Supporting Information

Hydroquinone-assisted assembly of coordination polymers from lanthanides and cucurbit[5]uril

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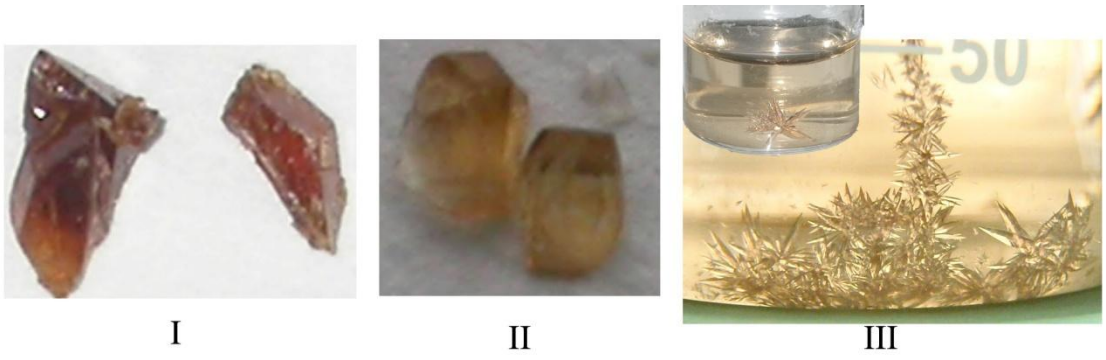
The detailed bond lengths and distances in the supramolecular assemblies of Q[5] with Lanthanides are showed in SI-Table 1 and SI-Figure 2.

SI-Table 1 The detailed bond lengths and distances in the supramolecular assemblies of Q[5] with Lanthanides

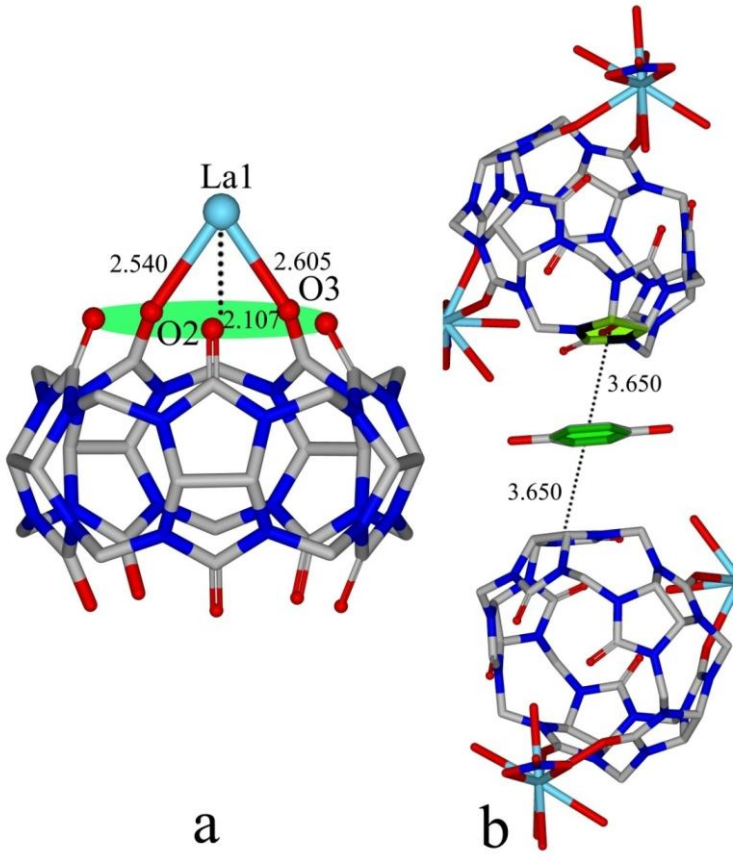
	$Ln\text{-}O_{(carbonyl)}$(Å)	$Ln\text{-}O_{(water)}$(Å)	$H_{Ln\text{-}plane}$(Å)
La	2.540-2.605	2.601-2.605	2.107
Sm	2.397-2.404	2.359-2.430	1.889
Eu	2.350-2.409	2.360-2.432	1.830-1.866
Gd	2.354-2.385	2.358-2.436	1.841-1.849
Dy	2.315-2.371	2.345-2.371	1.828-1.836
Er	2.302-2.349	2.302-2.337	1.812-1.813
Yb	2.280-2.335	2.285-2.333	1.785-1.803
Lu	2.275-2.332	2.286-2.329	1.766-1.813

