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A series of Ln-*p*-chlorobenzoic acid-terpyridine complexes: Lanthanide contraction effects, supramolecular interactions and luminescent behavior

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I. Powder X-ray diffraction data

For the following PXRD spectra it is important to note that calculated patterns are from low temperature (100K) data collections while observed patterns were collected at room temperature (298 K). This difference may result in slight shifts in two-theta values.

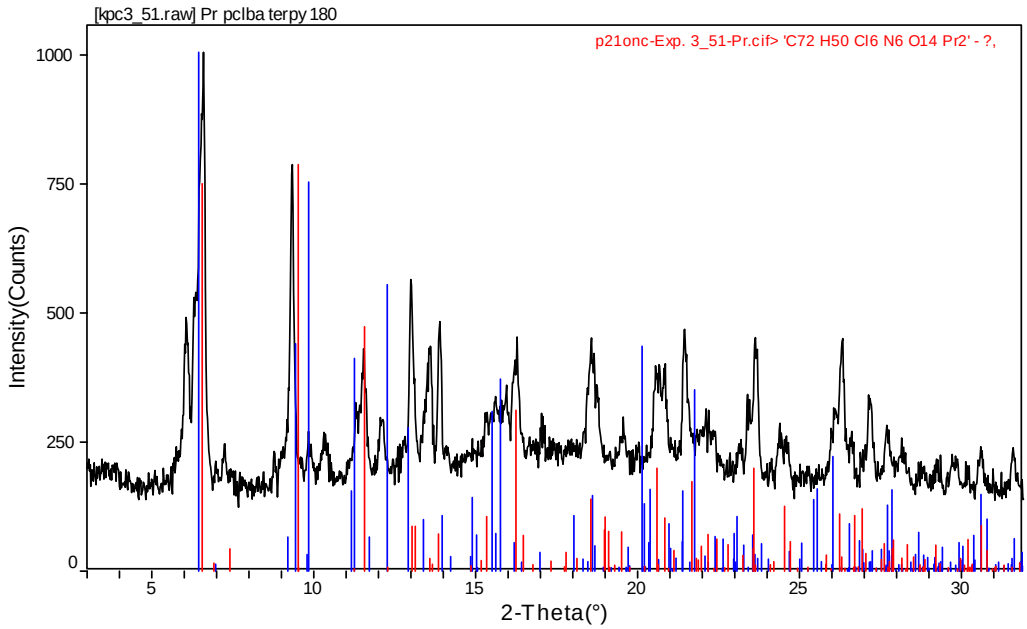

Figure S1: The PXRD pattern of structure **1 (**structure type **I**) with calculated pattern overlaid in red. The calculated pattern of structure **2** (structure type **II**) is also included in blue. We acknowledge that this sample contains impurities.

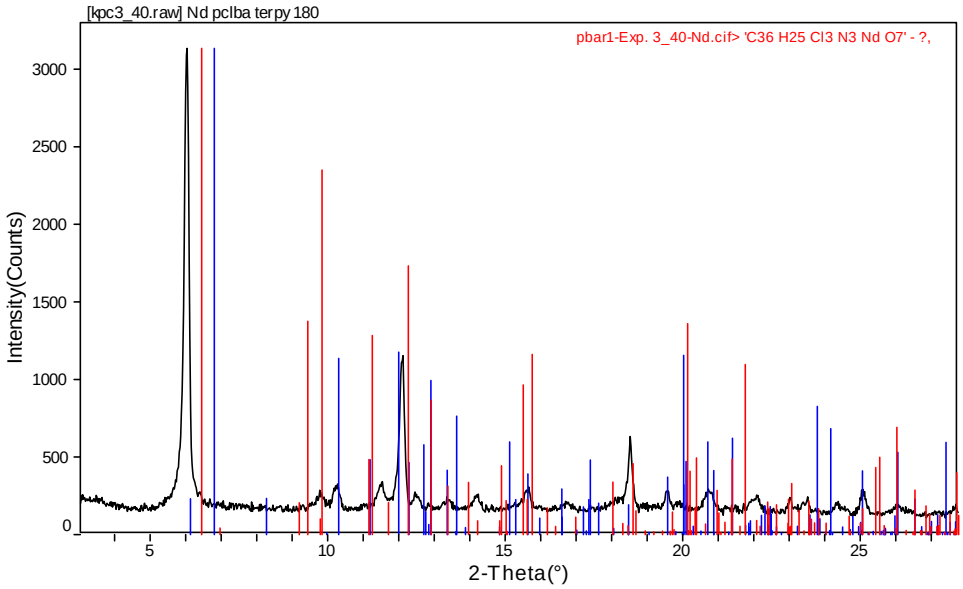

Figure S2: The PXRD pattern of structure **2 (**structure type **II**) with calculated pattern overlaid in red. The calculated pattern of structure **3'** (structure type **III**) is also included in blue. We acknowledge that this sample contains small impurities

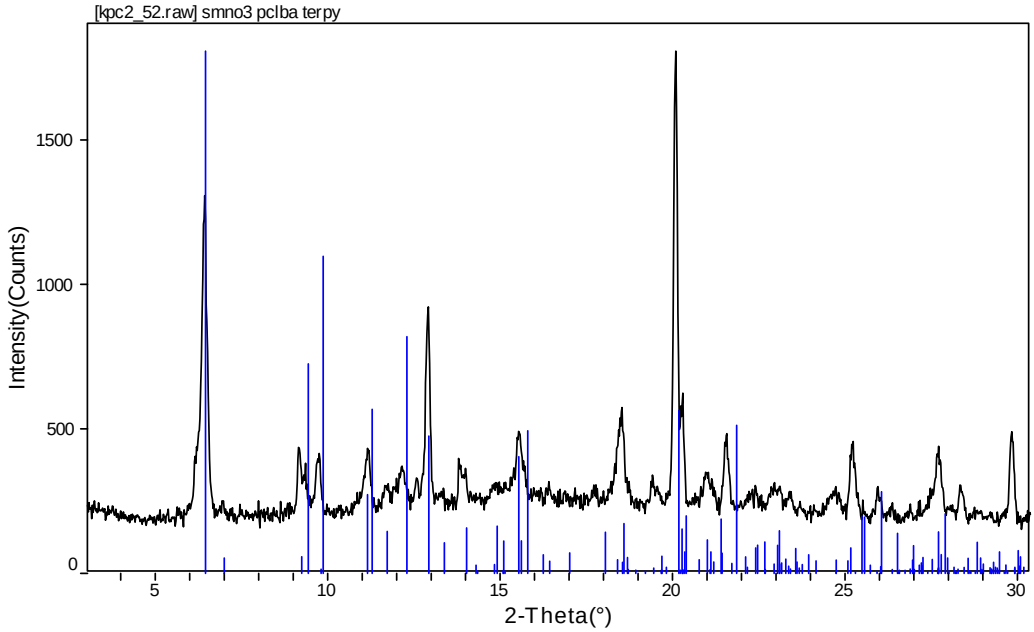

Figure S3: The PXRD pattern of structure **3** with calculated pattern overlaid in blue.

