RE-*p*-halobenzoic acid-terpyridine, Part II: structural diversity, supramolecular interactions, and luminescence properties in a series of *p*-bromobenzoic acid containing rare-earth complexes

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Supporting Info Section

I. Powder X-ray Diffraction data

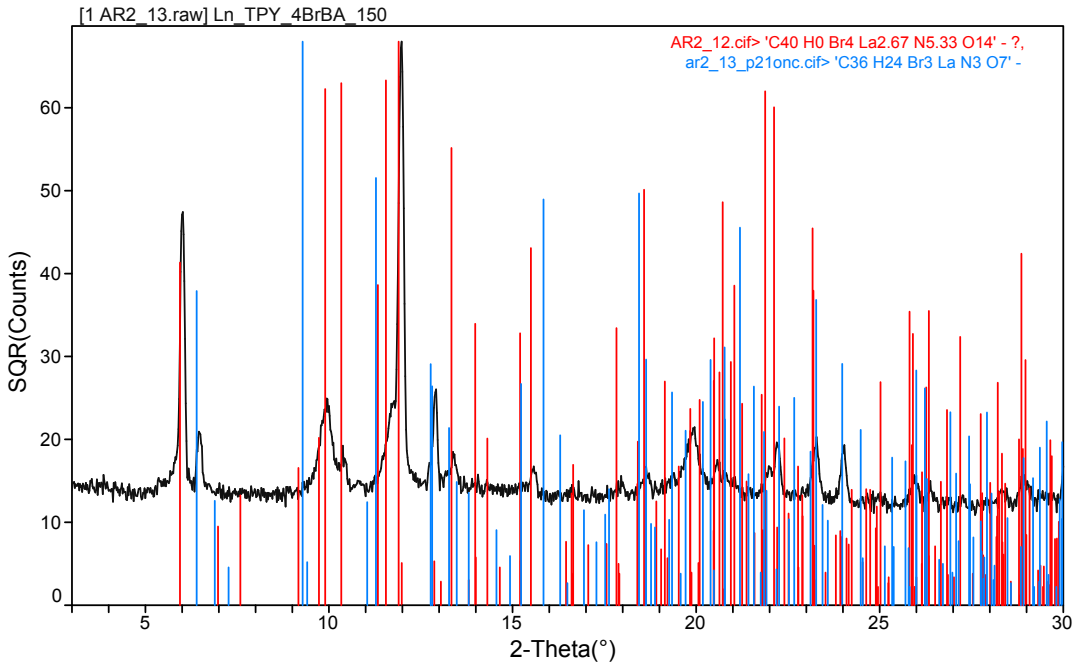

Figure S1: The PXRD pattern of Structure 1 (structure type I) with the calculated pattern overlaid in blue. The calculated pattern of structure 1' (structure type IV) is also included in red.

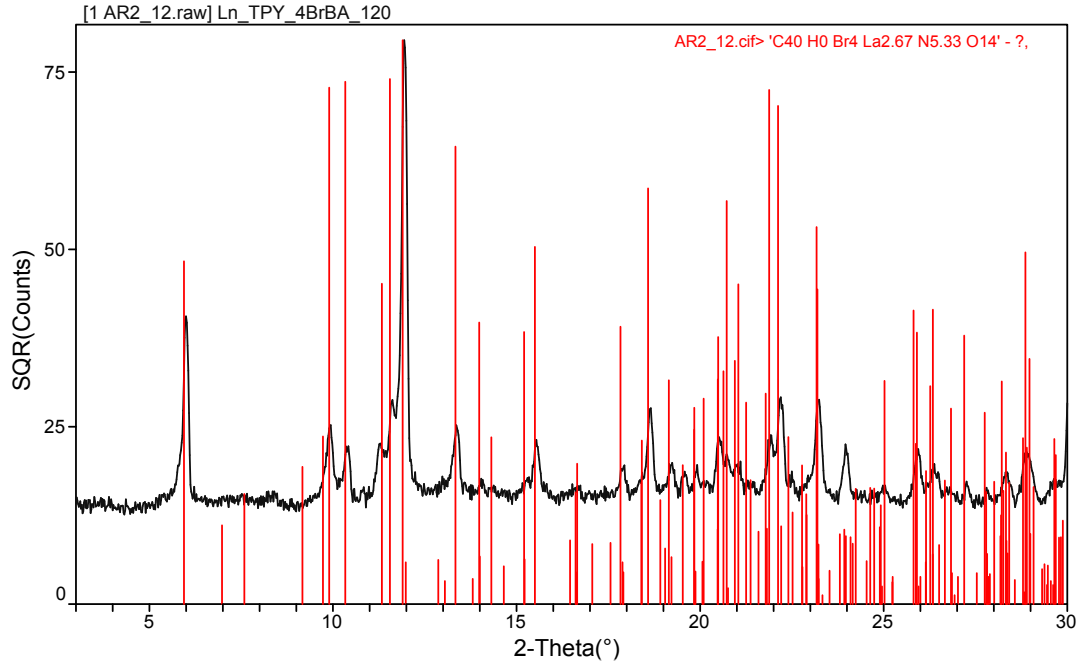

Figure S2: The PXRD pattern of Structure 1' (structure type IV) with the calculated pattern overlaid in blue.

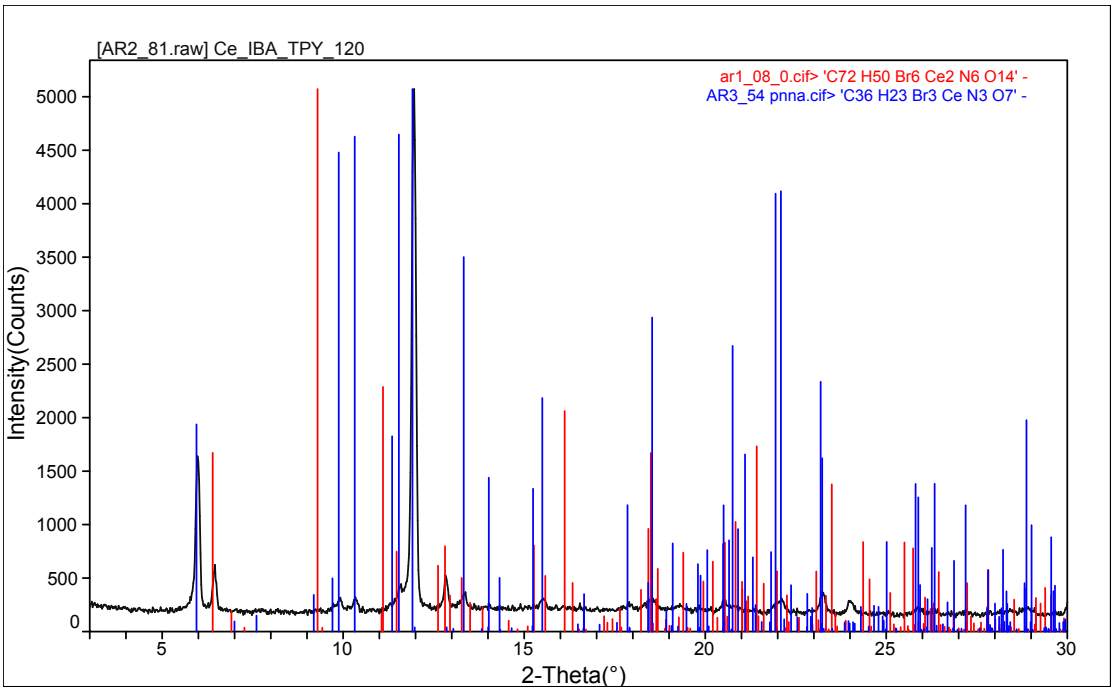

Figure S3: The PXRD pattern of Structure 2 and Structure 2' (structure type I and IV) with the calculated pattern overlaid in red. The calculated pattern of structure 2' (structure type IV) is also included in blue.

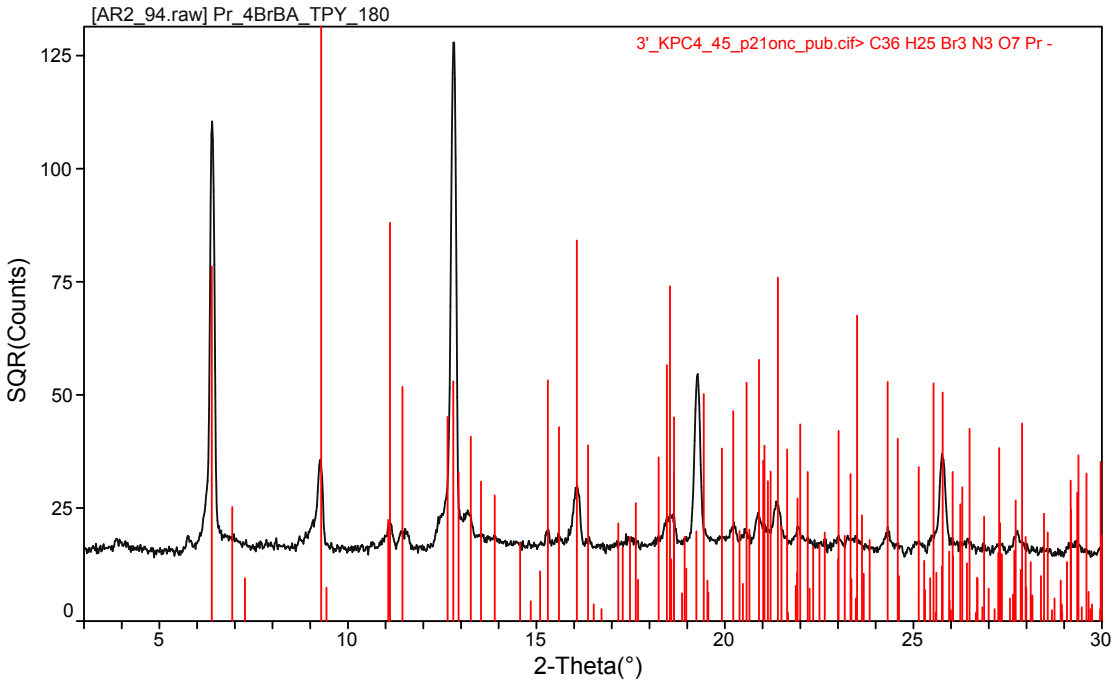

Figure S4: The PXRD pattern of Structure 3 (structure type IV) with the calculated pattern overlaid in red.

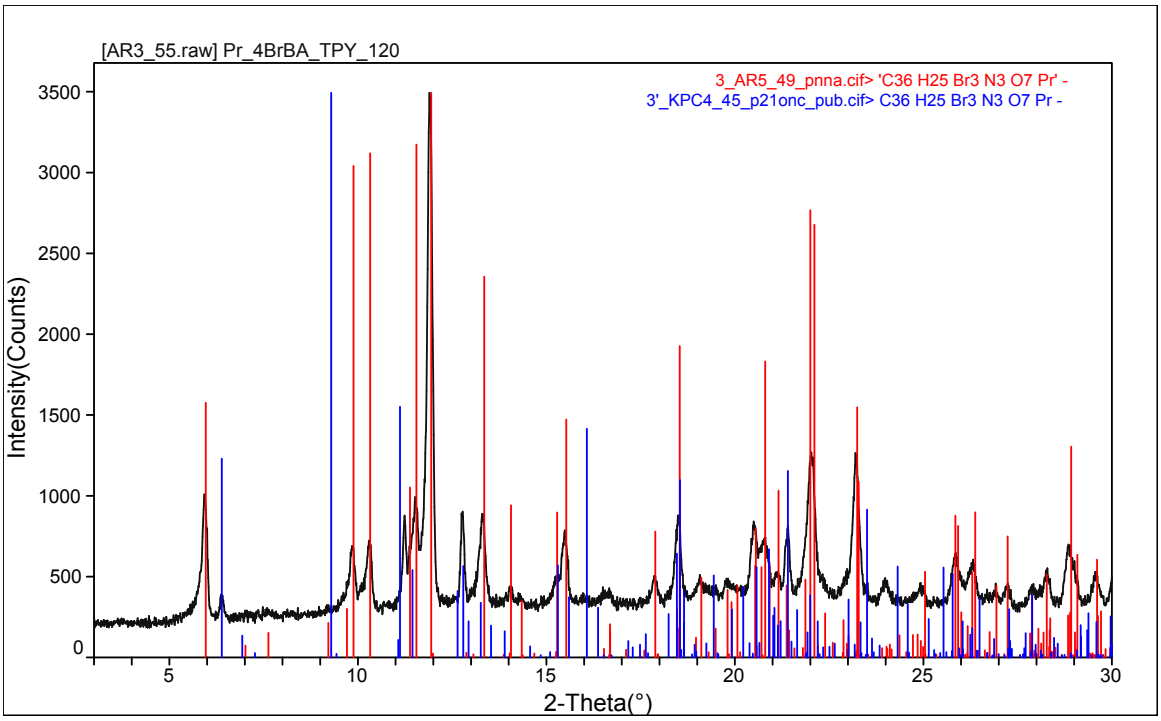

Figure S5: The PXRD pattern of Structure 3' (structure type IV) with the calculated pattern overlaid in red. The calculated pattern of structure 3 (structure type I) is also included in blue.

