

**Supramolecular assembly of molecular rare-earth-3,5-dichlorobenzoic acid-2,2':6',2''-terpyridine materials: structural systematics, luminescence properties, and magnetic behavior**

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**Supporting Info Section**

**I. Additional Figures**

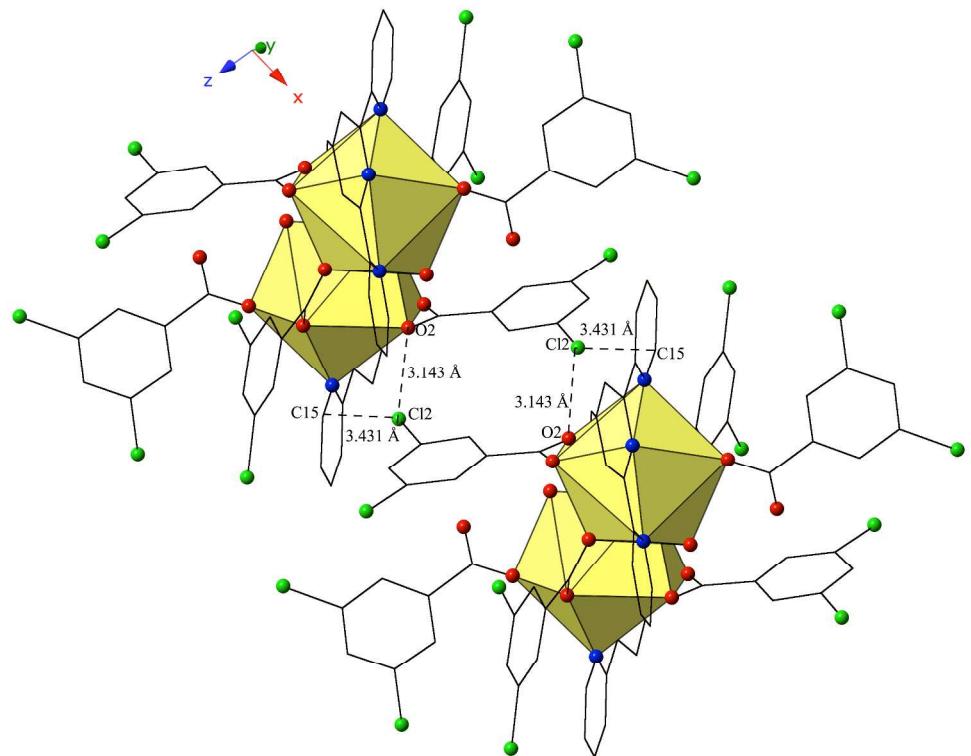
**II. Powder X-ray Diffraction data**

**III. Thermal Ellipsoid Plots**

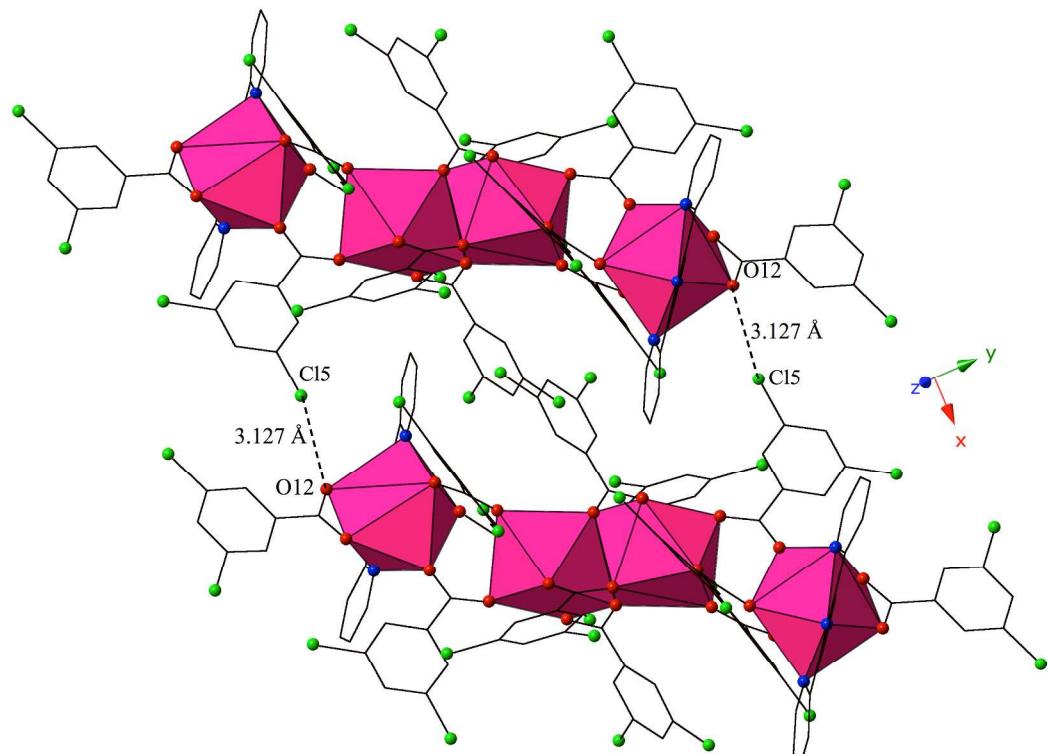
**IV. Tables of Bond Distances**

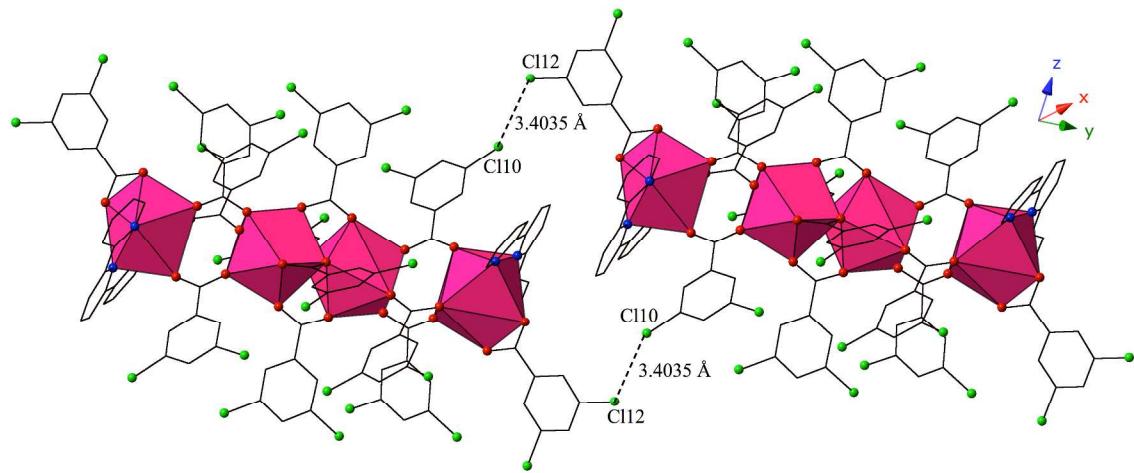
**V. Tables of Supramolecular Interactions**

## I. Additional Figures

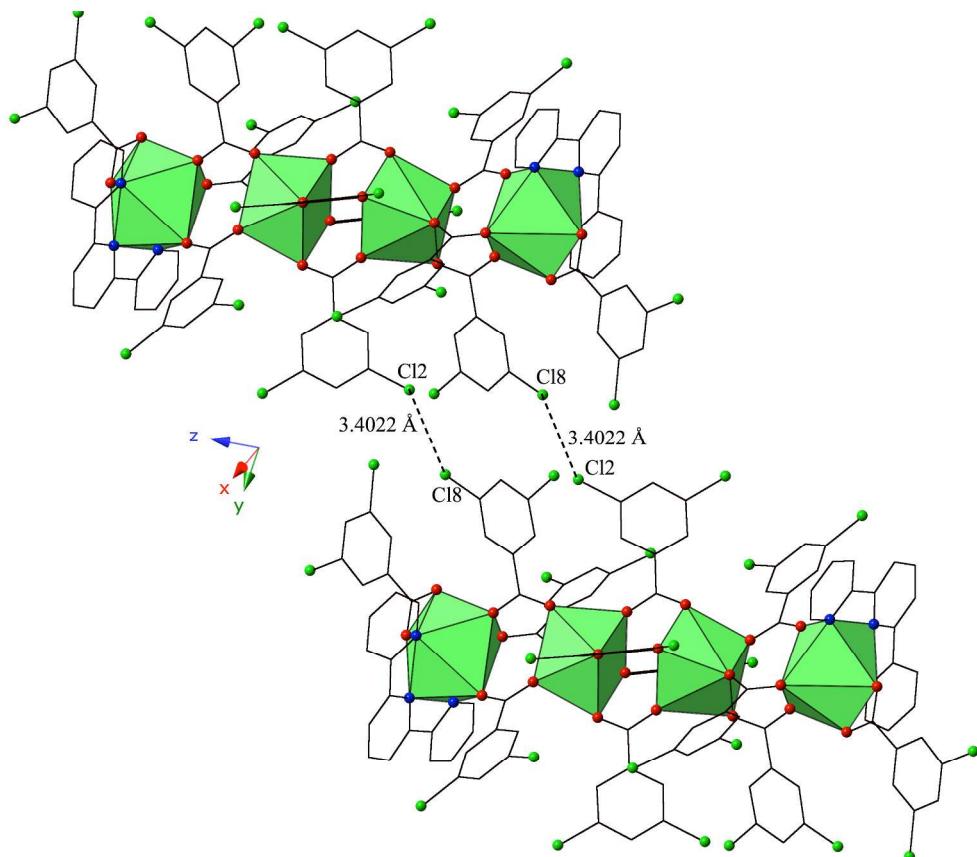


**Figure S1** Complex **3** viewed in approximately the (101) plane highlighting the halogen bonding and localized  $\text{Cl}-\pi$  interactions that further link  $\text{Ce}^{3+}$  tectons.

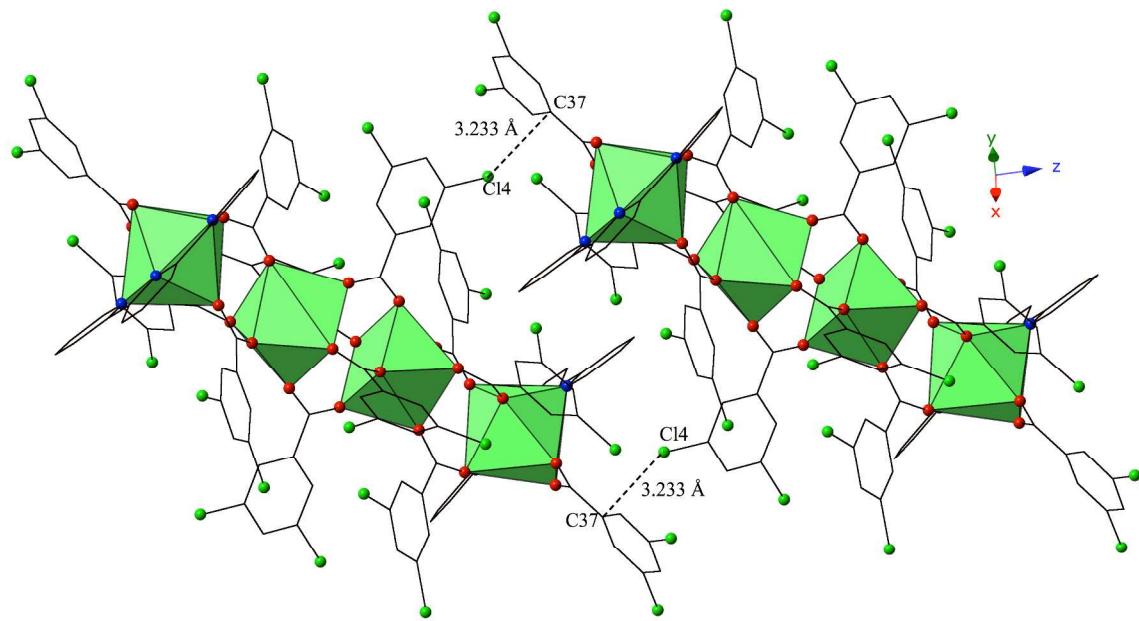




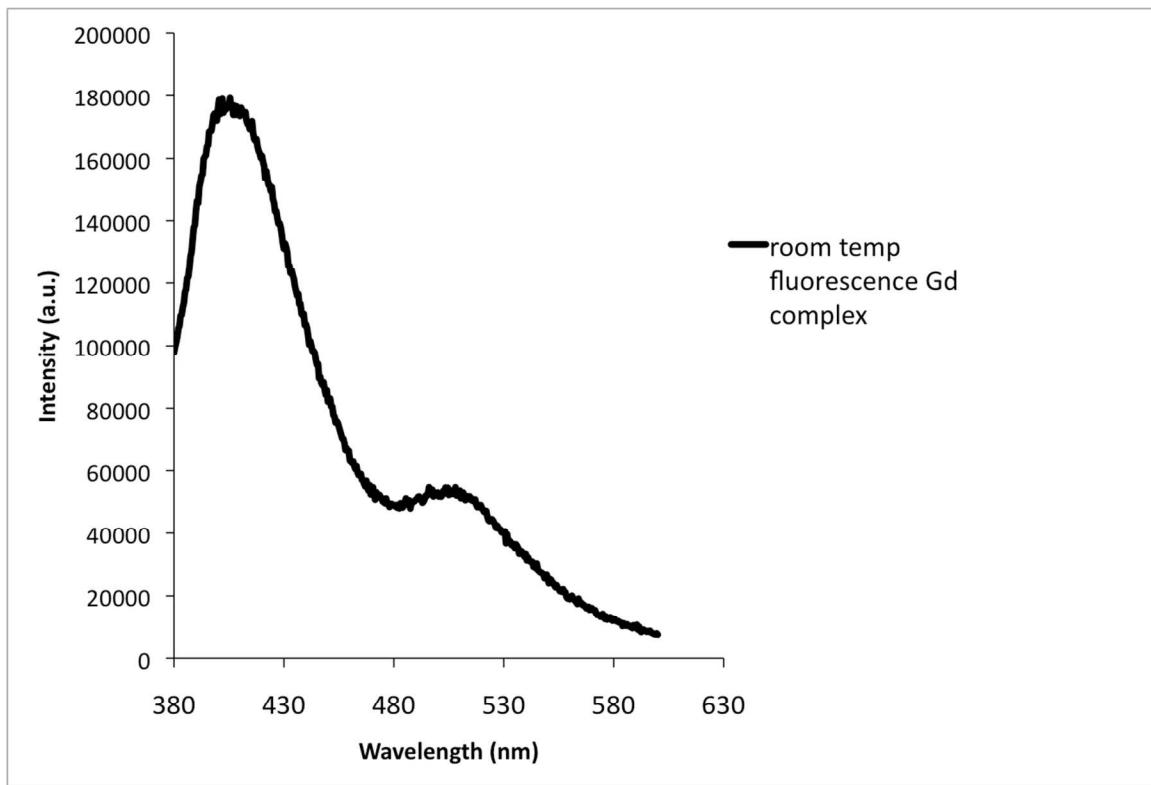
**Figure S2 (Top)** Complex **6** in approximately the (110) plane. Halogen bonding interactions that link tetramers into supramolecular 3D network are shown. **(Bottom)** Type II halogen-halogen interactions which supplement assembly into supramolecular 3D network are highlighted.