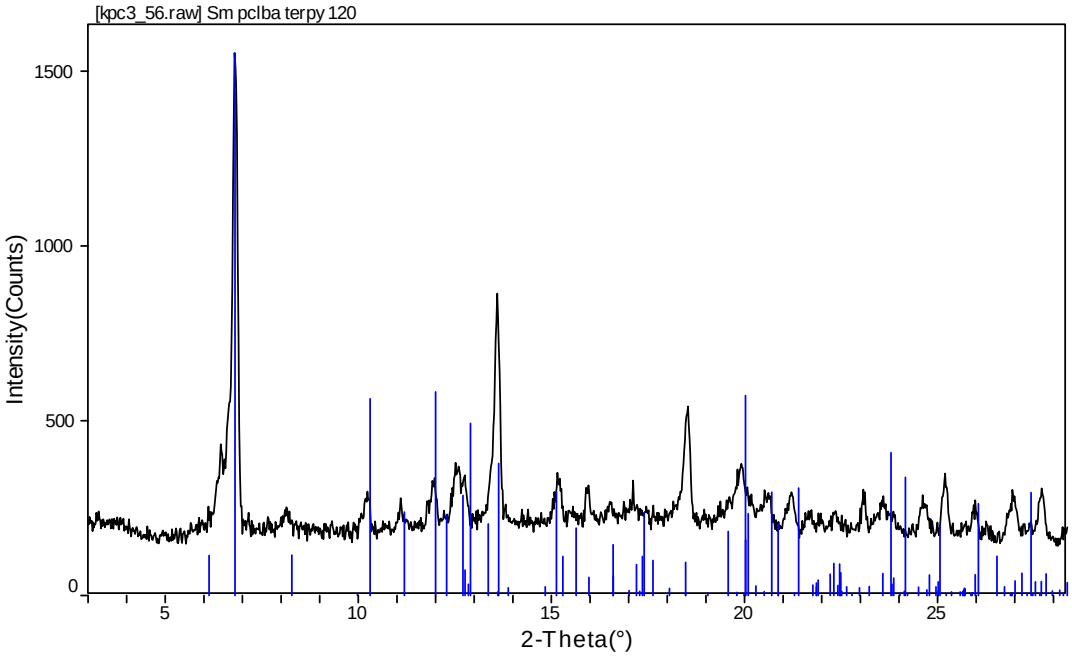

Figure S4: The PXRD pattern of **3'** with calculated pattern overlaid in blue

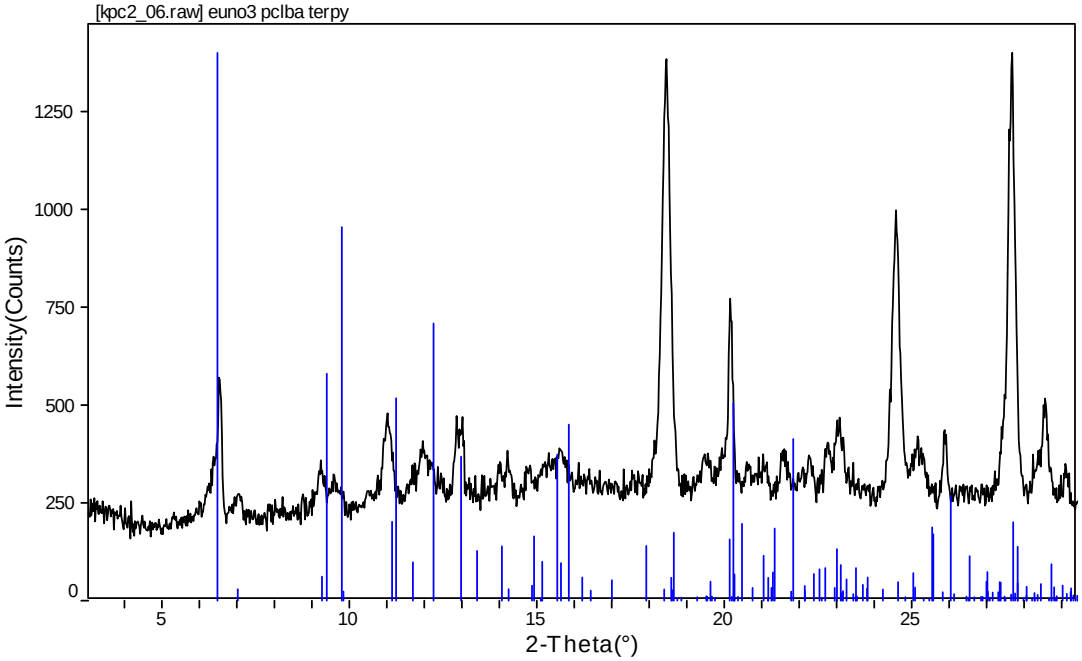

Figure S5: The PXRD pattern of **4** with calculated pattern overlaid in blue.

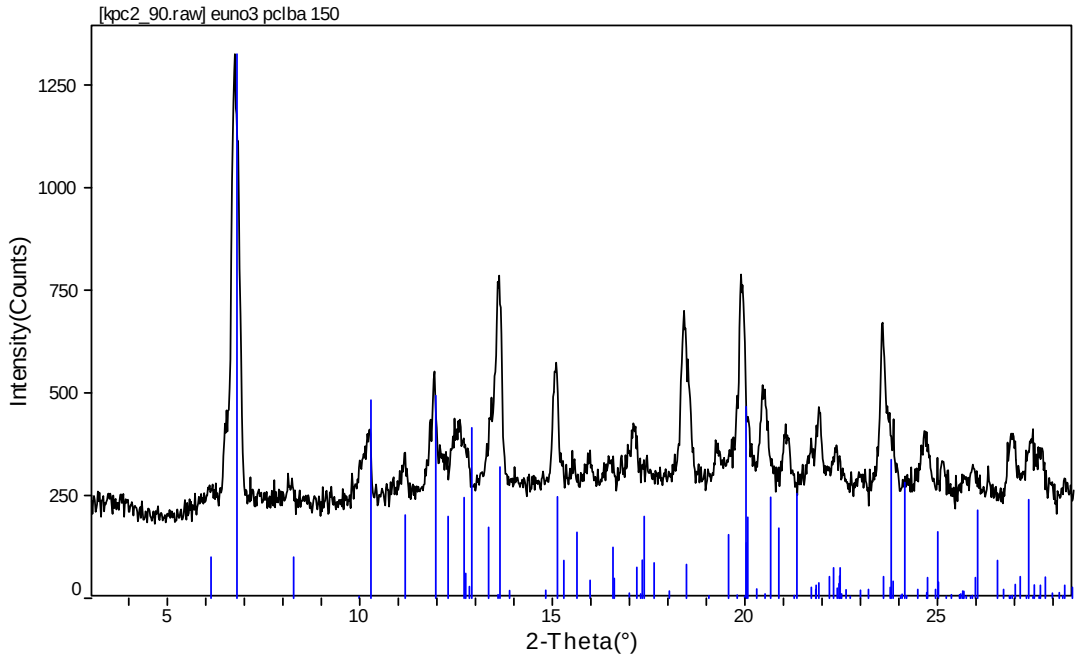

Figure S6: The PXRD pattern of **4'** with calculated pattern overlaid in blue.

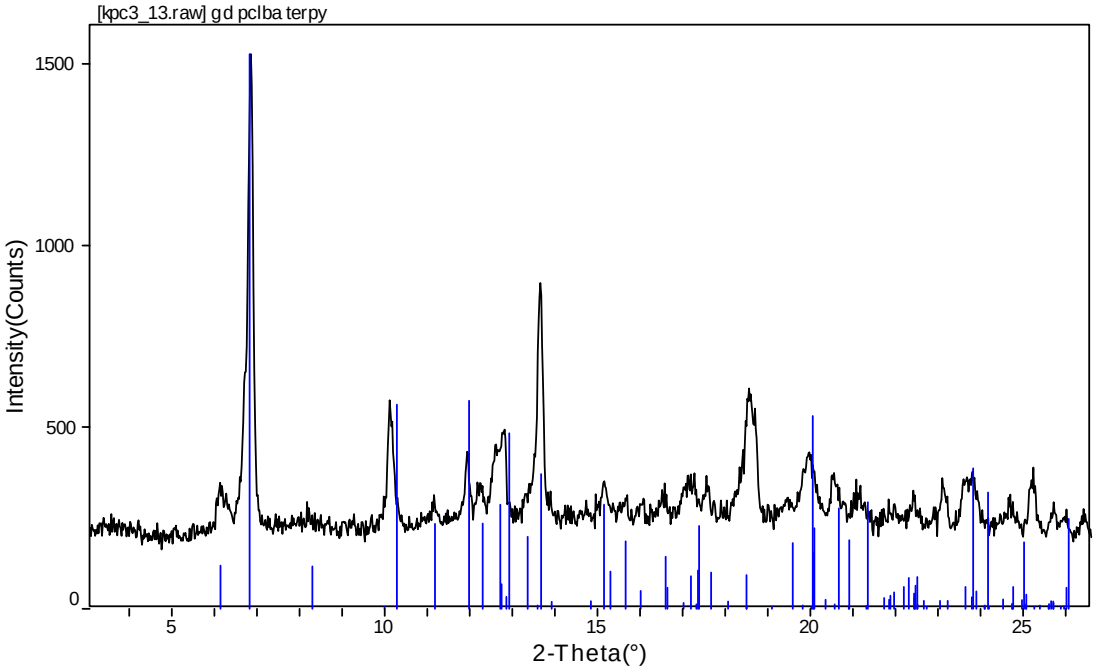

Figure S7: The PXRD pattern of **5** with calculated pattern overlaid in blue.