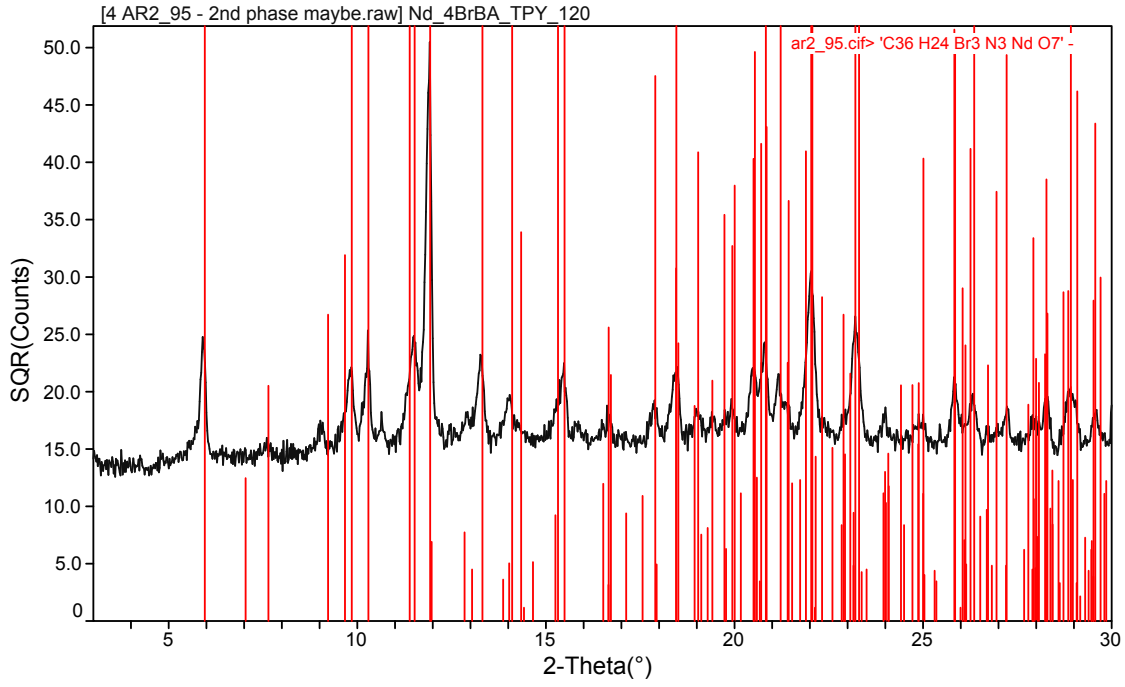

Figure S6: The PXRD pattern of Structure 4 (structure type I) with the calculated pattern overlaid in red.

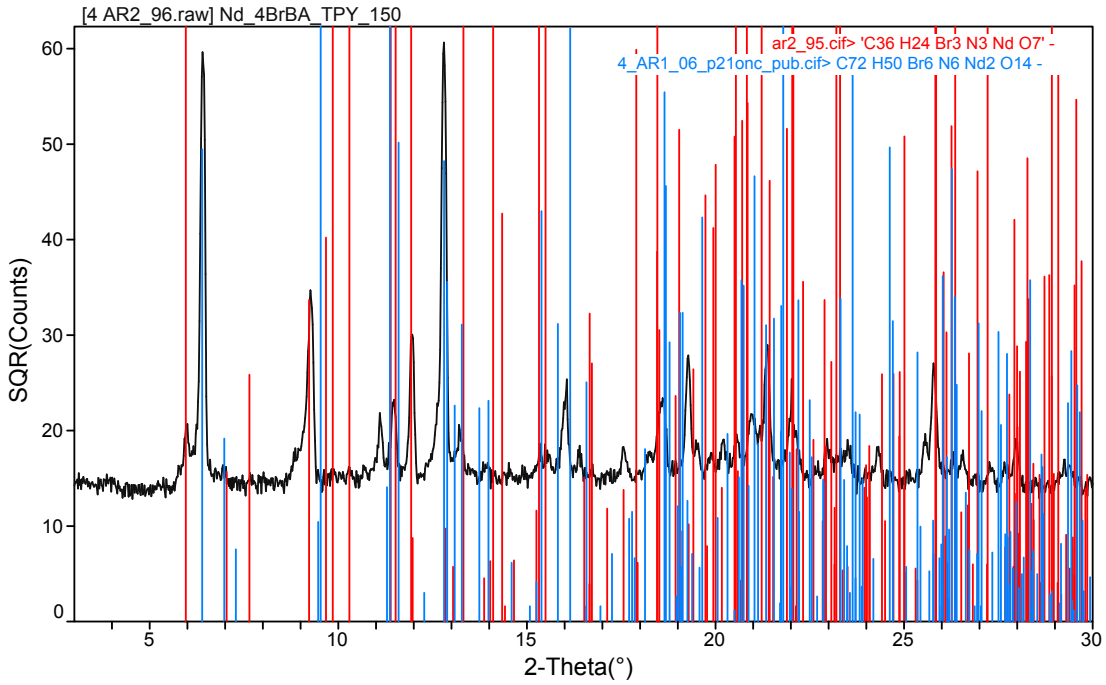

Figure S7: The PXRD pattern of Structure 4' (structure type IV) with the calculated pattern overlaid in red. The calculated pattern of structure 4 (structure type I) is also included in blue.

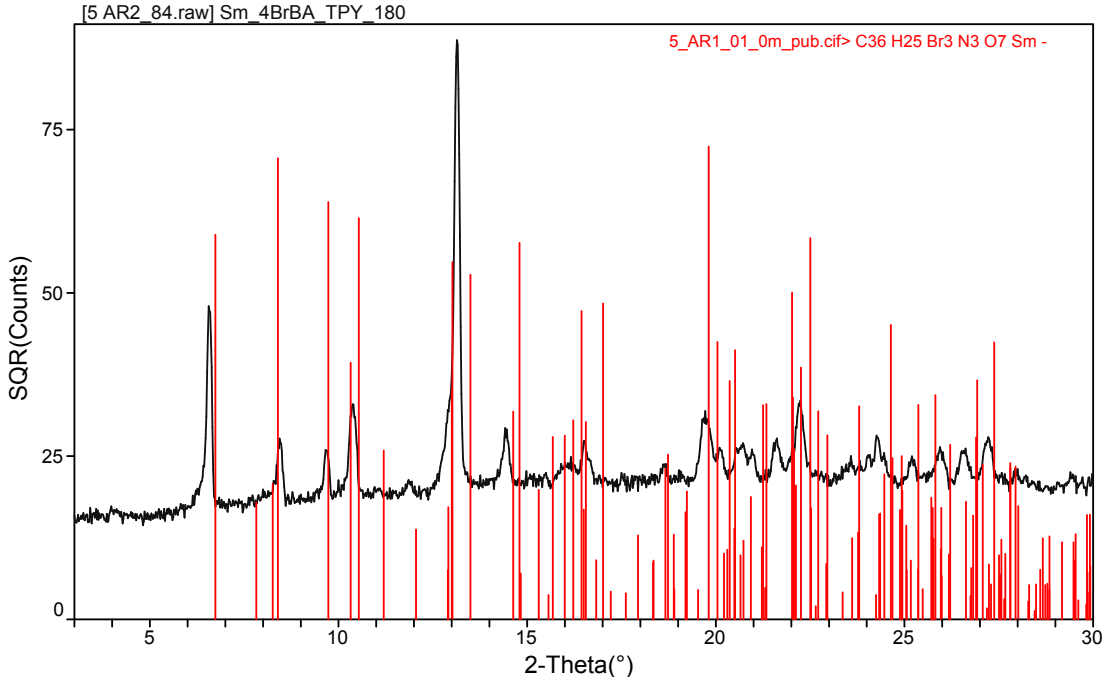

Figure S8: The PXRD pattern of Structure 5 (structure type V) with the calculated pattern overlaid in red.

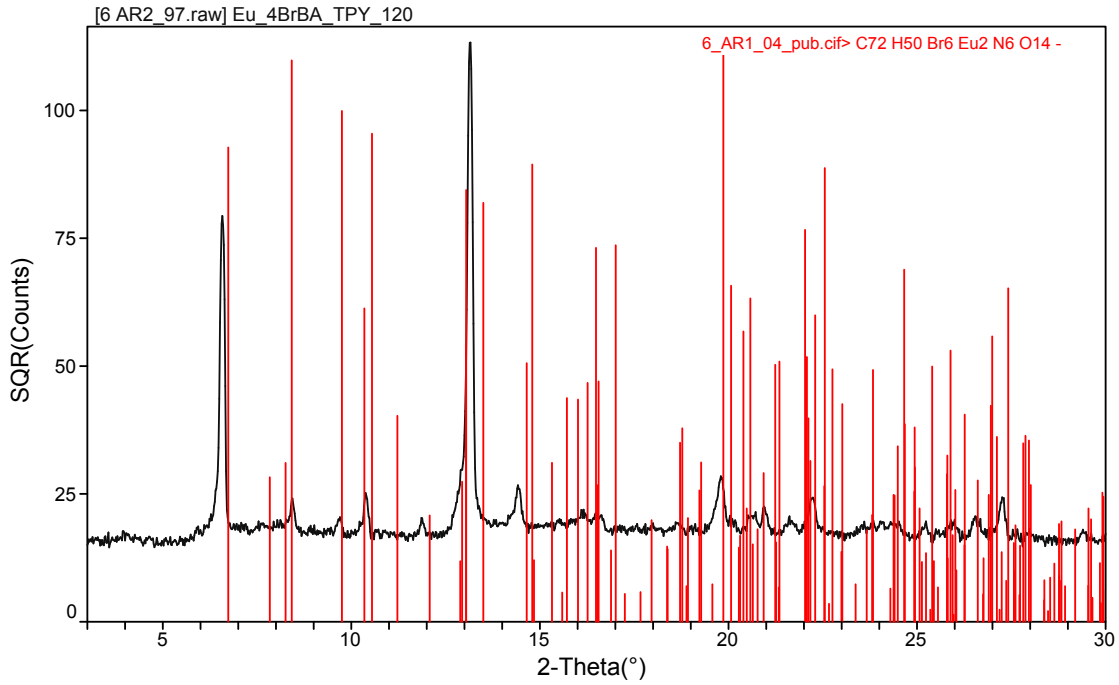

Figure S9: The PXRD pattern of Structure 6 (structure type V) with the calculated pattern overlaid in red.

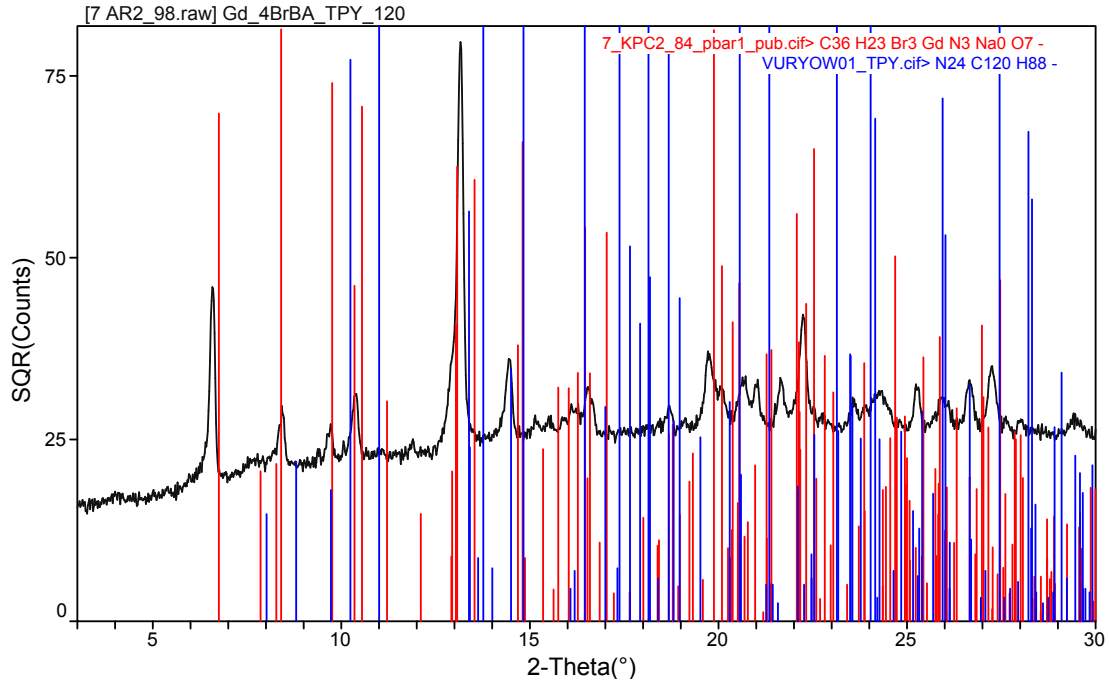

Figure S10: The PXRD pattern of Structure 7 (structure type V) with the calculated pattern overlaid in red. The calculated pattern of 2,2':6,2''-terpyridine is also included in blue.