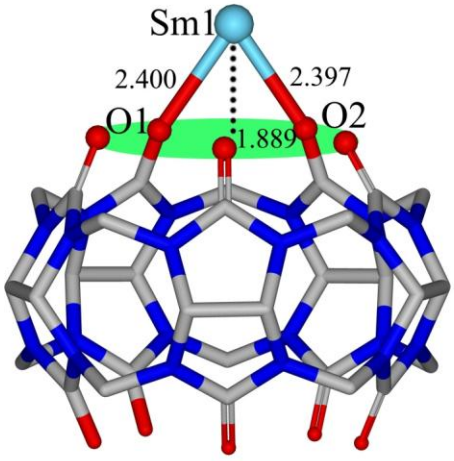
SI-Table 2 The Water molecules in Compound **1 – 8:** how many water molecules were found on Fourier maps and how many water molecules were introduced with SQUEEZE.

NO.	1	2	3	4	5	6	7	8
All Water molecules	14	19	52	58	13	14	16	19
Squeeze water molecules	10	8	32	48	9	10	12	15
Final water molecules	4	11	20	10	4	4	4	4



SI-Figure 1. The single-crystal photos of compounds corresponding to three different supramolecular assemblies.





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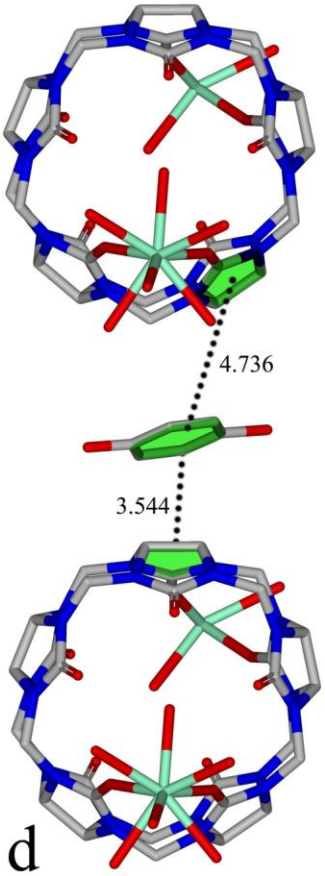

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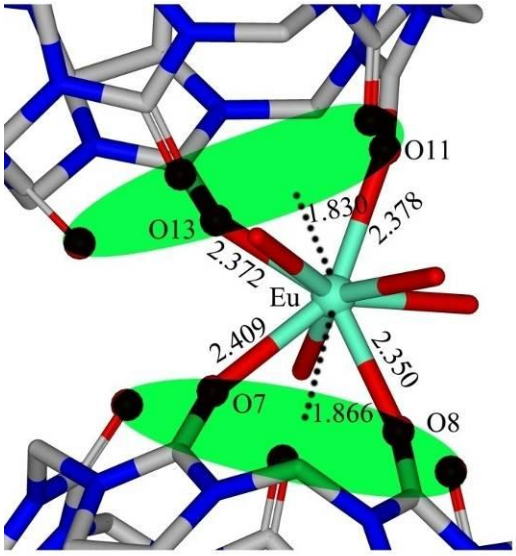

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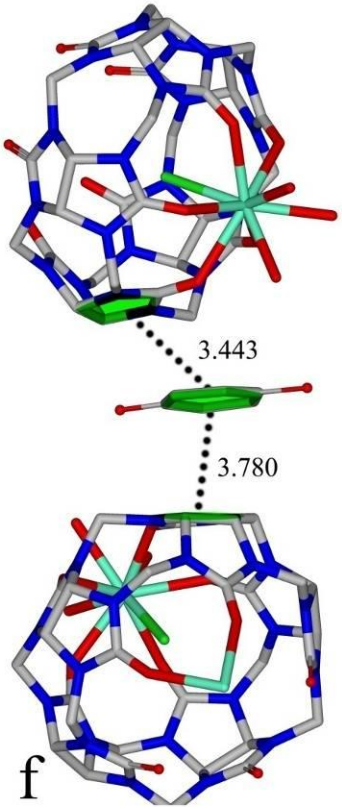

