

## SUPPORTING INFORMATION

### Metal-Organic Framework vs. Coordination Polymer—Influence of the Lanthanide on the Nature of the Heteroleptic Anilate/Terephthalate 3D Network

**Mariangela Oggianu<sup>1,2</sup>, Fabio Manna<sup>1,3</sup>, Suchithra Ashoka Sahadevan<sup>1,3</sup>, Narcis Avarvari<sup>3</sup>, Alexandre Abhervé<sup>3,\*</sup> and Maria Laura Mercuri<sup>1,2,\*</sup>**

<sup>1</sup> Dipartimento di Scienze Chimiche e Geologiche, Università degli Studi di Cagliari, I-09042 Monserrato, Cagliari, Italy; mari.oggianu@gmail.com (M.O.); fmanna@etud.univ-angers.fr (F.M.); suchithraiiserk@gmail.com (S.A.S.)

<sup>2</sup> INSTM, Cagliari Unit, Via Giuseppe Giusti, 9, 50121 Firenze, Italy

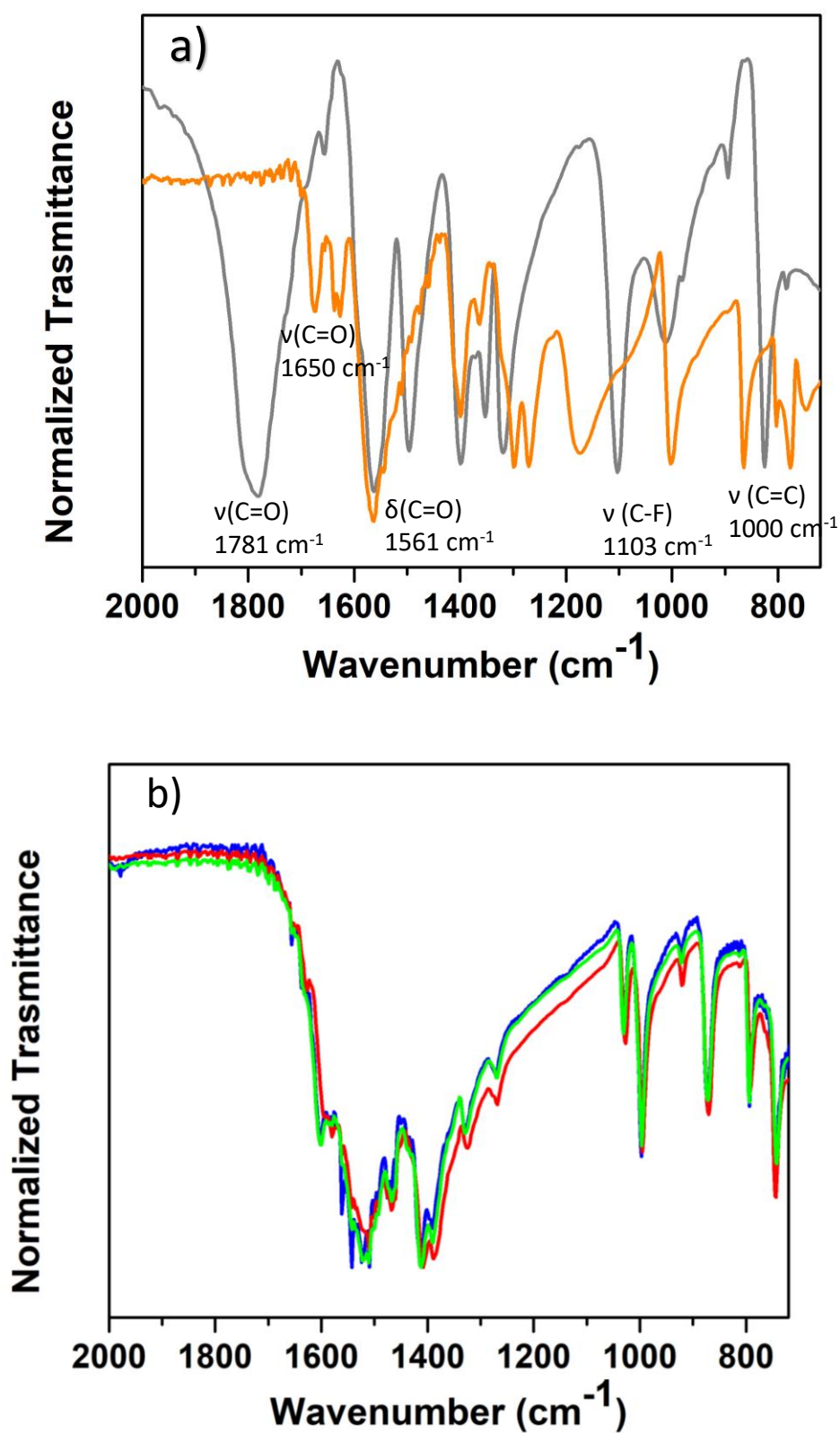
<sup>3</sup> Univ Angers, CNRS, MOLTECH-Anjou, SFR MATRIX, F-49000 Angers, France; narcis.avarvari@univ-angers.fr

\* Correspondence: alexandre.abherve@univ-angers.fr (A.A.); mercuri@unica.it (M.L.M.)