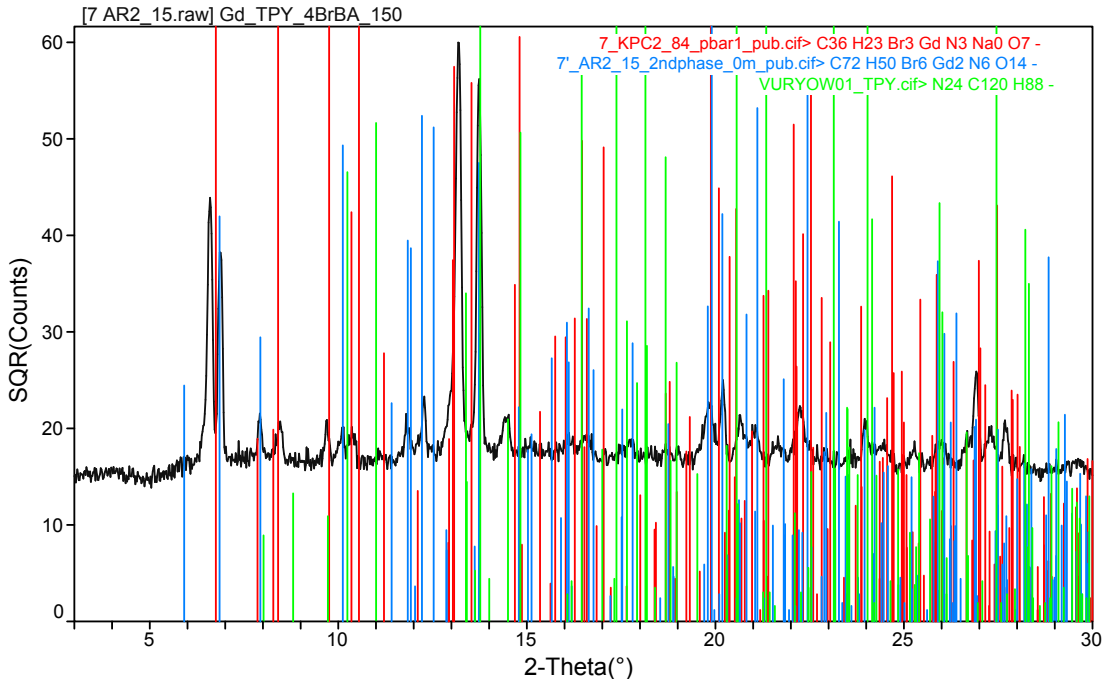

Figure S11: The PXRD pattern of Structure 7' (structure type III) with the calculated pattern overlaid in blue. The calculated pattern of Structure 7 (structure type V) and of 2':6,2''-terpyridine are also included in blue and green, respectively.

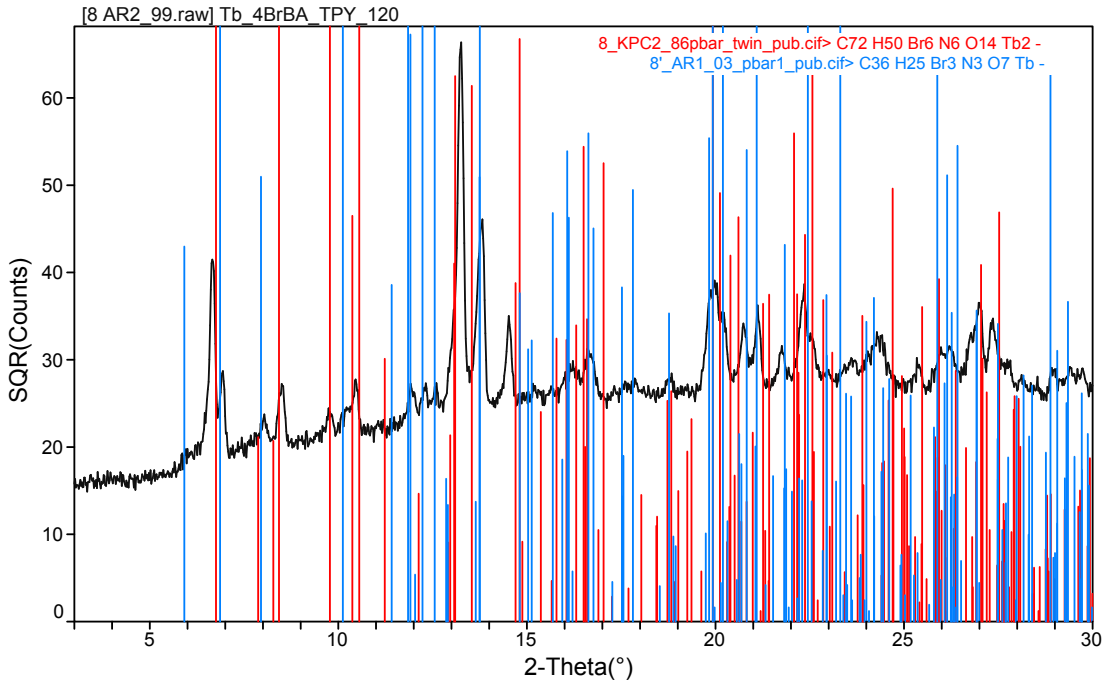

Figure S12: The PXRD pattern of Structure 8 (structure type V) with the calculated pattern overlaid in red. The calculated pattern of structure 8' (structure type III) is also included in blue.

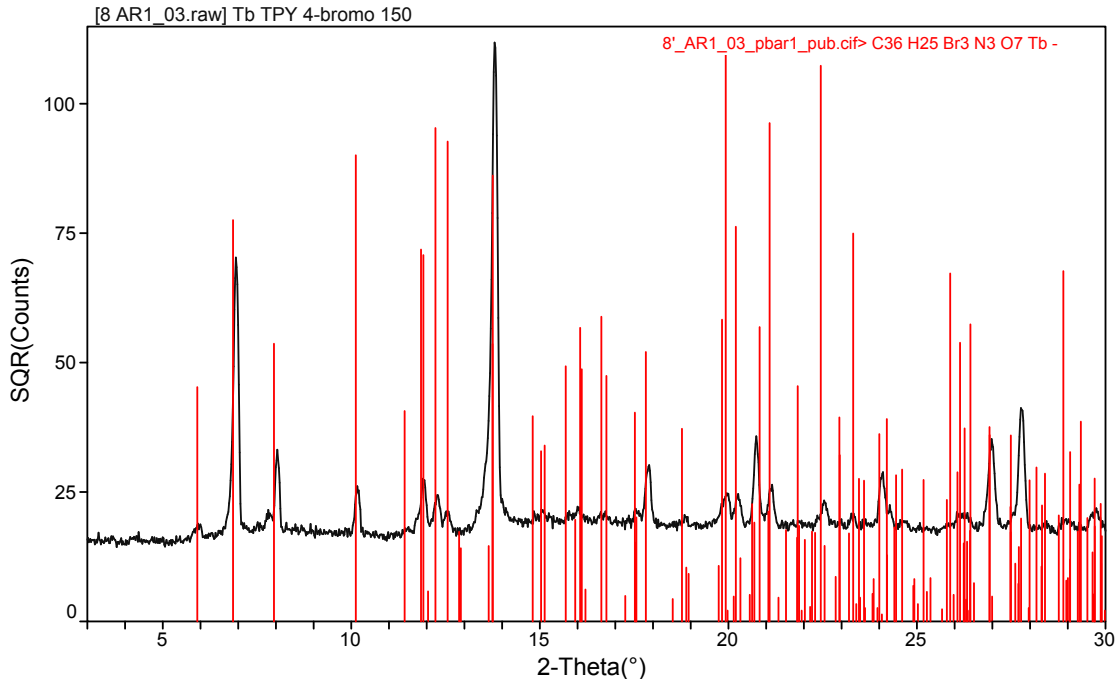

Figure S13: The PXRD pattern of Structure 8' (structure type III) with the calculated pattern overlaid in red.

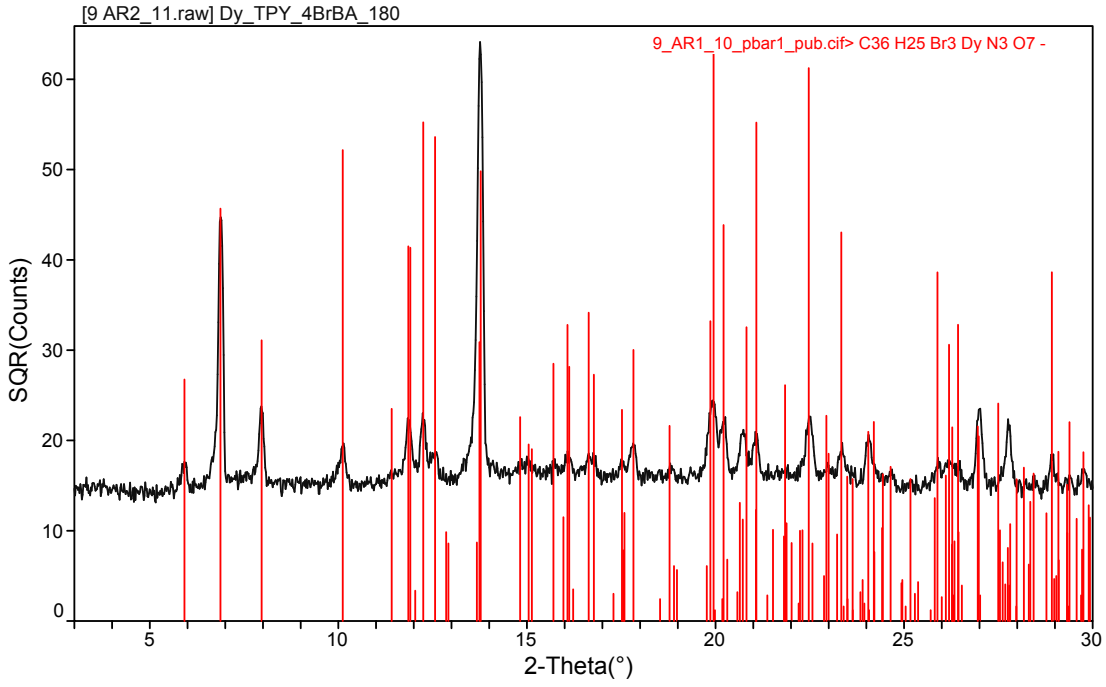

Figure S14: The PXRD pattern of Structure 9 (structure type III) with the calculated pattern overlaid in red.

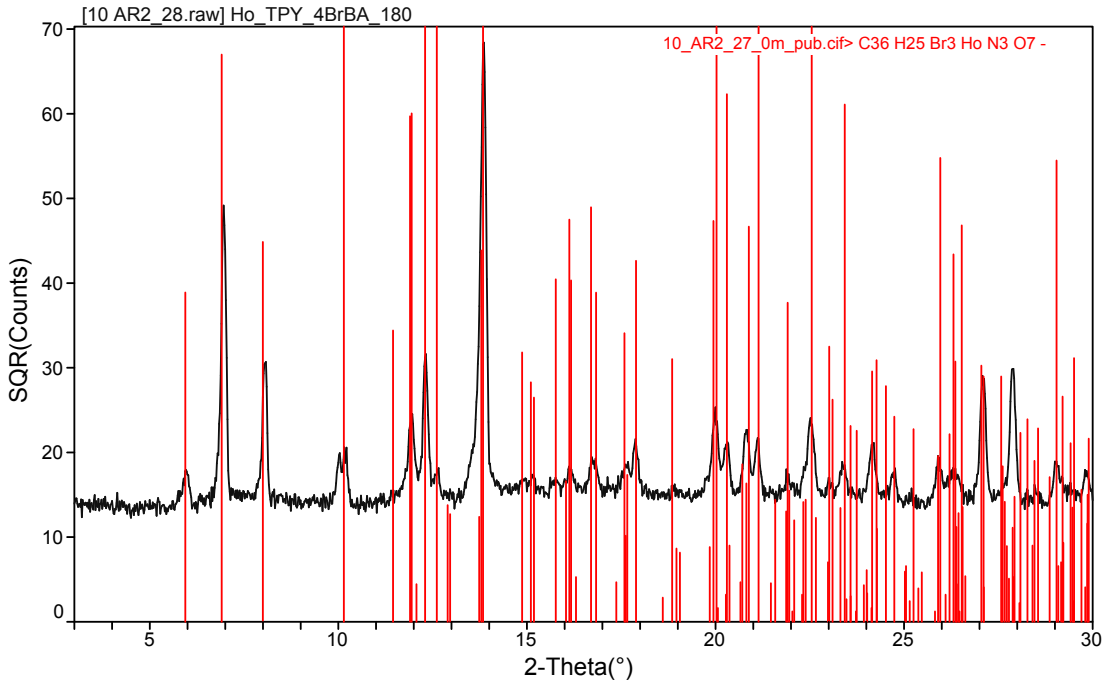

Figure S15: The PXRD pattern of Structure 10 (structure type III) with the calculated pattern overlaid in red.

