker

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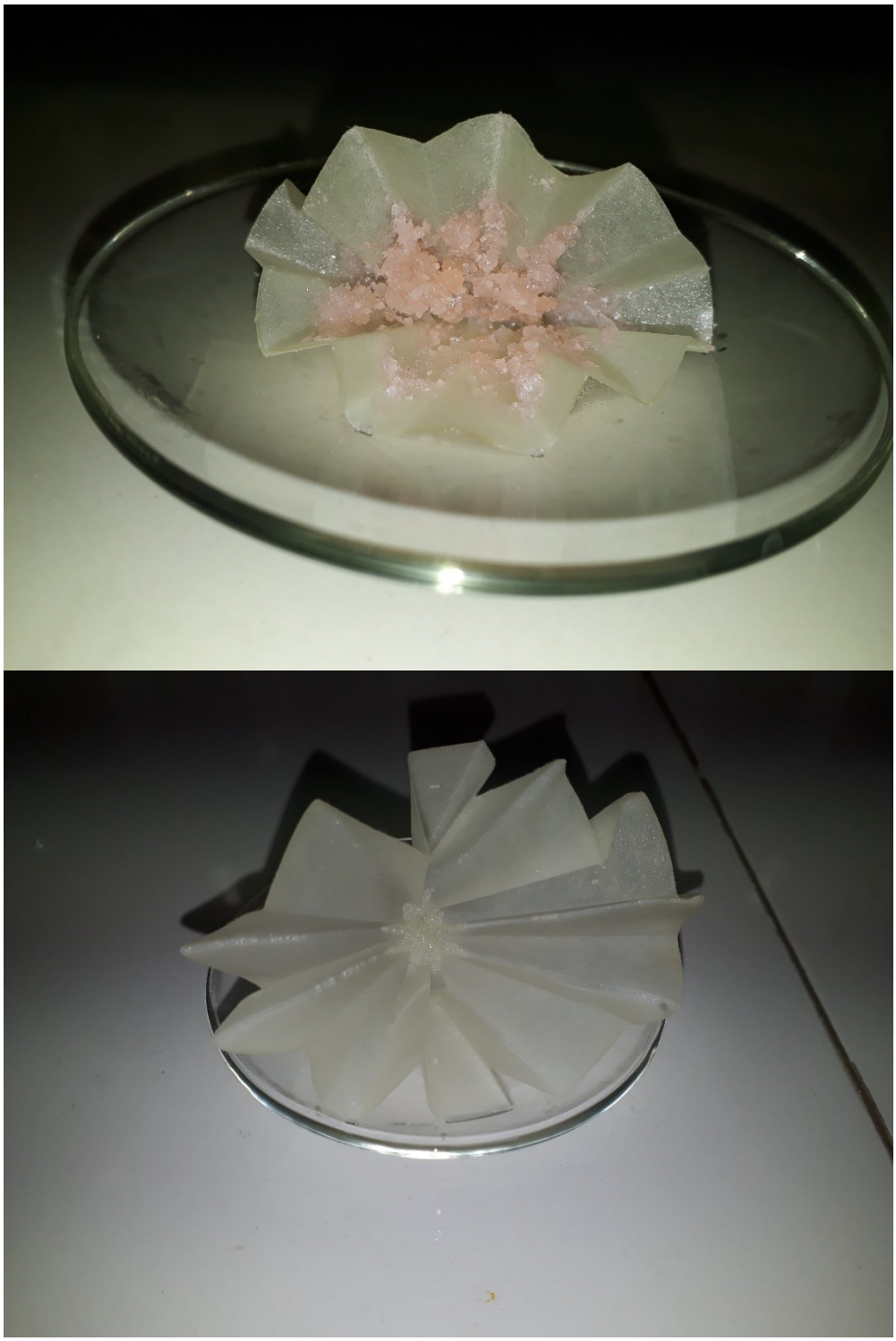
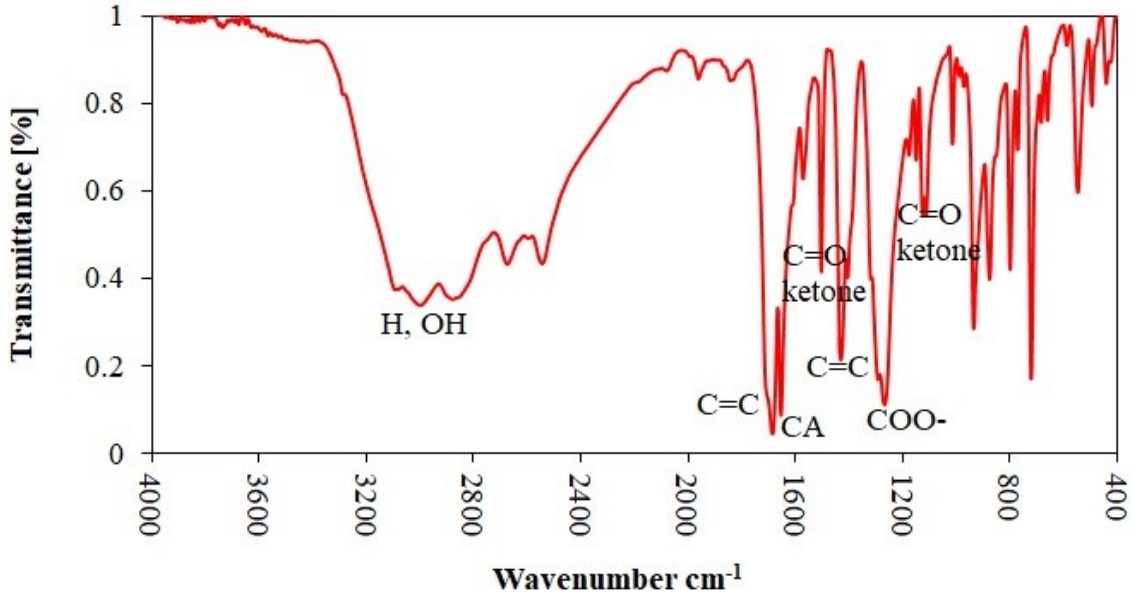
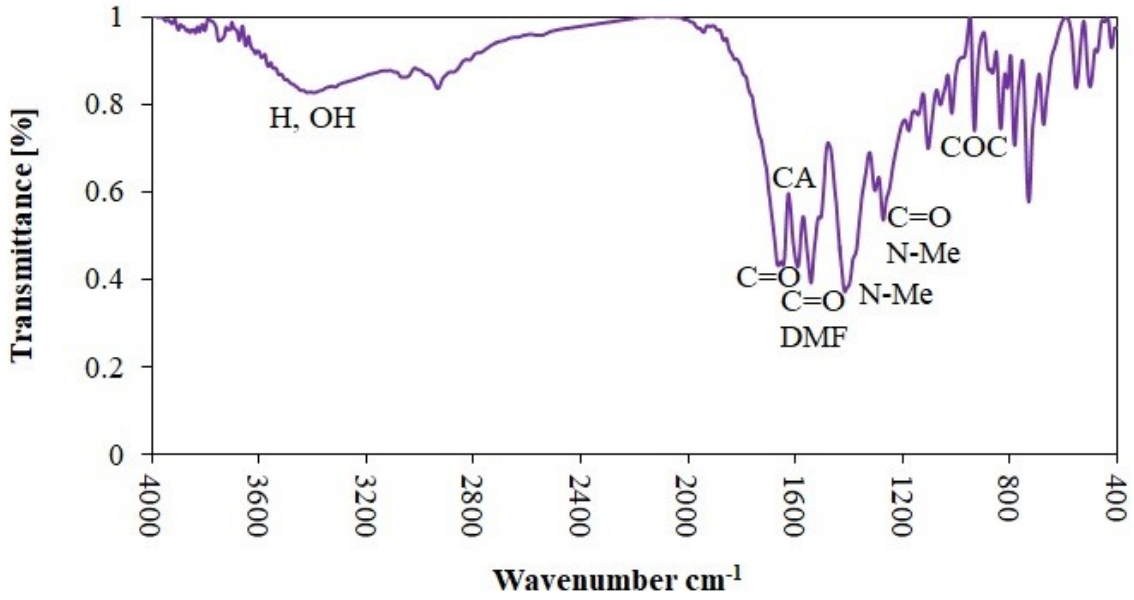