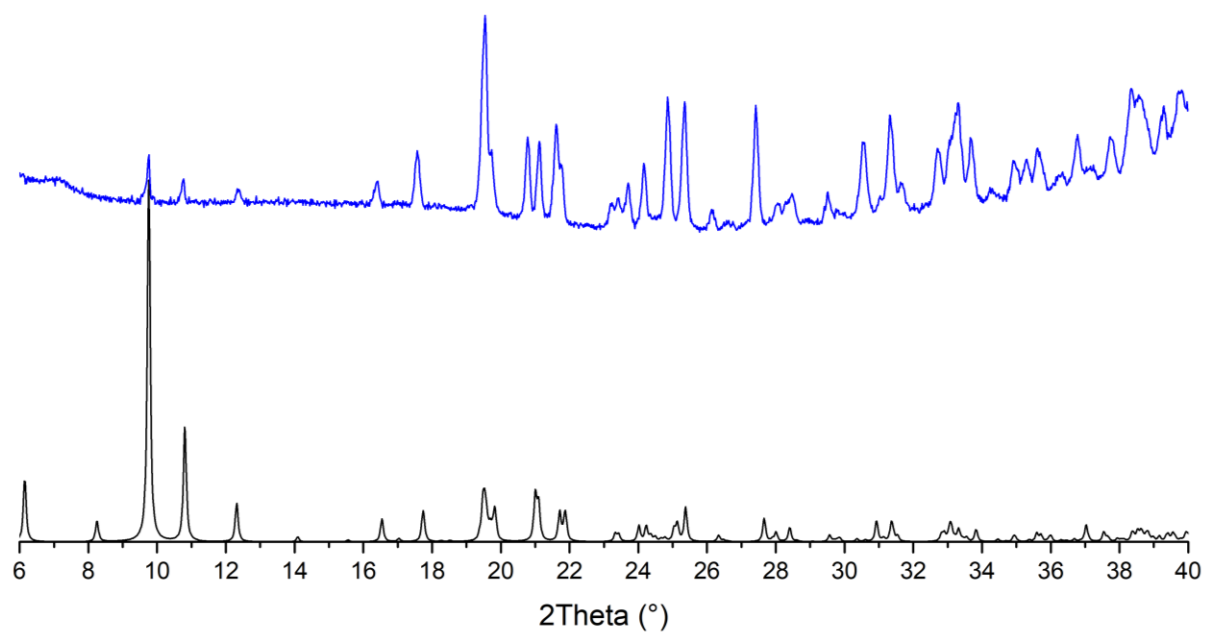
**Table S1.** Crystallographic data for **1–3**.

