Metal Organic Framework Assembled from Y(III), Li(I), and Terephthalate: Hydrothermal Synthesis, Crystal Structure, Thermal Decomposition and Topological Studies

Mohammed S. M. Abdelbaky,[1] Zakariae Amghouz,[1,2*] Santiago García-Granda,[1] José R. García[1]

[1]*Departamentos de Química Física y Analítica y Química Orgánica e Inorgánica, and*
[2]*Servicios Científico-Técnicos, Universidad de Oviedo-CINN, 33006 Oviedo, Spain*

Electronic Supporting Information

Table S1. Summary of trials carried out for the optimization of hydrothermal synthesis of **1**

H_2BDC (mmol)	**$YCl_3 \cdot 6H_2O$** (mmol)	**$LiOH \cdot H_2O$** (mmol)	**H_2Tart** (mmol)	**H_2O:Et*** **(mL)**	**Observation**
0.5	1	3.5	-	10:0	Single crystals of BDC ligand and/or microcrystalline powder of YBDC[¥] phase
0.5	1	3.5	-	5:5	Microcrystalline powder of YBDC phase
0.5	1	3.5	0.5	5:5	Microcrystalline powder of YBDC phase
0.5	1	3.5	1	5:5	Single phase (microcrystalline powder + single crystals) of compound **1**
0.5	1	3.5	1.5	5:5	Microcrystalline powder of YBDC phase

*Et = Ethanol

[¥] YBDC: Weng. D.; Zheng, X.; Jin, L . *Eur. J. Inorg. Chem.* **2006**, 20, 4184.

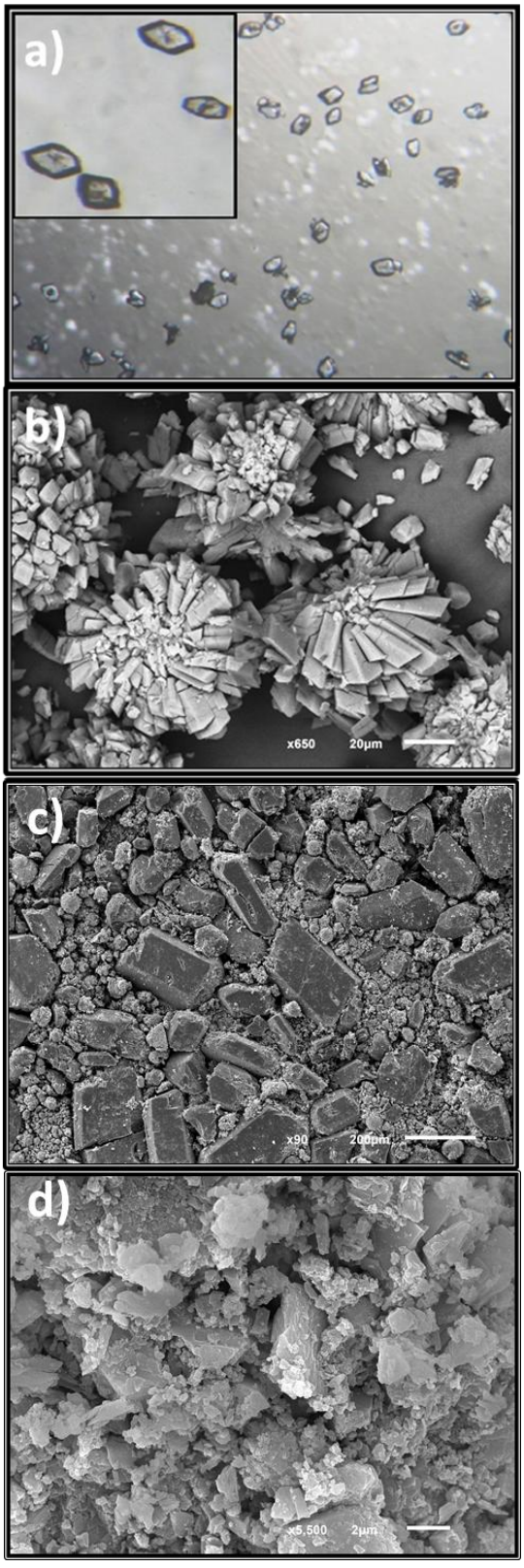

Figure S1. Optical microscopic images of single crystals (a) and SEM images of microcrystalline powder (b,c,d)