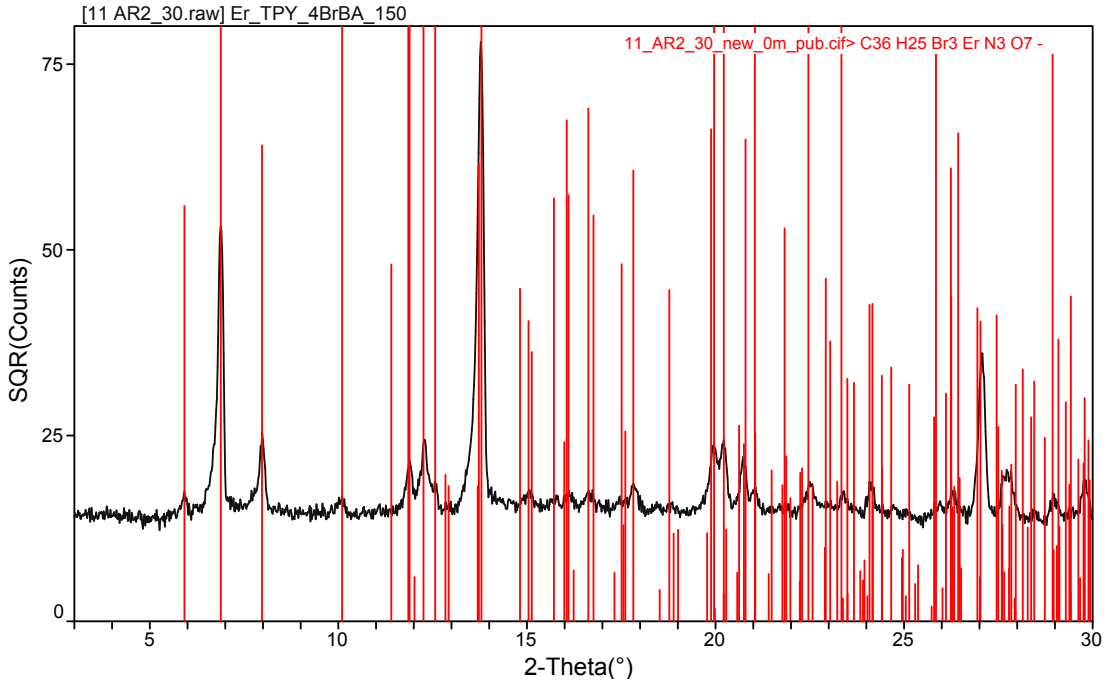

Figure S16: The PXRD pattern of Structure 11 (structure type III) with the calculated pattern overlaid in red.

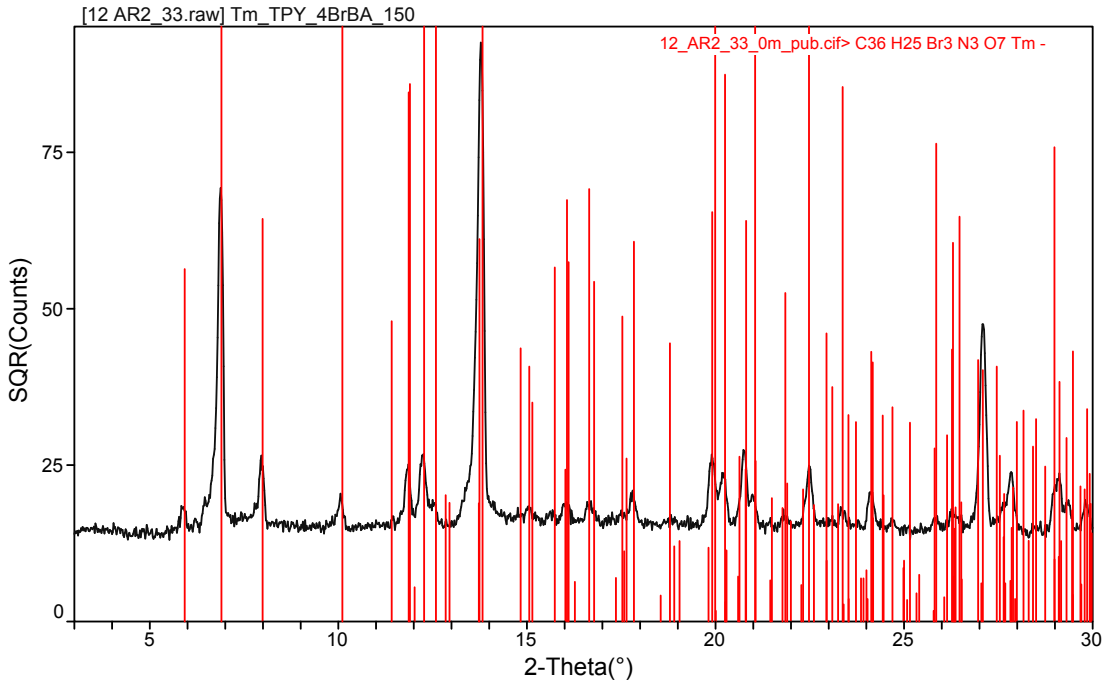

Figure S17: The PXRD pattern of Structure 12 (structure type III) with the calculated pattern overlaid in red.

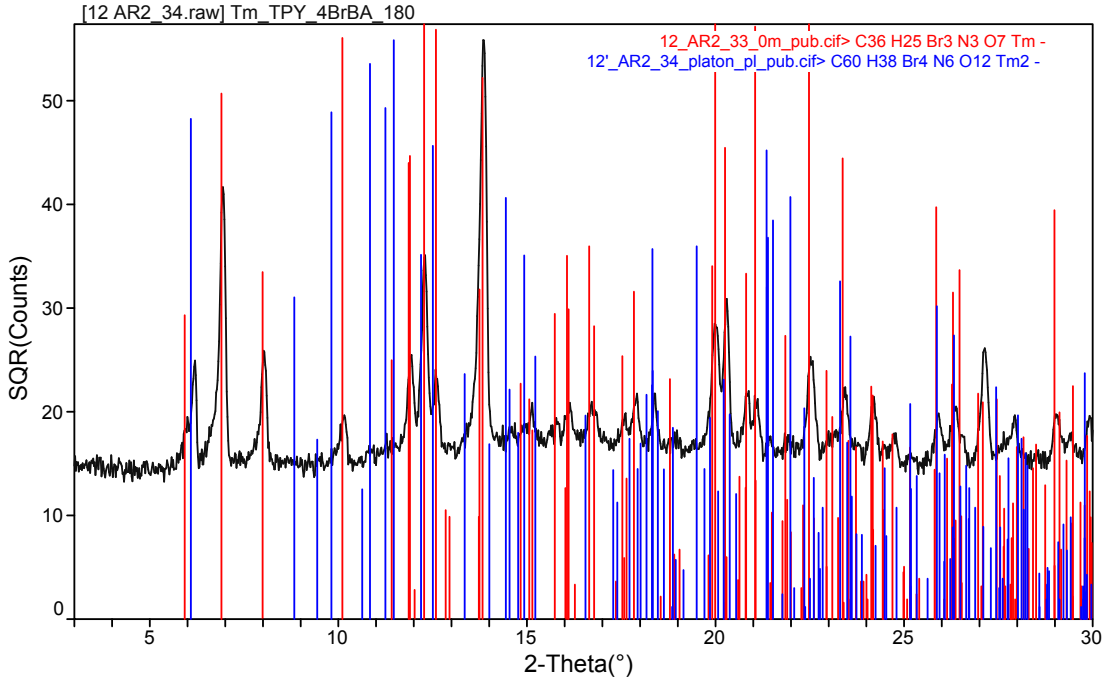

Figure S18: The PXRD pattern of Structure 12' (structure type VI) with the calculated pattern overlaid in blue. The calculated pattern of Structure 12 (structure type III) is also included in red.

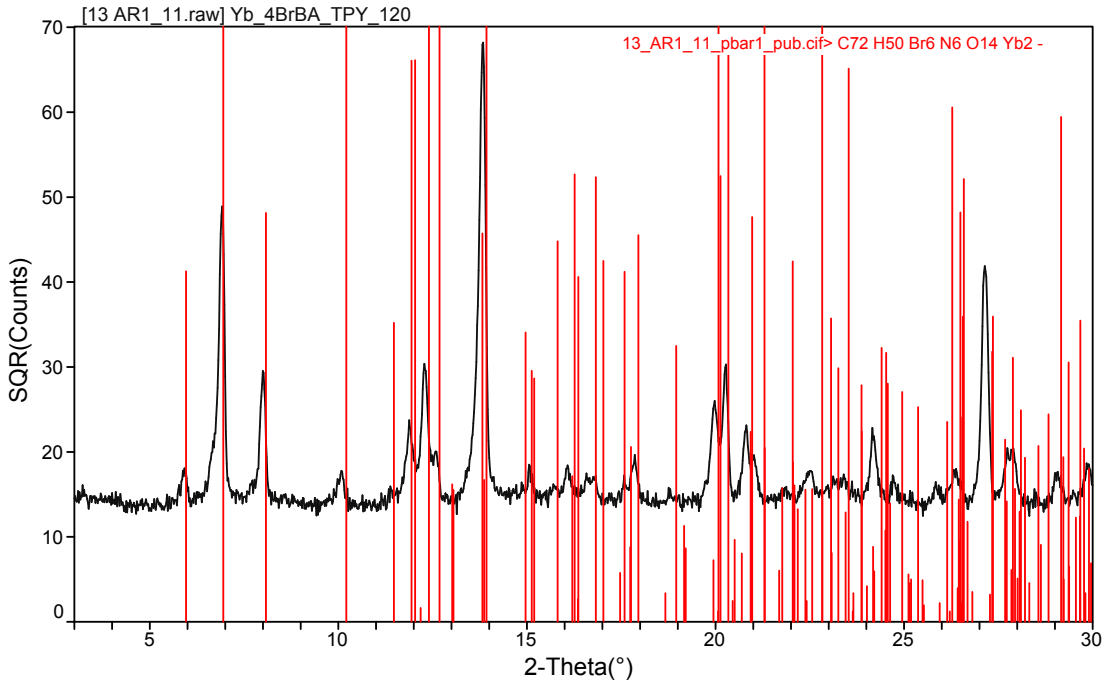

Figure S19: The PXRD pattern of Structure 13 (structure type III) with the calculated pattern overlaid in red.

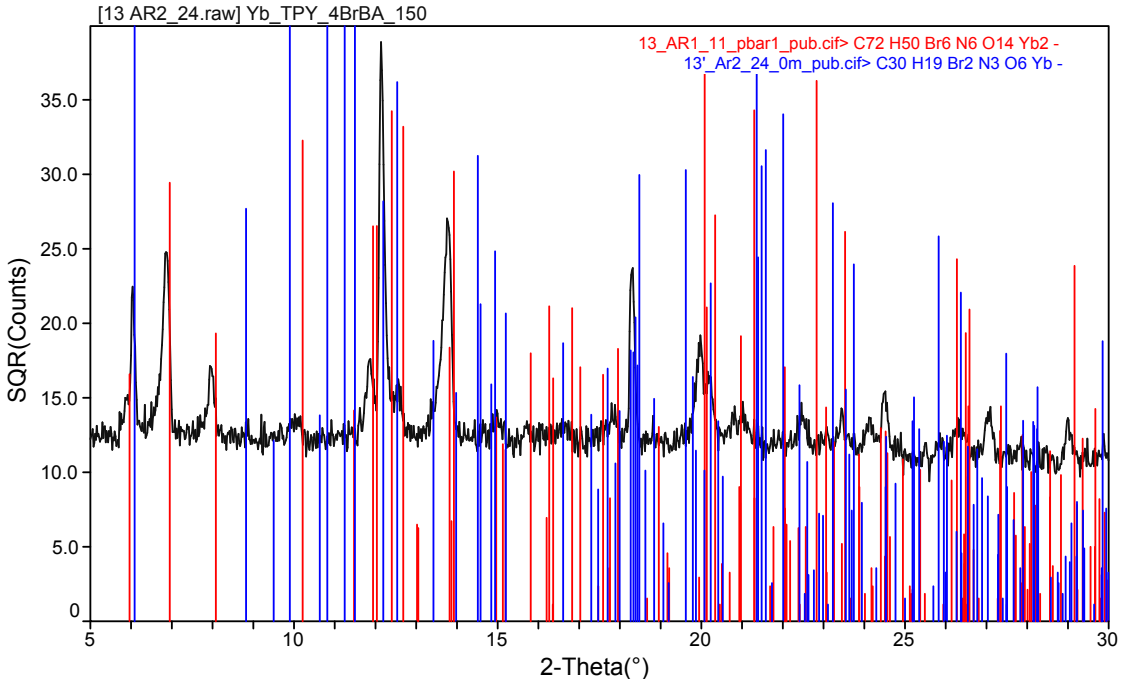

Figure S20: The PXRD pattern of Structure 13' (structure type VI) with the calculated pattern overlaid in blue. The calculated pattern of Structure 13 (structure type III) is also included in red.