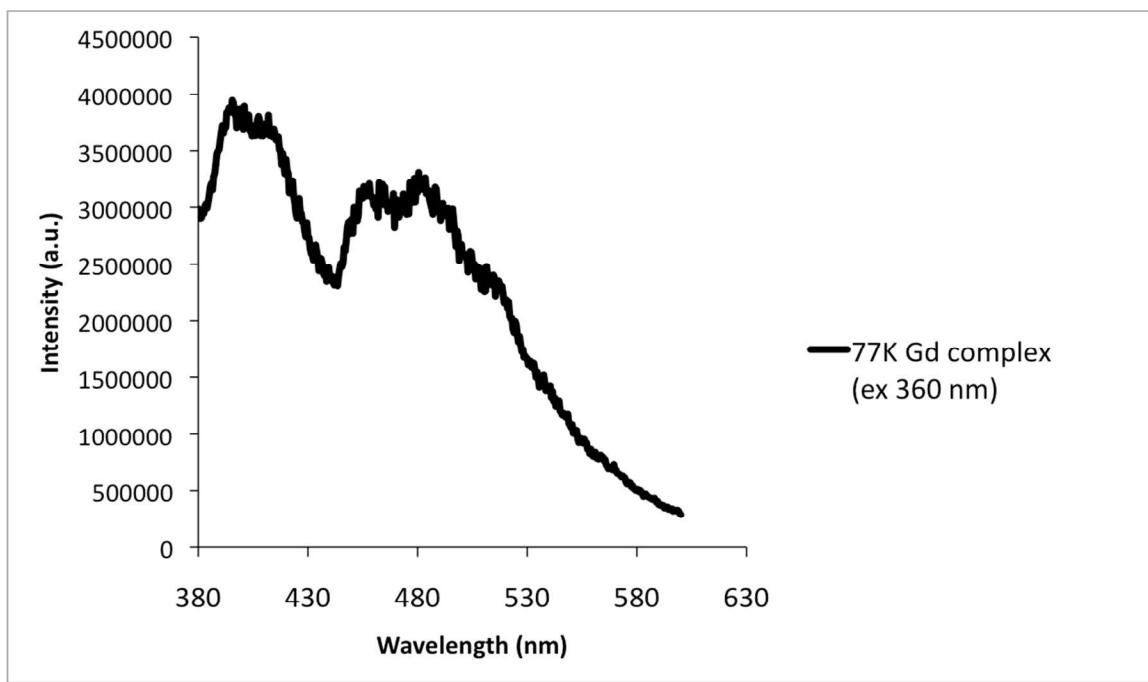
**Figure S3** Complex **12** in approximately the (011) plane. Type I halogen-halogen interactions that supplement assembly of **12** into 2D sheets are shown.



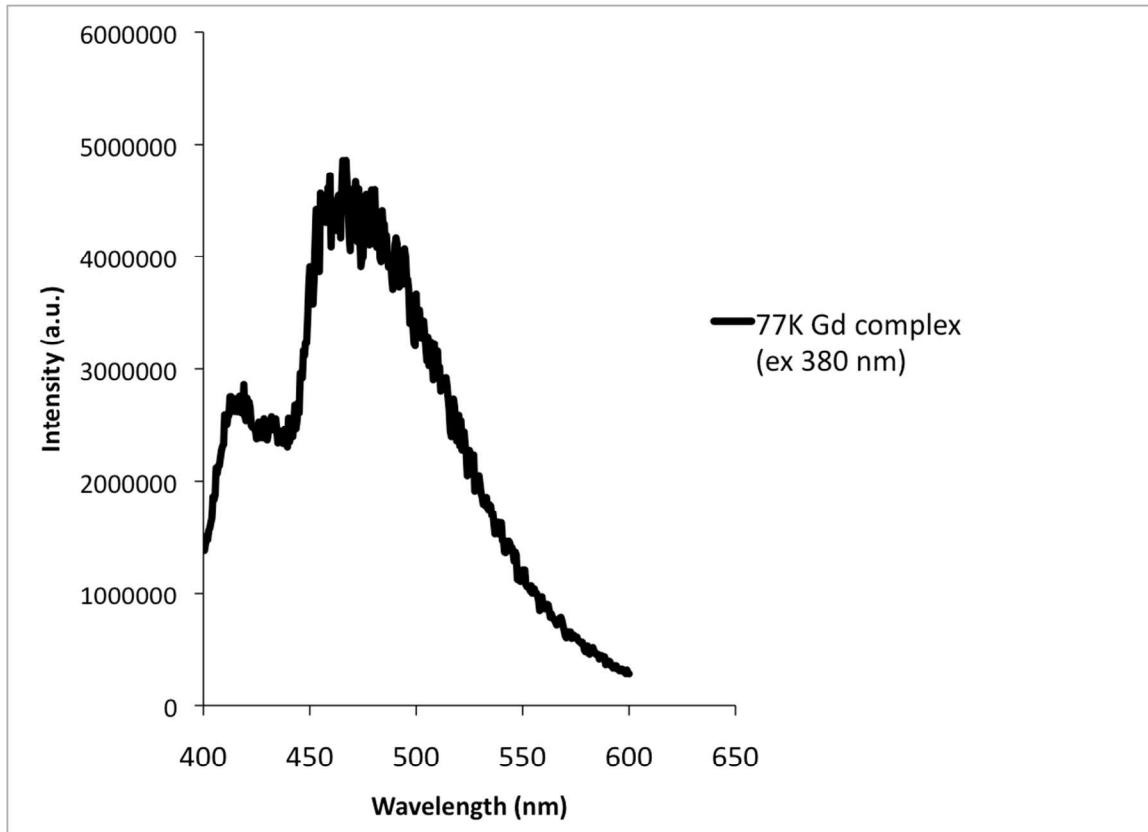
**Figure S4** Complex **12** in approximately the (101) plane. Localized  $\text{Cl}-\pi$  interactions, which tether tetramers of **12** into supramolecular 3D network are highlighted.



**Figure S5** Room temperature, solid state, emission spectrum for  $\text{Gd}^{3+}$  complex **8**.



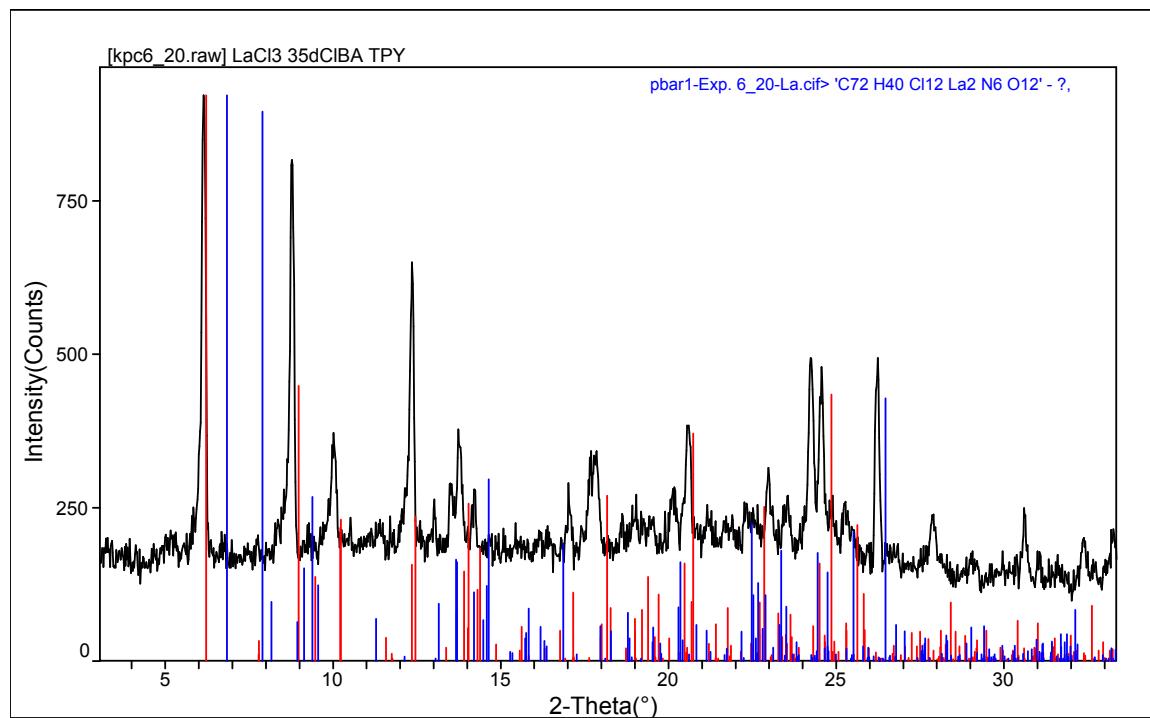
**Figure S6** Low temperature ( $77\text{K}$ ), solid state, emission spectrum for  $\text{Gd}^{3+}$  complex **8** upon excitation at  $360\text{ nm}$ .



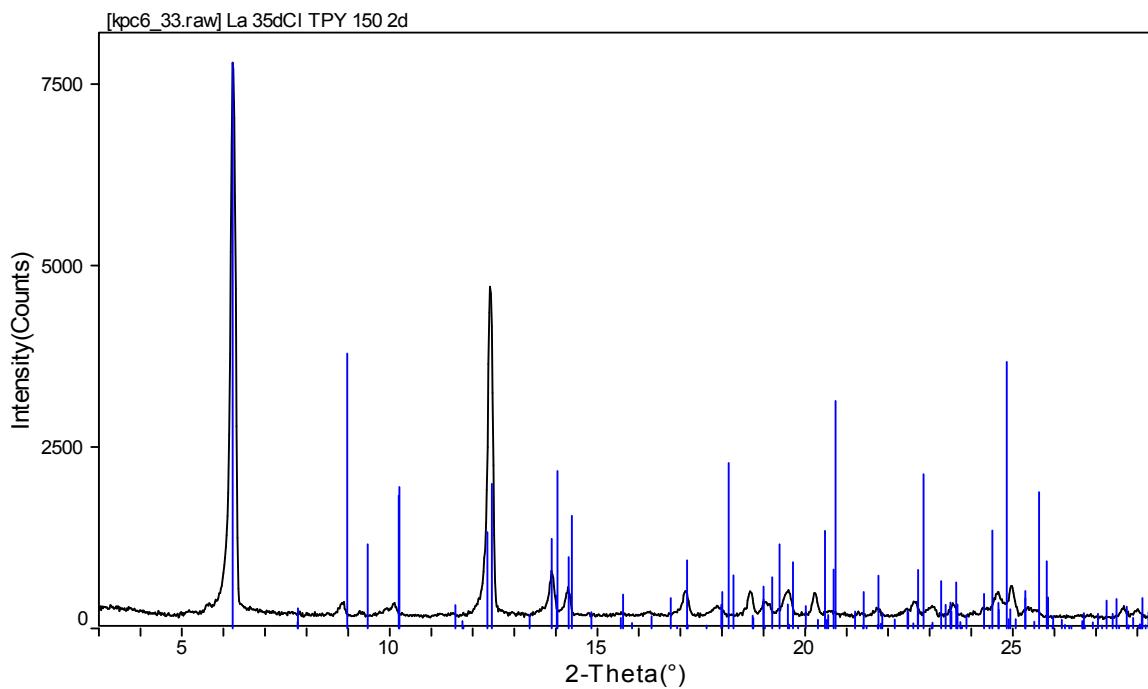
**Figure S7** Low temperature ( $77\text{K}$ ), solid state, emission spectrum for  $\text{Gd}^{3+}$  complex **8** upon excitation at  $380\text{ nm}$ .

## II. Powder X-ray diffraction data

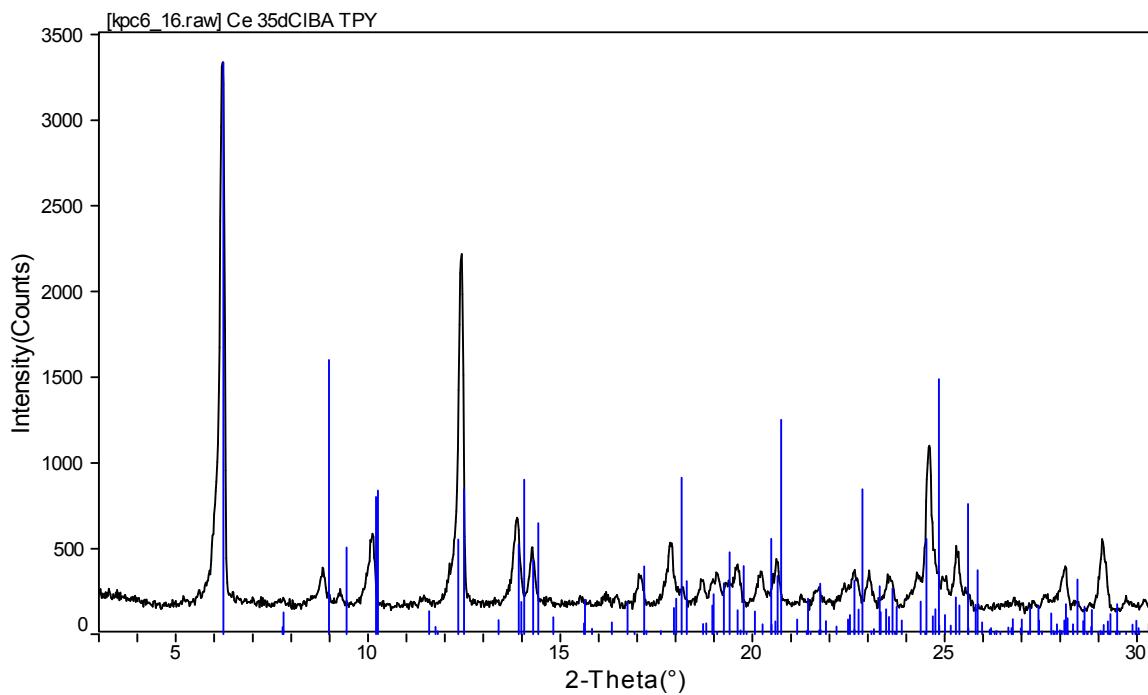
For the following PXRD spectra it is important to note that calculated patterns are from low temperature (100K) data collections while observed patterns were collected at room temperature (298 K). This difference may result in slight shifts in two-theta values.