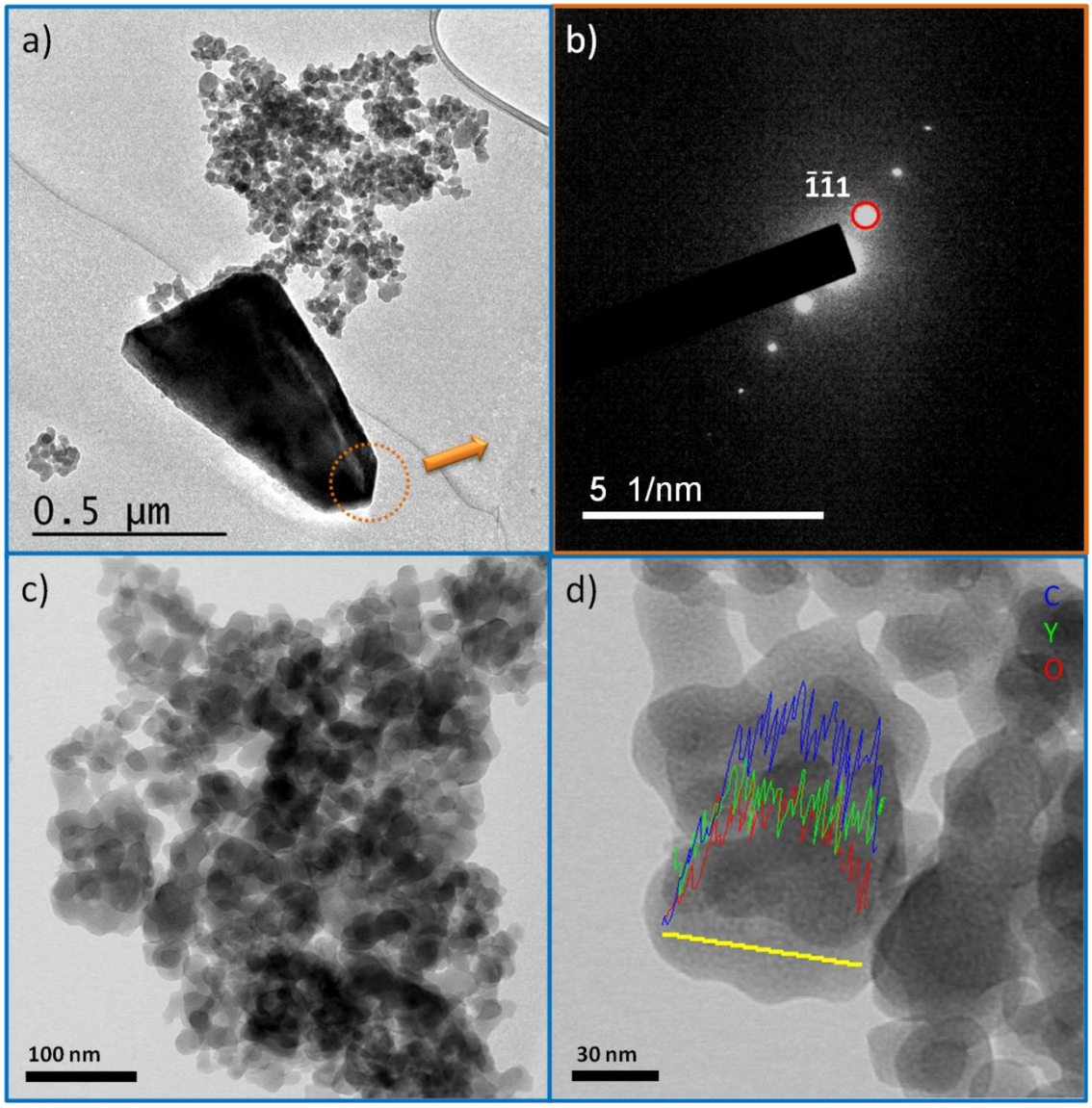

Figure S2. TEM image (a), SAED pattern (b), and BF-STEM image (c). BF-STEM EDX line scans (yellow line) along one particle (d).