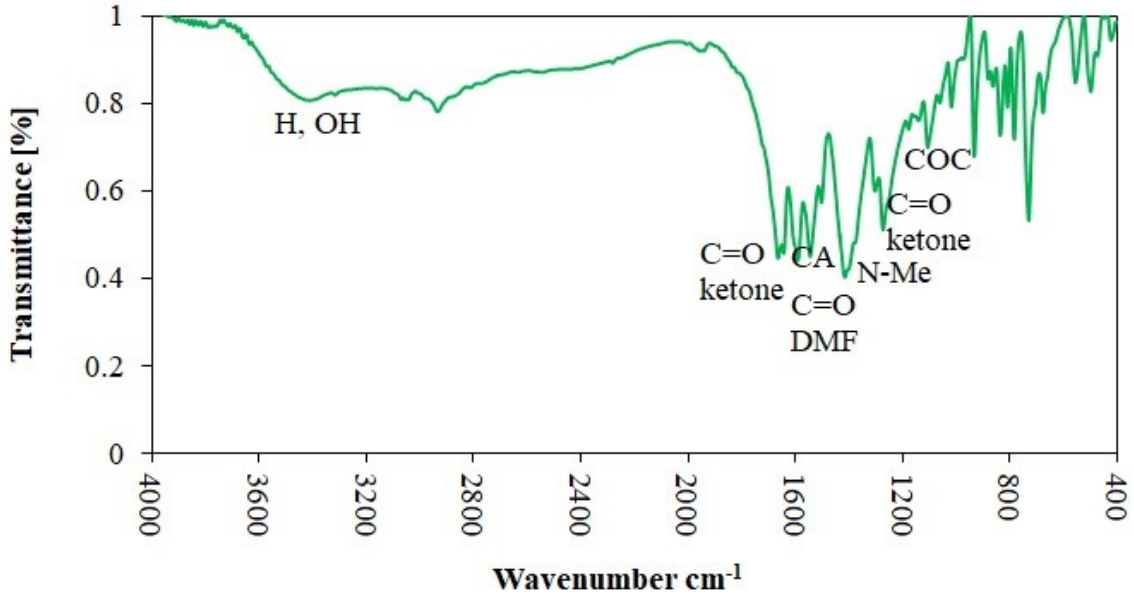
Figure S1. As-synthesized crystals of $[Er_2(bpndc)_3(DMF)_2]$ (top) and $[Yb_2(bpndc)_3(DMF)_2]$ (bottom)


Transmittance [%]
1
0.8
0.6
0.4
0.2
0
H, OH
C=C
CA
C=O
ketone
C=C
COO-
C=O
ketone
4000
3600
3200
2800
2400
2000
1600
1200
800
400
Wavenumber cm-1

(a)

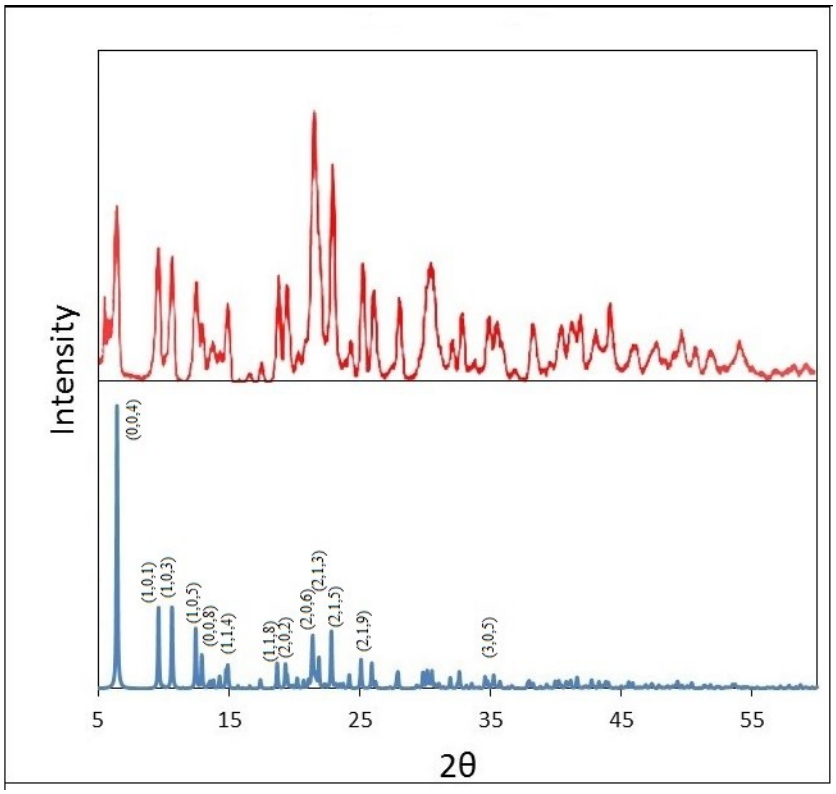

Transmittance [%]
1
0.8
0.6
0.4
0.2
0
H, OH
CA
C=O
C=O
DMF
N-Me
C=O
N-Me
COC
4000
3600
3200
2800
2400
2000
1600
1200
800
400
Wavenumber cm-1

(b)