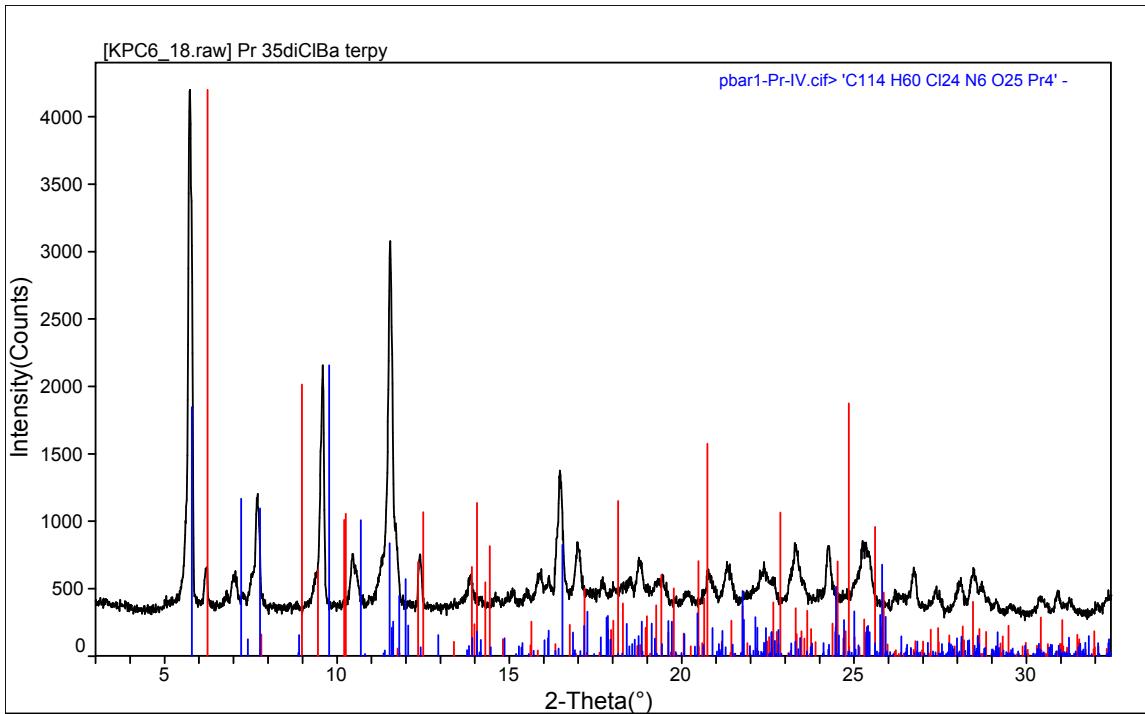
**Figure S8** The observed PXRD pattern of structure **1** with calculated pattern overlaid in blue. Impurities in **1** have been identified as complex **2** (CIF overlaid in red).



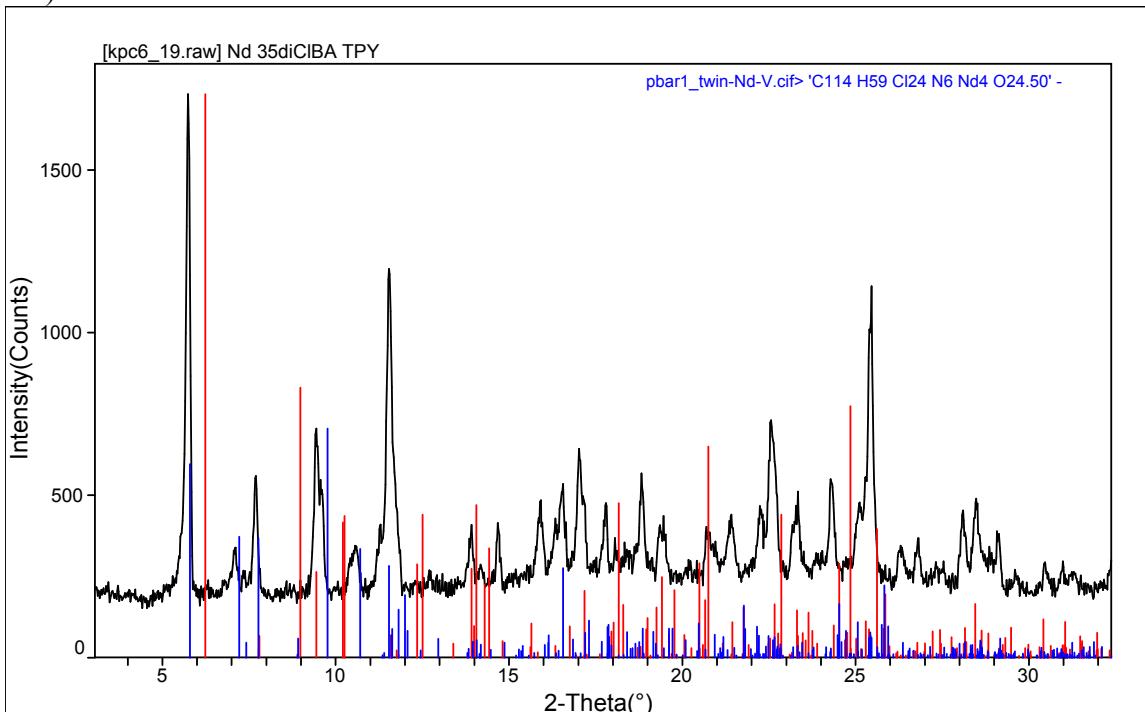
**Figure S9** The observed PXRD pattern of structure **2** with calculated pattern overlaid in blue.



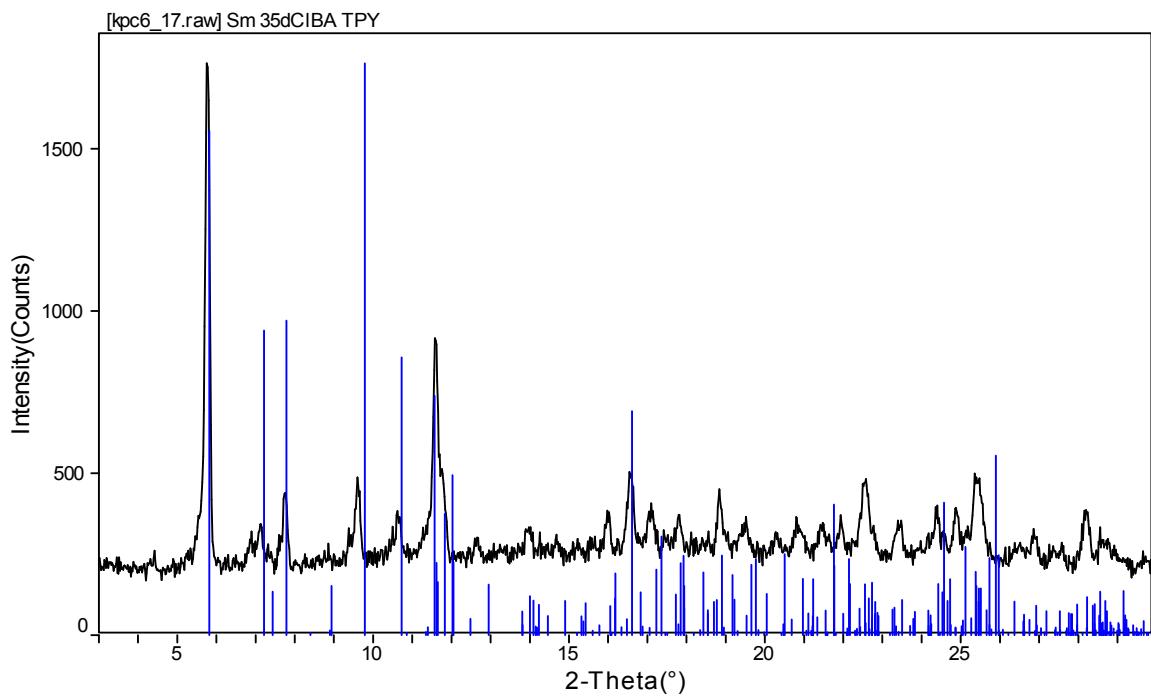
**Figure S10** The observed PXRD pattern of structure **3** with calculated pattern overlaid in blue.



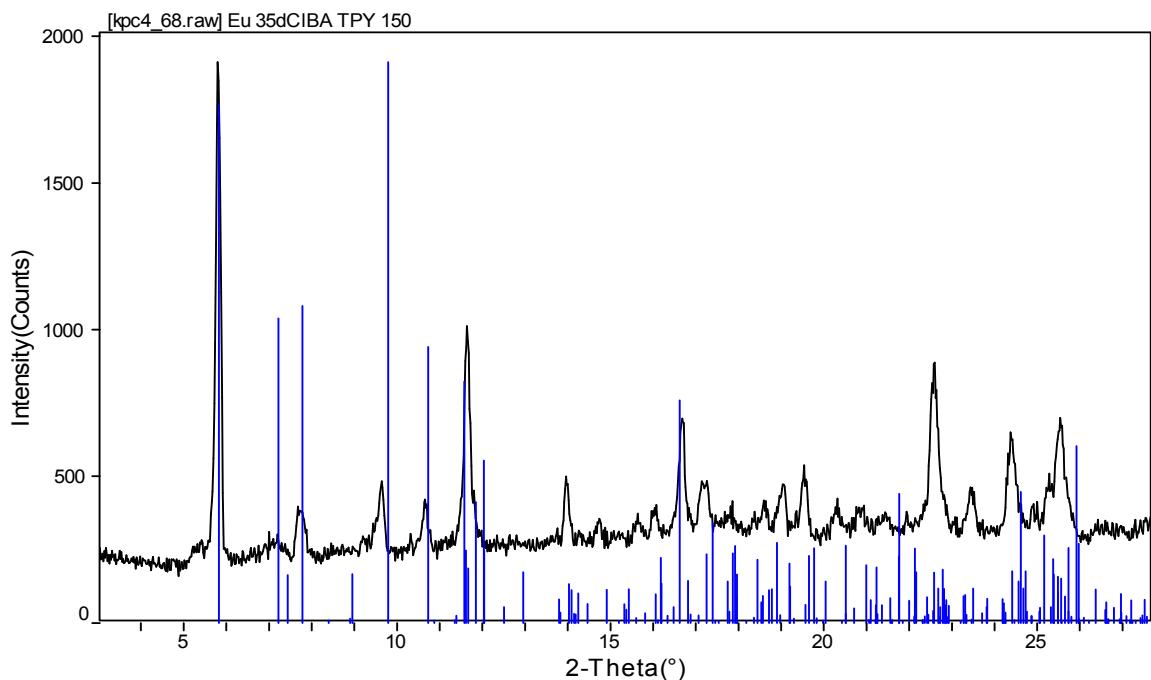
**Figure S11** The observed PXRD pattern of structure **4** with calculated pattern overlaid in blue. Minor impurities in **4** have been identified as the  $\text{Pr}^{3+}$  of complex **3** (CIF overlaid in red).



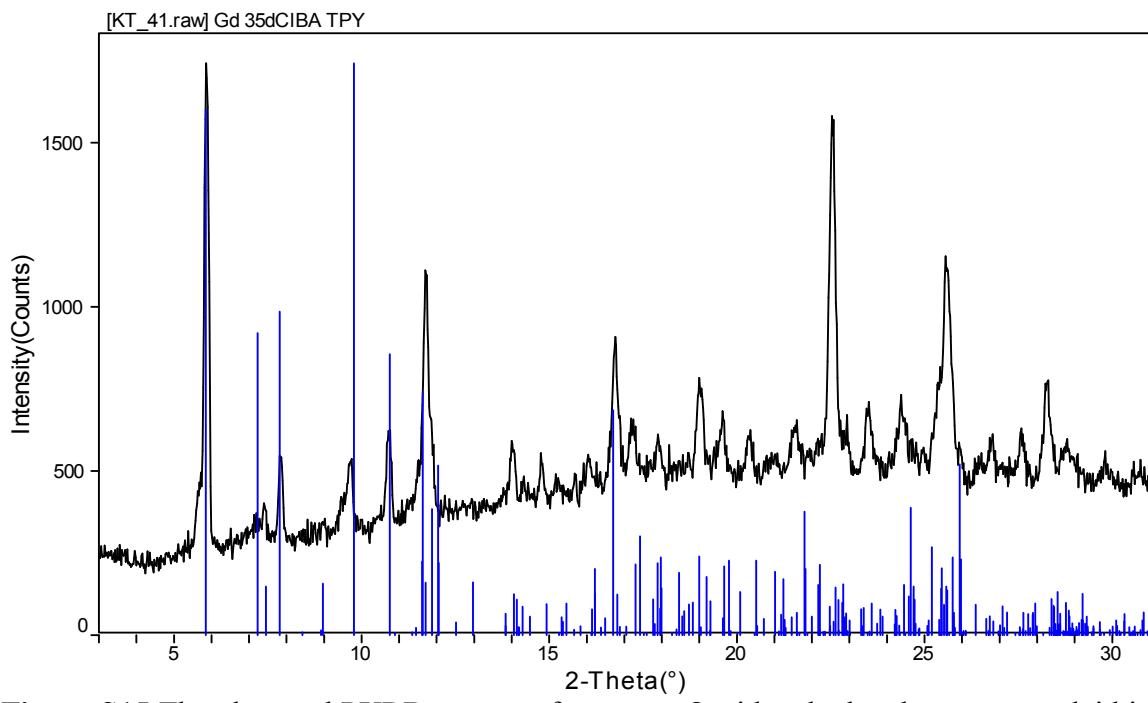
**Figure S12** The observed PXRD pattern of structure **5** with calculated pattern overlaid in blue. Minor impurities in **5** have been identified as the  $\text{Nd}^{3+}$  of complex **3** (CIF overlaid in red).