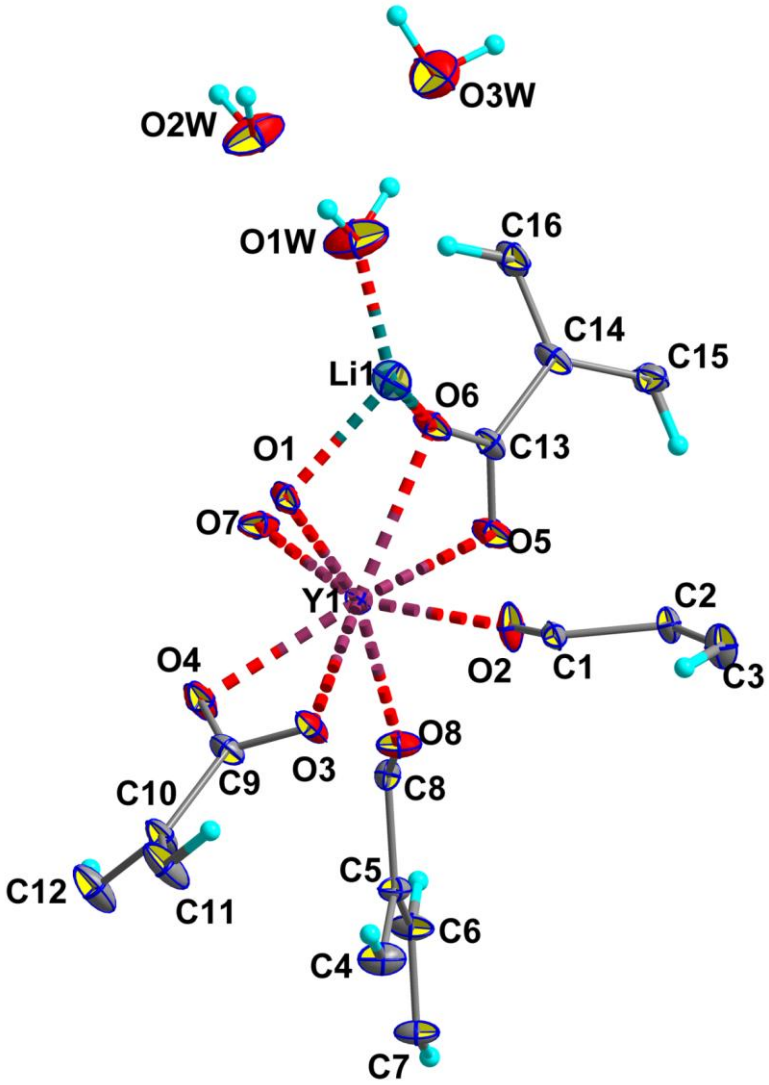

Figure S3. Asymmetric unit