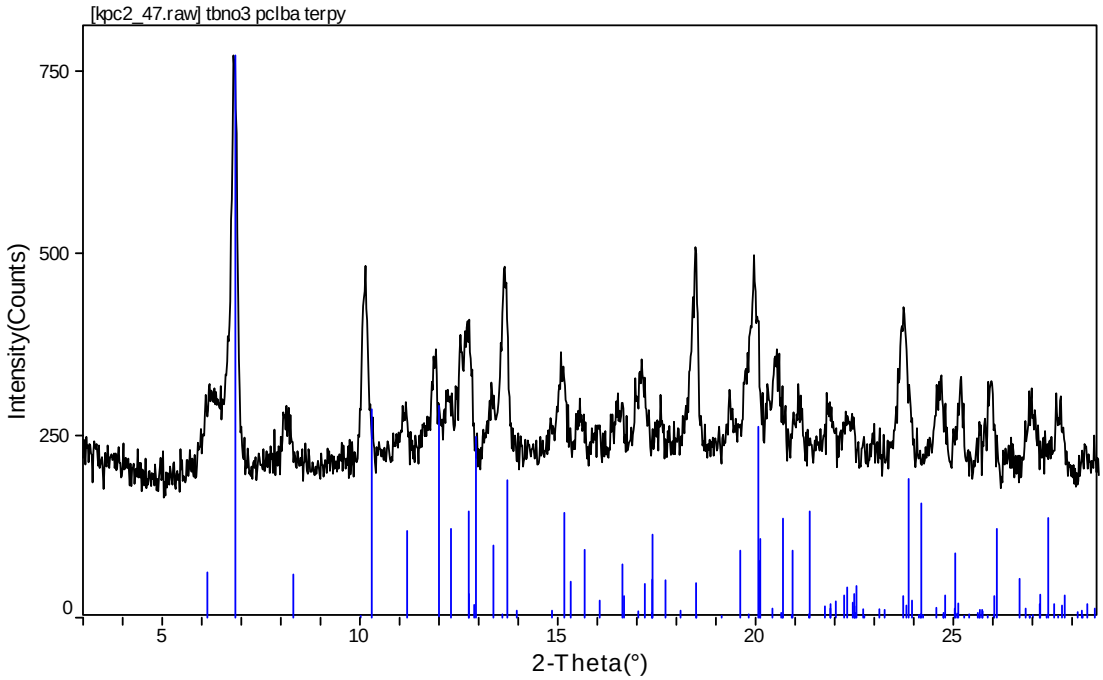

Figure S8: The PXRD pattern of **6** with calculated pattern overlaid in blue.

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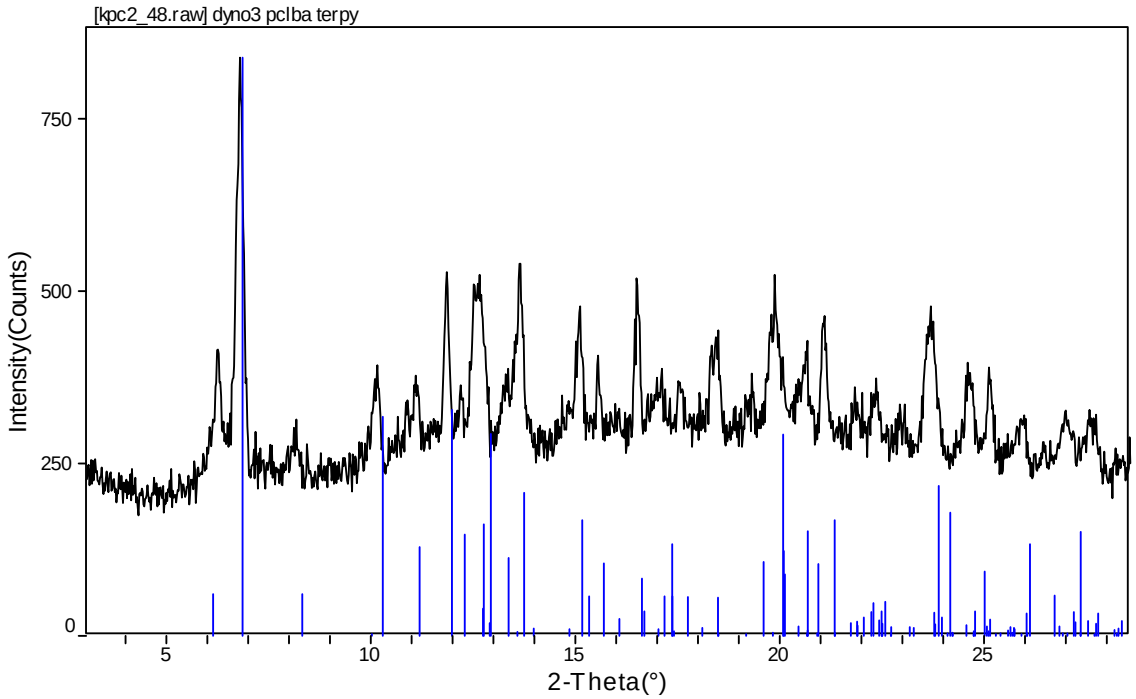

Figure S9: The PXRD pattern of **7** with calculated pattern overlaid in blue.

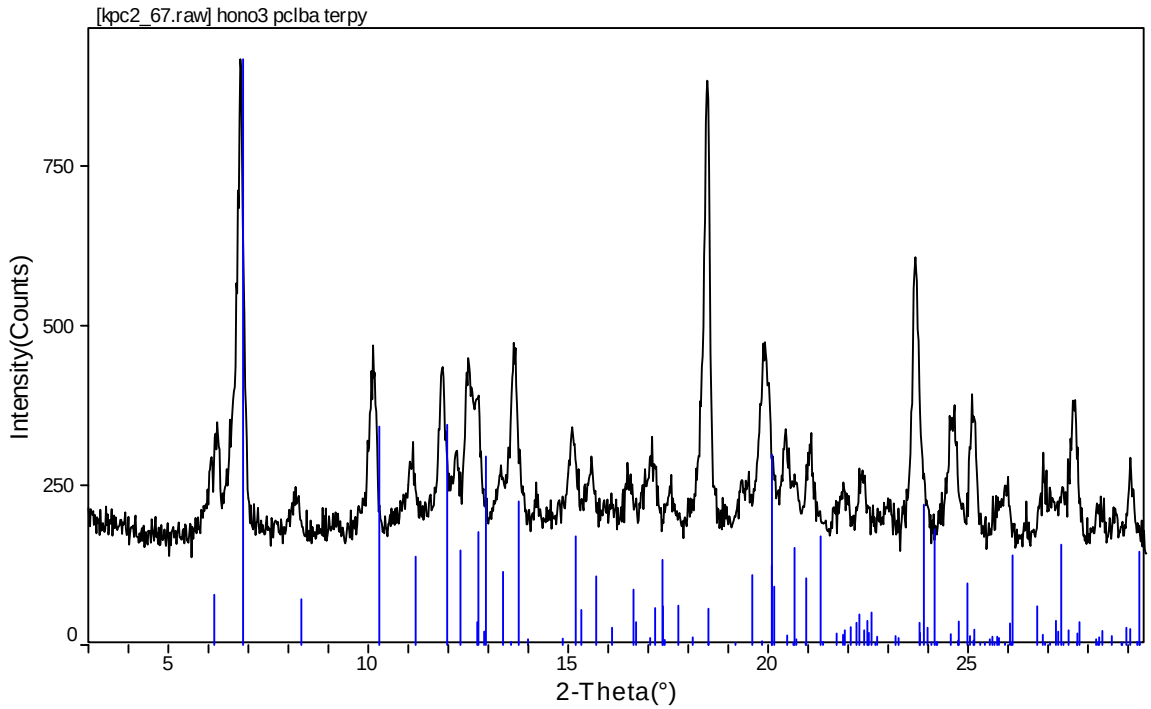

Figure S10: The PXRD pattern of **8** with calculated pattern overlaid in blue.