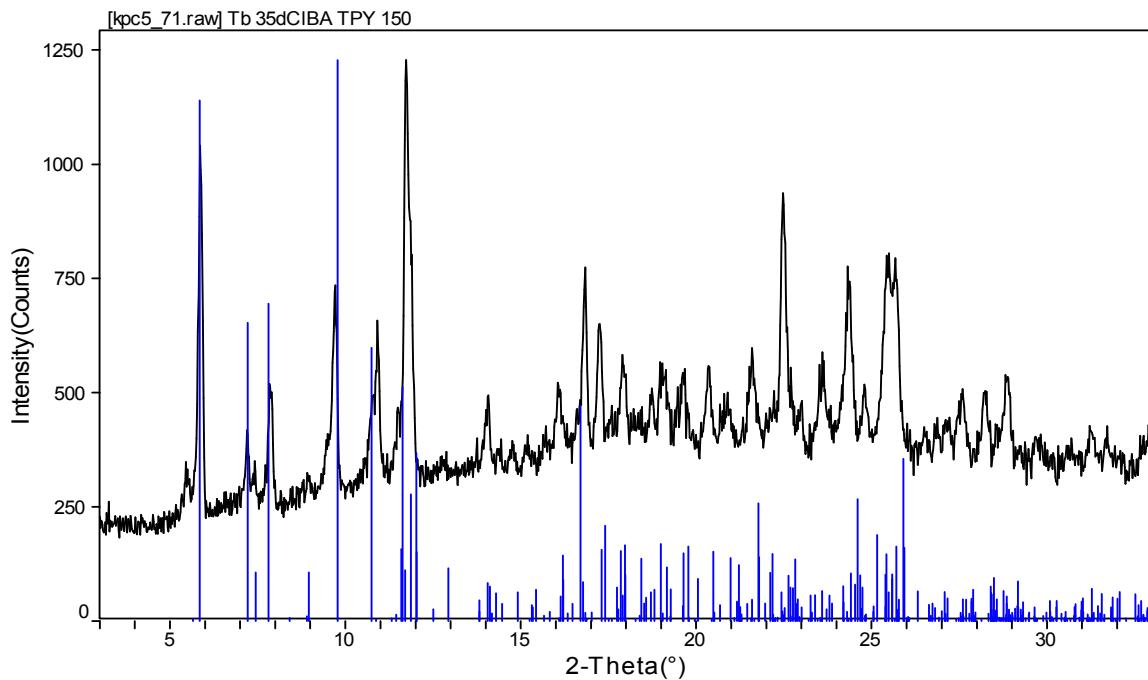
**Figure S13** The observed PXRD pattern of structure **6** with calculated pattern overlaid in blue.



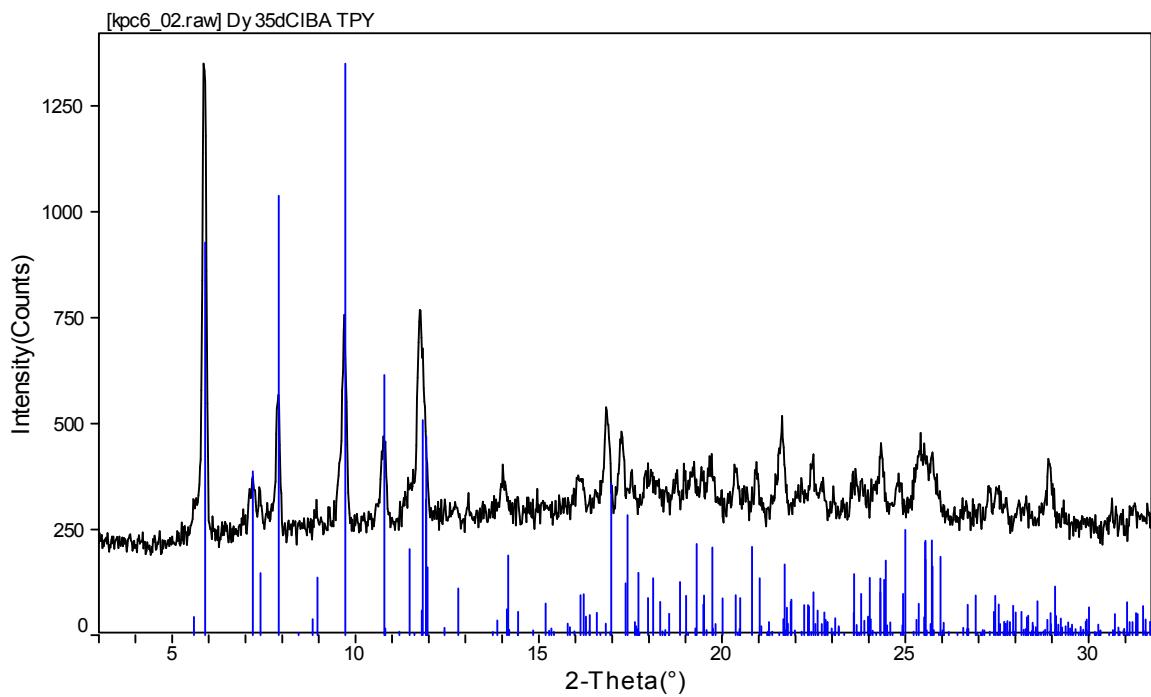
**Figure S14** The observed PXRD pattern of structure **7** with calculated pattern overlaid in blue.



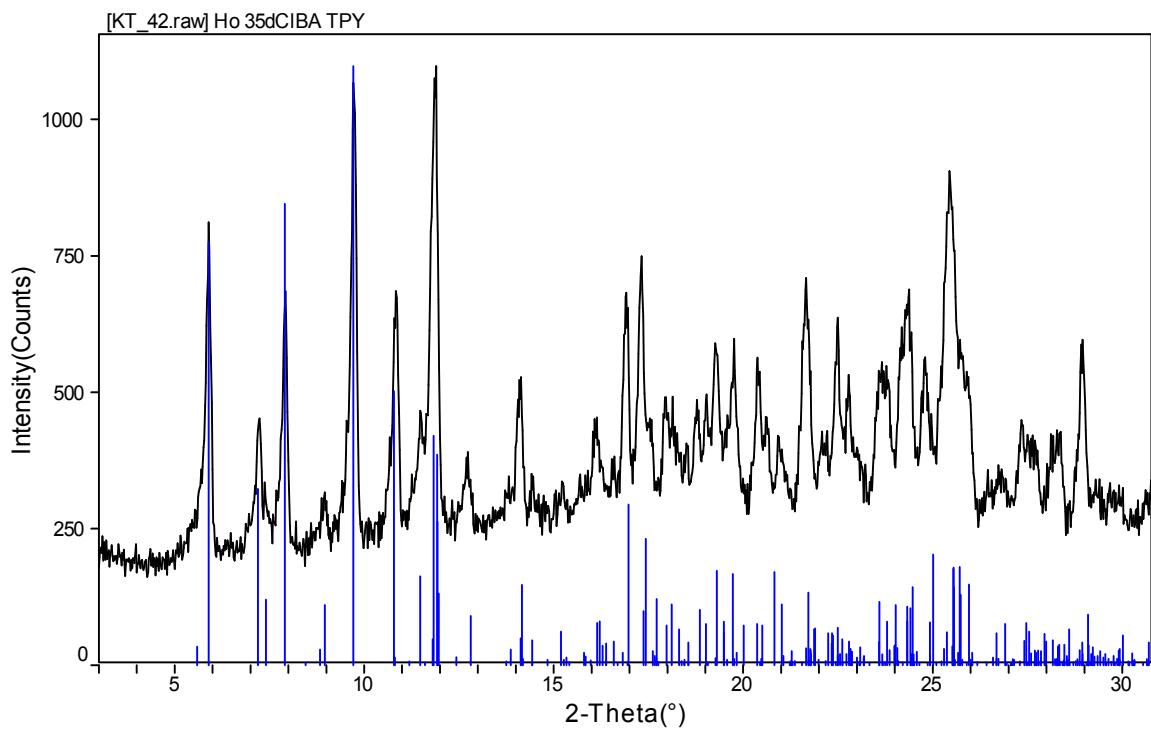
**Figure S15** The observed PXRD pattern of structure **8** with calculated pattern overlaid in blue.



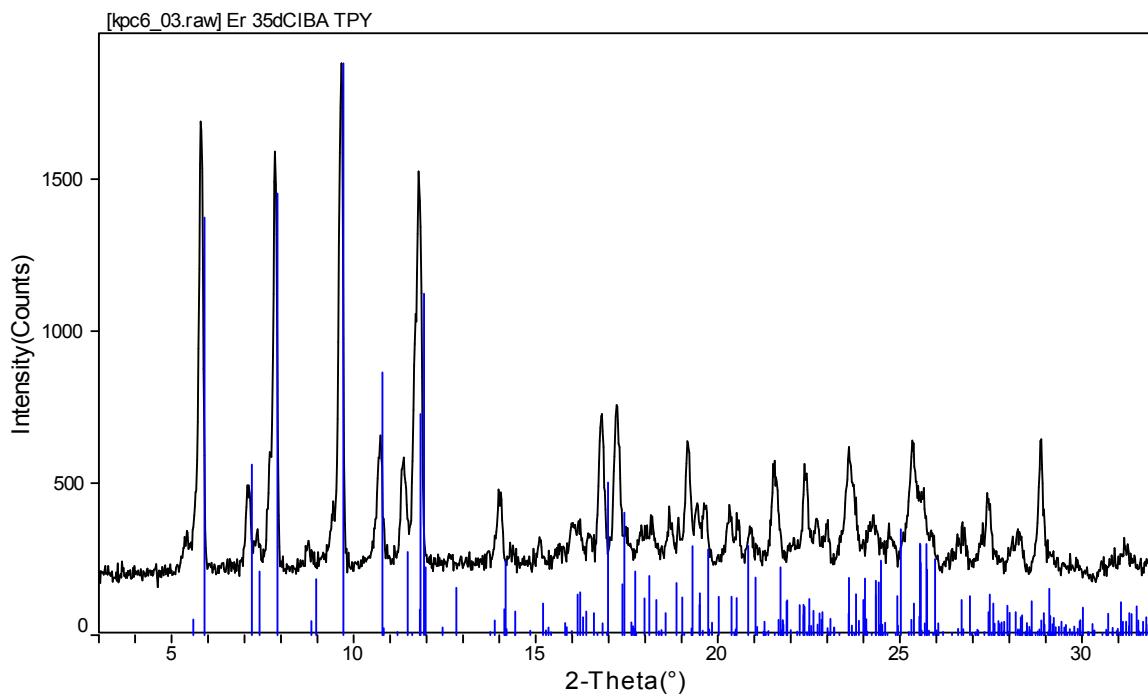
**Figure S16** The observed PXRD pattern of structure **9** with calculated pattern overlaid in blue.



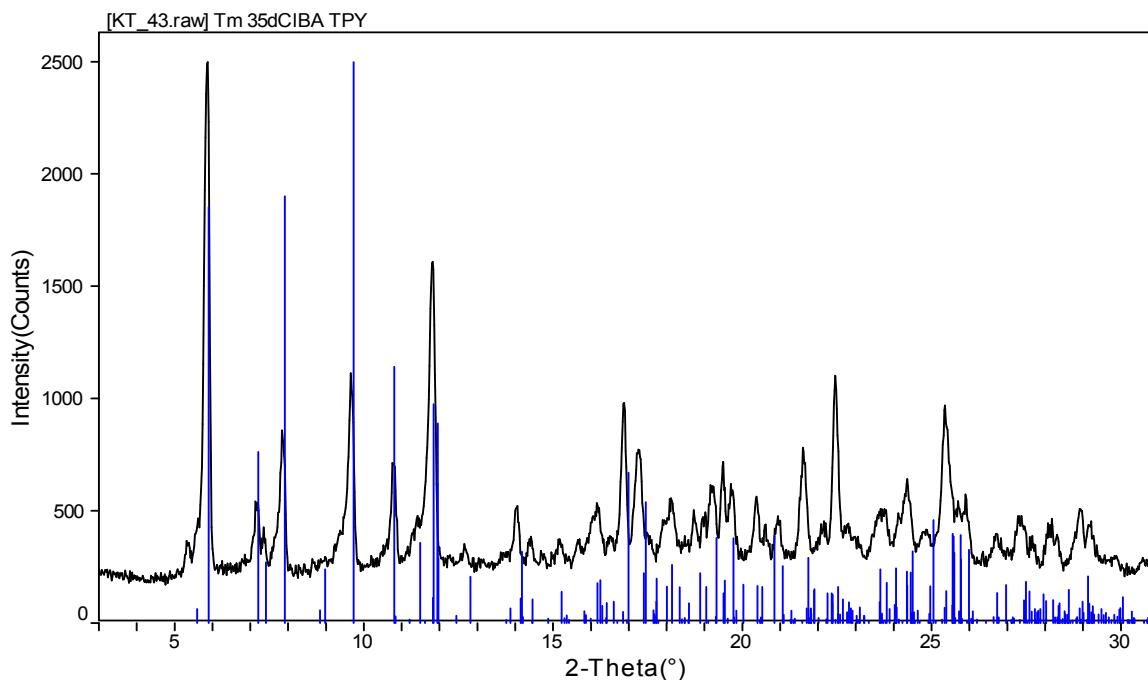
**Figure S17** The observed PXRD pattern of structure **10** with calculated pattern overlaid in blue.