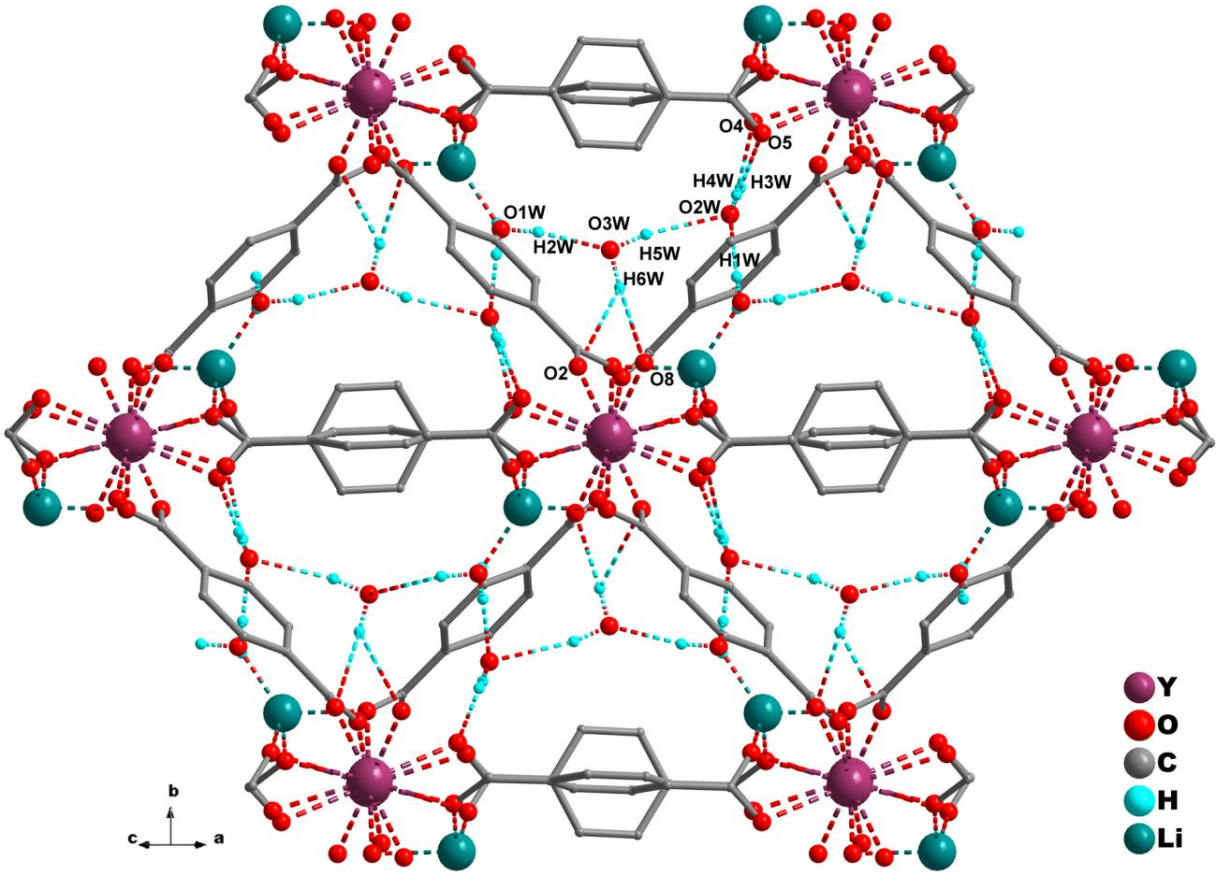

Figure S4. View of hydrogen bonds along [101]