	[Yb <sub>2</sub> (μ-CICNAn) <sub>2</sub> (μ-F <sub>4</sub> BDC)(H <sub>2</sub> O) <sub>4</sub> ·(H <sub>2</sub> O) <sub>3</sub> (1)	[Er <sub>2</sub> (μ-CICNAn) <sub>2</sub> (μ-F <sub>4</sub> BDC)(H <sub>2</sub> O) <sub>4</sub> ·(H <sub>2</sub> O) <sub>4</sub> (2)	[Eu <sub>2</sub> (μ-CICNAn) <sub>2</sub> (μ-F <sub>4</sub> BDC)(H <sub>2</sub> O) <sub>6</sub> ] (3)
Empirical formula	C <sub>22</sub> H <sub>14</sub> N <sub>2</sub> O <sub>19</sub> F <sub>4</sub> Cl <sub>2</sub> Yb <sub>2</sub>	C <sub>22</sub> H <sub>16</sub> N <sub>2</sub> O <sub>20</sub> F <sub>4</sub> Cl <sub>2</sub> Yb <sub>2</sub>	C <sub>22</sub> H <sub>12</sub> N <sub>2</sub> O <sub>18</sub> F <sub>4</sub> Cl <sub>2</sub> Eu <sub>2</sub>
Fw	1103.33	1109.79	1043.16
Crystal color	red	red	red
Crystal size (mm <sup>3</sup> )	0.03*0.03*0.02	0.12*0.05*0.04	0.10*0.08*0.05
Temperature (K)	150	270	220
Wavelength (Å)	1.54184	1.54184	1.54184
Crystal system, Z	Triclinic, 1	Triclinic, 1	Monoclinic, 4
Space group	<i>P</i> -1	<i>P</i> -1	<i>I</i> 2/ <i>a</i>
a (Å)	5.0711 (2)	5.1064 (2)	19.3998 (8)
b (Å)	10.7697 (7)	10.7800 (13)	9.2617 (3)
c (Å)	14.6511 (9)	14.7311 (14)	18.5209 (8)
α (°)	95.915 (5)	95.821 (9)	90
β (°)	99.675 (4)	99.673 (6)	121.571 (6)
γ (°)	90.477 (5)	90.532 (7)	90
V (Å <sup>3</sup> )	784.31 (8)	794.97 (13)	2835.2 (2)
ρ <sub>calc</sub> (g·cm <sup>-3</sup> )	2.336	2.318	2.444
μ(CuKα) (mm <sup>-1</sup> )	13.334	12.112	34.181
θ range (°)	3.077–73.515	3.060–71.980	5.353–72.002
Data collected	5935	5303	5883
Data unique	3033	5303	2714
Data observed	2830	4819	2530
R(int)	0.0337	0.1949	0.0418
Nb of parameters / restraints	244/32	225/10	267/18
R1( <i>F</i> ), <sup>a</sup> <i>I</i> > 2σ( <i>I</i> )	0.0728	0.1614	0.0355
wR2( <i>F</i> <sup>2</sup> ), <sup>b</sup> all data	0.2344	0.4610	0.0883
S( <i>F</i> <sup>2</sup> ), <sup>c</sup> all data	1.134	2.290	1.087
CCDC number	21708733	21708734	21708735

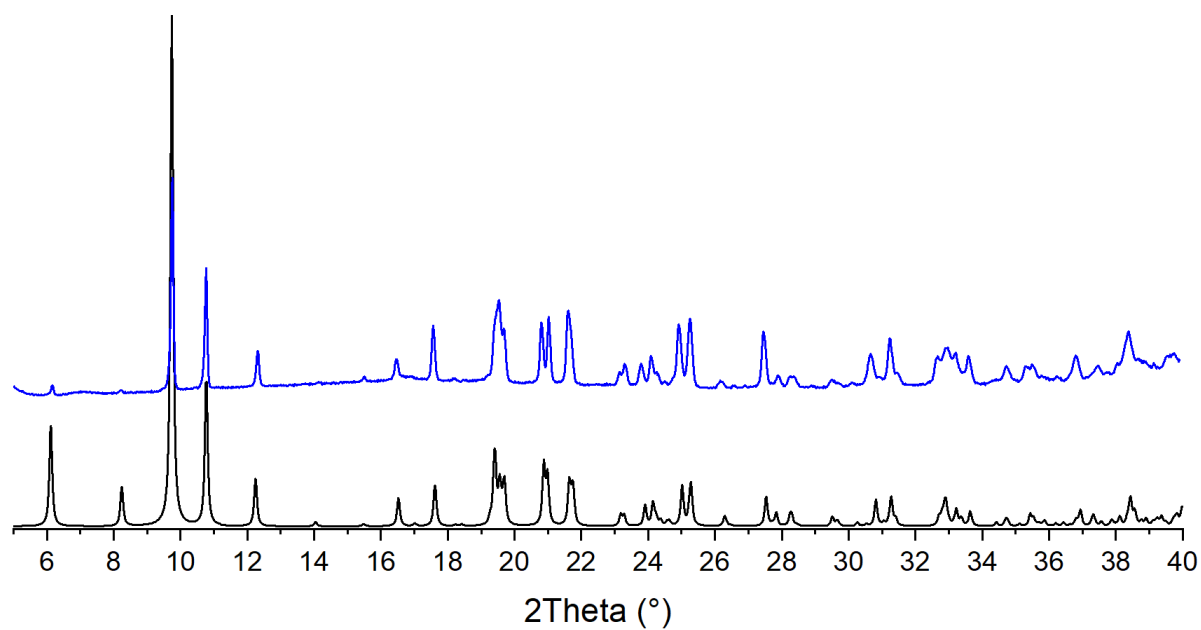
$$^a R1(F) = \sum \|F_0\| - \|F_C\| / \sum \|F_0\|; ^b wR2(F^2) = [\sum w(F_0^2 - F_C^2)^2 / \sum wF_0^4]^{1/2}; ^c S(F^2) = [\sum w(F_0^2 - F_C^2) / (n+r-p)]^{1/2}.$$