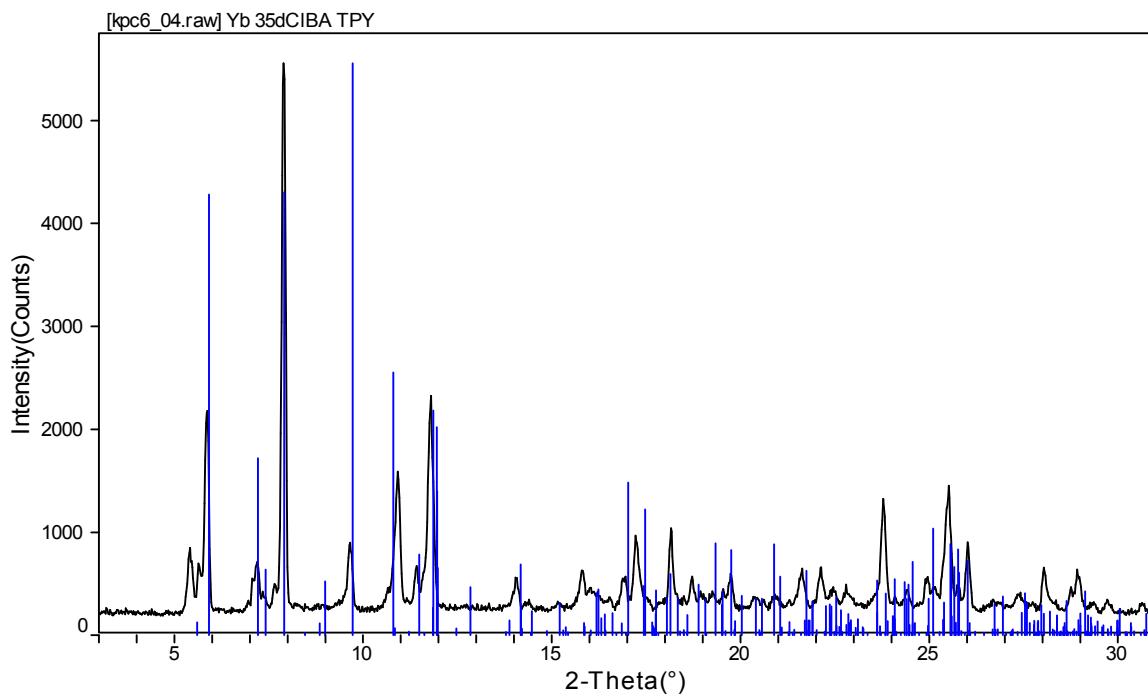
**Figure S18** The observed PXRD pattern of structure **11** with calculated pattern overlaid in blue.



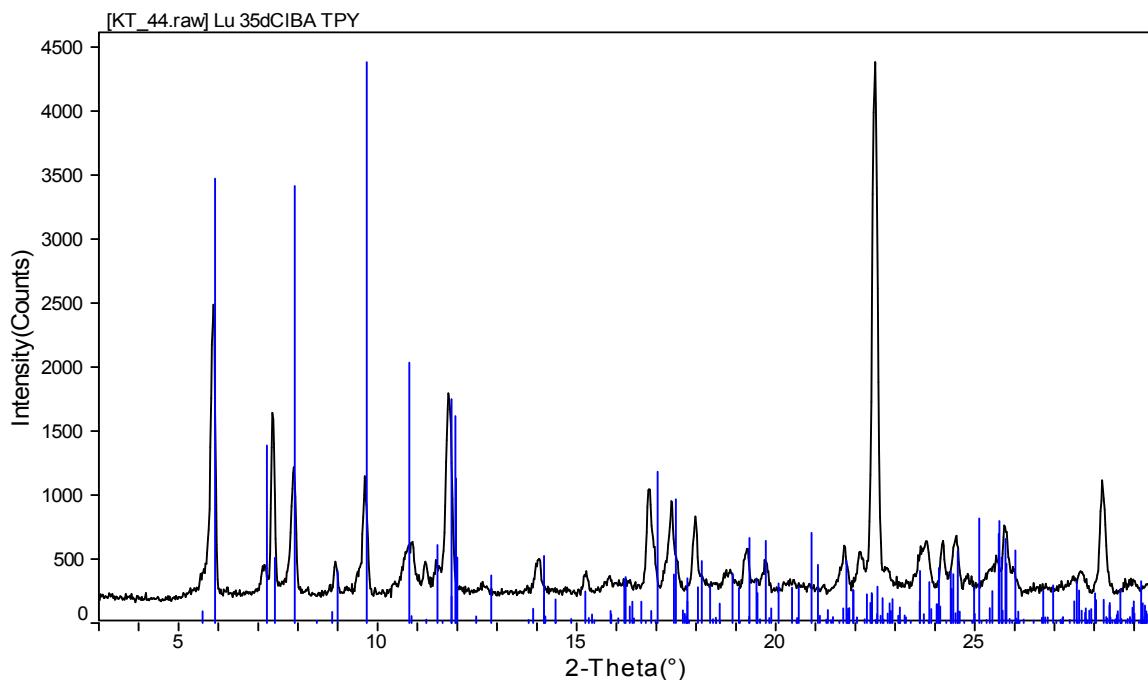
**Figure S19** The observed PXRD pattern of structure **12** with calculated pattern overlaid in blue.



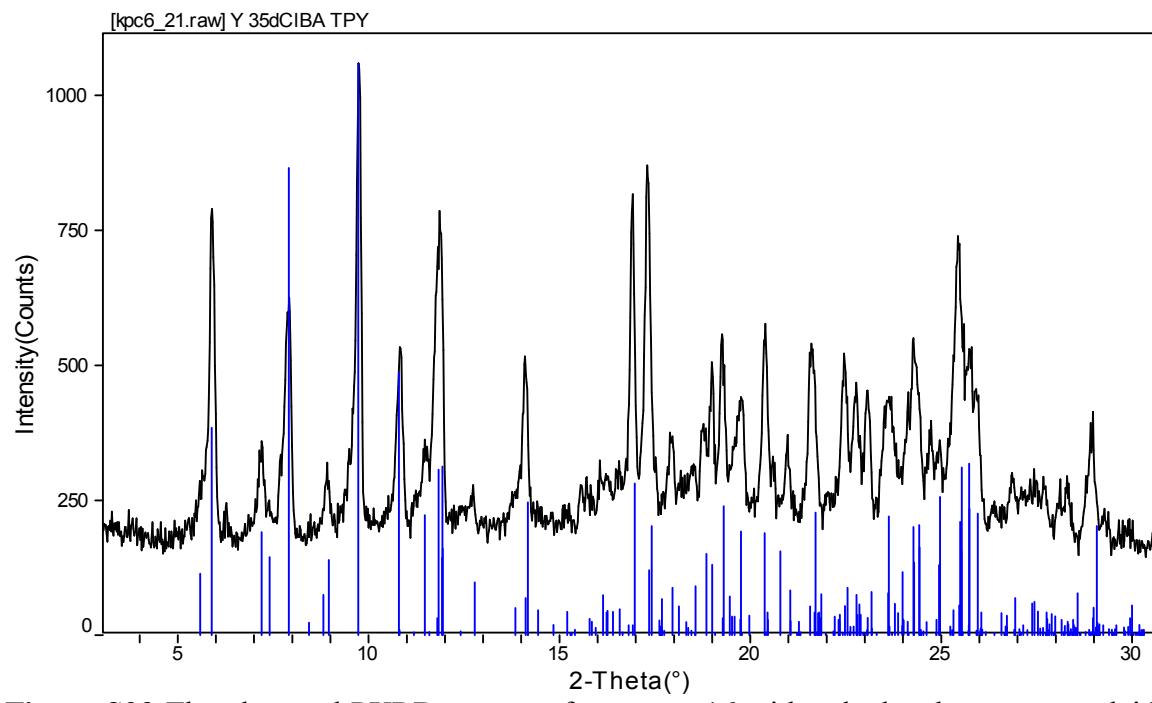
**Figure S20** The observed PXRD pattern of structure **13** with calculated pattern overlaid in blue.



**Figure S21** The observed PXRD pattern of structure **14** with calculated pattern overlaid in blue.

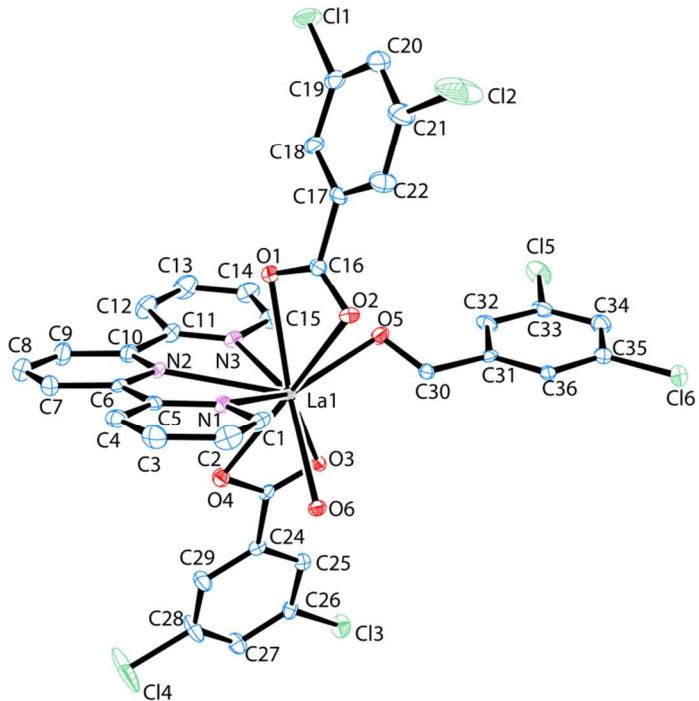


**Figure S22** The observed PXRD pattern of structure **15** with calculated pattern overlaid in blue.

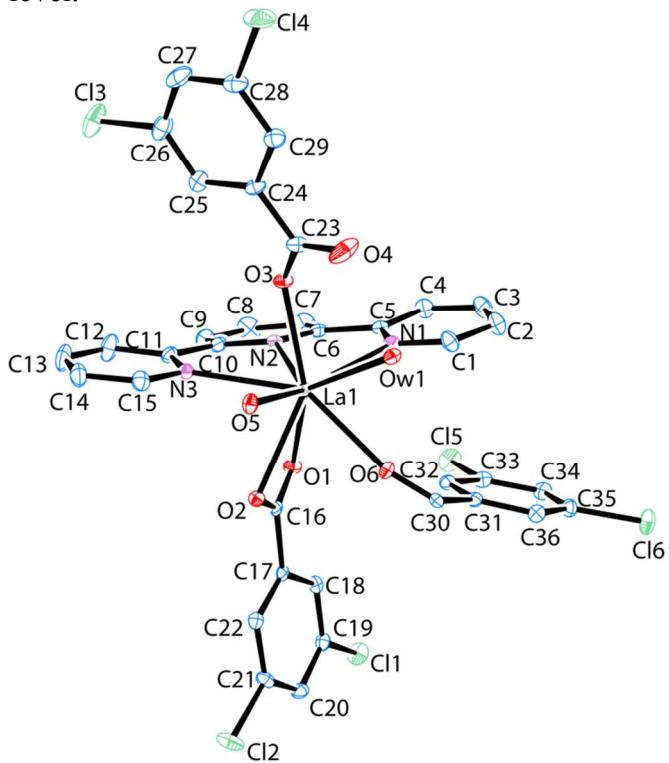


**Figure S23** The observed PXRD pattern of structure **16** with calculated pattern overlaid in blue.

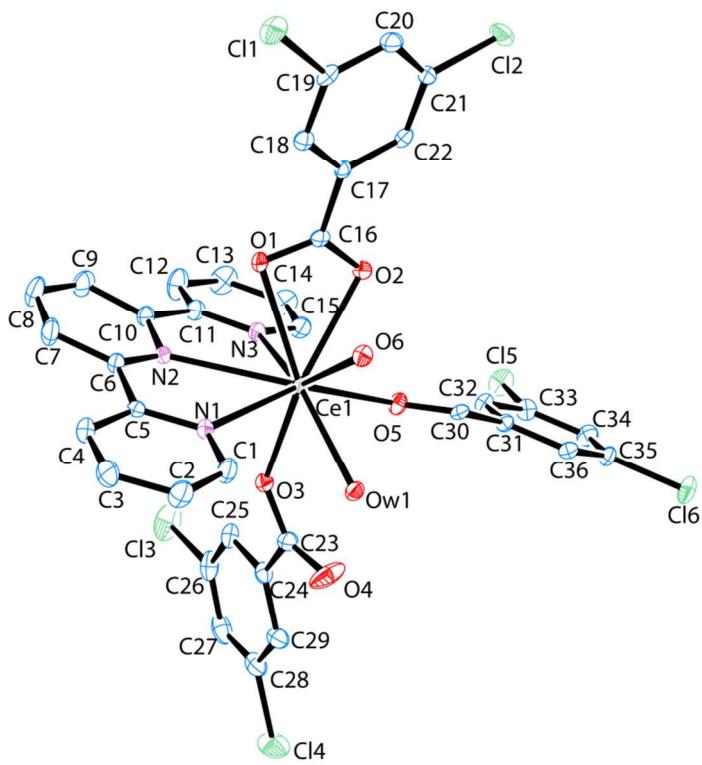
### III. Thermal Ellipsoid Plots



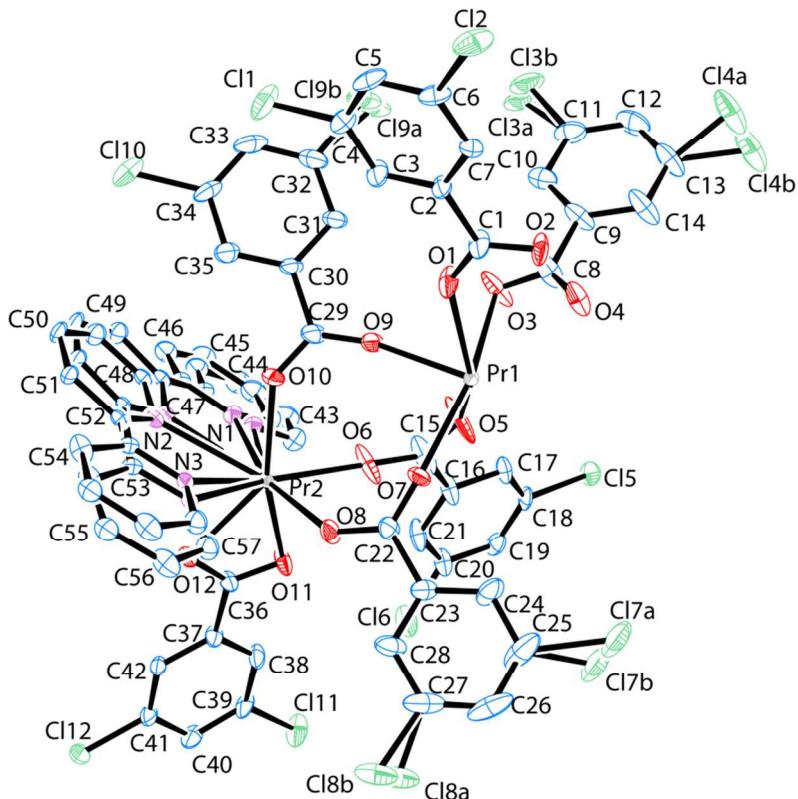
**Figure S24** ORTEP illustration of complex 1. Ellipsoids are shown at 50% probability level.