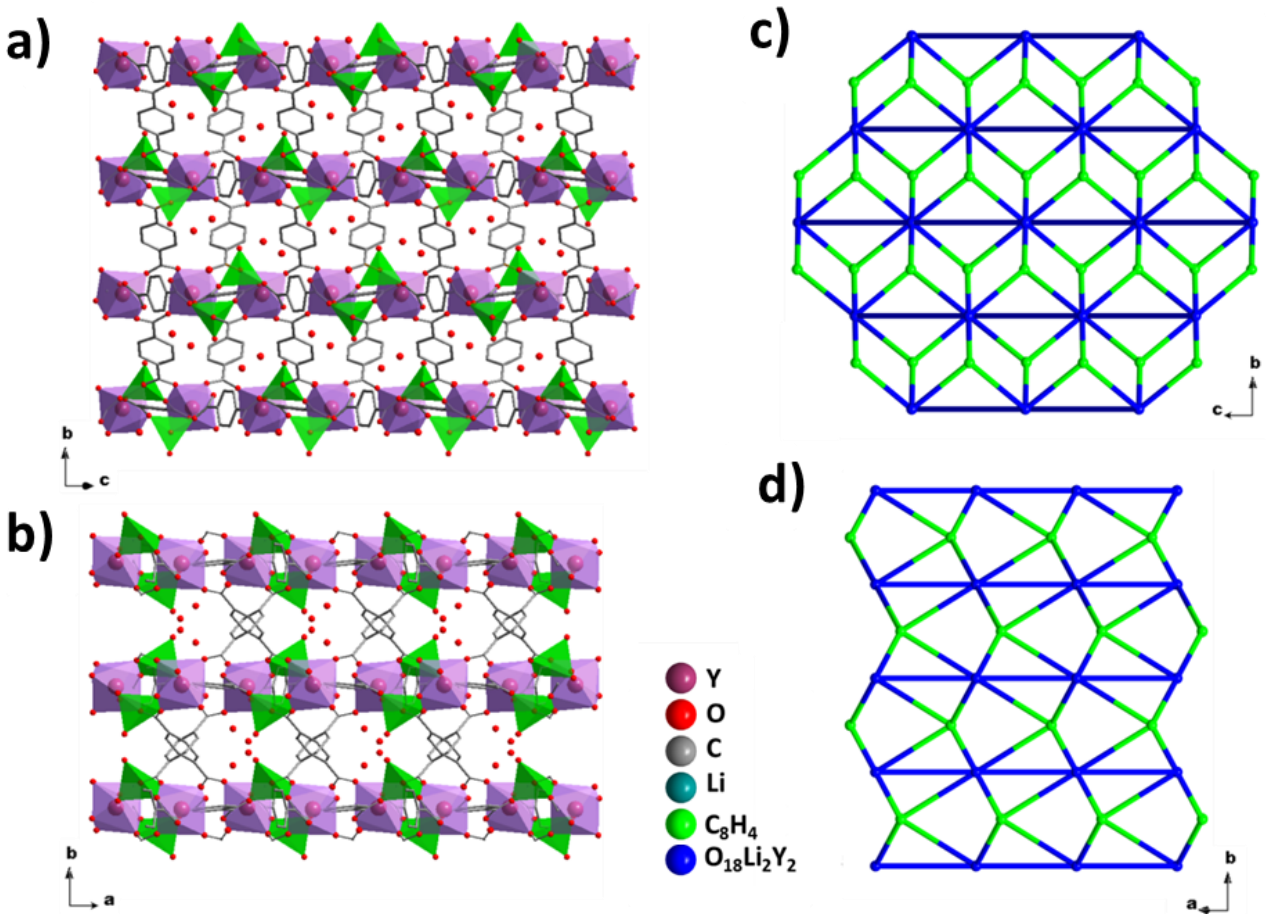

Figure S5. Projection of the structure along the *a*-axis and the *c*-axis (a,b) with the corresponding topological representations (c,d)

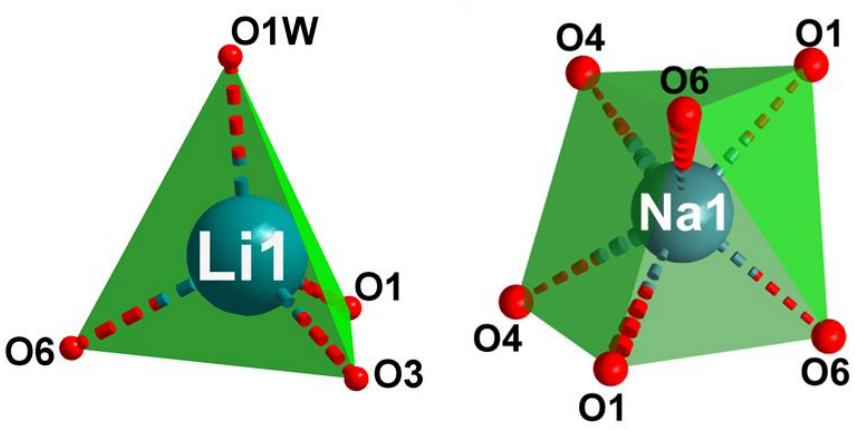

Figure S6.Comparison of Li^+ and Na^+ coordination environment in compound $[LiY(BDC)_2(H_2O)\cdot 2(H_2O)]$ (**1**) and the previously reported $[NaY(Tart)(BDC)(H_2O)_2]$[50].