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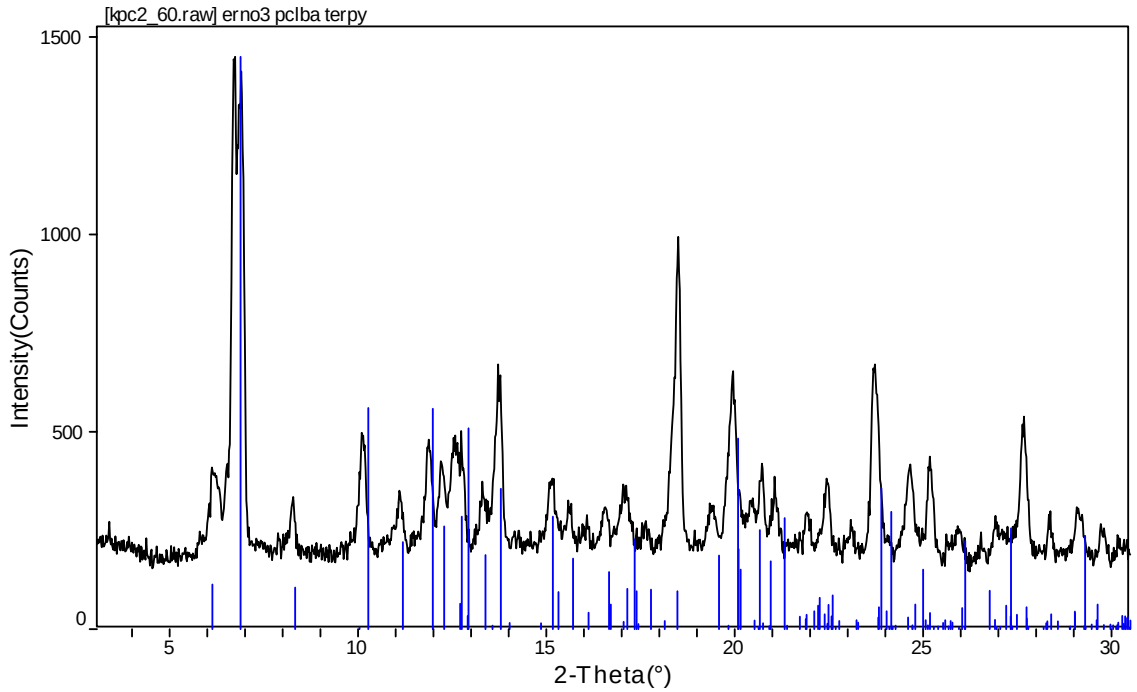

Figure S11: The PXRD pattern of **9** with calculated pattern overlaid in blue.

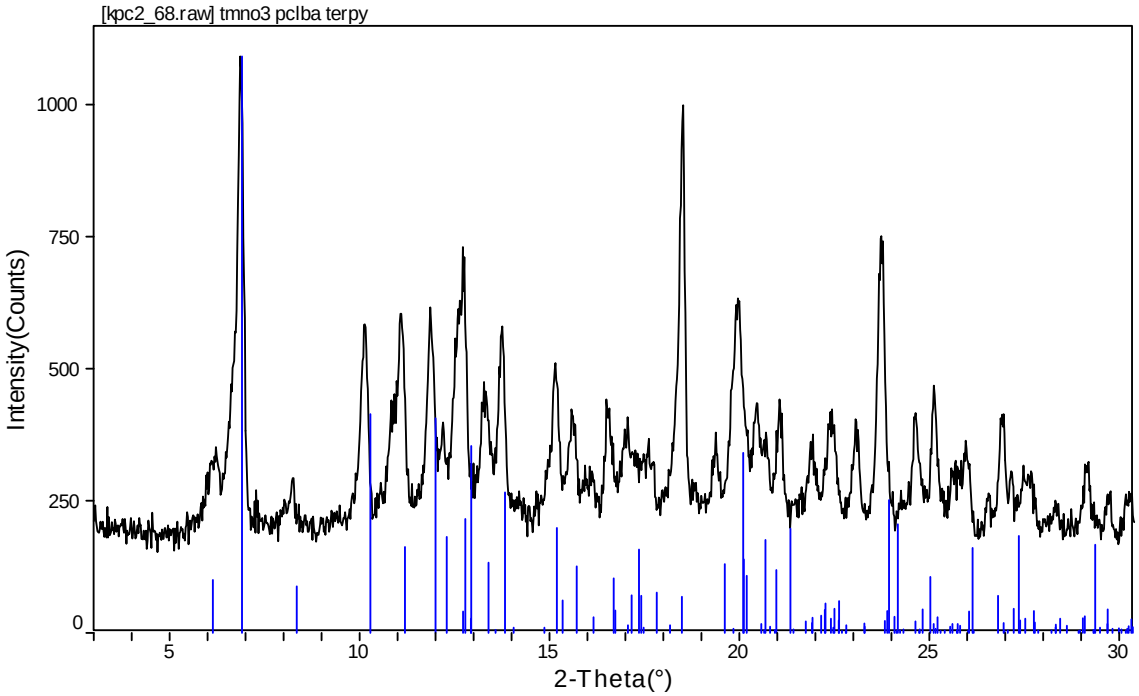

Figure S12: The PXRD pattern of **10** with calculated pattern overlaid in blue.

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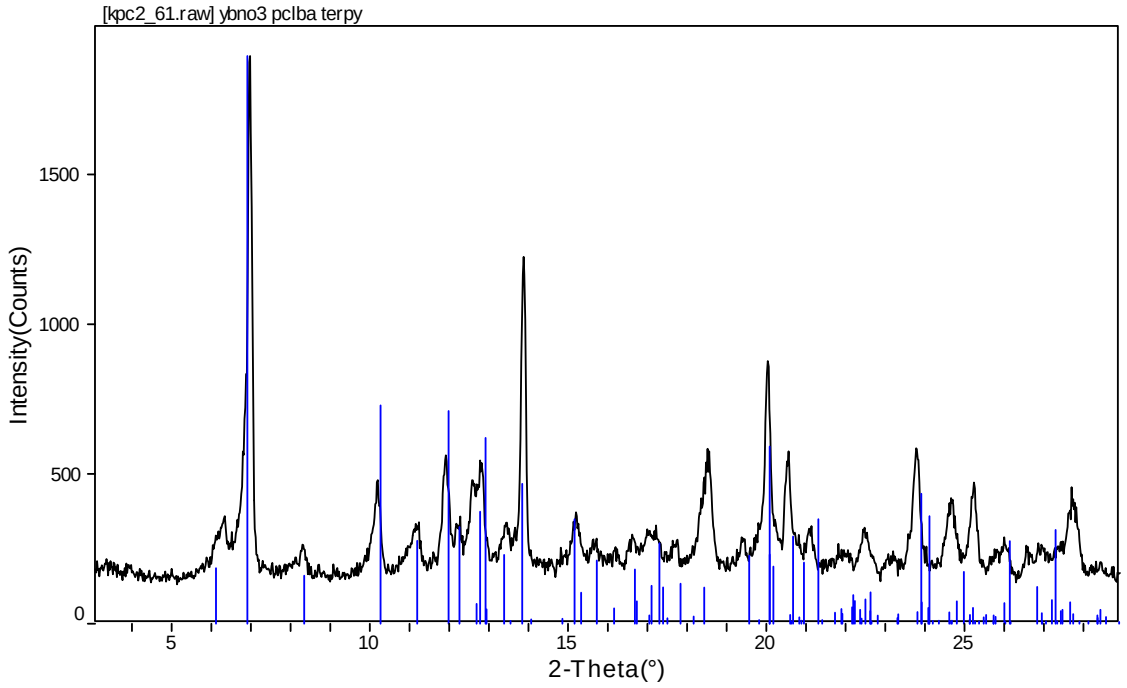

Figure S13: The PXRD pattern of **11** with calculated pattern overlaid in blue.