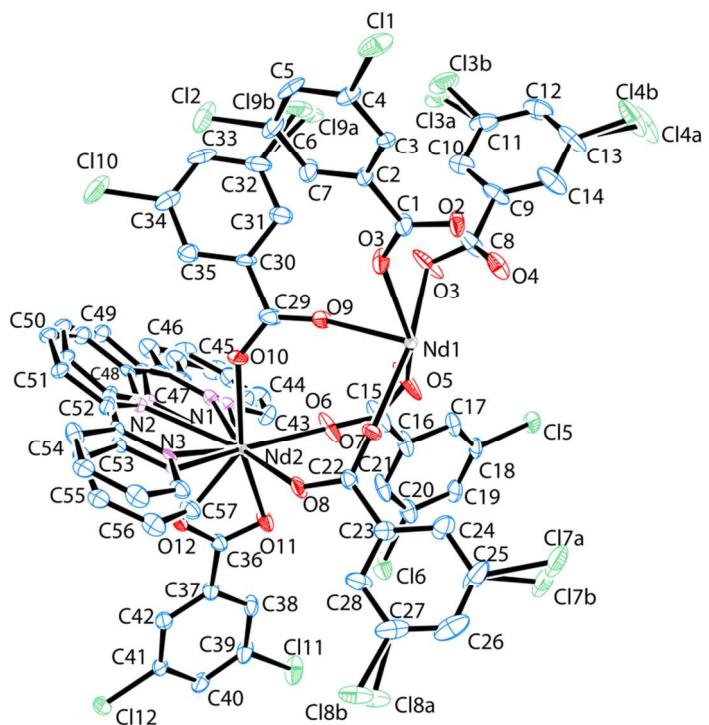
**Figure S25** ORTEP illustration of complex 2. Ellipsoids are shown at 50% probability level.



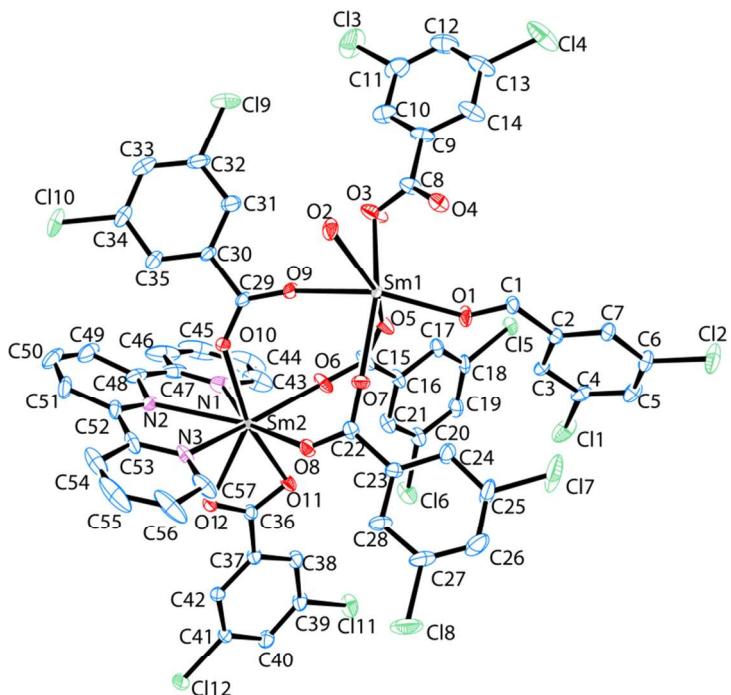
**Figure S26** ORTEP illustration of complex 3. Ellipsoids are shown at 50% probability level.



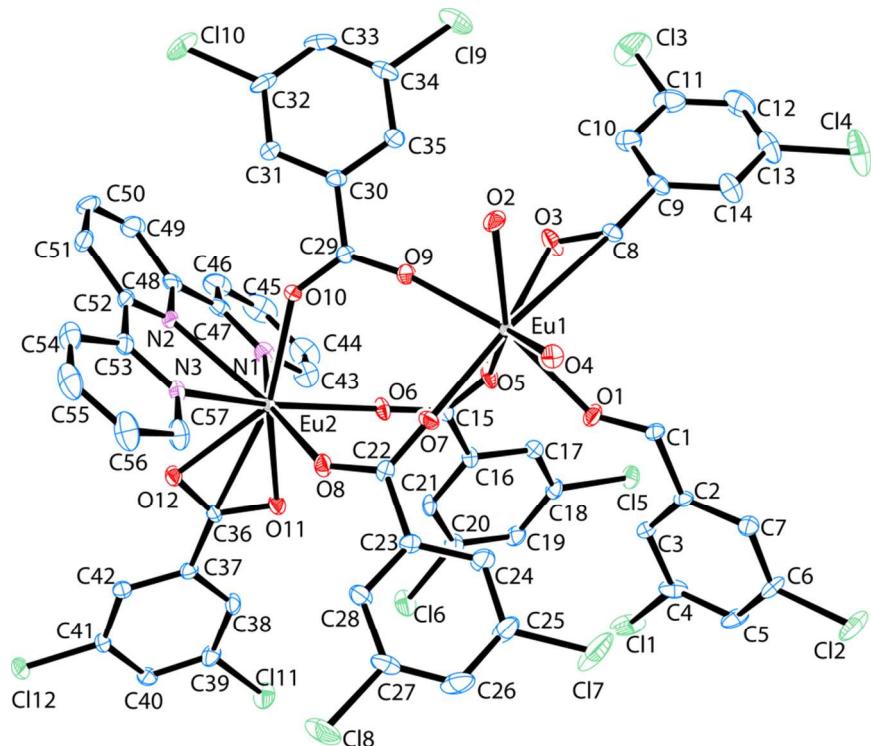
**Figure S27** ORTEP illustration of complex 4. Ellipsoids are shown at 50% probability level.



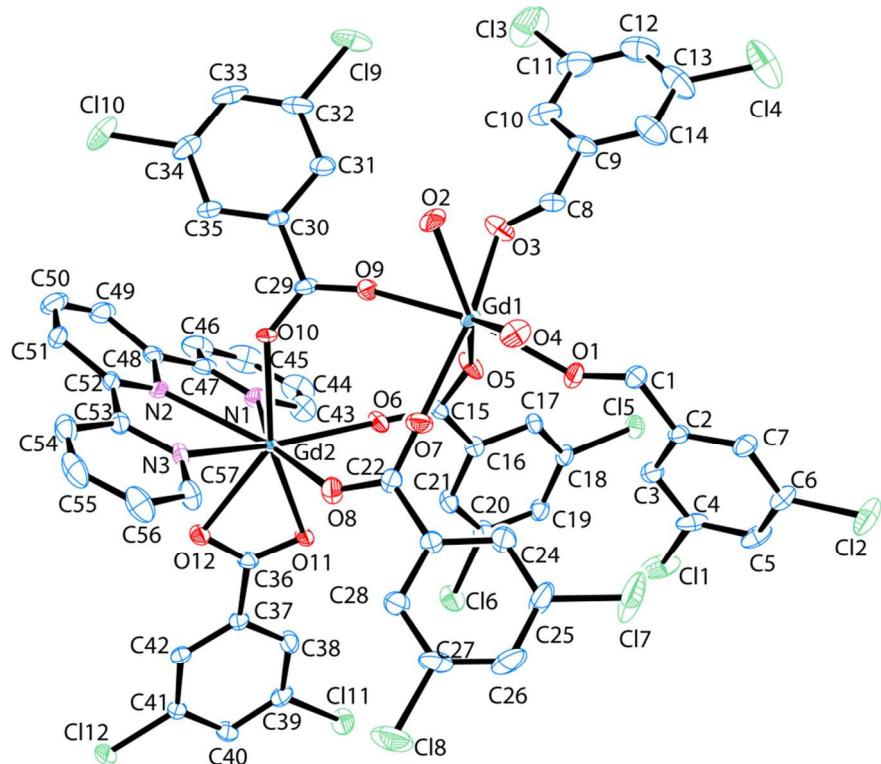
**Figure S28** ORTEP illustration of complex 5. Ellipsoids are shown at 50% probability level.



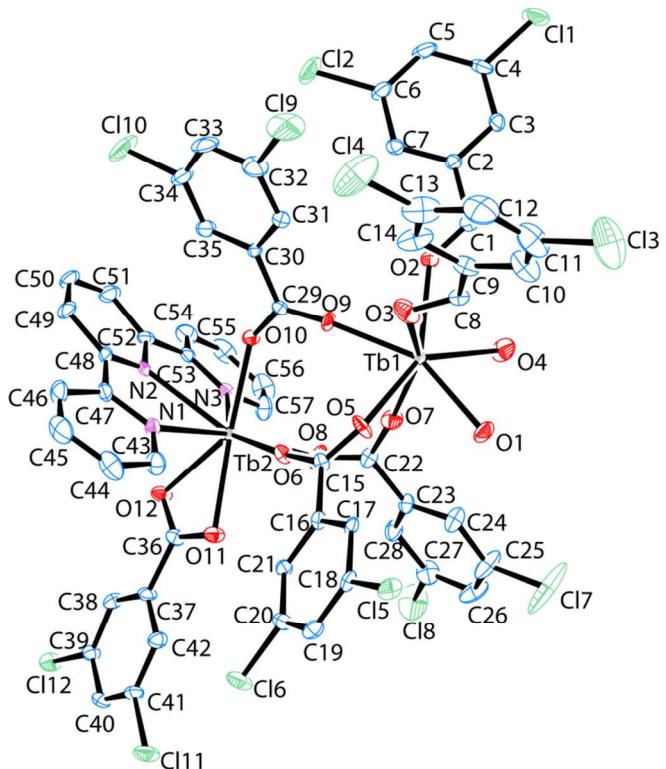
**Figure S29** ORTEP illustration of complex 6. Ellipsoids are shown at 50% probability level.



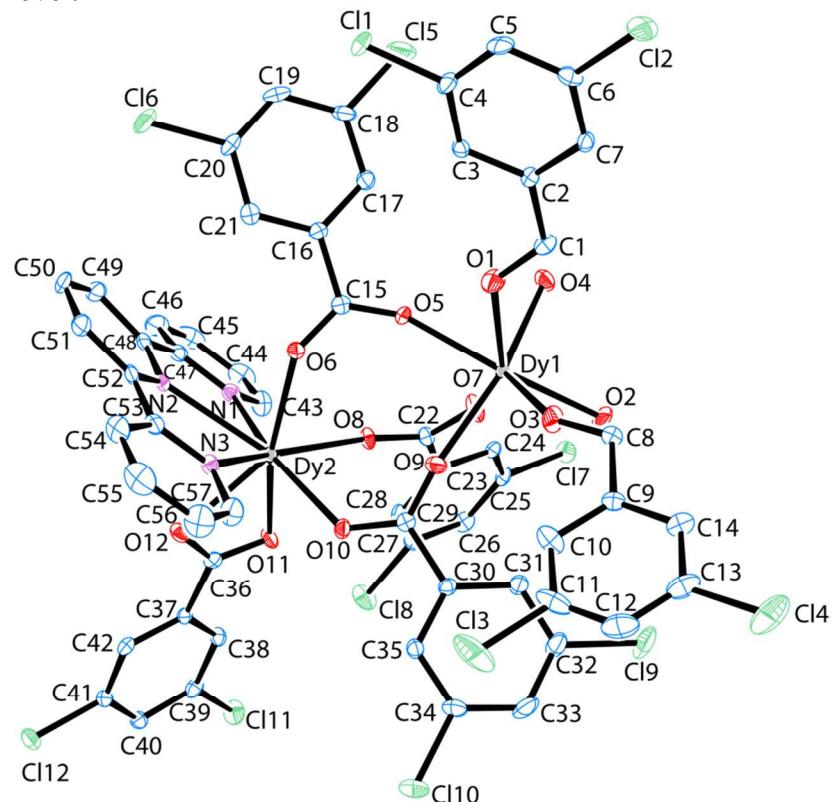
**Figure S30** ORTEP illustration of complex 7. Ellipsoids are shown at 50% probability level.



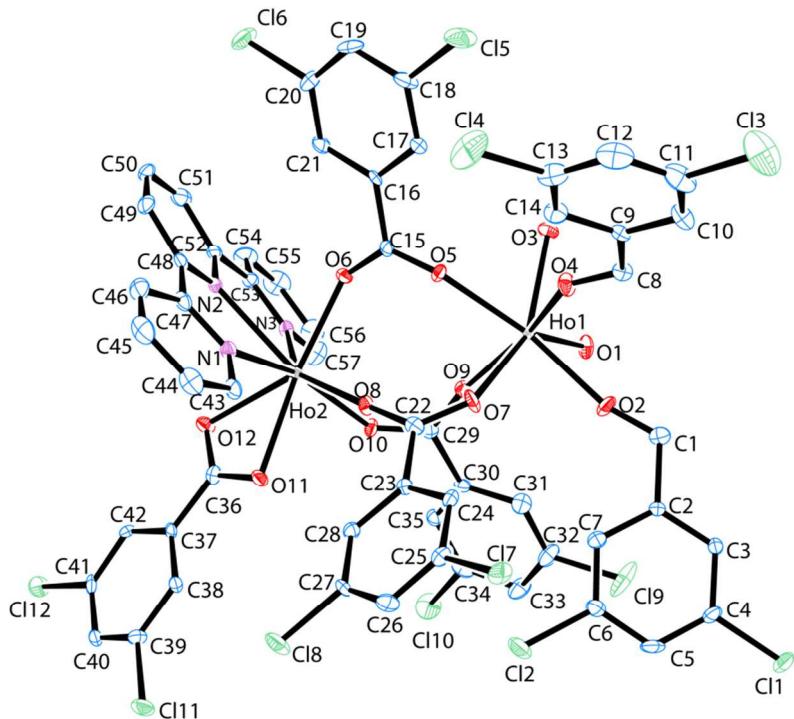
**Figure S31** ORTEP illustration of complex 8. Ellipsoids are shown at 50% probability level.