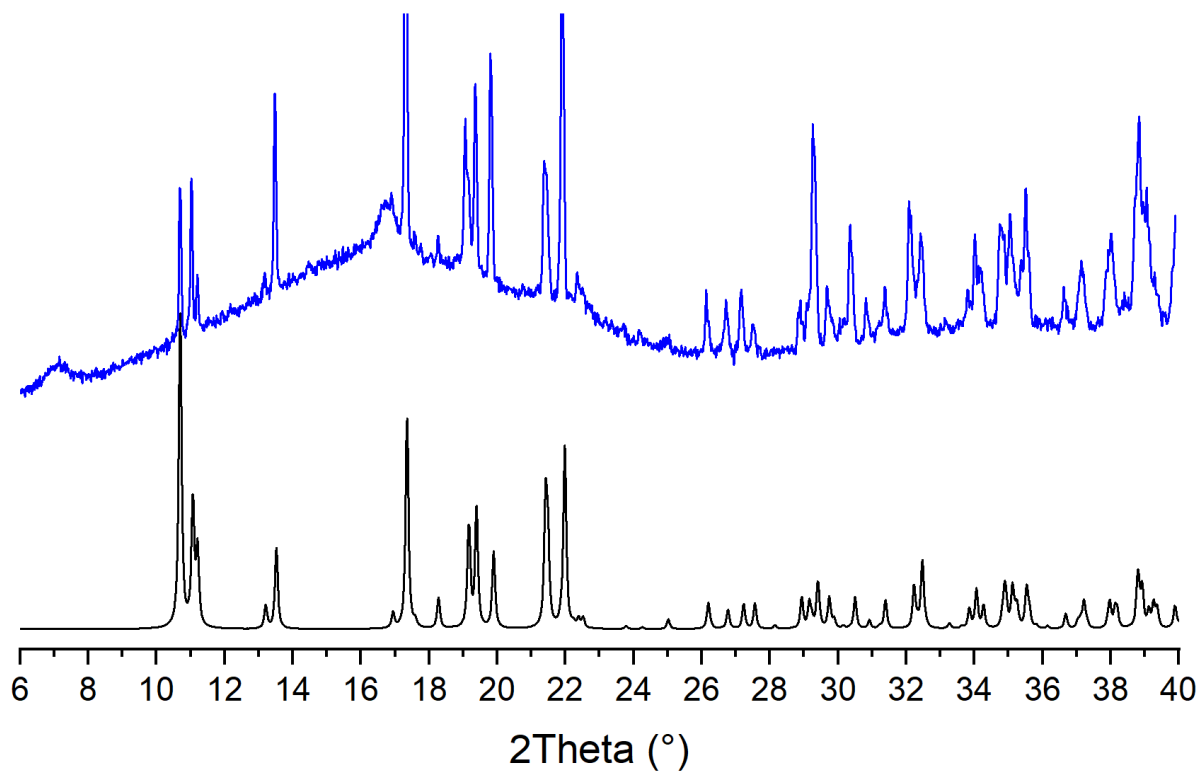
**Figure S1.** FT-IR spectra of: a) KHClCNAN (orange line),  $\text{H}_2\text{F}_4\text{BDC}$  (grey line) and b) **1** (red line), **2** (blue line) **3** (green line), in the 2000-700  $\text{cm}^{-1}$  region.



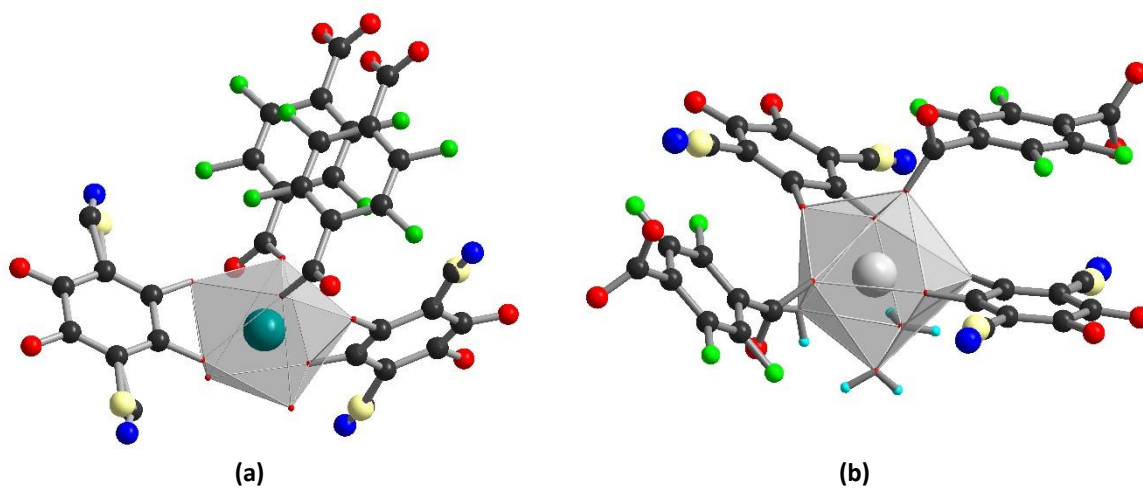
**Figure S2.** Simulated (black) and experimental (blue) X-ray powder patterns of **1**.