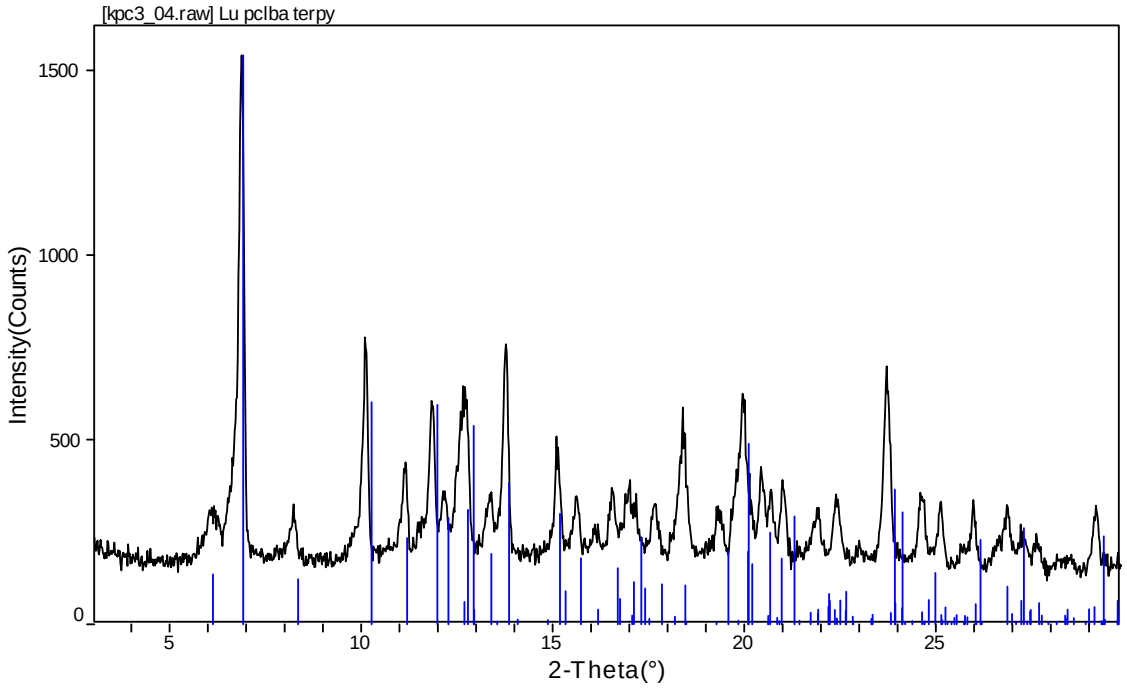

Figure S14: The PXRD pattern of **12** with calculated pattern overlaid in blue.

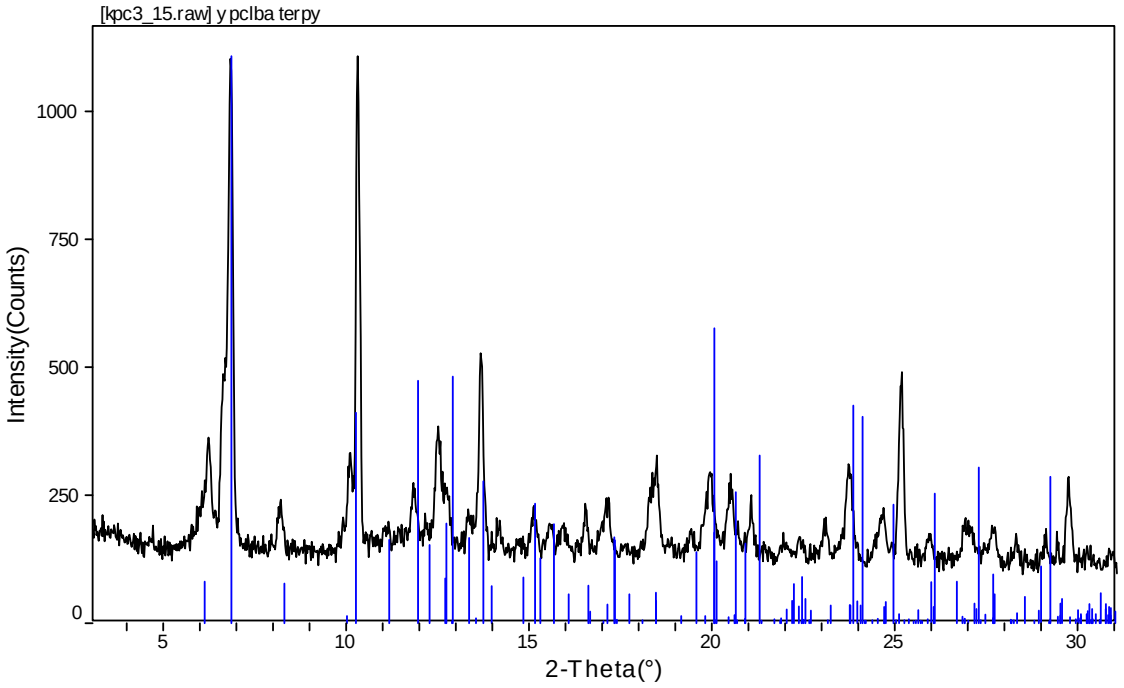

Figure S15: The PXRD pattern of **13** with calculated pattern overlaid in blue.

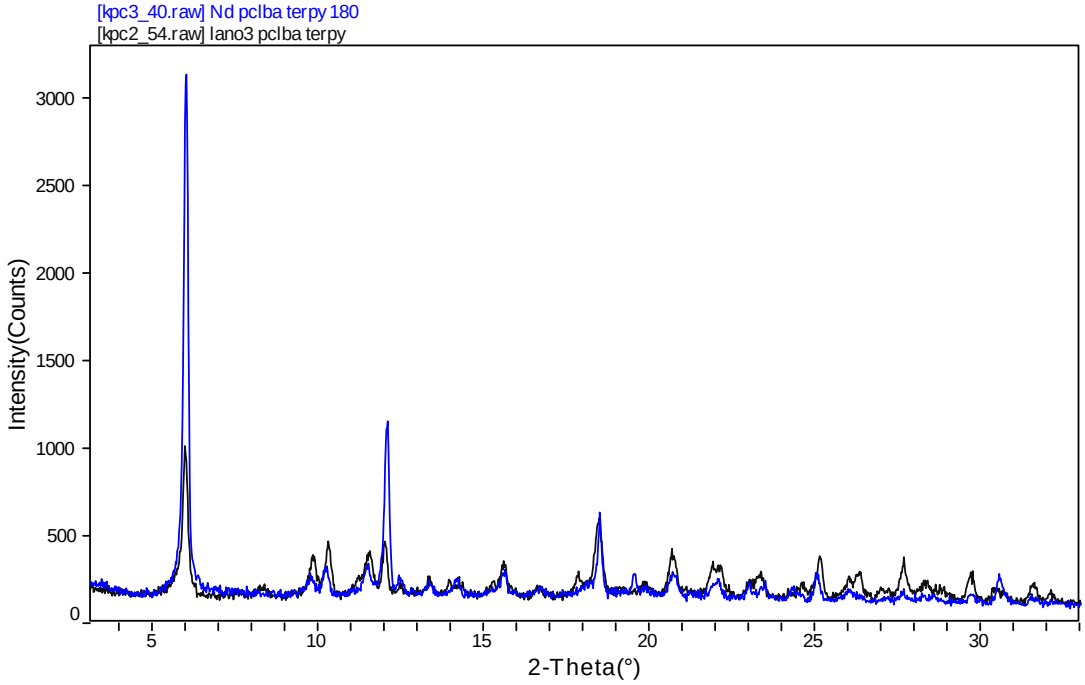

Figure S16: The PXRD pattern of La-*p*-chloro-TPY material with observed pattern of the bulk products of **2 (Nd)** overlaid in blue.