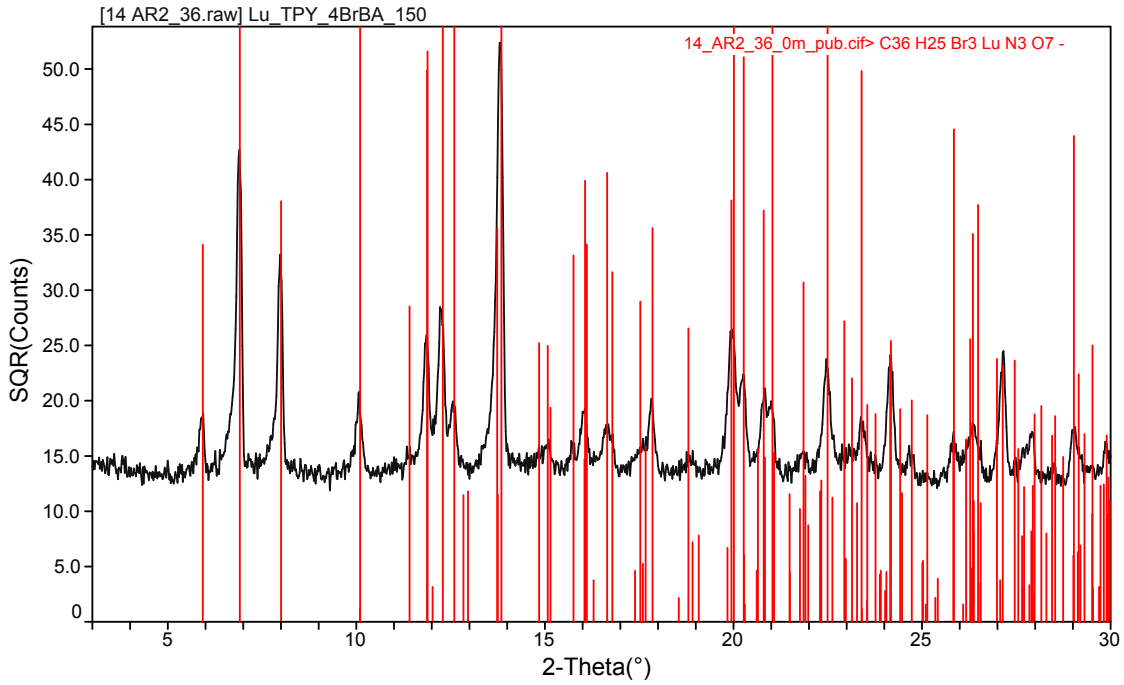

Figure S21: The PXRD pattern of Structure 14 (structure type III) with the calculated pattern overlaid in red.

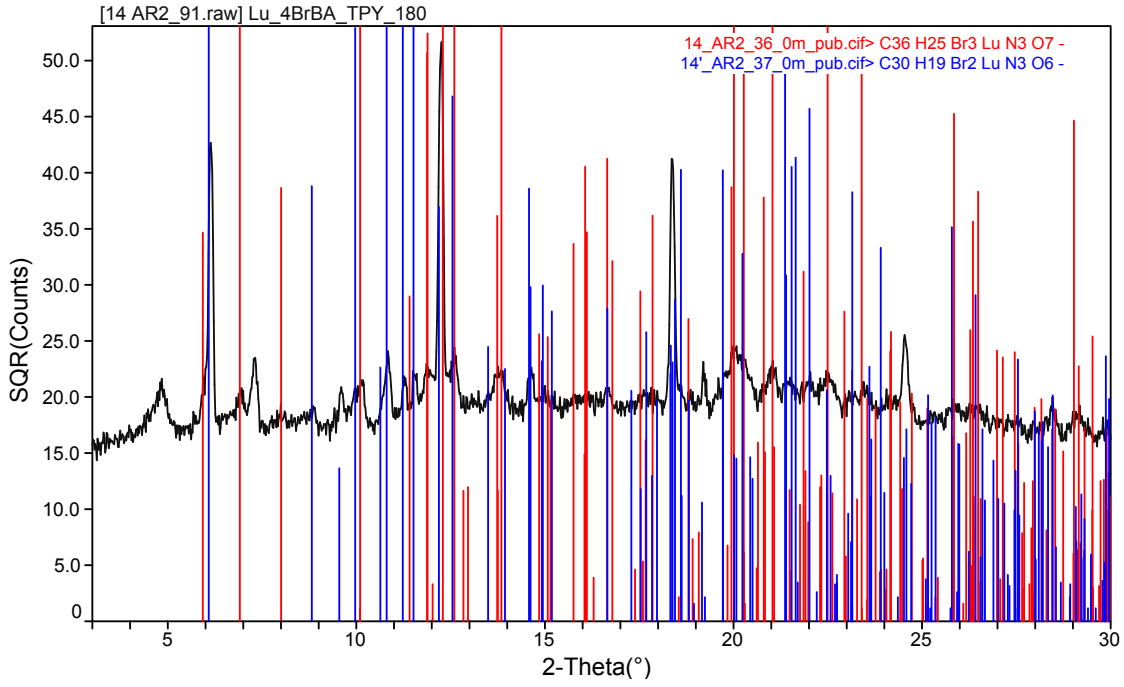

Figure S22: The PXRD pattern of Structure 14' (structure type VI) with the calculated pattern overlaid in blue. The calculated pattern of Structure 14 (structure type III) is also included in red. We acknowledge that this sample contains impurities.

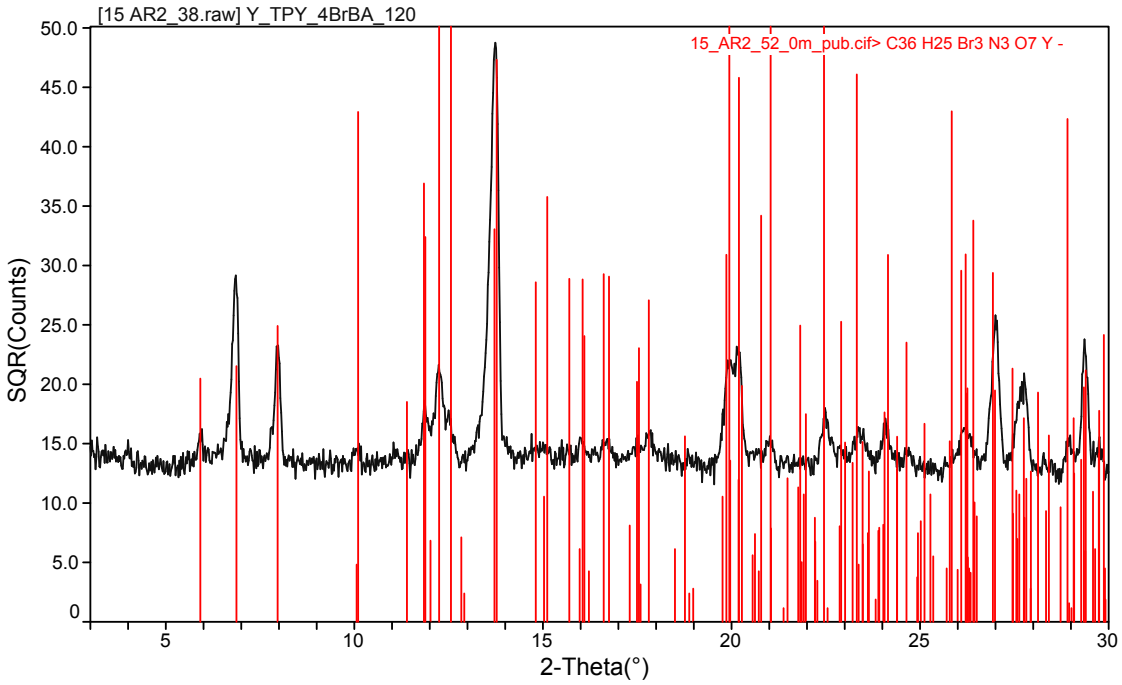

Figure S23: The PXRD pattern of Structure 15 (structure type III) with the calculated pattern overlaid in red.

II. Thermal Ellipsoid Plots

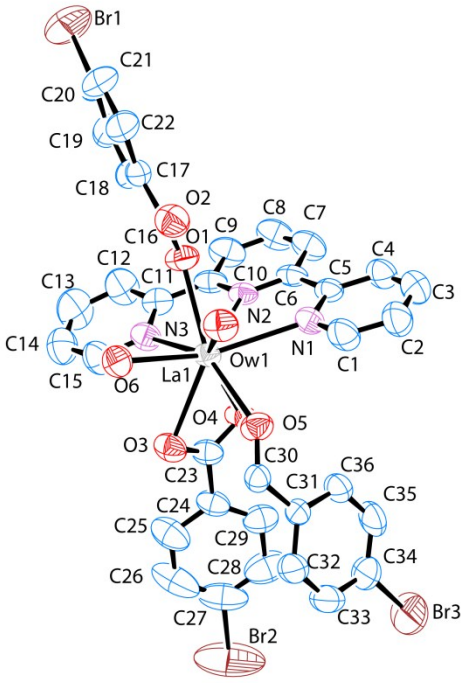

Figure S24: ORTEP illustration of structure **1**. Ellipsoids are shown at 50% probability level.

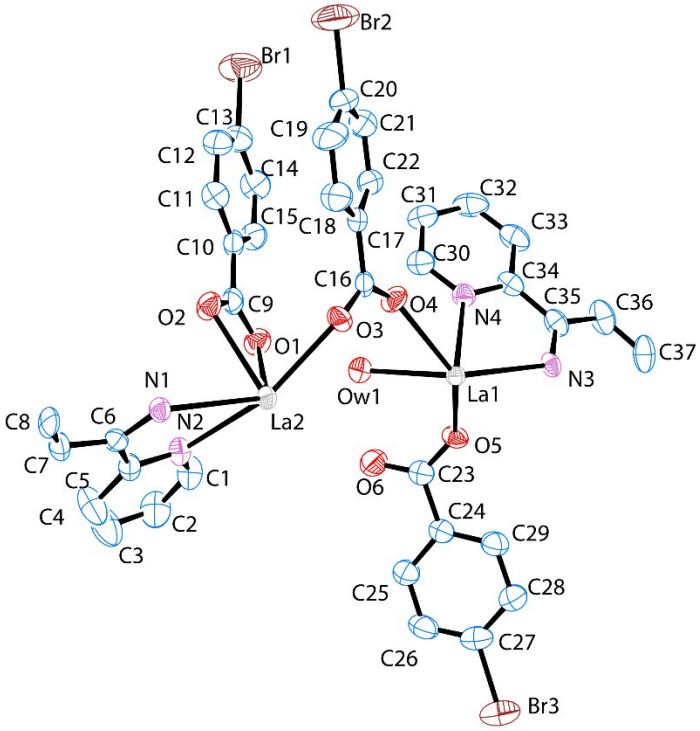

Figure S25: ORTEP illustration of structure **1'**. Ellipsoids are shown at 50% probability level.

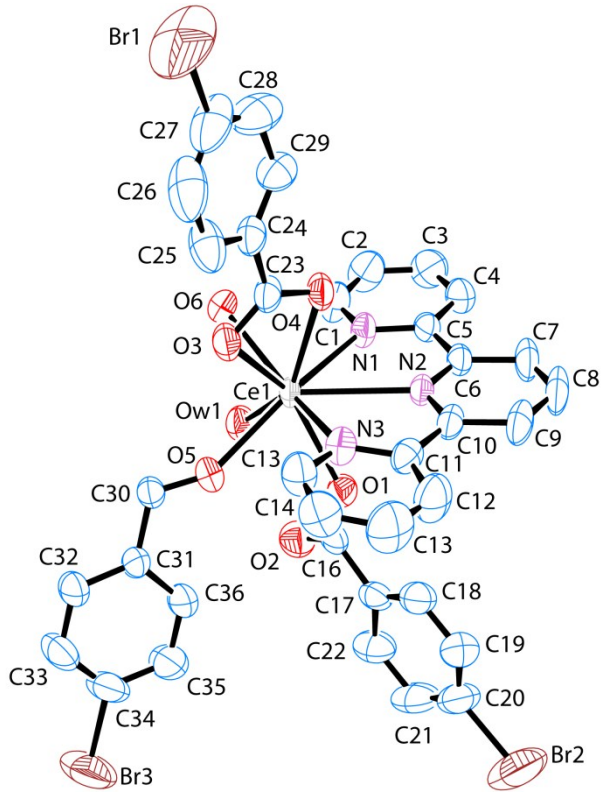

Figure S26: ORTEP illustration of structure **2**. Ellipsoids are shown at 50% probability level.

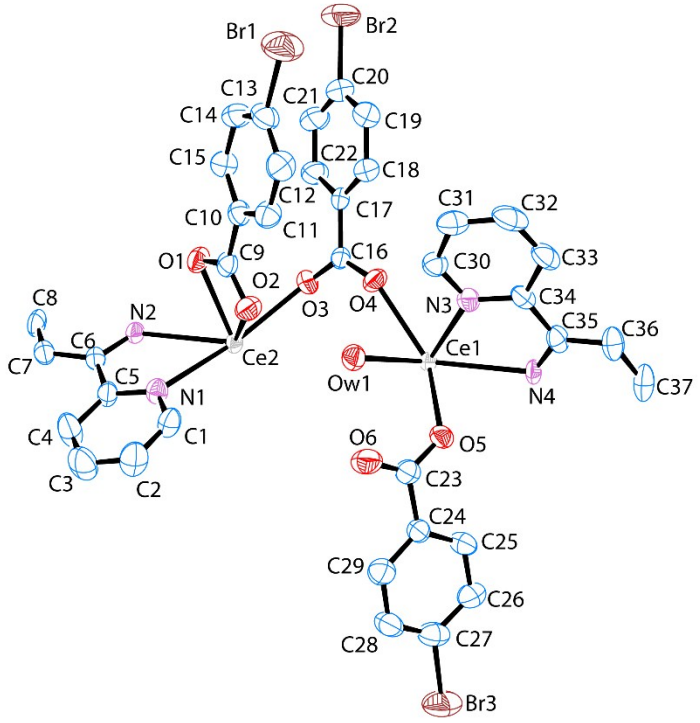

Figure S27: ORTEP illustration of structure **2'**. Ellipsoids are shown at 50% probability level.