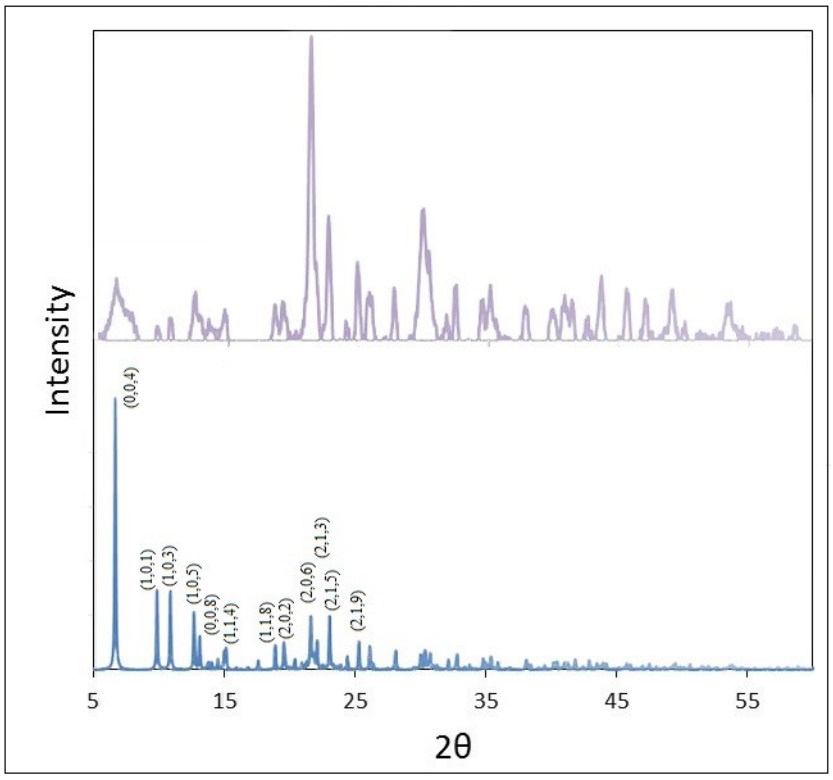


(c)

Figure S2. FT-IR spectra of Benzophenone-4,4′-dicarboxylic acid (a) $[Er_2(bpndc)_3(DMF)_2]$ (b) and $[Yb_2(bpndc)_3(DMF)_2]$ (c)



(a)



(b)

Figure S3. Powder X-ray Diffraction of $[Er_2(bpndc)_3(DMF)_2]$ (a) and $[Yb_2(bpndc)_3(DMF)_2]$ (b) simulated (bottom), as synthesized (top) by solvothermal method.

Hkl	Multiplicity	dhkl	Distance	Total facet area	% Total facet area
{0 0 4}	2	13.66625000	7.31729626	722.69832423	36.74104347
{1 0 1}	8	9.17066195	10.90433827	934.37697279	47.50251083
{1 0 2}	8	8.80642509	11.35534555	303.48731526	15.42890065

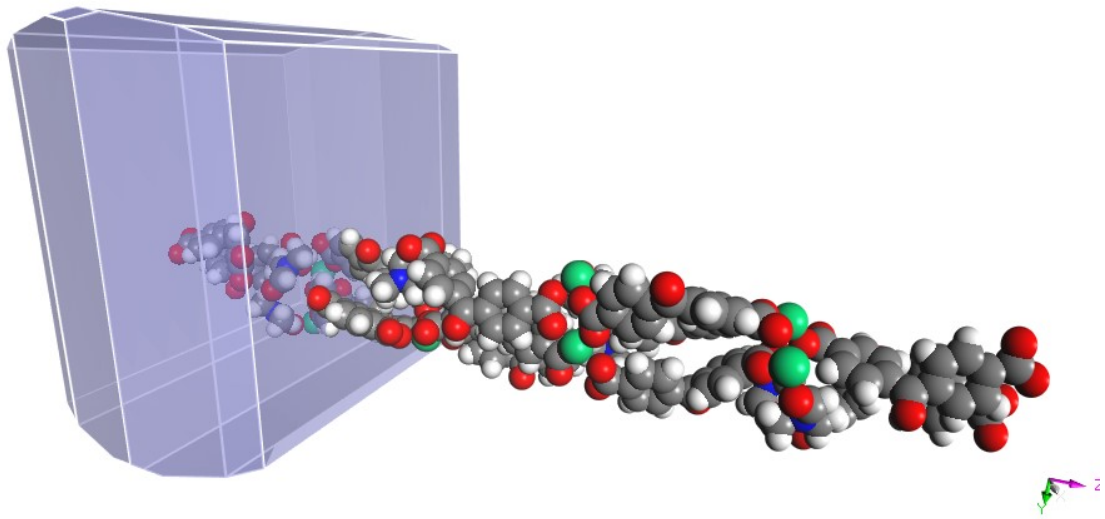
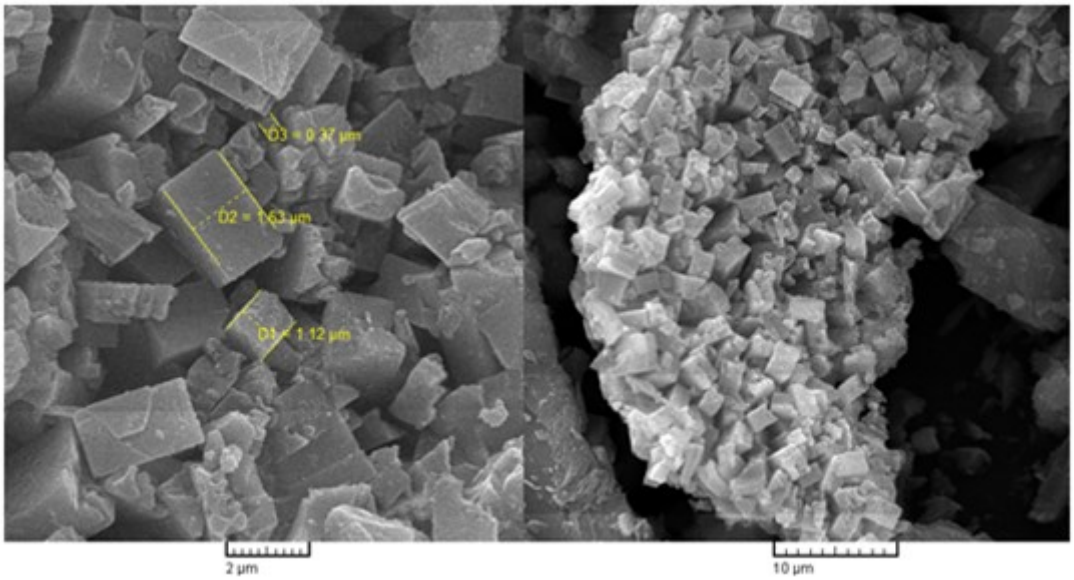
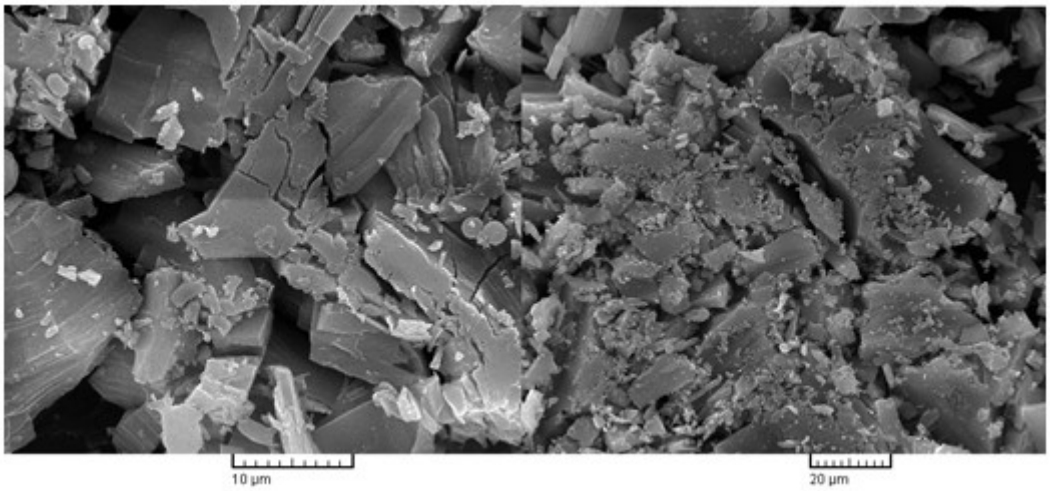