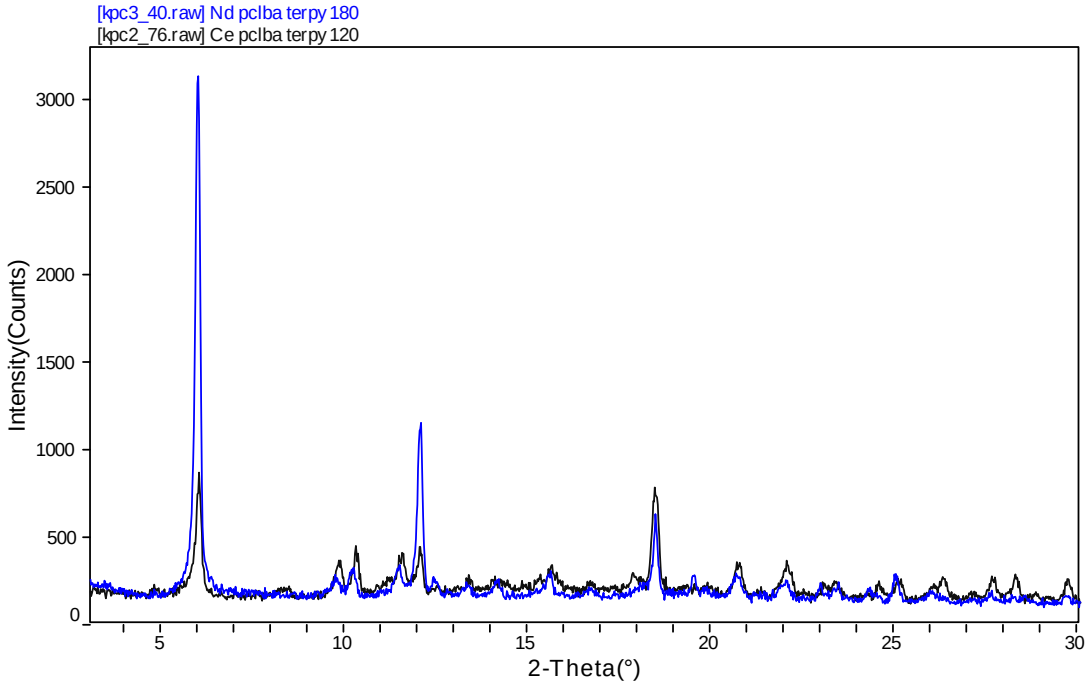

Figure S17: The PXRD pattern of Ce-*p*-chloro-TPY material with observed pattern of the bulk products of **2 (Nd)** overlaid in blue.

II. Thermal Ellipsoid Plots

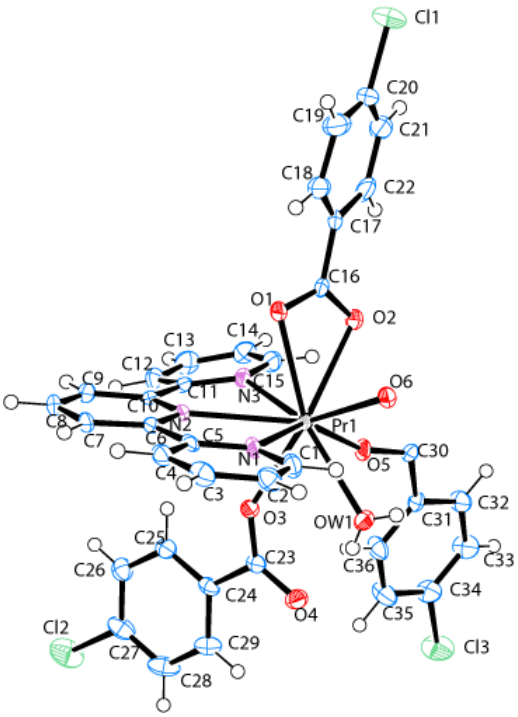

Figure S18: ORTEP illustration of structure **1**. Ellipsoids are shown at 50% probability level.

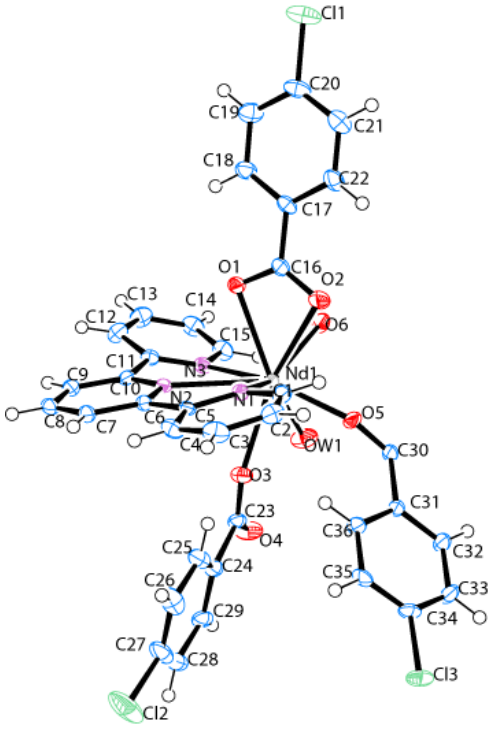

Figure S19: ORTEP illustration of structure **2**. Ellipsoids are shown at 50% probability level.

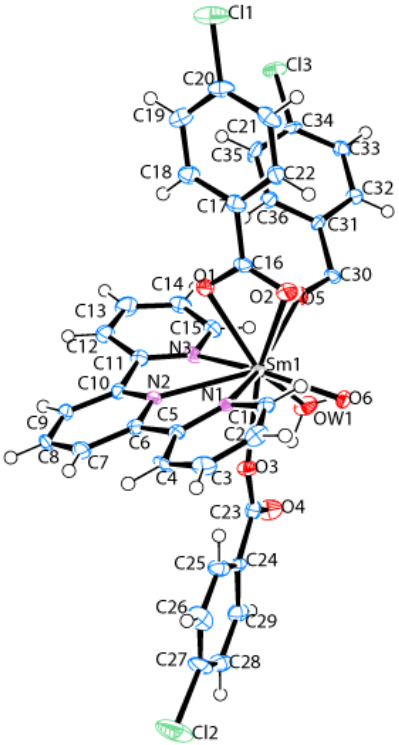

Figure S20: ORTEP illustration of structure **3**. Ellipsoids are shown at 50% probability level.

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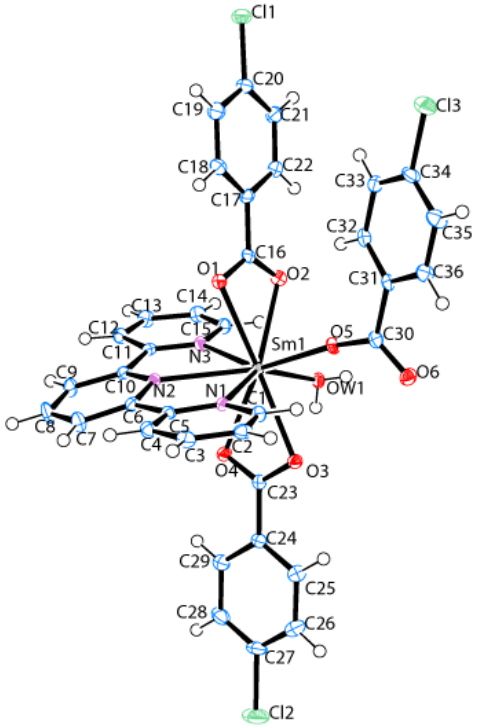

Figure S21: ORTEP illustration of structure **3'**. Ellipsoids are shown at 50% probability level.

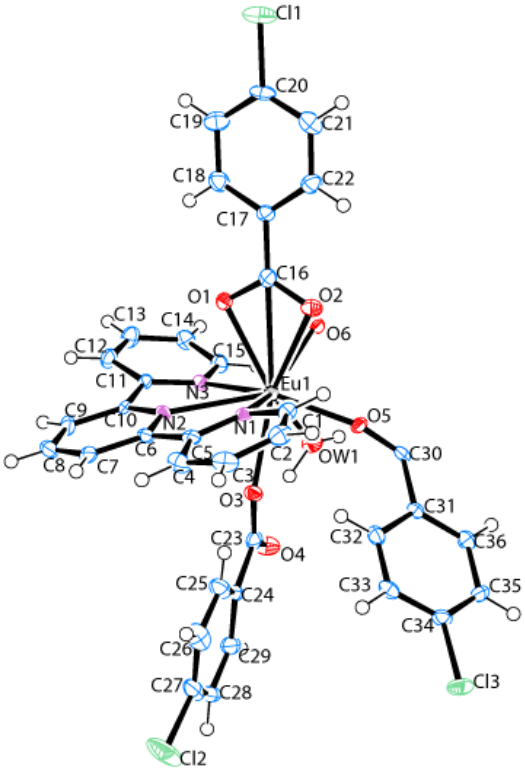

Figure S22: ORTEP illustration of structure **4**. Ellipsoids are shown at 50% probability level.