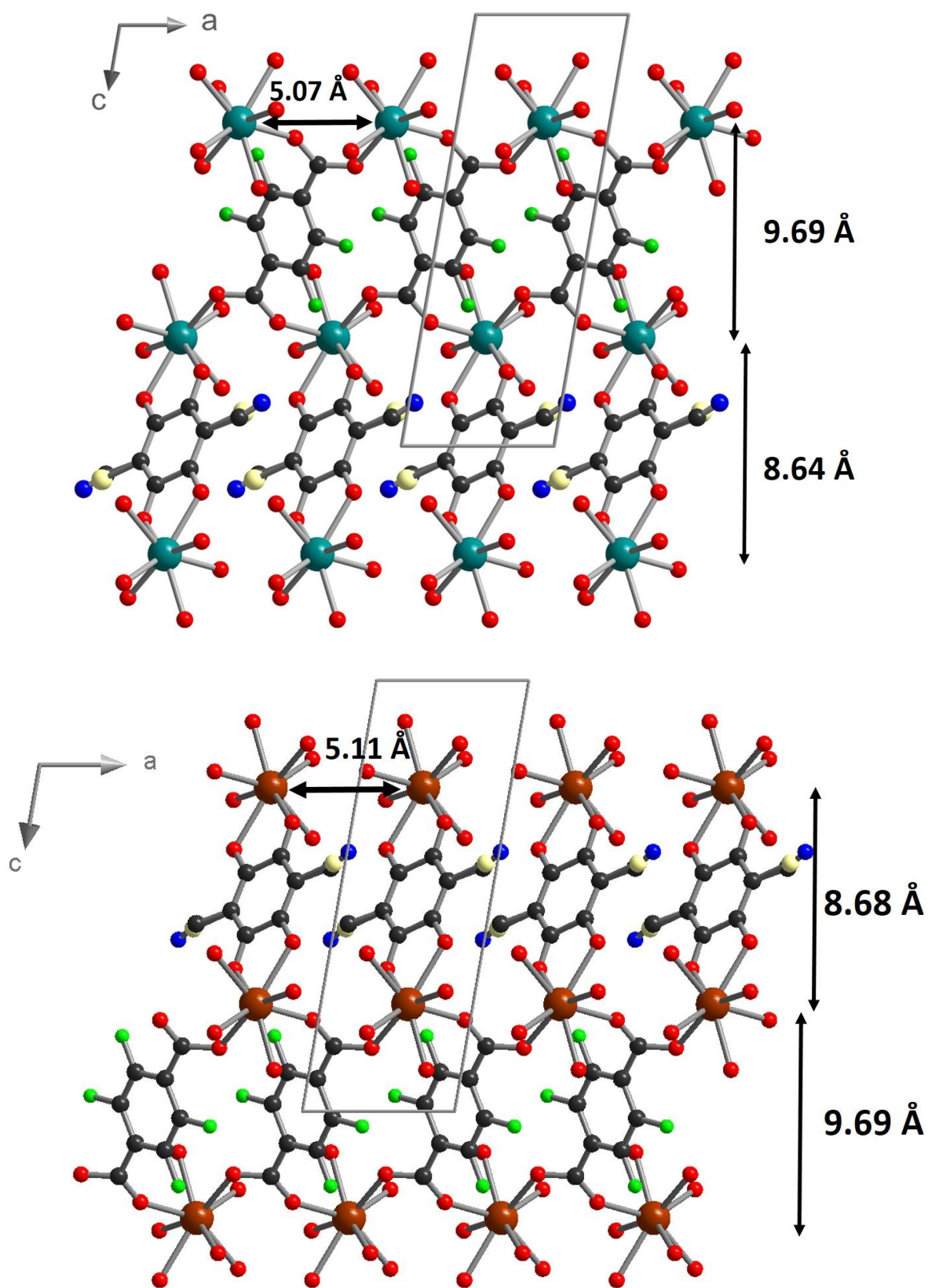
**Figure S3.** Simulated (black) and experimental (blue) X-ray powder patterns of **2**.