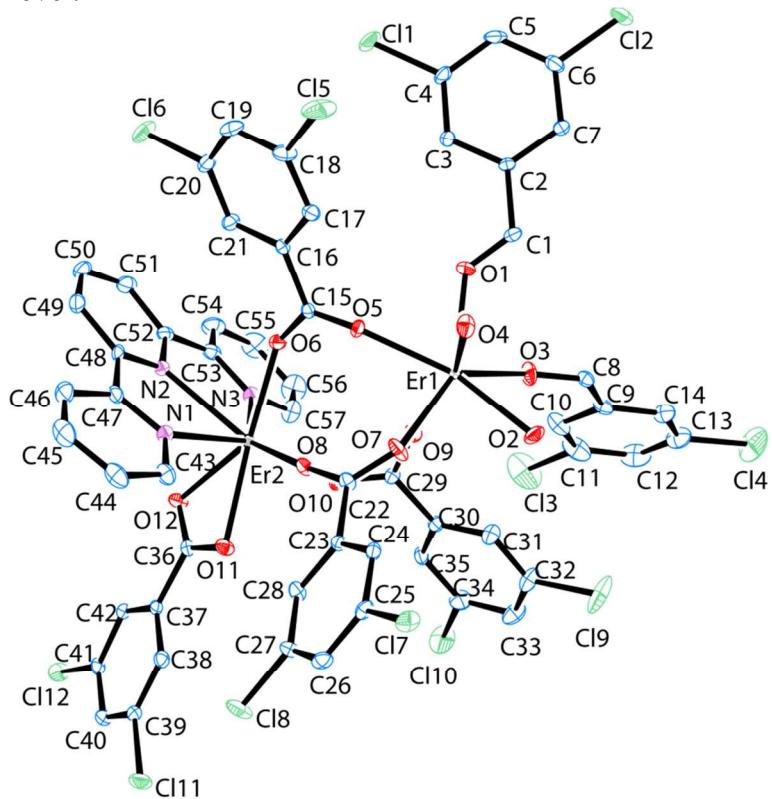
**Figure S32** ORTEP illustration of complex **9**. Ellipsoids are shown at 50% probability level.



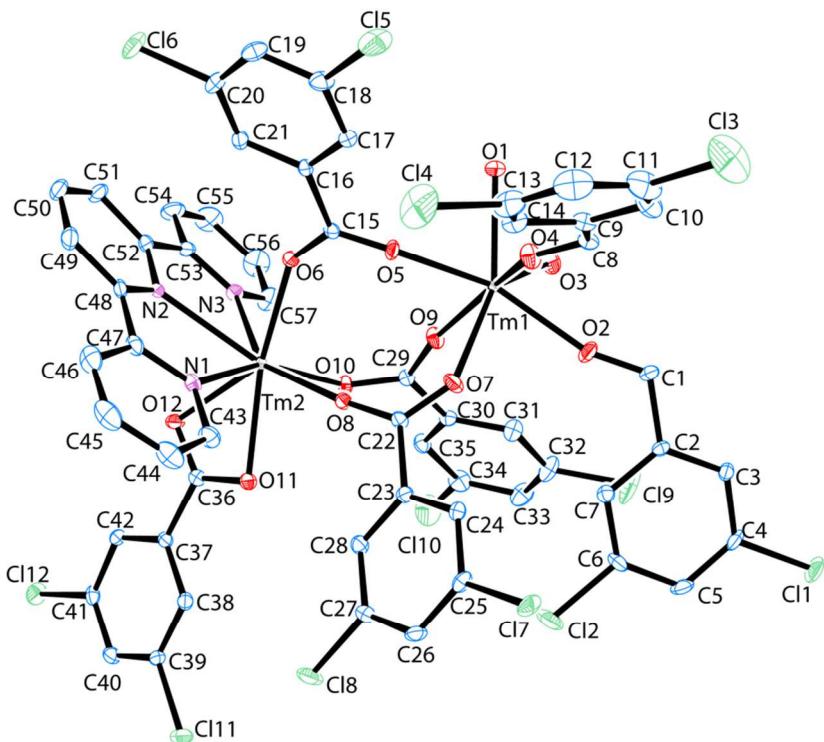
**Figure S33** ORTEP illustration of complex **10**. Ellipsoids are shown at 50% probability level.



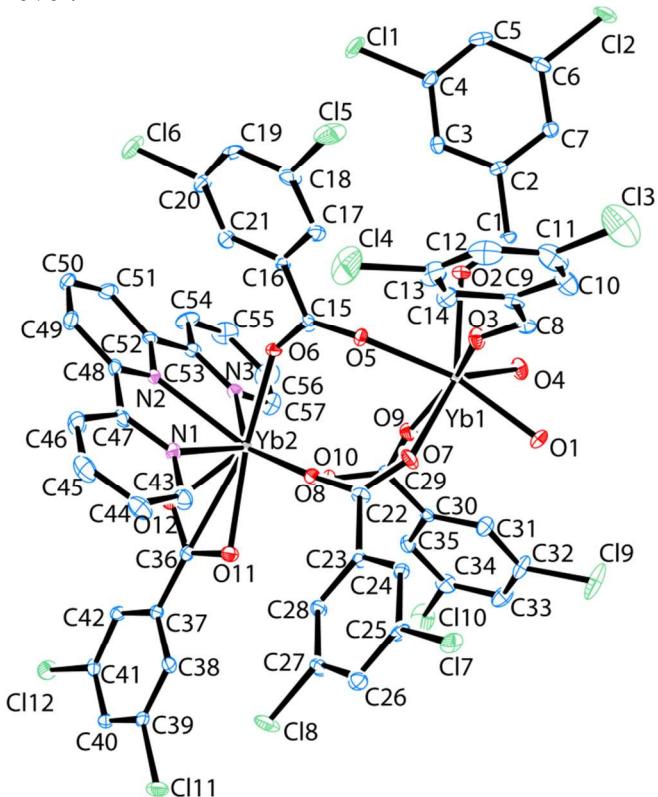
**Figure S34** ORTEP illustration of complex **11**. Ellipsoids are shown at 50% probability level.



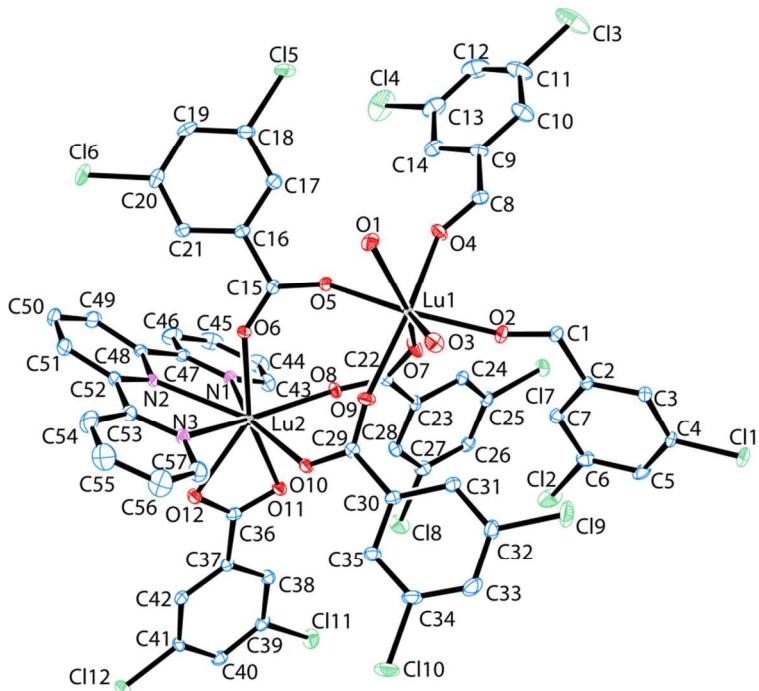
**Figure S35** ORTEP illustration of complex **12**. Ellipsoids are shown at 50% probability level.



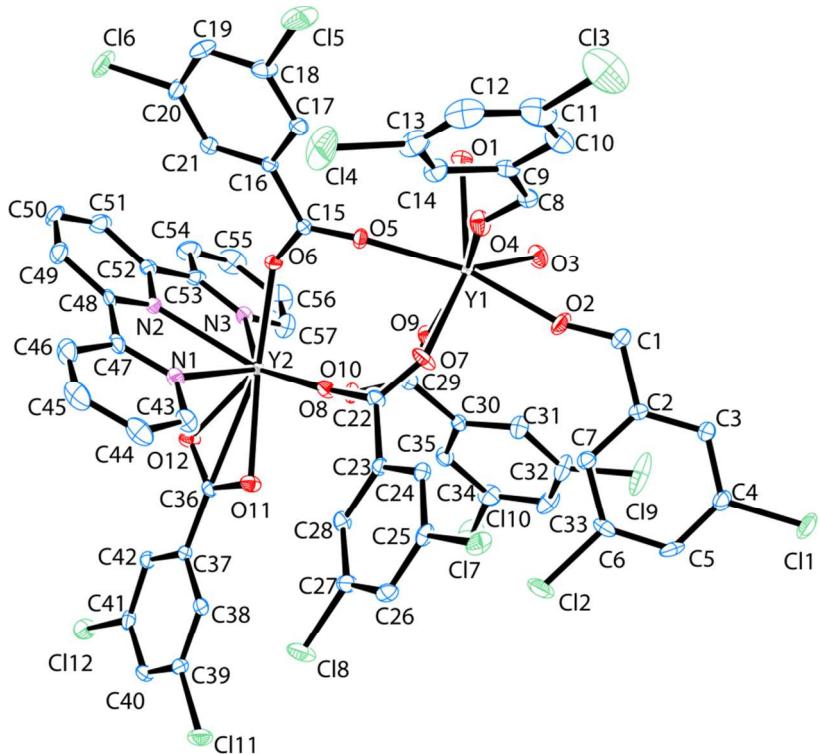
**Figure S36** ORTEP illustration of complex **13**. Ellipsoids are shown at 50% probability level.



**Figure S37** ORTEP illustration of complex **14**. Ellipsoids are shown at 50% probability level.



**Figure S38** ORTEP illustration of complex **15**. Ellipsoids are shown at 50% probability level.



**Figure S39** ORTEP illustration of complex **16**. Ellipsoids are shown at 50% probability level.

#### IV. Tables of Bond Distances

**Table S1** Ln-O bond lengths in dinuclear complexes **1-3** with 3,5-dichlorobenzoic acid and 2,2':6',2''-terpyridine. (structure types **I** and **II**)

Complex (Ln <sup>3+</sup> )	$d_{\text{Ln}1-\text{O}1}$ [Å]	$d_{\text{Ln}1-\text{O}2}$ [Å]	$d_{\text{Ln}1-\text{O}3}$ [Å]	$d_{\text{Ln}1-\text{O}4}$ [Å]	$d_{\text{Ln}1-\text{O}5}$ [Å]	$d_{\text{Ln}1-\text{O}6}$ [Å]	$d_{\text{Ln}1-\text{O}6'}$ [Å]	$d_{\text{Ln}1-\text{OW}1}$ [Å]
<b>1 (La<sup>3+</sup>-I)</b>	2.536(2)	2.662(2)	2.6039 (19)	2.585(2)	2.536 (2)	2.5734 (19)	2.760(2)	
<b>2 (La<sup>3+</sup>-II)</b>	2.6500 (17)	2.5811 (17)	2.4831 (17)		2.5131 (17)	2.4761 (18)		2.5133 (18)
<b>3 (Ce<sup>3+</sup>-II)</b>	2.6163 (17)	2.5688 (17)	2.4544 (17)		2.4813 (17)	2.4584 (17)		2.4872 (18)

**Table S2** Ln-O bond lengths in tetranuclear complexes **4-9** with 3,5-dichlorobenzoic acid and 2,2':6',2''-terpyridine. (structure type **III**)

Complex Ln <sup>3+</sup>	$d_{\text{Ln}1-\text{O}1}$ [Å]	$d_{\text{Ln}1-\text{O}2}$ [Å]	$d_{\text{Ln}1-\text{O}3}$ [Å]	$d_{\text{Ln}1-\text{O}4}$ [Å]	$d_{\text{Ln}1-\text{O}4'}$ [Å]	$d_{\text{Ln}1-\text{O}5}$ [Å]	$d_{\text{Ln}1-\text{O}7}$ [Å]	$d_{\text{Ln}1-\text{O}9}$ [Å]	$d_{\text{Ln}2-\text{O}6}$ [Å]	$d_{\text{Ln}2-\text{O}8}$ [Å]	$d_{\text{Ln}2-\text{O}10}$ [Å]	$d_{\text{Ln}2-\text{O}11}$ [Å]	$d_{\text{Ln}2-\text{O}12}$ [Å]
<b>4 Pr<sup>3+</sup></b>	2.396 (3)	2.423 (3)	2.512 (3)	2.777 (3)	2.450 (2)	2.413 (3)	2.366 (2)	2.330 (3)	2.388 (3)	2.381 (3)	2.420 (2)	2.459 (3)	2.543 (2)
<b>5 Nd<sup>3+</sup></b>	2.383 (2)	2.407 (2)	2.492 (2)	2.761 4 (19)	2.438 7 (19)	2.397 7 (19)	2.350 7 (19)	2.320 9 (19)	2.372 3 (19)	2.373 1 (18)	2.404 4 (18)	2.448 4 (18)	2.522 1 (18)
<b>6 Sm<sup>3+</sup></b>	2.360 (2)	2.378 (2)	2.463 (2)	2.734 (2)	2.415 (2)	2.374 (2)	2.317 (2)	2.290 (2)	2.349 (2)	2.348 (2)	2.363 (2)	2.428 (2)	2.492 (2)
<b>7 Eu<sup>3+</sup></b>	2.346 3 (19)	2.368 9 (19)	2.447 0 (18)	2.721 8 (19)	2.406 5 (19)	2.366 1 (18)	2.306 1 (18)	2.281 6 (18)	2.342 1 (18)	2.341 8 (18)	2.339 2 (18)	2.420 9 (19)	2.476 7 (19)
<b>8 Gd<sup>3+</sup></b>	2.325 (3)	2.356 (3)	2.421 (4)	2.802 (4)	2.380 (4)	2.347 (3)	2.288 (3)	2.265 (3)	2.326 (3)	2.322 (3)	2.327 (3)	2.414 (3)	2.465 (3)
<b>9 Tb<sup>3+</sup></b>	2.314 (4)	2.340 (4)	2.407 (4)	2.828 (5)	2.366 (4)	2.346 (3)	2.275 (4)	2.254 (3)	2.316 (3)	2.310 (4)	2.317 (3)	2.404 (4)	2.450 (4)