Figure S4. Face lists generated according to the BFDH and The predicted morphology of corresponding compounds **1** and **2**

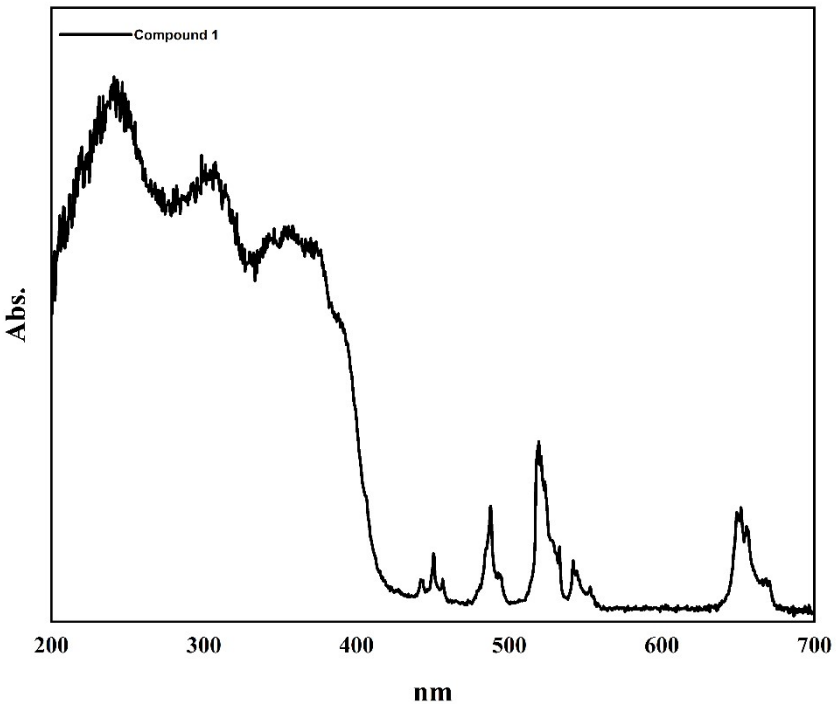


(a)

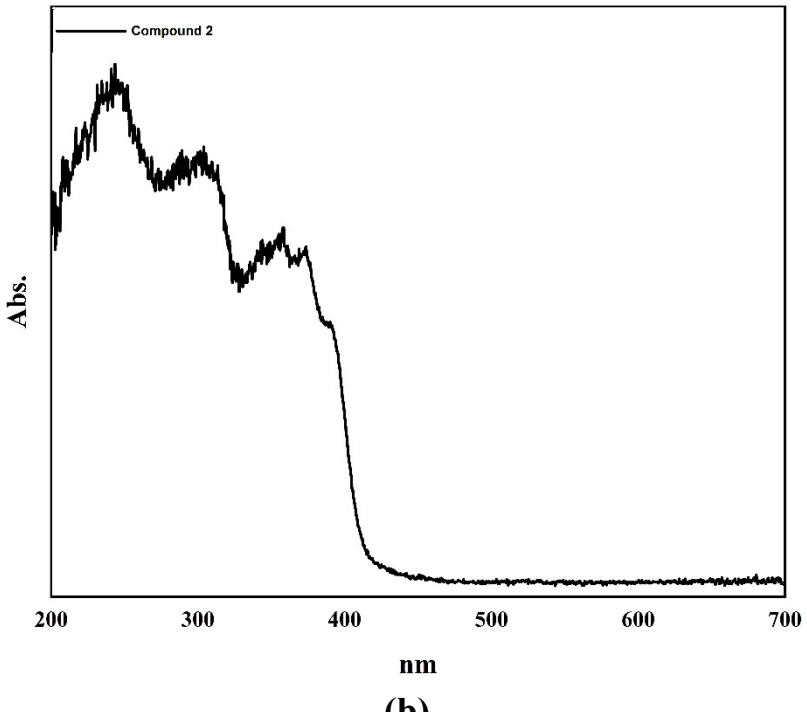


(b)

Figure S5. FE-SEM images of $[Er_2(bpndc)_3(DMF)_2]$ (a) and $[Yb_2(bpndc)_3(DMF)_2]$ (b) at two different magnifications with different locations



(a)



(b)

Figure S6. excitation wavelength of compounds **1** (a) and **2** (b) in the solid state at room temperature.