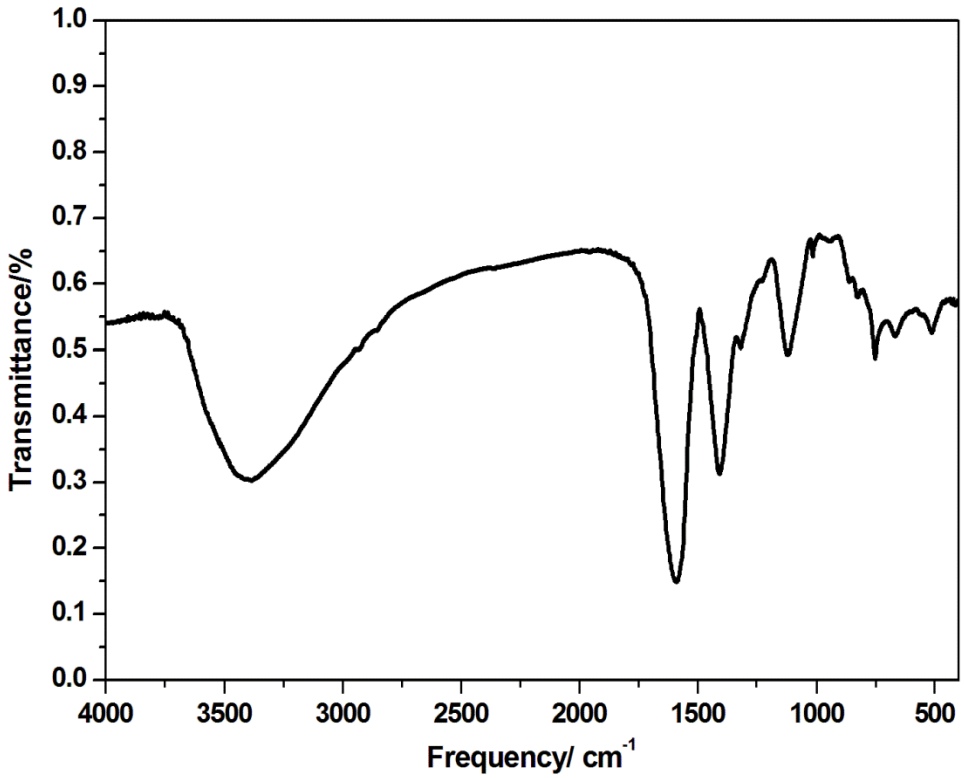

Figure S7. Infrared spectra

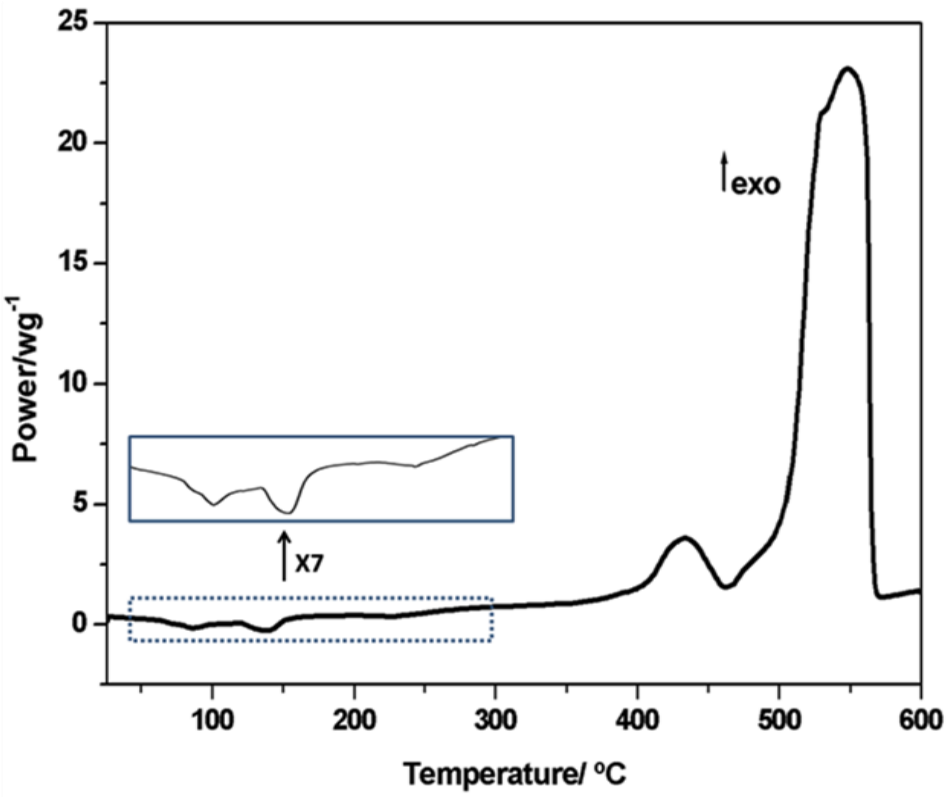

Figure S8. DSC curve