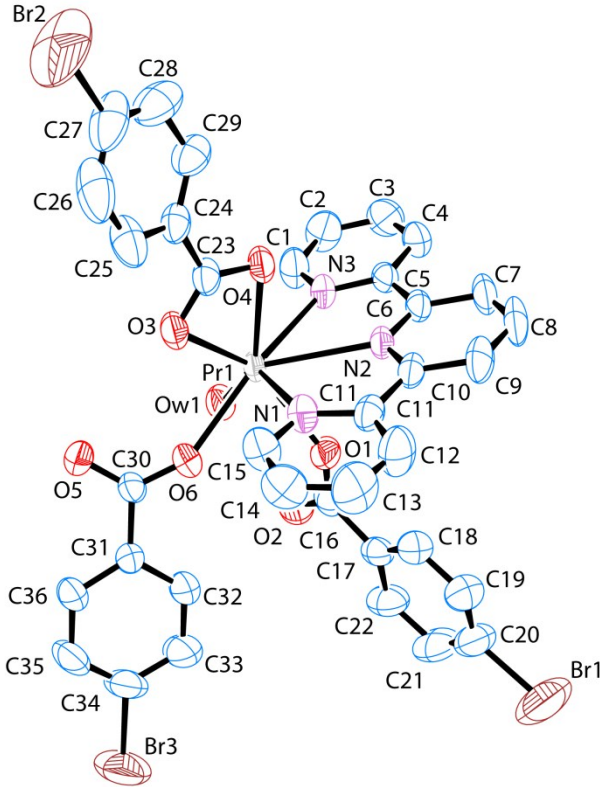

Figure S28: ORTEP illustration of structure **3**. Ellipsoids are shown at 50% probability level.

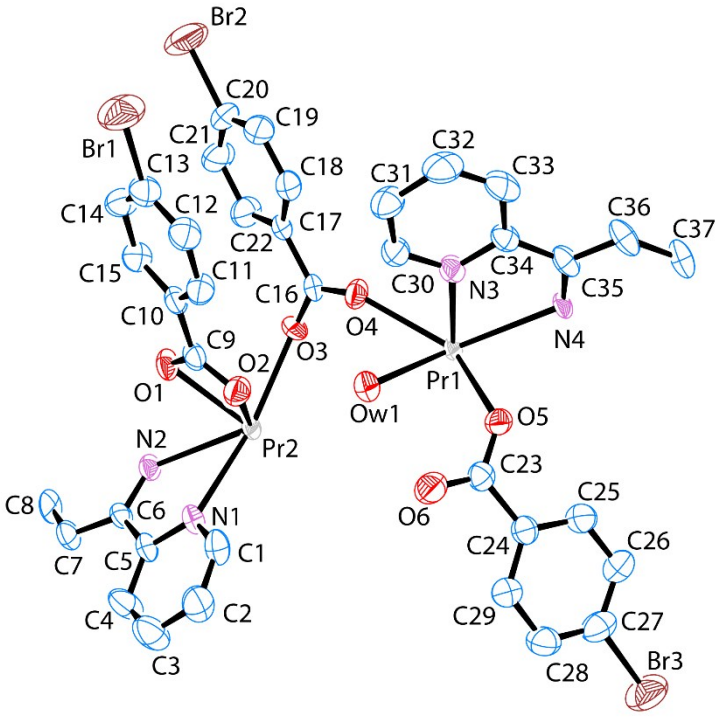

Figure S29: ORTEP illustration of structure **3'**. Ellipsoids are shown at 50% probability level.

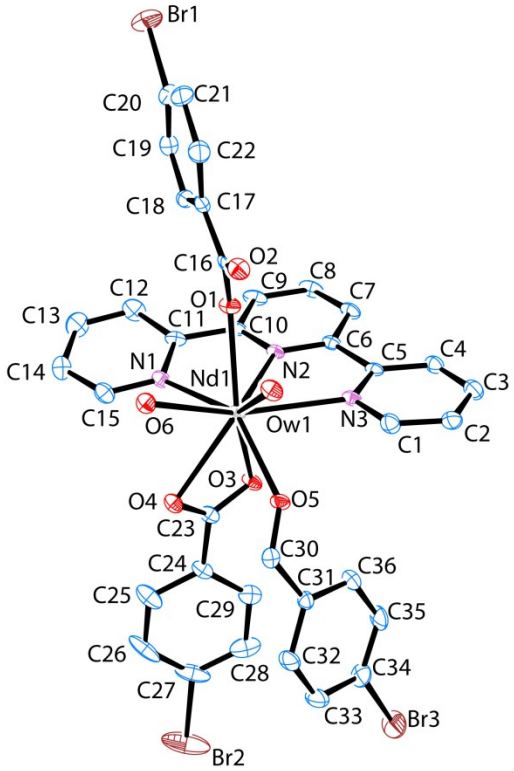

Figure S30: ORTEP illustration of structure **4**. Ellipsoids are shown at 50% probability level.

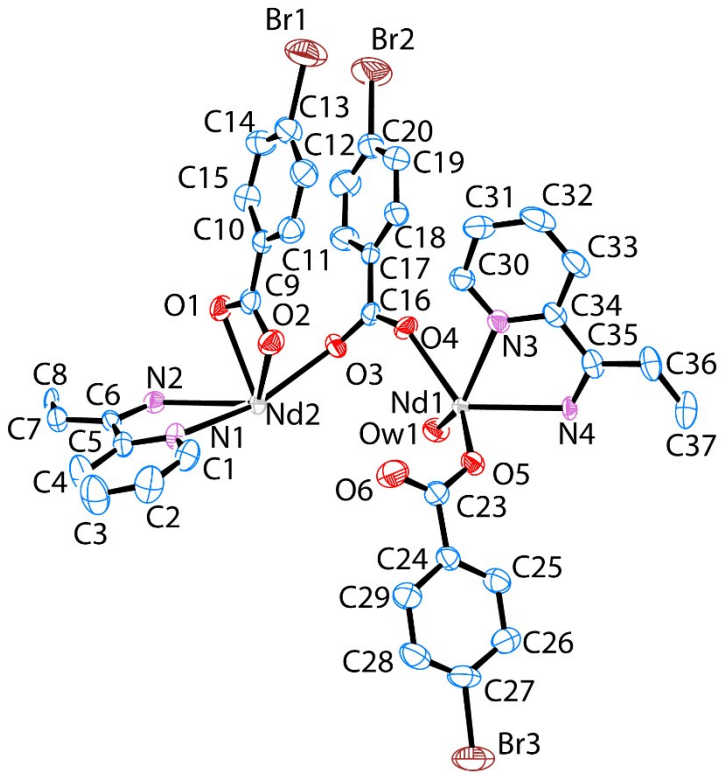

Figure S31: ORTEP illustration of structure **4'**. Ellipsoids are shown at 50% probability level.

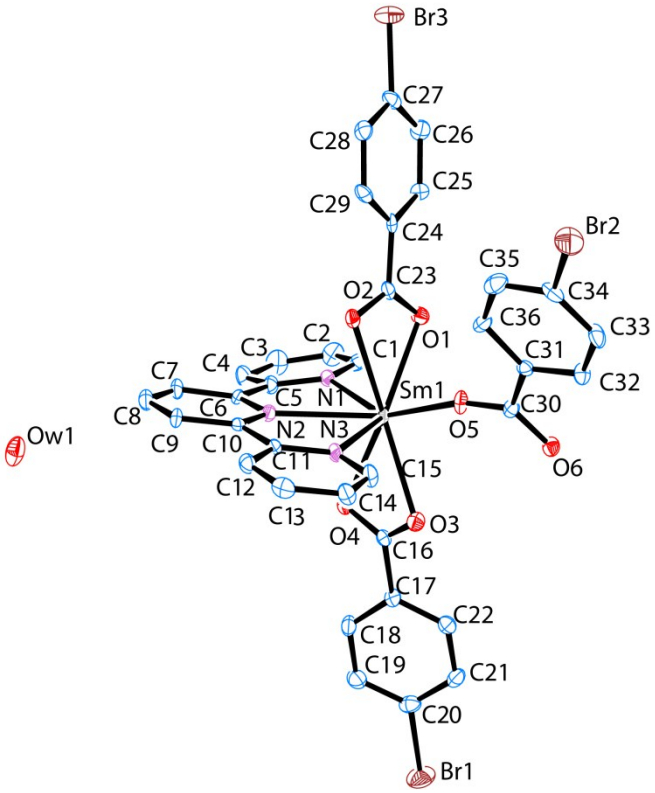

Figure S32: ORTEP illustration of structure **5**. Ellipsoids are shown at 50% probability level.

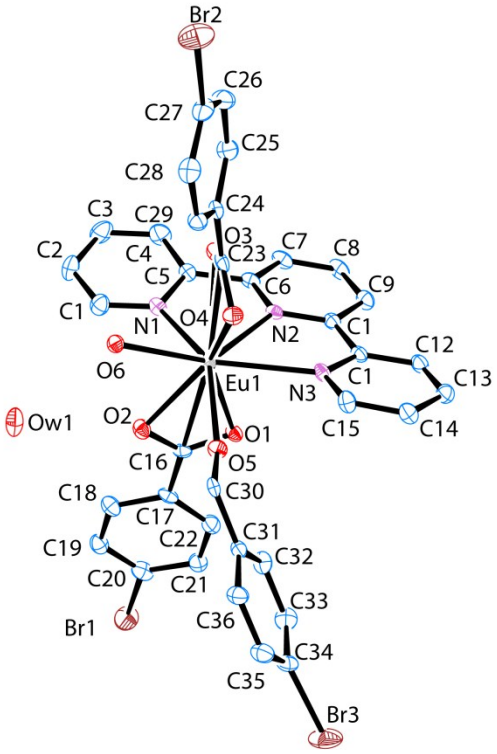

Figure S33: ORTEP illustration of structure **6**. Ellipsoids are shown at 50% probability level.

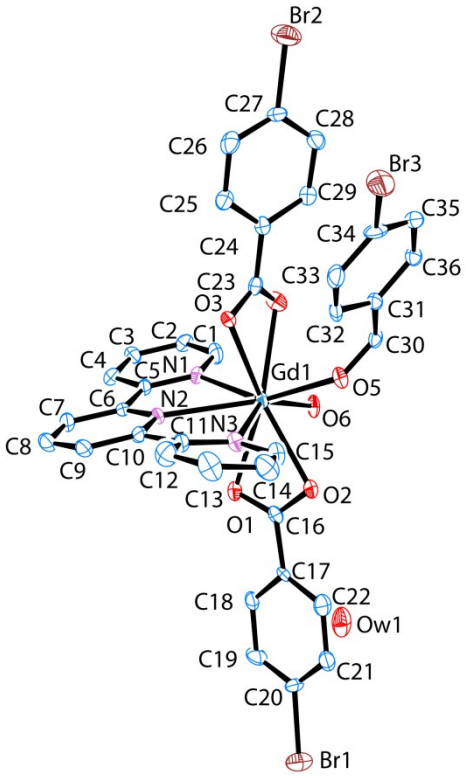

Figure S34: ORTEP illustration of structure **7**. Ellipsoids are shown at 50% probability level.

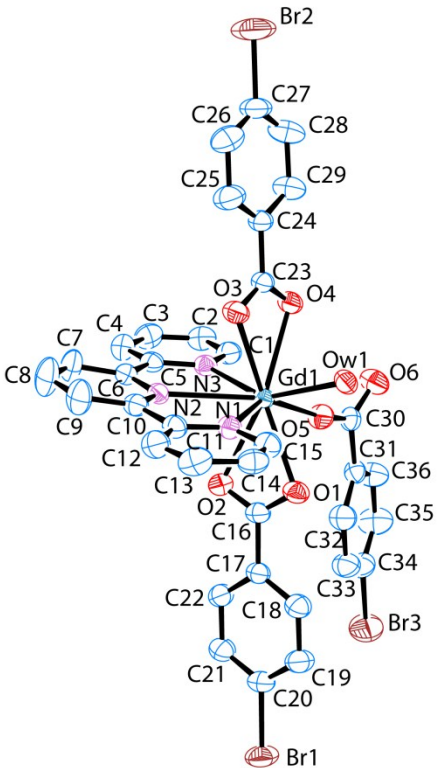

Figure S35: ORTEP illustration of structure **7'**. Ellipsoids are shown at 50% probability level.

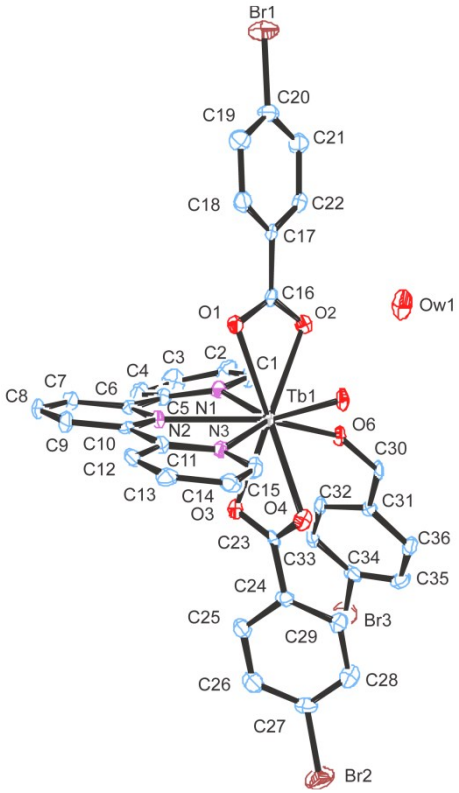

Figure S36: ORTEP illustration of structure **8**. Ellipsoids are shown at 50% probability level.