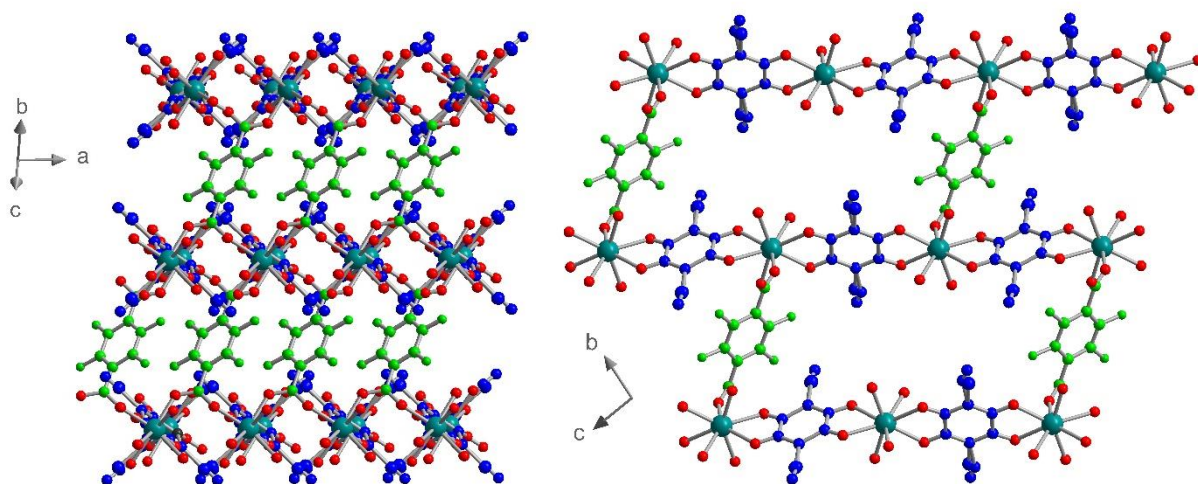
**Figure S4.** Simulated (black) and experimental (blue) X-ray powder patterns of **3**.



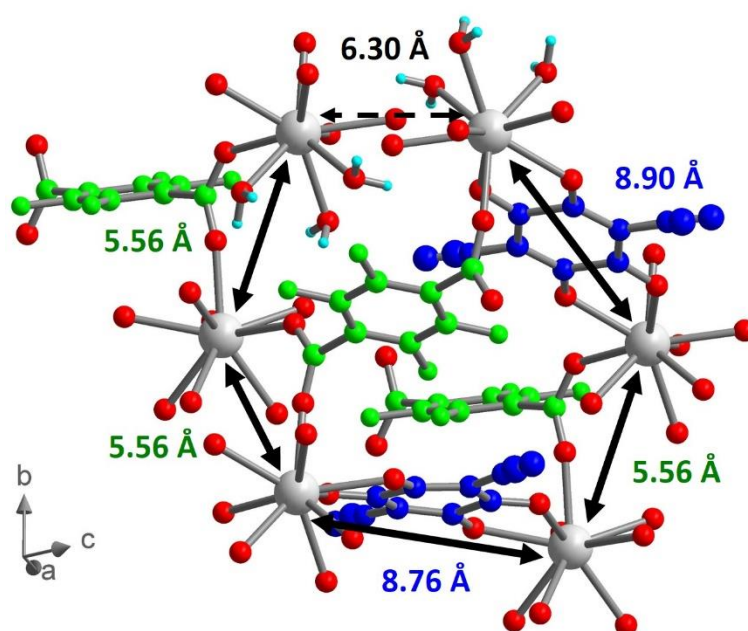
**Figure S5.** Coordination environment of the metal ion in **1** (a) and **3** (b). Color code: C (black), H (cyan), O (red), N (blue), F (green), Cl (light yellow), Yb (teal), Eu (grey).



**Figure S6.** View of the crystal structures of **1** (top) and **2** (bottom) in the *ac* plane highlighting the shortest Ln(III)···Ln(III) distances. Color code: C (black), O (red), N (blue), F (green), Cl (light yellow), Yb (teal), Er (brown).