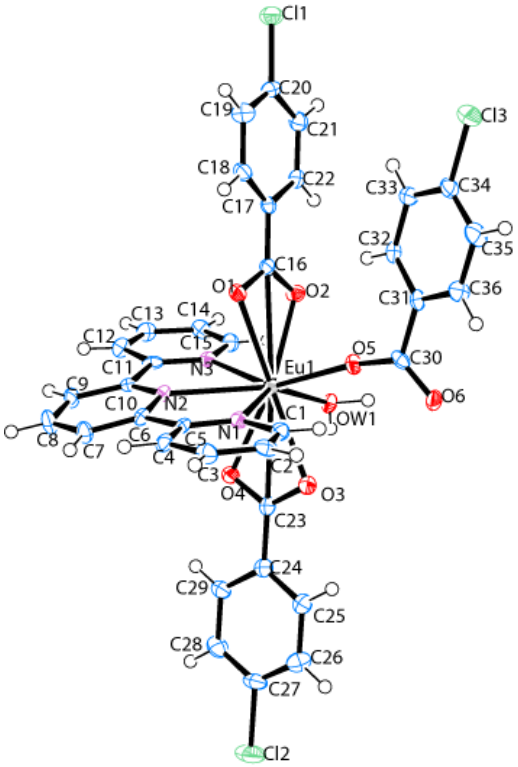

Figure S23: ORTEP illustration of structure **4'**. Ellipsoids are shown at 50% probability level.

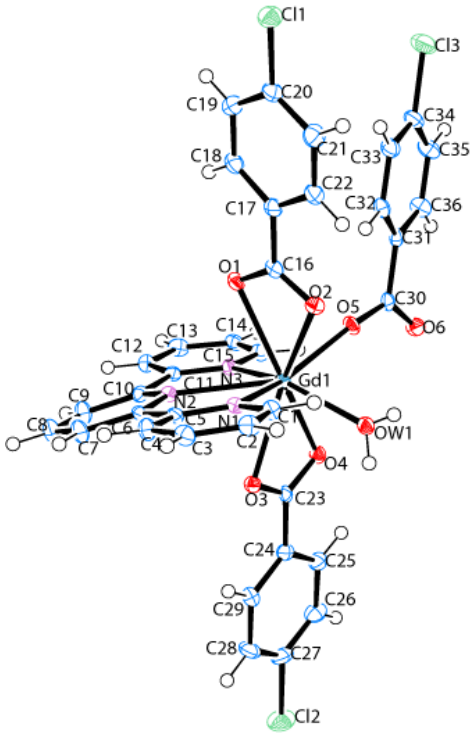

Figure S24: ORTEP illustration of structure **5**. Ellipsoids are shown at 50% probability level.

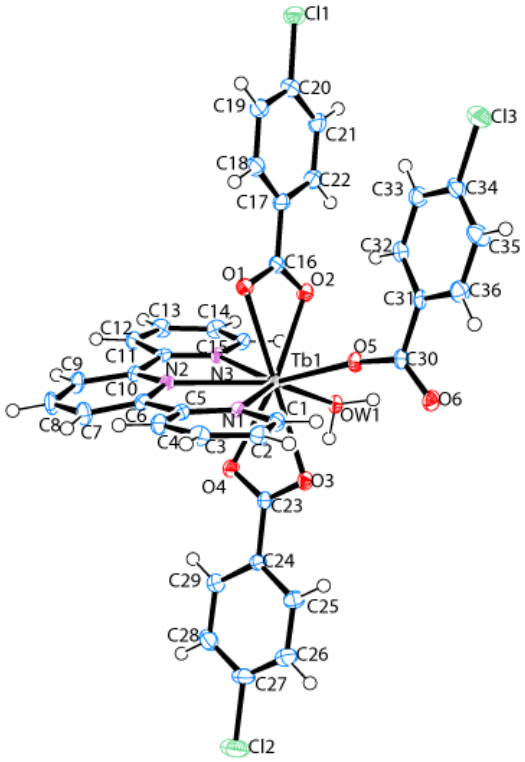

Figure S25: ORTEP illustration of structure **6**. Ellipsoids are shown at 50% probability level.

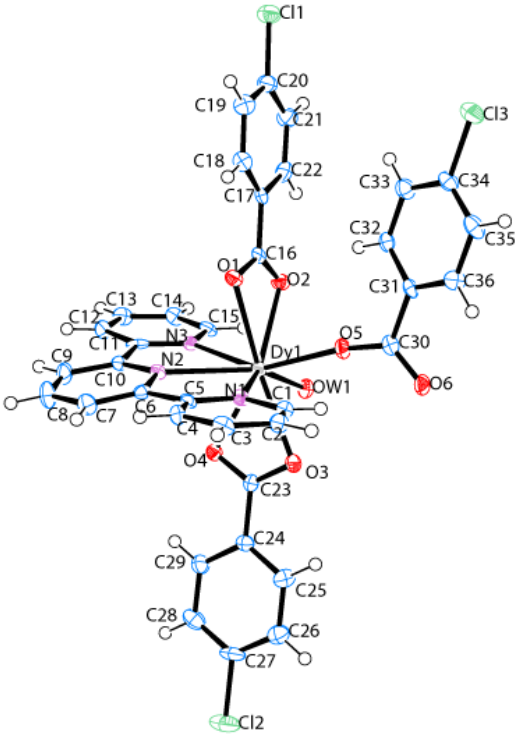

Figure S26: ORTEP illustration of structure **7**. Ellipsoids are shown at 50% probability level.

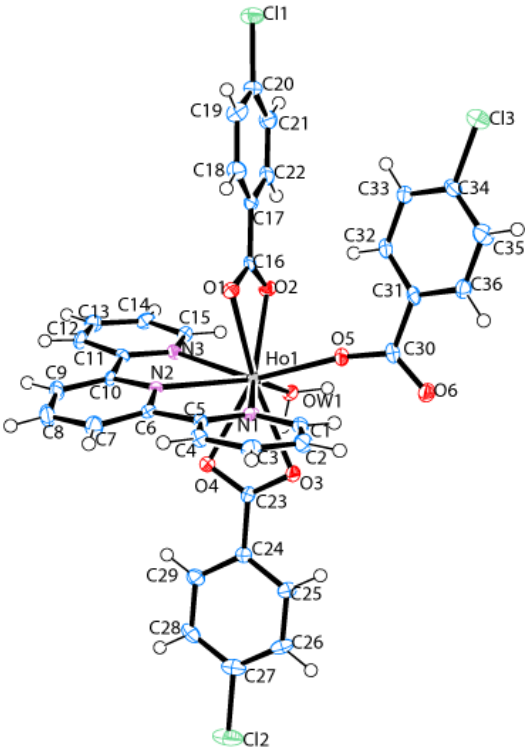

Figure S27: ORTEP illustration of structure **8**. Ellipsoids are shown at 50% probability level.

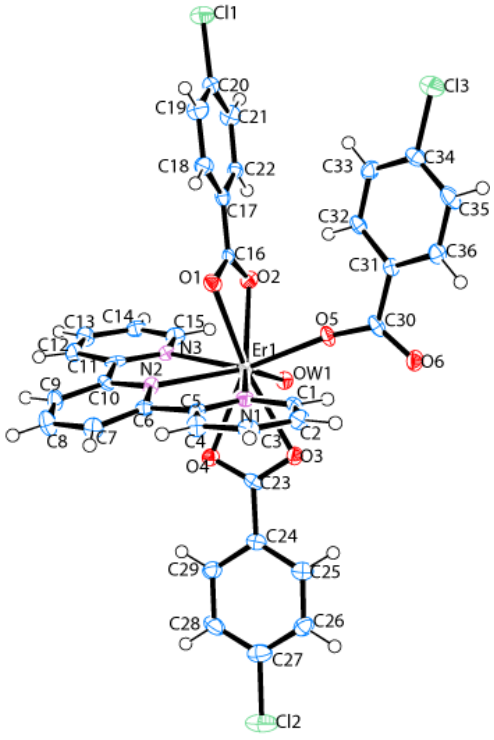

Figure S28: ORTEP illustration of structure **9**. Ellipsoids are shown at 50% probability level.