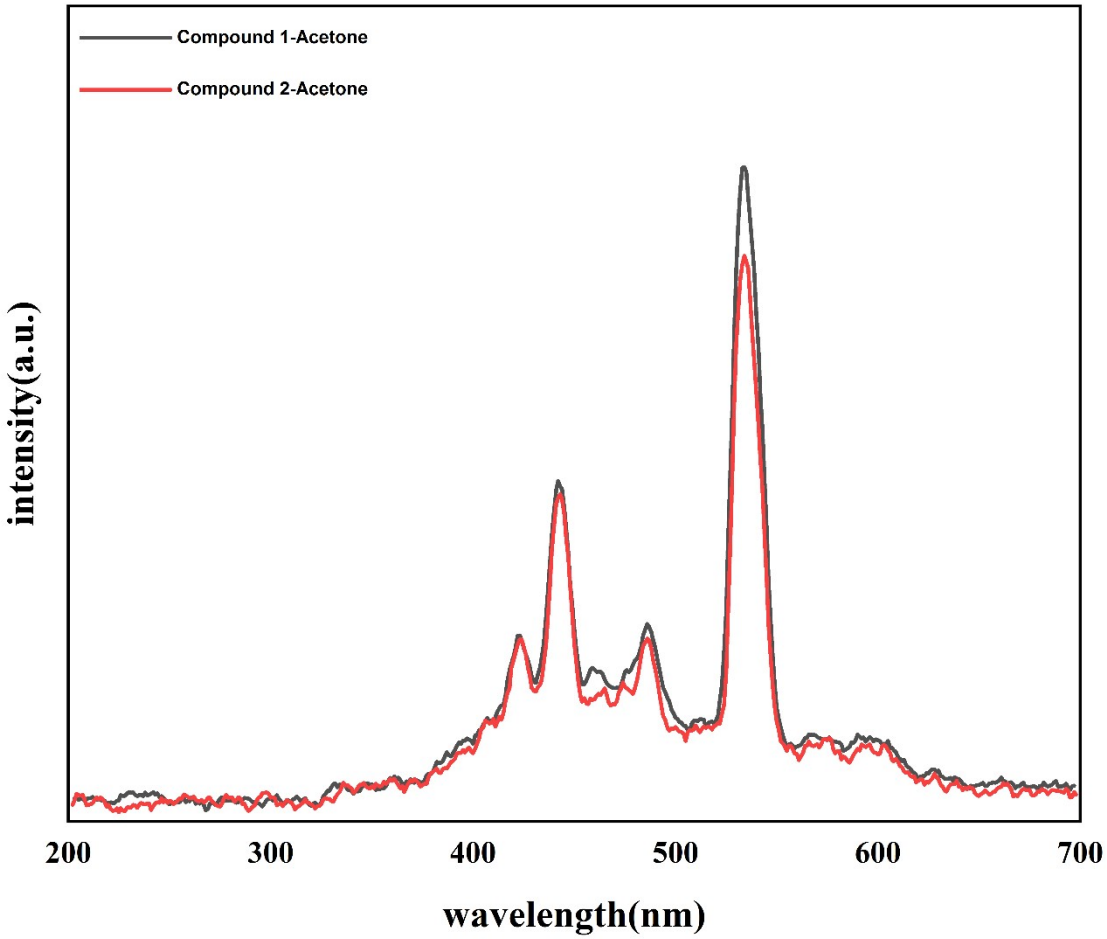
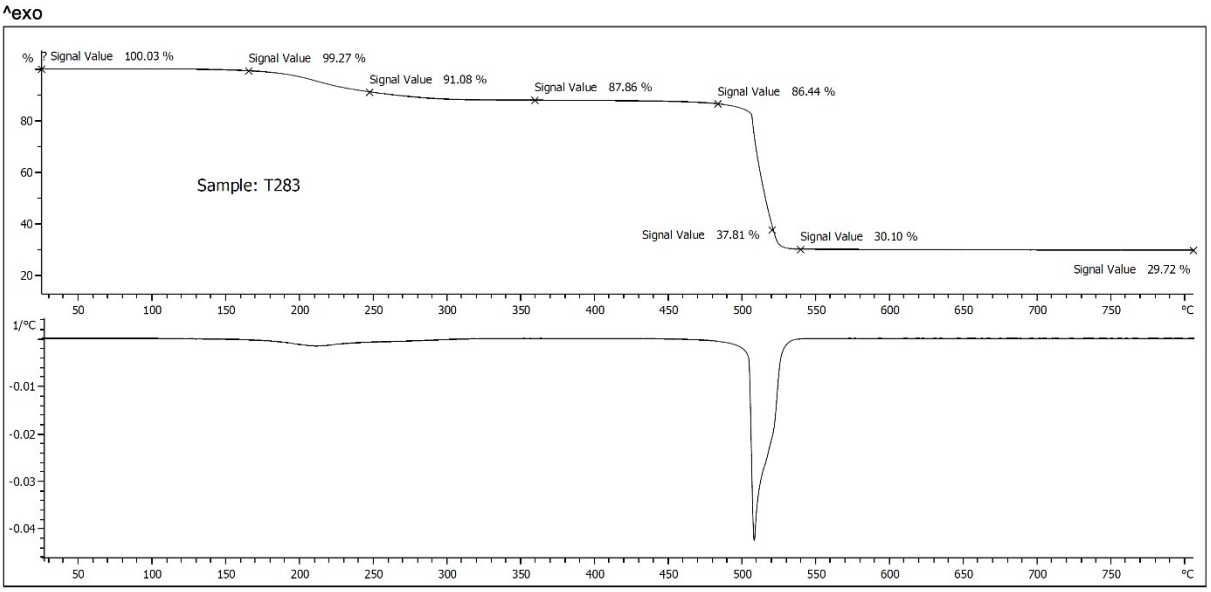
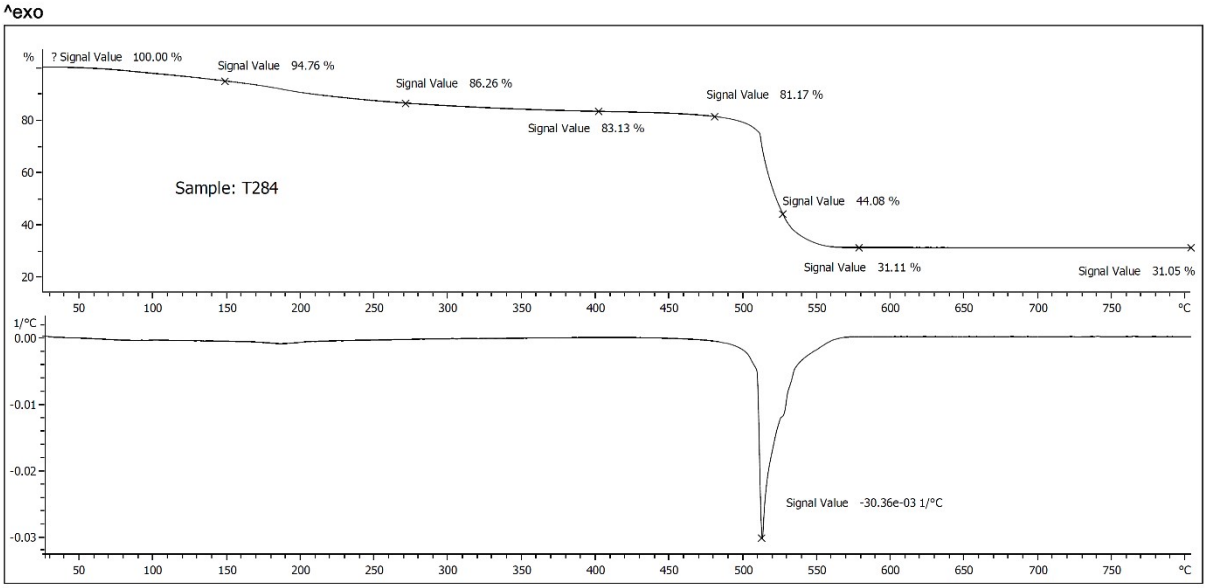


Figure S7. The emission spectrum of 4 mg compounds **1** and **2** dispersed in 5 ml of acetone at room temperature