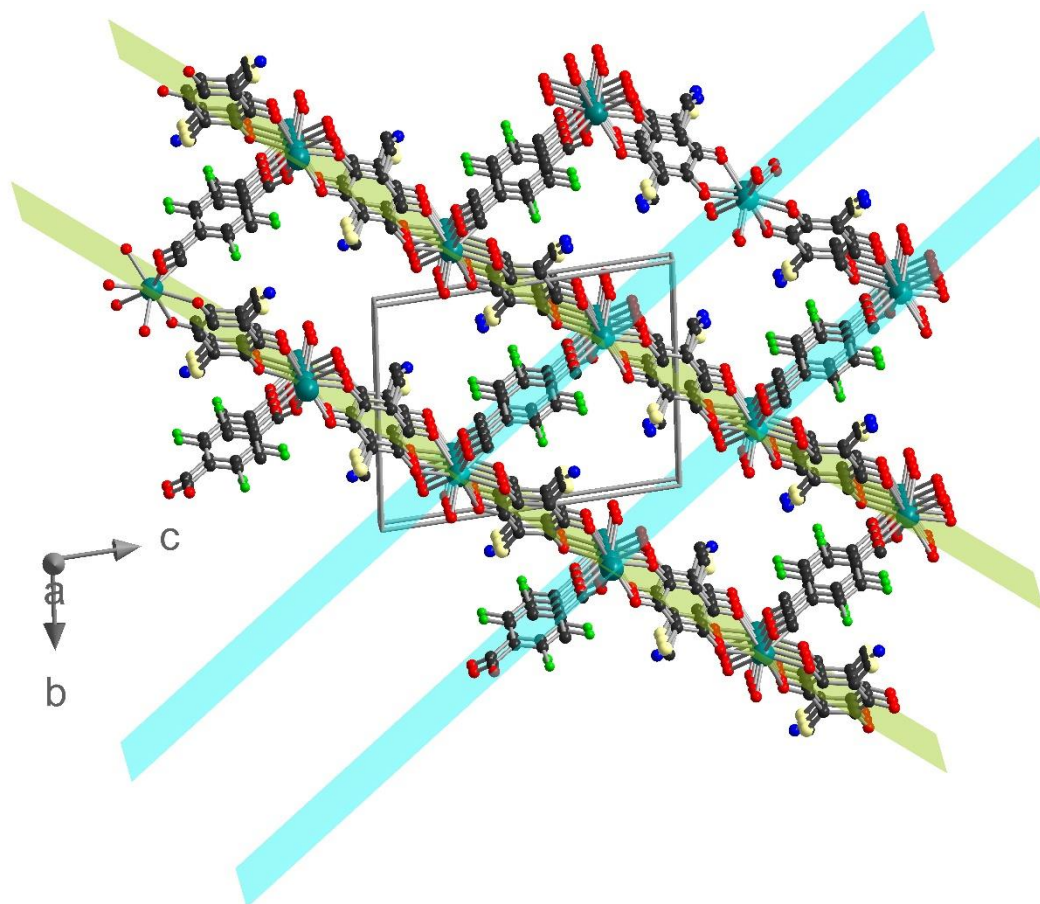


**Figure S7.** Views of the extended structure in **1**. ClCNAn<sup>2-</sup> and F<sub>4</sub>BDC<sup>2-</sup> are highlighted in blue and green respectively.

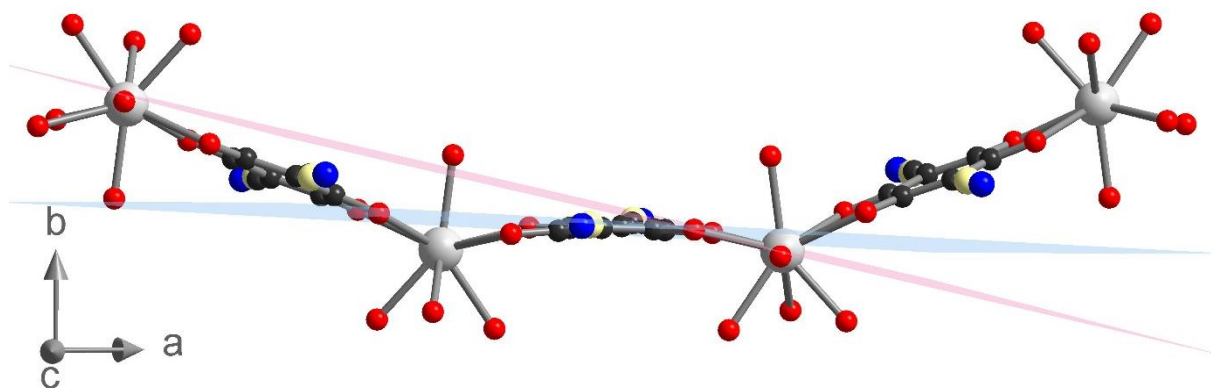


**Figure S8.** View of the crystal structure of **3** highlighting the shortest Eu...Eu distances. ClCNAn<sup>2-</sup> and F<sub>4</sub>BDC<sup>2-</sup> are highlighted in blue and green respectively.