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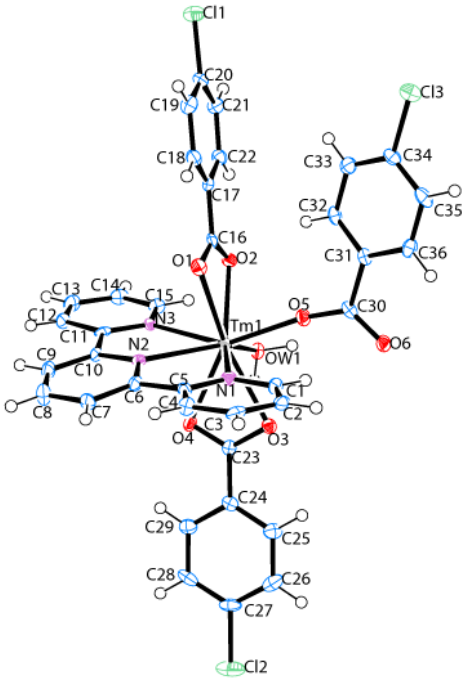

Figure S29: ORTEP illustration of structure **10**. Ellipsoids are shown at 50% probability level.

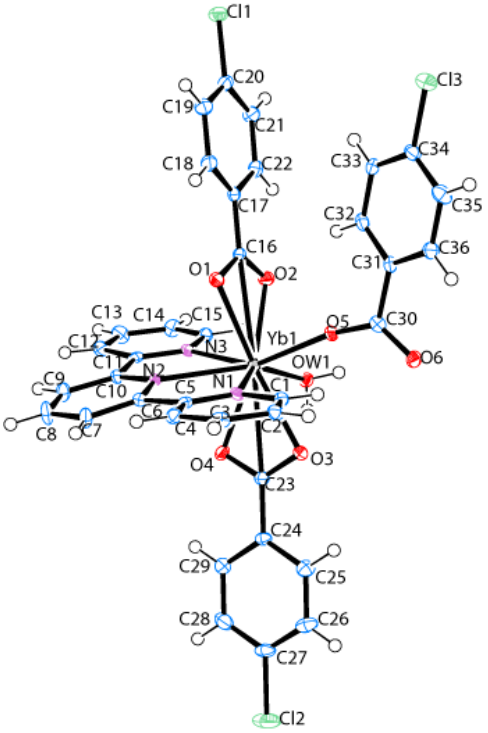

Figure S30: ORTEP illustration of structure **11**. Ellipsoids are shown at 50% probability level.

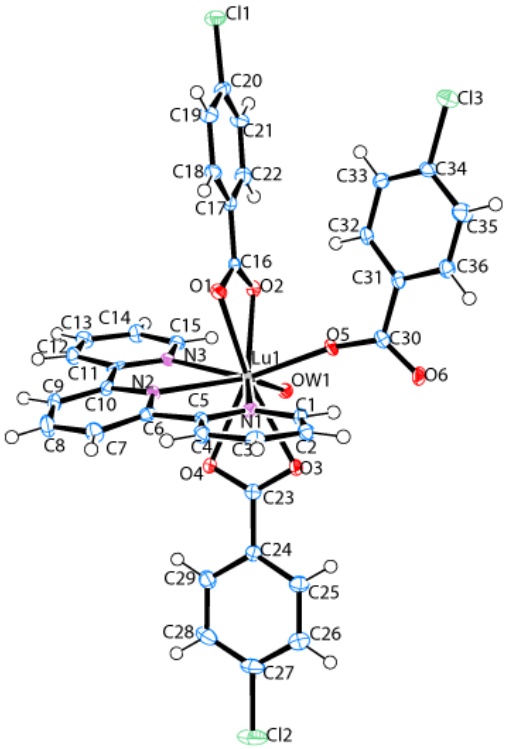

Figure S31: ORTEP illustration of structure **12**. Ellipsoids are shown at 50% probability level.

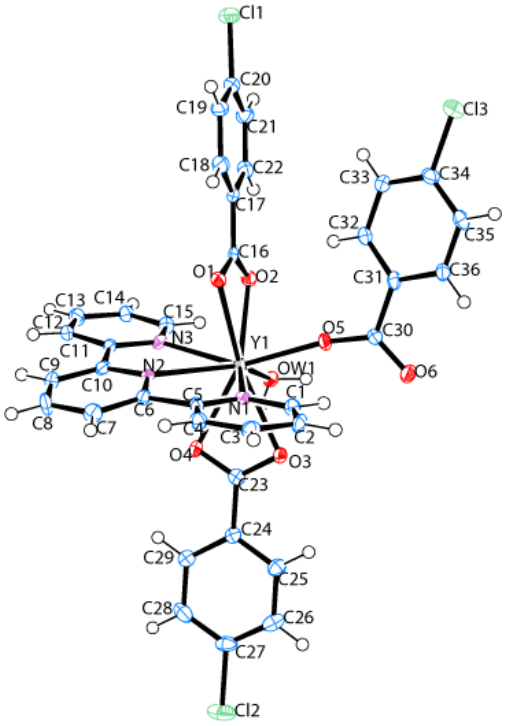

Figure S32: ORTEP illustration of structure **13**. Ellipsoids are shown at 50% probability level.

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III. Table of Bond Distances

Table S1: Bond Lengths Ln-O in Lanthanide Complexes (**1-13**) with *p*-chlorobenzoic acid and 2,2':6',2''-terpyridine

f electrons (Ln^{3+})	d_{Ln-O1} [Å]	d_{Ln-O2} [Å]	d_{Ln-O3} [Å]	d_{Ln-O4} [Å]	d_{Ln-O5} [Å]	d_{Ln-O6} [Å]	d_{Ln-OW1} [Å]
2 (Pr)	2.560(2)	2.619(2)	2.436(2)		2.397(2)	2.411(2)	2.561(2)
3 (Nd)	2.495(3)	2.609(3)	2.418(3)		2.357(3)	2.384(3)	2.546(3)
4 (Pm)							
5 (Sm)	2.458(4)	2.600(4)	2.389(4)		2.354(4)	2.325(4)	2.507(4)
5' (Sm)	2.536(2)	2.480(2)	2.521(2)	2.484(2)	2.319(2)		2.395(2)
6 (Eu)	2.457(3)	2.581(3)	2.376(3)		2.348(3)	2.321(3)	2.502(3)
6' (Eu)	2.517(3)	2.470(4)	2.518(4)	2.472(3)	2.305(3)		2.392(3)
7 (Gd)	2.510(2)	2.459(3)	2.507(3)	2.465(2)	2.299(2)		2.373(2)
8 (Tb)	2.497(2)	2.446(2)	2.498(2)	2.442(2)	2.282(2)		2.356(2)
9 (Dy)	2.484(4)	2.441(4)	2.485(4)	2.427(4)	2.273(4)		2.354(4)
10 (Ho)	2.476(3)	2.425(3)	2.478(3)	2.429(3)	2.266(3)		2.331(3)
11 (Er)	2.463(4)	2.421(4)	2.470(4)	2.416(4)	2.255(4)		2.329(4)
12 (Tm)	2.450(3)	2.409(3)	2.469(3)	2.396(3)	2.246(3)		2.303(3)
13 (Yb)	2.439(2)	2.408(2)	2.466(2)	2.385(2)	2.232(2)		2.298(2)
14 (Lu)	2.435(3)	2.398(3)	2.463(3)	2.382(3)	2.224(3)		2.291(3)
0 (Y)	2.473(3)	2.425(3)	2.477(3)	2.427(3)	2.262 (3)		2.329(3)

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IV. Tables of Supramolecular Interaction Distances

Table S2: Intermolecular Non-Covalent Interaction Distances in Structure Type II Complexes (**2-4**) (where Ln=Nd, Sm and Eu)

Compound	d(Cl1-Cl3) [Å]	d(π-π) [Å]
2 (Nd)	3.4495(19)	3.3710(16)
3 (Sm)	3.437(3)	3.374(2)
4 (Eu)	3.445(2)	3.392(2)

Table S3: Intermolecular Non-Covalent Interaction Distances in Structure Type III Complexes (**3', 4', 5-13**) (where Ln=Sm→Lu+Y)

Compound	d(Cl2-π) [Å]
3' (Sm)	3.570(2)
4' (Eu)	3.564(3)
5 (Gd)	3.5536(19)
6 (Tb)	3.528(3)
7 (Dy)	3.521(3)
8 (Ho)	3.521(3)
9 (Er)	3.502(3)
10 (Tm)	3.489(3)
11 (Yb)	3.4894(15)
12 (Lu)	3.485(2)
13 (Y)	3.519(2)