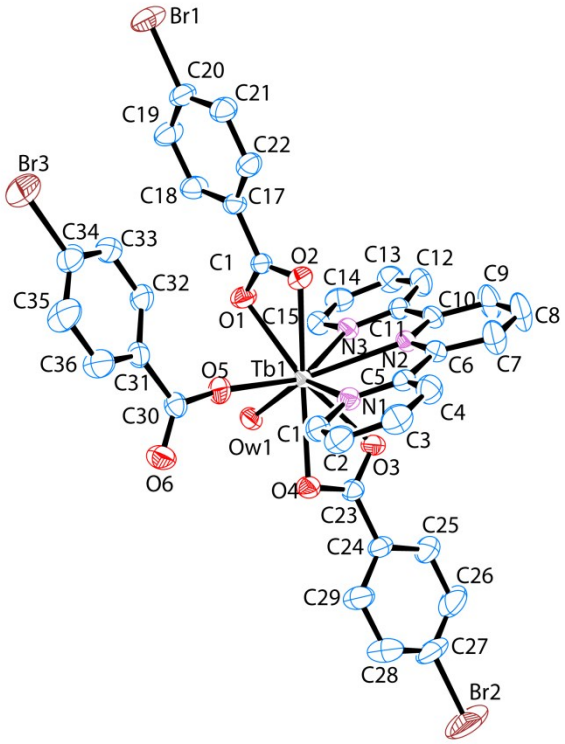

Figure S37: ORTEP illustration of structure **8'**. Ellipsoids are shown at 50% probability level.

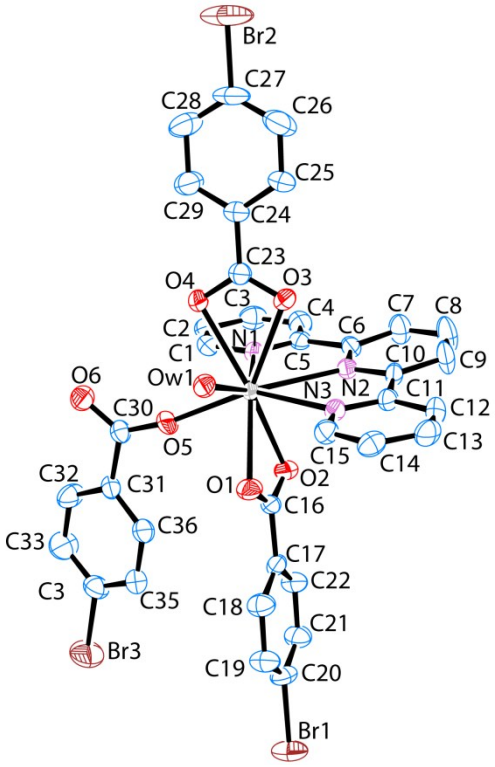

Figure S38: ORTEP illustration of structure **9**. Ellipsoids are shown at 50% probability level.

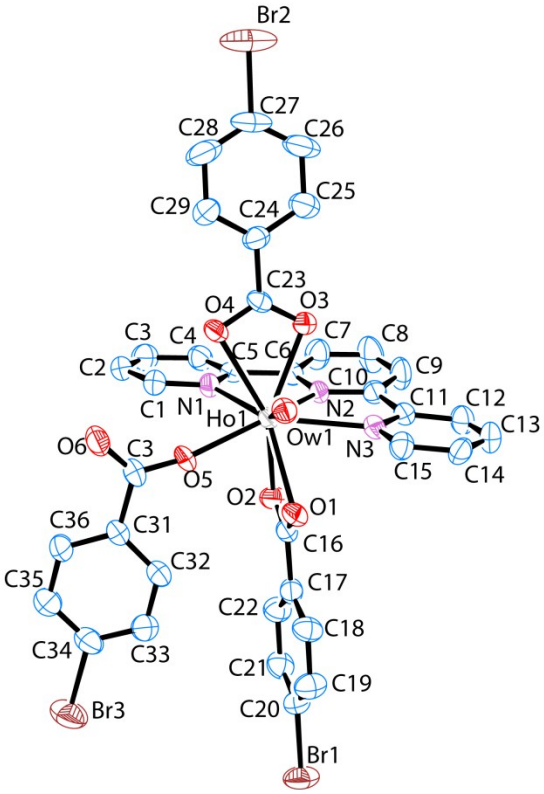

Figure S39: ORTEP illustration of structure **10**. Ellipsoids are shown at 50% probability level.

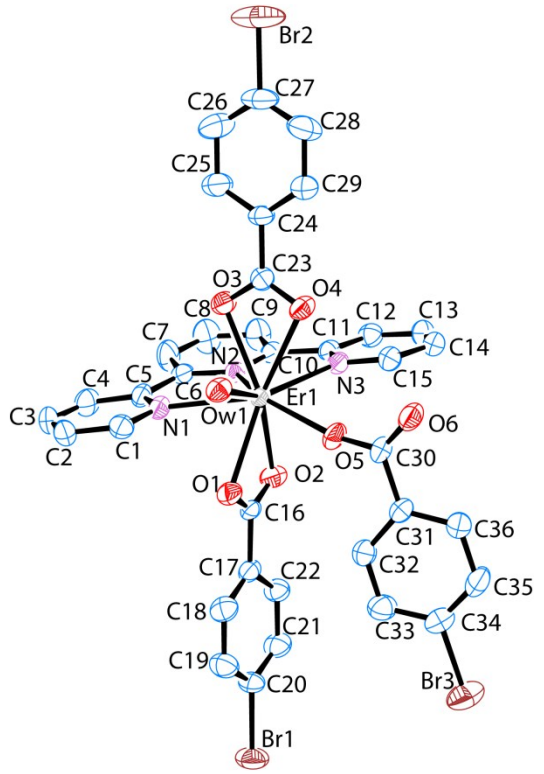

Figure S40: ORTEP illustration of structure **11**. Ellipsoids are shown at 50% probability level.

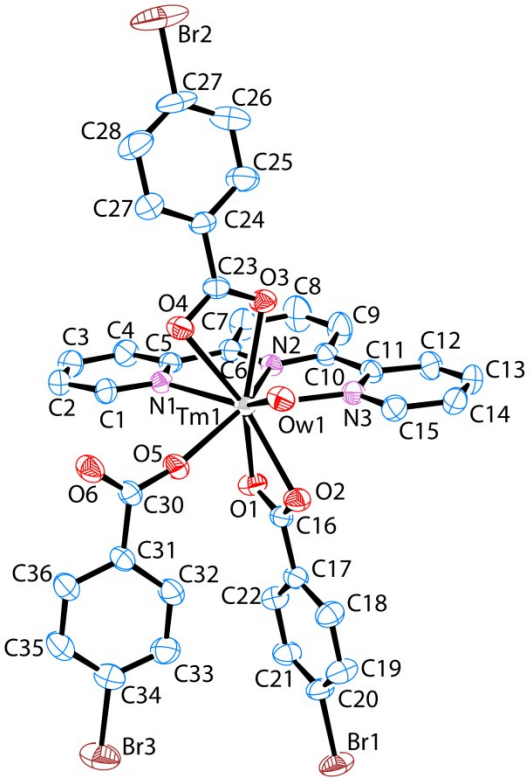

Figure S41: ORTEP illustration of structure **12**. Ellipsoids are shown at 50% probability level.

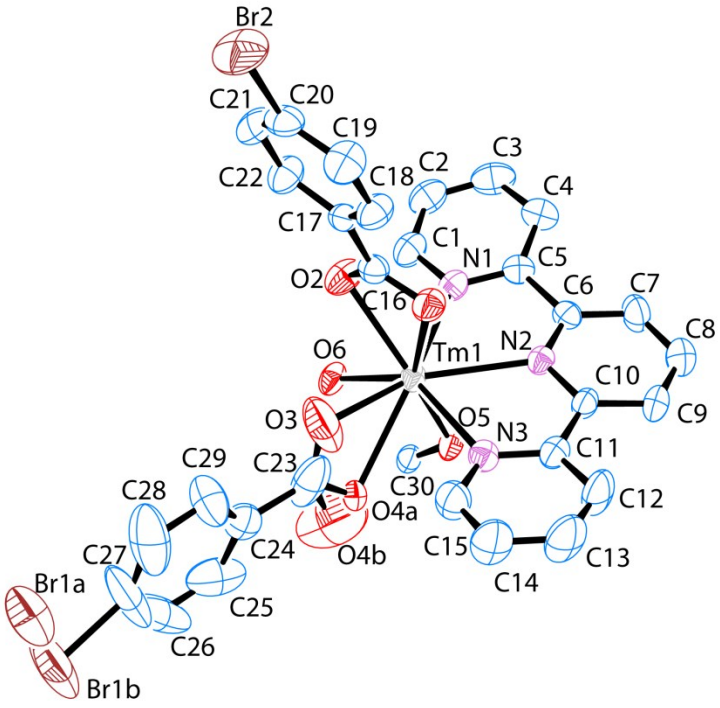

Figure S42: ORTEP illustration of structure **12'**. Ellipsoids are shown at 50% probability level.

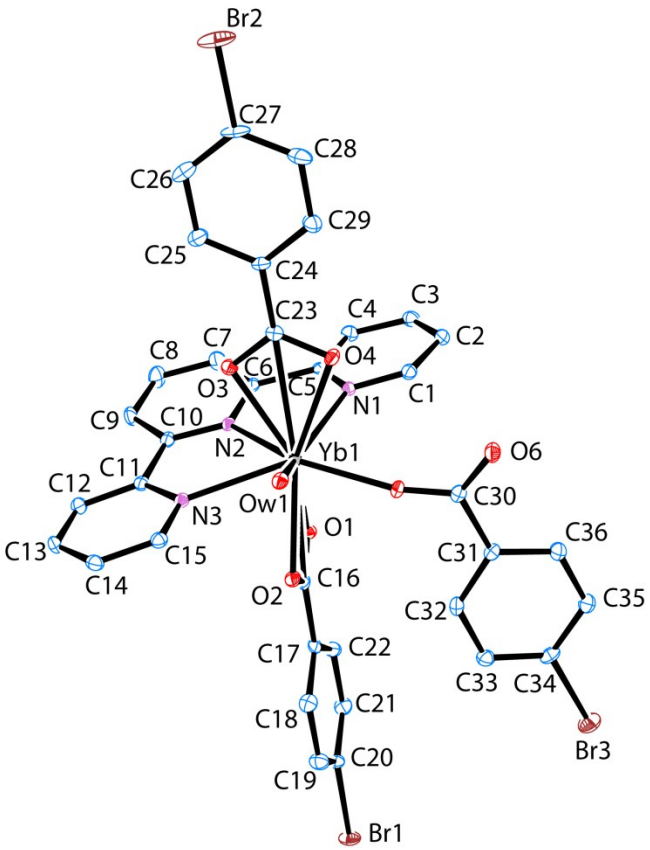

Figure S43: ORTEP illustration of structure **13**. Ellipsoids are shown at 50% probability level.

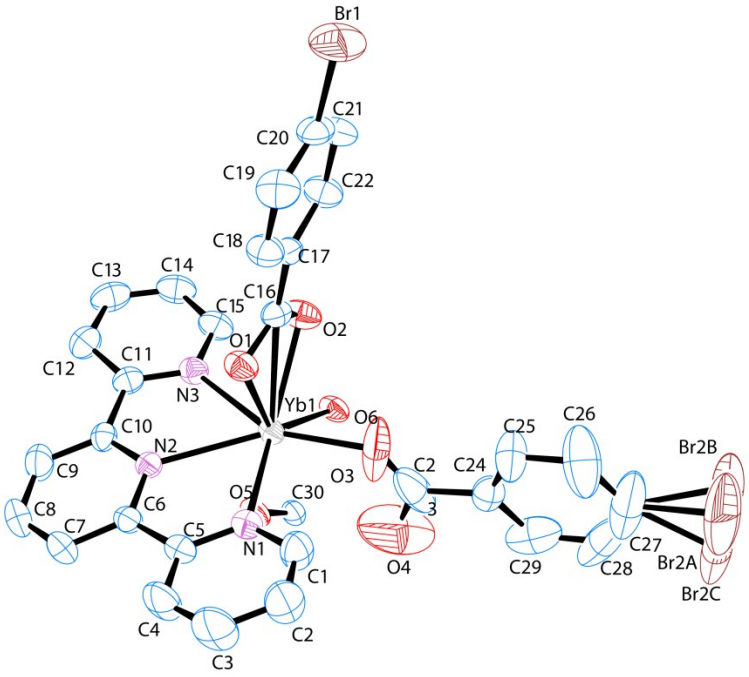

Figure S44: ORTEP illustration of structure **13'**. Ellipsoids are shown at 50% probability level.