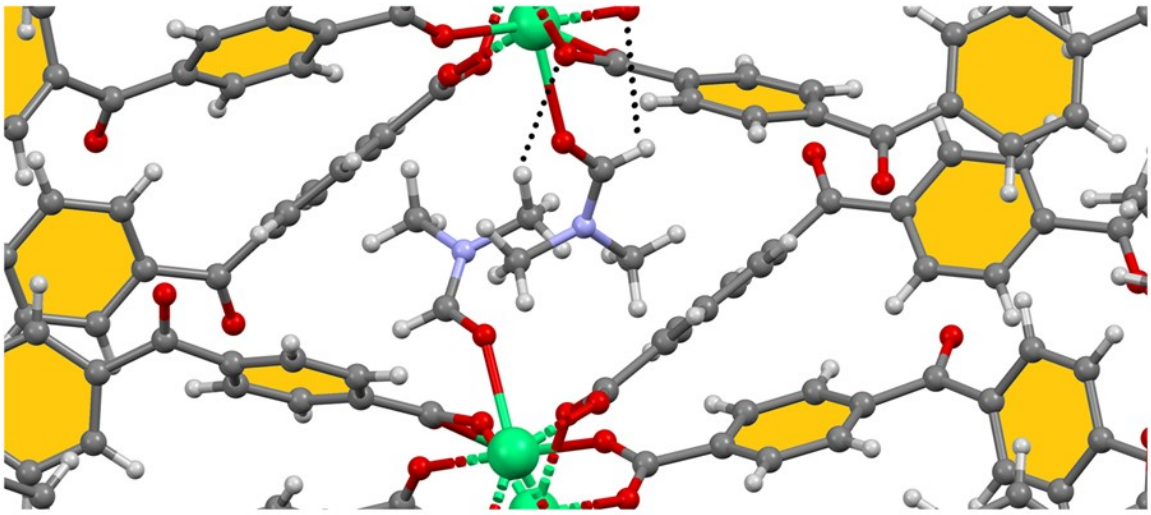


(a)

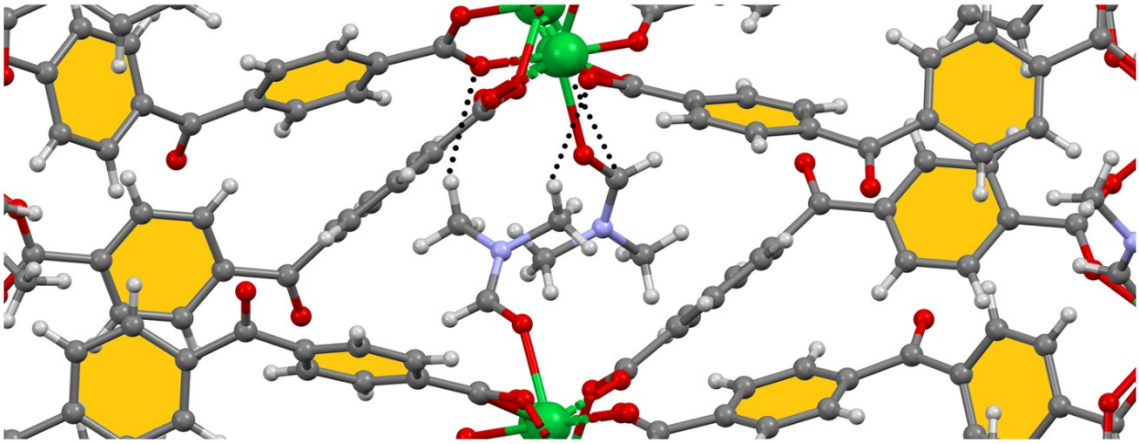


(b)

Figure S8. Thermogravimetric analyses of $[Er_2(bpndc)_3(DMF)_2]$ (a) and $[Yb_2(bpndc)_3(DMF)_2]$ (b)



(a)



(b)

Figure S9. Hydrogen bonding interactions between the coordinated DMF solvent molecules and the carboxylate oxygen atoms in the crystal structure of compounds **1** and **2**