**Table S3** Ln-O bond lengths in tetranuclear complexes **10-16** with 3,5-dichlorobenzoic acid and 2,2':6',2''-terpyridine. (structure type **IV**)

Complex (Ln <sup>3+</sup> )	$d_{\text{Ln}1-\text{O}1}$ [Å]	$d_{\text{Ln}1-\text{O}2}$ [Å]	$d_{\text{Ln}1-\text{O}3}$ [Å]	$d_{\text{Ln}1-\text{O}4}$ [Å]	$d_{\text{Ln}1-\text{O}5}$ [Å]	$d_{\text{Ln}1-\text{O}7}$ [Å]	$d_{\text{Ln}1-\text{O}9}$ [Å]	$d_{\text{Ln}2-\text{O}6}$ [Å]	$d_{\text{Ln}2-\text{O}8}$ [Å]	$d_{\text{Ln}2-\text{O}10}$ [Å]	$d_{\text{Ln}2-\text{O}11}$ [Å]	$d_{\text{Ln}2-\text{O}12}$ [Å]
<b>10 Dy<sup>3+</sup></b>	2.330 (2)	2.268 (2)	2.317 (2)	2.306 (2)	2.269 (2)	2.334 (2)	2.267 (2)	2.289 (2)	2.309 (2)	2.315 (2)	2.385 (2)	2.415 (2)
<b>11 Ho<sup>3+</sup></b>	2.312 (3)	2.255 (3)	2.317 (3)	2.291 (3)	2.265 (3)	2.326 (3)	2.258 (3)	2.285 (3)	2.301 (3)	2.298 (3)	2.377 (3)	2.408 (3)
<b>12 Er<sup>3+</sup></b>	2.305 9 (19)	2.245 2 (18)	2.303 5 (19)	2.283 9 (19)	2.252 2 (18)	2.314 2 (18)	2.249 8 (19)	2.276 1 (18)	2.291 3 (17)	2.286 8 (18)	2.372 2 (18)	2.398 0 (18)
<b>13</b>	2.293	2.237	2.290	2.271	2.234	2.302	2.232	2.263	2.280	2.277	2.355	2.389

<b>Tm<sup>3+</sup></b>	7 (18)	8 (18)	3 (18)	1 (18)	2 (17)	2 (18)	4 (17)	5 (17)	4 (17)	4 (17)	0 (17)	1 (17)
<b>14 Yb<sup>3+</sup></b>	2.287 (2)	2.224 (2)	2.281 (2)	2.264 (2)	2.232 (2)	2.289 (2)	2.226 (2)	2.243 (2)	2.275 (2)	2.272 (2)	2.349 (2)	2.374 (2)
<b>15 Lu<sup>3+</sup></b>	2.276 1 (18)	2.216 0 (18)	2.272 9 (18)	2.252 9 (18)	2.222 3 (17)	2.282 1 (18)	2.218 1 (17)	2.235 7 (17)	2.273 4 (17)	2.253 4 (17)	2.348 1 (18)	2.368 6 (18)
<b>16 Y<sup>3+</sup></b>	2.315 (2)	2.253 (2)	2.309 (2)	2.293 (2)	2.255 (2)	2.321 (2)	2.252 (2)	2.283 (2)	2.295 8 (19)	2.296 (2)	2.377 (2)	2.406 (2)

**Table S4** Ln-N bond lengths in dinuclear and tetranuclear complexes **1-16** with 3,5-dichlorobenzoic acid and 2,2':6',2''-terpyridine. (structure types **I-IV**)

<b>Complex (Ln<sup>3+</sup>)</b>	<i>d</i> <sub>Ln1-N1</sub> [Å]	<i>d</i> <sub>Ln1-N2</sub> [Å]	<i>d</i> <sub>Ln1-N3</sub> [Å]	<i>d</i> <sub>Ln2-N1</sub> [Å]	<i>d</i> <sub>Ln2-N2</sub> [Å]	<i>d</i> <sub>Ln2-N3</sub> [Å]
<b>1 (La<sup>3+</sup>--I)</b>	2.640(2)	2.738(2)	2.681(2)			
<b>2 (La<sup>3+</sup>--II)</b>	2.692(20)	2.770(2)	2.707(2)			
<b>3 (Ce<sup>3+</sup>--III)</b>	2.673(2)	2.745(2)	2.682(2)			
<b>4 (Pr<sup>3+</sup>--III)</b>				2.606(3)	2.720(4)	2.633(4)
<b>5 (Nd<sup>3+</sup>--III)</b>				2.574(3)	2.705(6)	2.618(3)
<b>6 (Sm<sup>3+</sup>--III)</b>				2.539(3)	2.613(3)	2.557(3)
<b>7 (Eu<sup>3+</sup>--III)</b>				2.531(2)	2.607(2)	2.547(2)
<b>8 (Gd<sup>3+</sup>--III)</b>				2.516(4)	2.586(4)	2.530(4)
<b>9 (Tb<sup>3+</sup>--III)</b>				2.508(4)	2.581(4)	2.526(4)
<b>10 (Dy<sup>3+</sup>--IV)</b>				2.506(3)	2.557(3)	2.529(3)
<b>11 (Ho<sup>3+</sup>--IV)</b>				2.502(3)	2.539(3)	2.521(3)
<b>12 (Er<sup>3+</sup>--IV)</b>				2.489(2)	2.531(2)	2.510(2)
<b>13 (Tm<sup>3+</sup>--IV)</b>				2.480(2)	2.522(2)	2.498(2)
<b>14 (Yb<sup>3+</sup>--IV)</b>				2.474(3)	2.519(3)	2.493(3)
<b>15 (Lu<sup>3+</sup>--IV)</b>				2.460(2)	2.504(2)	2.488(2)
<b>16 (Y<sup>3+</sup>--IV)</b>				2.508(3)	2.551(2)	2.522(2)

## V. Tables of Supramolecular Interactions

**Table S5** Halogen bonding (halogen-halogen, halogen- $\pi$ , halogen bonding) interaction distances in structure type **II**  $\text{Ln}^{3+}$  complexes (**2**, **3**) with 3,5-dichlorobenzoic acid and 2,2':6',2''-terpyridine (where  $\text{Ln}^{3+}=\text{La}^{3+}$ ,  $\text{Ce}^{3+}$ ).

Complex	d(Cl1-Cl1) (X-X) [Å]	d(Cl1-Cl3) (X-X) [Å]	d(Cl2-C15) (X- $\pi$ ) [Å]	d(Cl2-O2) (X-O) [Å]
<b>2 (La<sup>3+</sup>)</b>	3.2226(11)	3.3111(13)	3.458(3)	3.140(2)
<b>3 (Ce<sup>3+</sup>)</b>	3.2217(11)	3.3229(12)	3.431(3)	3.143(2)

**Table S6** Halogen-halogen interaction distances in structure type **III**  $\text{Ln}^{3+}$  complexes (**4-9**) with 3,5-dichlorobenzoic acid and 2,2':6',2''-terpyridine (where  $\text{Ln}^{3+}=\text{Pr}^{3+}$ ,  $\text{Nd}^{3+}$ ,  $\text{Sm}^{3+}$ ,  $\text{Eu}^{3+}$ ,  $\text{Gd}^{3+}$ ,  $\text{Tb}^{3+}$ ).

Complex	d(Cl1-Cl6) (X-X) [Å]	d(Cl2-Cl7) (X-X) [Å]	d(Cl7-Cl8) (X-X) [Å]	d(Cl8-Cl9) (X-X) [Å]	d(Cl10-Cl12) (X-X) [Å]
<b>4 (Pr<sup>3+</sup>)</b>	3.2836(16)	3.432(6)	3.534(6)	3.267(11)	3.4283(17)
<b>5 (Nd<sup>3+</sup>)</b>	3.2732(12)	3.430(5)	3.527(5)	3.274(9)	3.4194(12)
<b>6 (Sm<sup>3+</sup>)</b>	3.2623(14)	3.4016(19)	3.499(2)	3.2710(18)	3.4035(10)
<b>7 (Eu<sup>3+</sup>)</b>	3.2617(12)	3.4197(16)	3.5083(19)	3.2621(15)	3.3945(13)
<b>8 (Gd<sup>3+</sup>)</b>	3.247(3)	3.415(3)	3.486(4)	3.274(3)	3.399(3)
<b>9 (Tb<sup>3+</sup>)</b>	3.253(2)	3.419(3)	3.495(4)	3.273(3)	3.402(2)

**Table S7** Additional halogen bonding interaction (Cl-O) distances in structure type **III**  $\text{Ln}^{3+}$  complexes (**4-9**) with 3,5-dichlorobenzoic acid and 2,2':6',2''-terpyridine (where  $\text{Ln}^{3+}=\text{Pr}^{3+}$ ,  $\text{Nd}^{3+}$ ,  $\text{Sm}^{3+}$ ,  $\text{Eu}^{3+}$ ,  $\text{Gd}^{3+}$ ,  $\text{Tb}^{3+}$ ).

Complex	d(Cl5-O12) (X-O) [Å]
<b>4 (Pr<sup>3+</sup>)</b>	3.134(3)
<b>5 (Nd<sup>3+</sup>)</b>	3.132(2)
<b>6 (Sm<sup>3+</sup>)</b>	3.127(3)
<b>7 (Eu<sup>3+</sup>)</b>	3.116(2)
<b>8 (Gd<sup>3+</sup>)</b>	3.095(4)
<b>9 (Tb<sup>3+</sup>)</b>	3.113(4)

**Table S8** Halogen-halogen interaction distances in structure type **IV**  $\text{RE}^{3+}$  complexes (**10-16**) with 3,5-dichlorobenzoic acid and 2,2':6',2''-terpyridine (where  $\text{Ln}^{3+}=\text{Dy}^{3+}$ ,  $\text{Ho}^{3+}$ ,  $\text{Er}^{3+}$ ,  $\text{Tm}^{3+}$ ,  $\text{Yb}^{3+}$ ,  $\text{Lu}^{3+}$ ,  $\text{Y}^{3+}$ ).

Complex	d(Cl1-Cl3) (X-X) [Å]	d(Cl2-Cl8) (X-X) [Å]	d(Cl5-Cl10) (X-X) [Å]	d(Cl6-Cl12) (X-X) [Å]
<b>10 (Dy<sup>3+</sup>)</b>	3.4207(17)	3.4070(14)	3.4786(16)	3.4901(14)
<b>11 (Ho<sup>3+</sup>)</b>	3.413(2)	3.4078(17)	3.4786(19)	3.4886(17)
<b>12 (Er<sup>3+</sup>)</b>	3.4119(15)	3.4022(12)	3.4688(14)	3.4796(12)
<b>13 (Tm<sup>3+</sup>)</b>	3.4068(13)	3.3896(10)	3.4606(13)	3.4724(11)
<b>14 (Yb<sup>3+</sup>)</b>	3.3986(17)	3.3866(14)	3.4449(15)	3.4691(14)
<b>15 (Lu<sup>3+</sup>)</b>	3.3973(13)	3.3889(10)	3.4488(13)	3.4641(11)
<b>16 (Y<sup>3+</sup>)</b>	3.4225(16)	3.4029(12)	3.4649(15)	3.4787(13)

**Table S9** Additional halogen bonding interaction (Cl-O, Cl- $\pi$ ) distances in structure type **IV** RE<sup>3+</sup> complexes (**10-16**) with 3,5-dichlorobenzoic acid and 2,2':6',2''-terpyridine (where Ln<sup>3+</sup>=Dy<sup>3+</sup>, Ho<sup>3+</sup>, Er<sup>3+</sup>, Tm<sup>3+</sup>, Yb<sup>3+</sup>, Lu<sup>3+</sup>, Y<sup>3+</sup>).

Complex	d(Cl7-O12) (X-O) [Å]	d(Cl4-C37) (X- $\pi$ ) [Å]
<b>10 (Dy<sup>3+</sup>)</b>	3.053(3)	3.231(3)
<b>11 (Ho<sup>3+</sup>)</b>	3.054(3)	3.240(4)
<b>12 (Er<sup>3+</sup>)</b>	3.055(2)	3.233(3)
<b>13 (Tm<sup>3+</sup>)</b>	3.062(2)	3.233(3)
<b>14 (Yb<sup>3+</sup>)</b>	3.062(3)	3.235(3)
<b>15 (Lu<sup>3+</sup>)</b>	3.059(2)	3.232(3)
<b>16 (Y<sup>3+</sup>)</b>	3.051(2)	3.239(3)

**Table S10** Offset  $\pi$ - $\pi$  interaction distances and angles in structure type **IV** RE<sup>3+</sup> complexes (**10-16**) with 3,5-dichlorobenzoic acid and 2,2':6',2''-terpyridine (where Ln<sup>3+</sup>=Dy<sup>3+</sup>, Ho<sup>3+</sup>, Er<sup>3+</sup>, Tm<sup>3+</sup>, Yb<sup>3+</sup>, Lu<sup>3+</sup>, Y<sup>3+</sup>).

Complex	Cg $\bullet\bullet\bullet$ Cg [Å]	Cg $\perp$ $\bullet\bullet\bullet$ Cg $\perp$ [Å]	Beta [deg]
<b>10 (Dy<sup>3+</sup>)</b>	3.529(2)	3.3439(14)	18.65
<b>11 (Ho<sup>3+</sup>)</b>	3.540(3)	3.3391(19)	19.40
<b>12 (Er<sup>3+</sup>)</b>	3.5509(18)	3.3442(12)	19.64
<b>13 (Tm<sup>3+</sup>)</b>	3.5572(16)	3.3393(11)	20.20
<b>14 (Yb<sup>3+</sup>)</b>	3.561(2)	3.3365(14)	20.50
<b>15 (Lu<sup>3+</sup>)</b>	3.5713(16)	3.3373(11)	20.92
<b>16 (Y<sup>3+</sup>)</b>	3.5469(19)	3.3488(13)	19.28