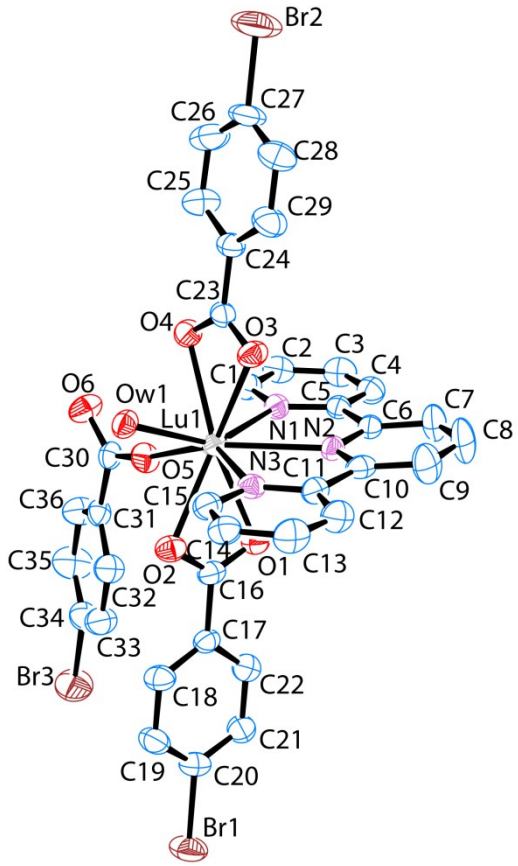

Figure S45: ORTEP illustration of structure **14**. Ellipsoids are shown at 50% probability level.

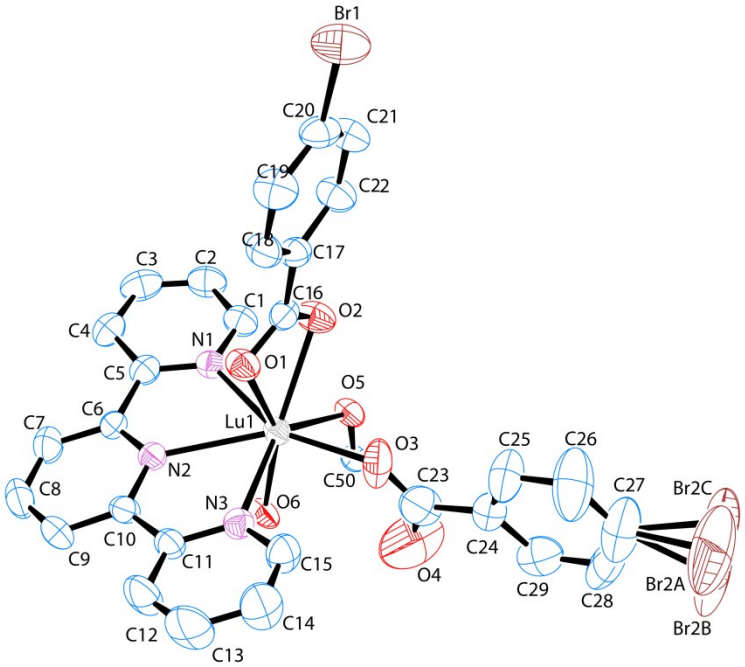

Figure S46: ORTEP illustration of structure **14'**. Ellipsoids are shown at 50% probability level.

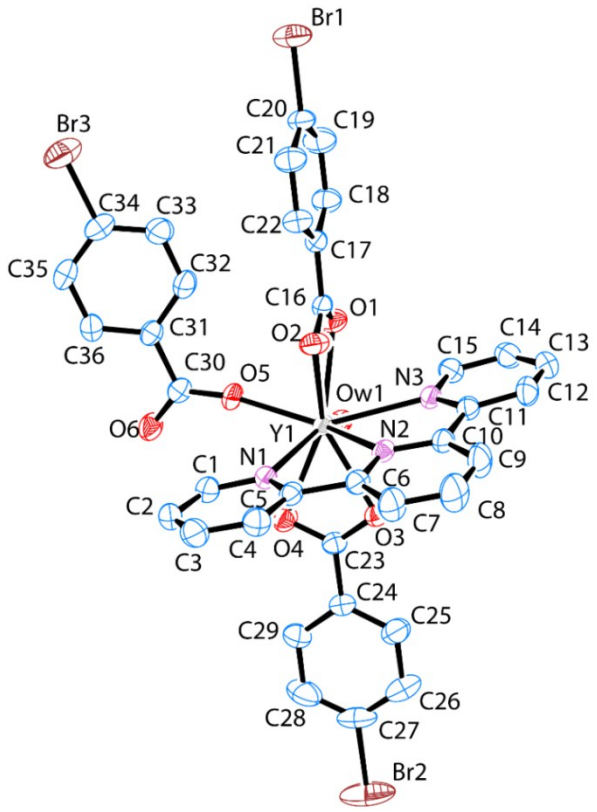

Figure S47: ORTEP illustration of structure **15**. Ellipsoids are shown at 50% probability level.

III. Tables of Bond Distance

Table S1: Bond Lengths RE-N in Rare Earth Complexes **1-15** with *p*-bromobenzoic acid and 2,2':6'2"-terpyridine.

RE(III) Complex	d_{Ln-N1} [Å]	d_{Ln-N2} [Å]	d_{Ln-N3} [Å]	d_{Ln-N4} [Å]
1 (La)	2.696(4)	2.747(3)	2.677(4)	
1' (La)	2.688(3)	2.739(4)	2.684(3)	2.738(4)
2 (Ce)	2.680(3)	2.722(3)	2.656(4)	
2' (Ce)	2.665(4)	2.714(4)	2.663(4)	2.710(4)
3 (Pr)	2.644(4)	2.699(3)	2.663(4)	
3' (Pr)	2.644(5)	2.696(6)	2.643(5)	2.691(6)
4 (Nd)	2.616(3)	2.669(3)	2.631(3)	
4 (Nd)	2.630(4)	2.678(5)	2.636(4)	2.667(4)
5 (Sm)	2.595(3)	2.624(3)	2.579(3)	
6 (Eu)	2.584(4)	2.607(3)	2.569(3)	
7 (Gd)	2.567(6)	2.609(5)	2.564(6)	
7' (Gd)	2.576(3)	2.613(3)	2.550(3)	
8 (Tb)	2.556(5)	2.576(4)	2.547(5)	
8' (Tb)	2.537(2)	2.595(2)	2.559(2)	
9 (Dy)	2.529(3)	2.576(3)	2.553(3)	
10 (Ho)	2.515(5)	2.555(4)	2.539(4)	
11 (Er)	2.529(4)	2.548(4)	2.508(4)	
12 (Tm)	2.498(2)	2.548(2)	2.522(2)	
12' (Tm)	2.519(4)	2.511(4)	2.529(4)	
13 (Yb)	2.483(2)	2.532(2)	2.501(2)	
13' (Yb)	2.517(4)	2.500(3)	2.499(4)	
14 (Lu)	2.481(3)	2.522(3)	2.512(3)	
14' (Lu)	2.489(4)	2.489(4)	2.509(4)	
15 (Y)	2.523(2)	2.575(2)	2.551(2)	

Table S2: Bond Lengths RE-O in Rare Earth Complexes **1-15** with *p*-bromobenzoic acid and 2,2':6'2"-terpyridine.

RE(III) Complex	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]
1 (La)	2.468(3)		2.643(3)	2.616(3)	2.441(3)	2.428(3)	2.602(4)
1' (La)	2.622(3)	2.545(3)	2.456(3)	2.472(3)	2.493(3)		2.626(4)
2 (Ce)	2.442(3)		2.625(3)	2.589(3)	2.408(3)	2.427(3)	2.580(3)
2' (Ce)	2.523(3)	2.596(3)	2.435(3)	2.448(3)	2.472(3)		2.616(3)
3 (Pr)	2.422(3)		2.607(3)	2.567(3)	2.407(3)	2.390(3)	2.564(3)
3' (Pr)	2.508(4)	2.579(4)	2.419(4)	2.431(4)	2.452(4)		2.586(5)
4 (Nd)	2.421(3)		2.545(2)	2.598(2)	2.396(2)	2.375(3)	2.526(3)
4' (Nd)	2.496(3)	2.566(3)	2.405(3)	2.419(3)	2.444(3)		2.569(4)
5 (Sm)	2.495(3)	2.508(3)	2.500(3)	2.538(3)	2.332(3)	2.342(3)	
6 (Eu)	2.496(3)	2.476(3)	2.527(3)	2.493(3)	2.324(3)	2.327(3)	
7 (Gd)	2.477(5)	2.469(5)	2.516(5)	2.478(5)	2.317(5)	2.303(5)	
7' (Gd)	2.483(2)	2.488(2)	2.459(2)	2.523(2)	2.302(2)		2.381(3)
8 (Tb)	2.468(4)	2.456(4)	2.497(4)	2.471(4)	2.296(4)	2.295(4)	
8' (Tb)	2.476(2)	2.475(2)	2.443(2)	2.510(2)	2.285(2)		2.369(2)
9 (Dy)	2.459(3)	2.455(3)	2.428(3)	2.500(3)	2.275(3)		2.352(3)
10 (Ho)	2.446(4)	2.450(4)	2.410(4)	2.489(4)	2.261(4)		2.340(4)
11 (Er)	2.450(3)	2.439(3)	2.409(3)	2.493(3)	2.262(3)		2.333(3)
12 (Tm)	2.432(2)	2.438(2)	2.395(2)	2.491(2)	2.246(2)		2.315(2)
12' (Tm)	2.356(3)	2.401(3)	2.263(5)		2.292(3)	2.329(3)	
13 (Yb)	2.401(2)	2.435(2)	2.379(2)	2.473(2)	2.240(2)		2.303(2)
13' (Yb)	2.348(3)	2.386(3)	2.204(4)		2.270(3)	2.319(3)	
14 (Lu)	2.417(3)	2.425(3)	2.375(3)	2.484(3)	2.233(3)		2.295(3)
14' (Lu)	2.339(3)	2.374(3)	2.203(4)		2.308(3)	2.252(3)	
15 (Y)	2.456(2)	2.454(2)	2.419(2)	2.501(2)	2.263(2)		2.340(2)

Table S3: Intermolecular Non-Covalent Interactions Distances in Structure Type I Complexes (**1**, **2**, **3**, **4)**

Compound	d(Br3-π) localized [Å]/%VdW	d(π- π) [Å]
1 (La)	3.4362(1)/[96.79%]	3.5856(2)
2 (Ce)	3.4271(1)/[96.54%]	3.5843(1)
3 (Pr)	3.4263(1)/[96.52%]	3.5881(1)
4 (Nd)	3.4260(2)/[97.52%]	3.5114(3)

Table S4: Intermolecular Non-Covalent Interactions Distances in Structure Type IV Complexes (**1'**, **2'**, **3'**, **4')**

Compound	d(Br3-π) localized [Å]/%VdW	d(π- π) [Å]
1' (La)	3.3726(2)/[95.00%]	3.5303(2) and 3.7372(2)
2' (Ce)	3.3898(7)/[95.49%]	3.5328(7) and 3.7381(7)
3' (Pr)	3.383(6)/[95.29%]	3.533(3) and 3.729(4)
4' (Nd)	3.3925(2)/[95.56%]	3.5347(3) and 3.7315(3)

Table S5: Intermolecular Non-Covalent Interactions Distances in Structure Type V Complexes (**5**, **6**, **7**, **8**)

Compound	d(Br1-π) delocalized [Å]	d(π- π) [Å]
5 (Sm)	3.3762(7)	3.7136(8)
6 (Eu)	3.3689(5)	3.7121(6)
7 (Gd)	3.3776(10)	3.7105(11)
8 (Tb)	3.3782(5)	3.7142(5)

Table S6: Intermolecular Non-Covalent Interactions Distances in Structure Type III Complexes (**7'**, **8'**, **9**, **10**, **11**, **12**, **13**, **14**, **15)**

Compound	d(Br1-π) localized [Å]/%VdW	d(Br2-π) localized [Å]/%VdW	d(π- π) [Å]
7' (Gd)	3.3552(3)/[94.51%]	3.4195(3)[96.32%]	3.5643(3)
8' (Tb)	3.3504(1)/[94.38%]	3.4117(1)/[96.10%]	3.5610(1)
9 (Dy)	3.3469(2)/[94.28%]	3.4110(2)/[96.08%]	3.5590(3)
10 (Ho)	3.3406(7)/[94.10%]	3.4006(7)/[95.79%]	3.5432(7)
11 (Er)	3.3510(3)/[94.39%]	3.4093(3)/[96.04%]	3.5632(3)
12 (Tm)	3.3522(1)/[94.42%]	3.4102(1)/[96.06%]	3.5567(1)

13 (Yb)	3.2988(5)/[92.92%]	3.3736(5)/[95.03%]	3.4941(5)
14 (Lu)	3.3556(2)/[94.52%]	3.4069(2)/[95.97%]	3.5534(2)
15 (Y)	3.3535(11)/[94.46%]	3.4140(12)/[96.27%]	3.5624(12)

Table S7: Intermolecular Non-Covalent Interactions Distances in Structure Type VI Complexes (**12'**, **13'**, **14'**) [Interaction distances calculated from a centroid created by the two or three disordered parts of the halogen atom]

Compound	d(Br2-π) localized [Å]/%VdW
12' (Tm)	3.3644(1)/[94.77%]
13' (Yb)	3.3499(1)/[94.36%]
14' (Lu)	3.3927(1)/[95.57%]