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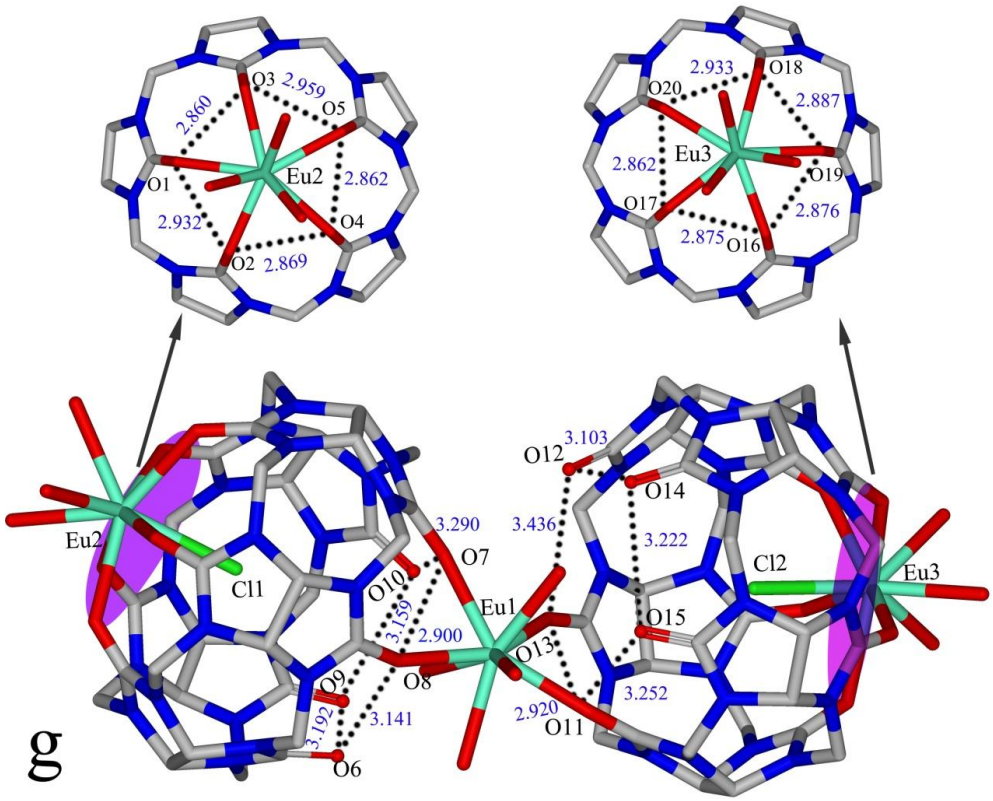