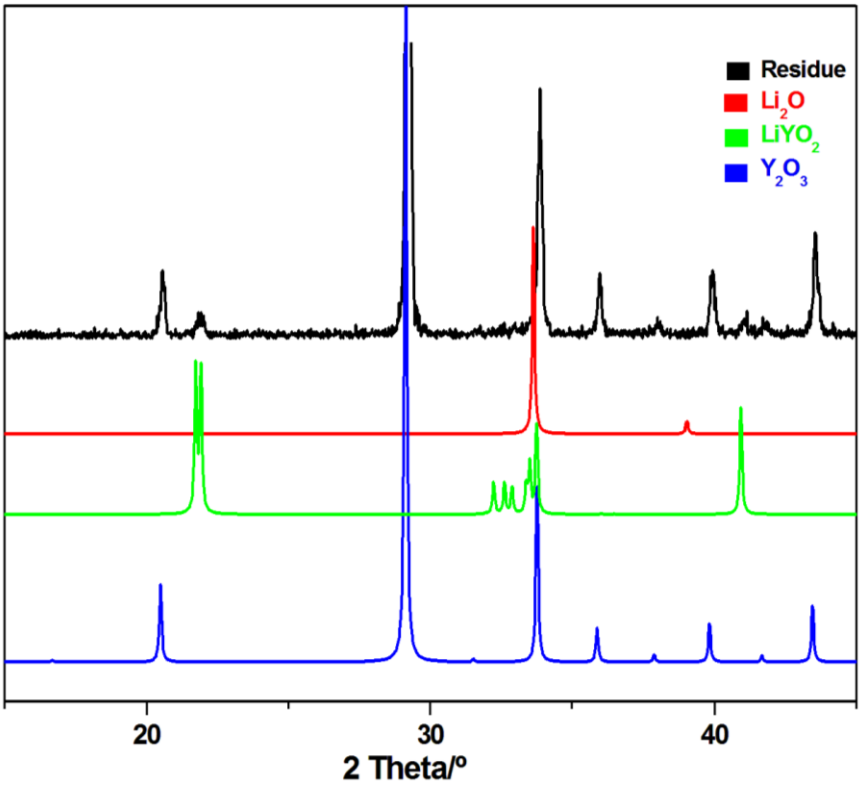

Figure S9. A typical PXRD pattern of thermal decomposition residue compared with the theoretical ones.