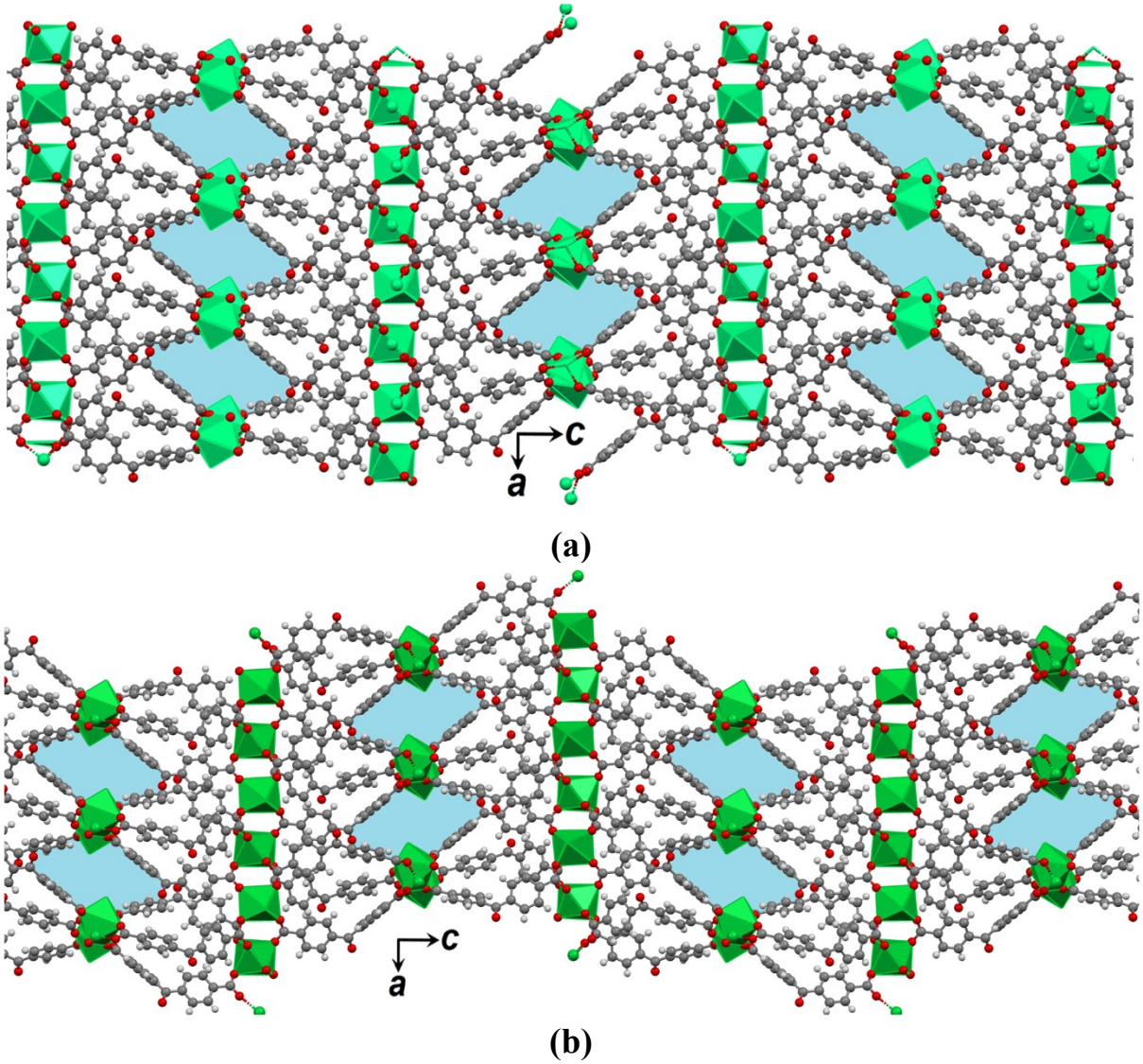
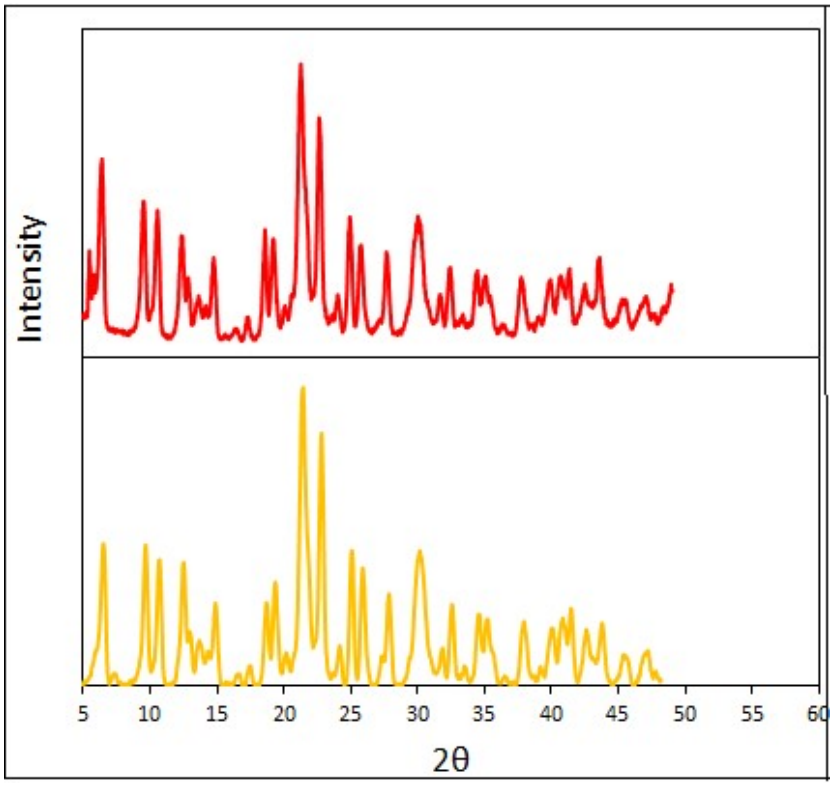
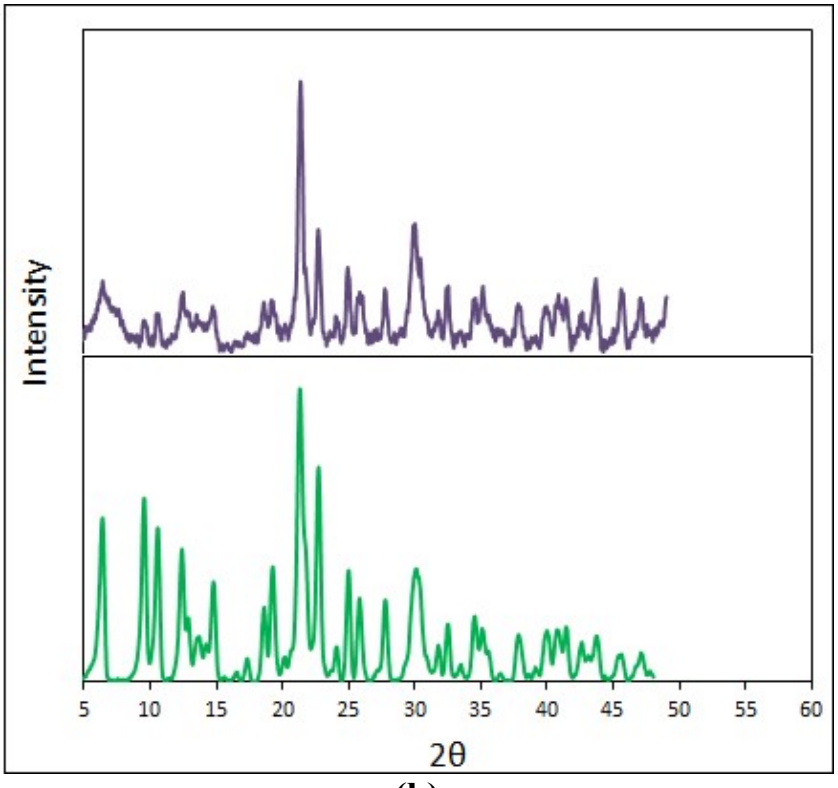


Figure S10. The 3D coordination polymer chains of **1** and **2** pack closely to build a dense crystal structure without any free solvent molecules between them and contain no void spaces. These frameworks would have unsaturated lanthanide centers and possess narrow pore channels running along the *a*- and *b*-axis without coordinated DMF molecules.

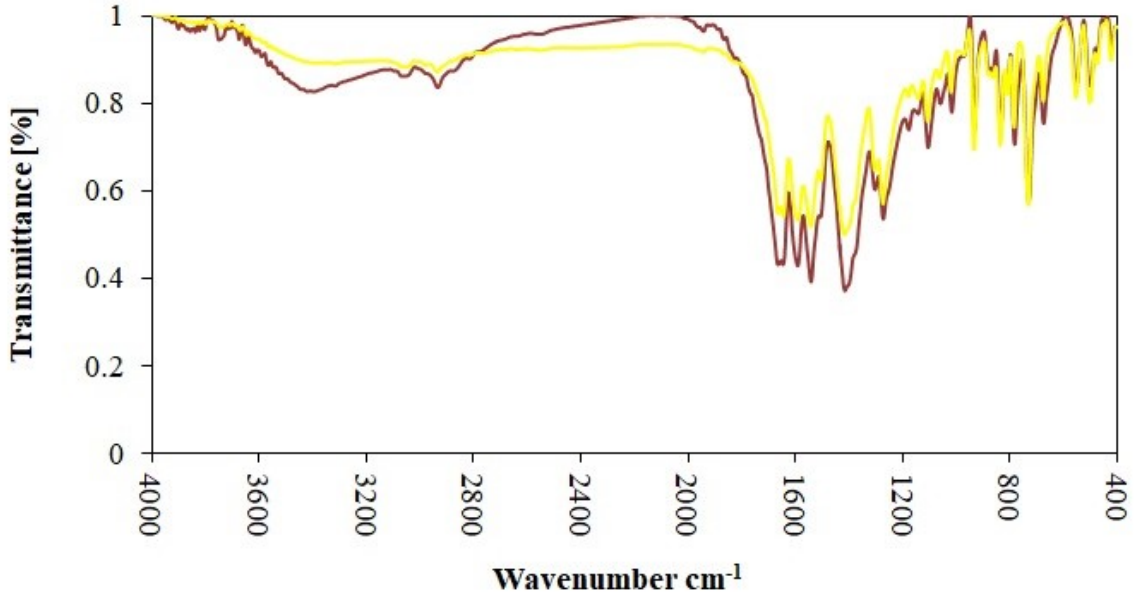


(a)