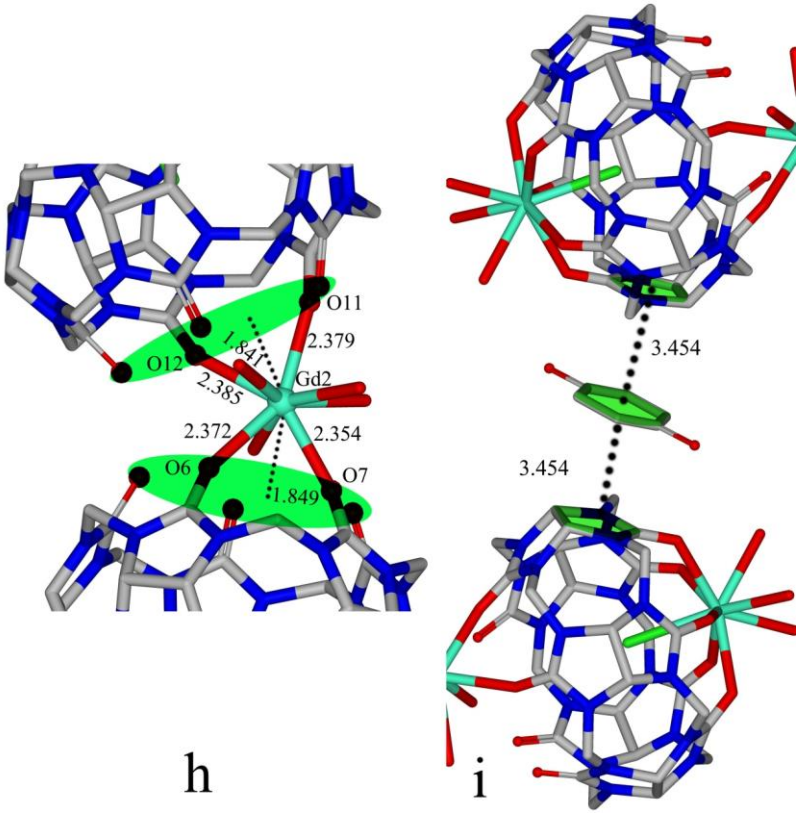
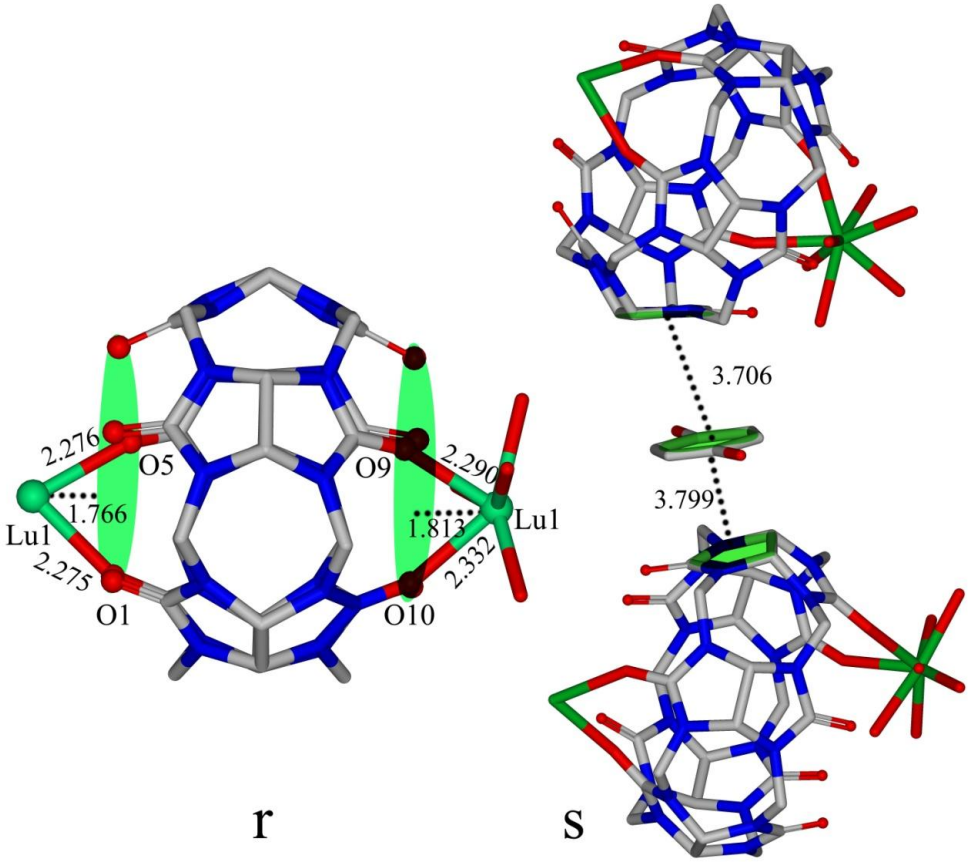
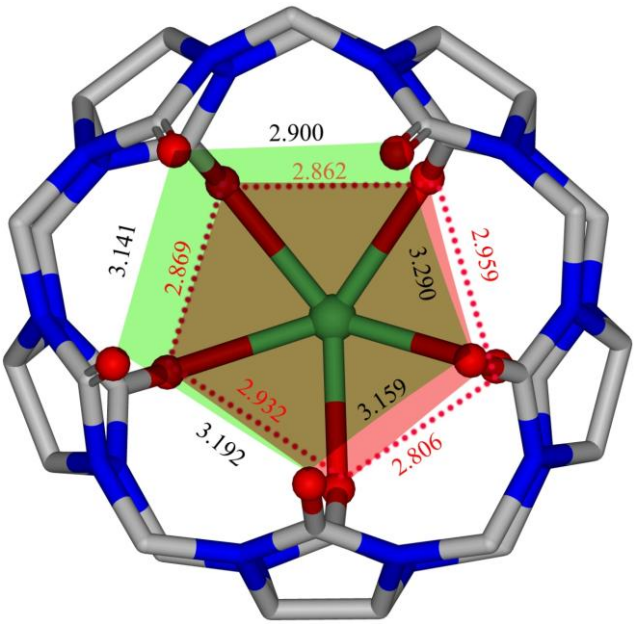