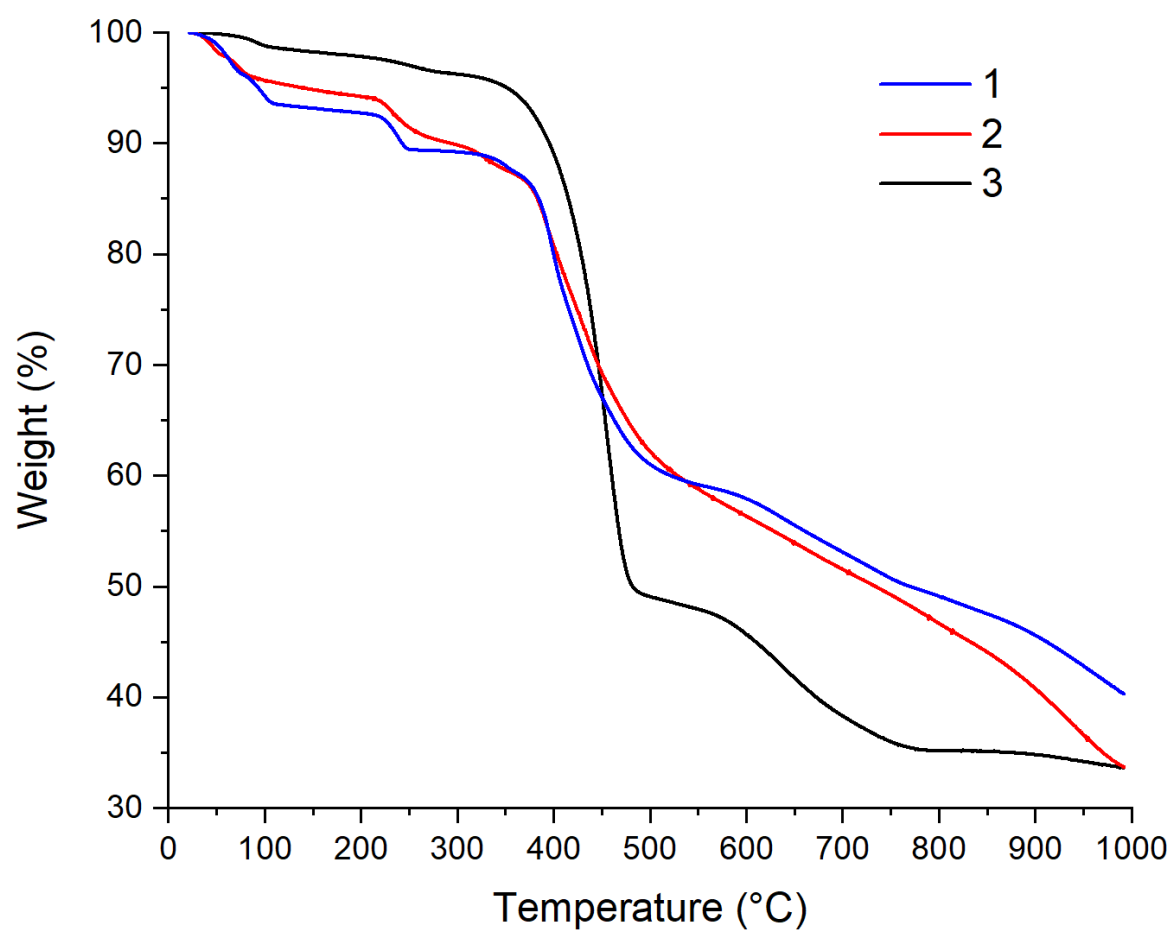




**Figure S9.** View of the crystal structure of **1** highlighting the (011) and (0-11) lattice planes in cyan and green respectively. Color code: C (black), O (red), N (blue), F (green), Cl (light yellow), Yb (teal).



**Figure S10.** View of the Eu-anilate 1D chain of **3** highlighting the plane of the ligand (in blue) and the plane made by the Ln metal centre and the two coordinated O atoms (in red). Color code: C (black), O (red), N (blue), F (green), Cl (light yellow), Eu (gray).



**Figure S11.** TGA of compounds **2** and **3**.