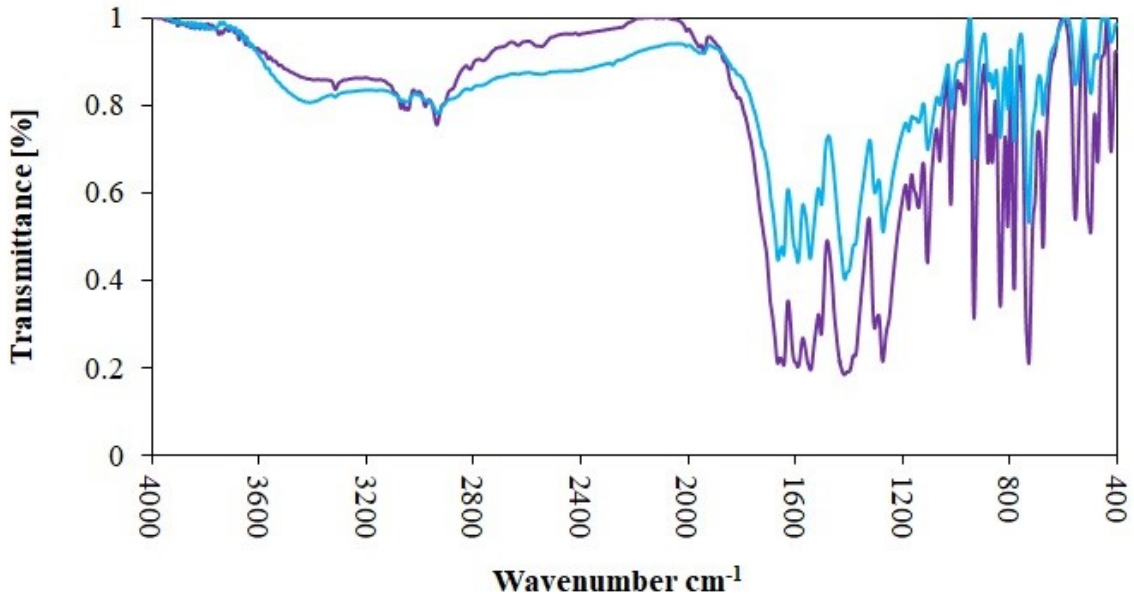


(b)

Figure S11. Powder X-ray Diffraction of $[Er_2(bpndc)_3(DMF)_2]$ (a) and $[Yb_2(bpndc)_3(DMF)_2]$ (b) as-synthesized (top), and after being dispersed in acetone for 10 h (bottom)

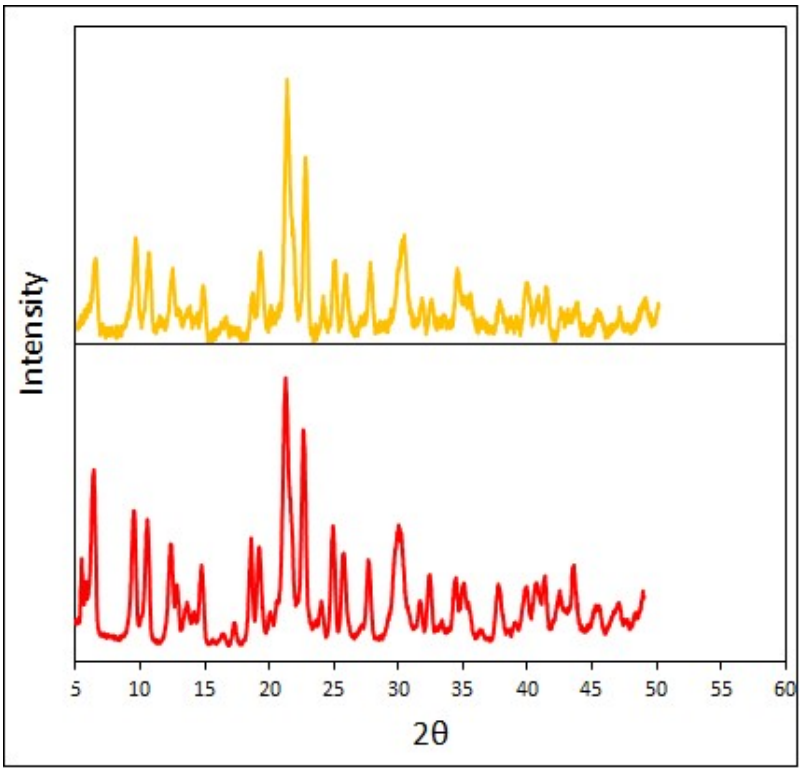


(a)

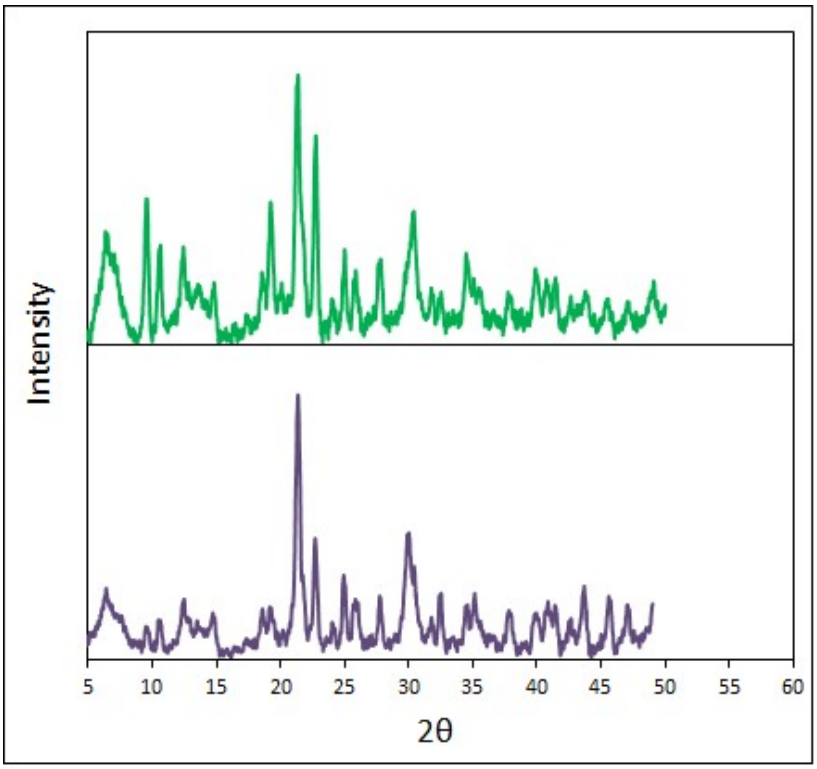


(b)

Figure S12. FT-IR spectra of $[Er_2(bpndc)_3(DMF)_2]$ (brown:as-synthesized; yellow: after being dispersed in acetone for 10 h) (a) and $[Yb_2(bpndc)_3(DMF)_2]$ (purple:as-synthesized; blue: after being dispersed in acetone for 10 h) (b)



(a)



(b)

Figure S13. Powder X-ray Diffraction of $[Er_2(bpndc)_3(DMF)_2]$ (a) and $[Yb_2(bpndc)_3(DMF)_2]$ (b) as-synthesized (top), and after the catalytic activity in the acetalization of glycerol (bottom)