O3
2.959
O5
2.860
O1
Eu2
2.862
2.932
O4
O2
2.869
2.933
O18
O20
2.887
Eu3
2.862
O19
O17
2.876
2.875
O16
Eu2
Cl1
3.290
O7
O10
3.159
2.900
Eu1
O9
O8
3.192
3.141
O6
O12
3.103
O14
3.436
3.222
Cl2
Eu3
O15
O13
3.252
2.920
O11
g

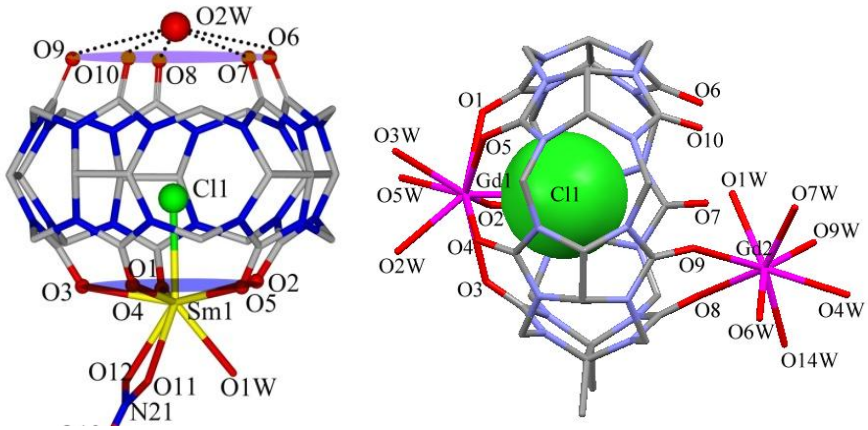

O11
2.379
1.841
O12
2.385
Gd2
2.372
2.354
O6
O7
1.849
h
3.454
3.454
i



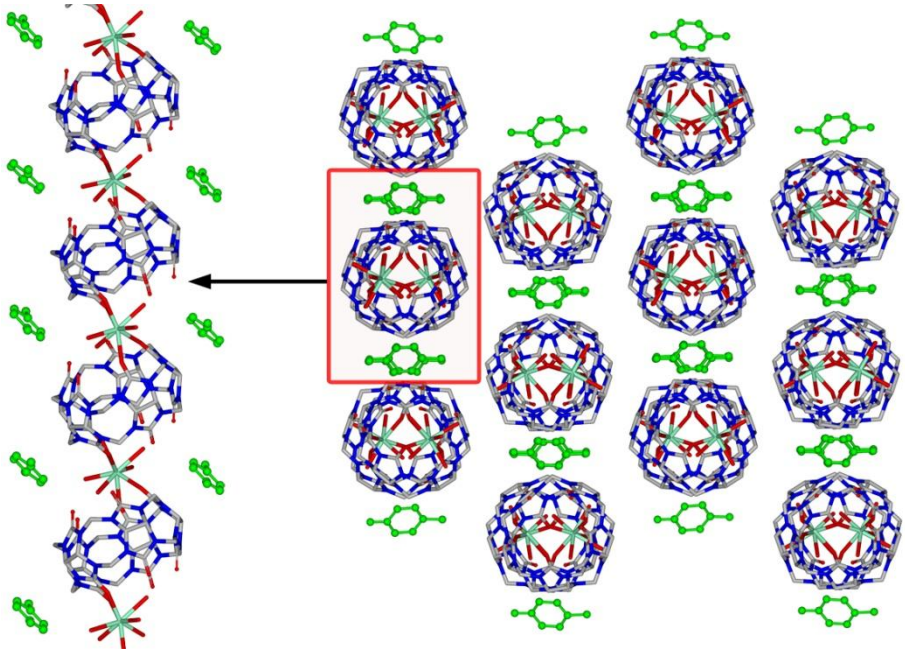
SI-Figure 2. The detailed bond lengths and distances in the supramolecular assemblies of Q[5] incorporating lanthanides



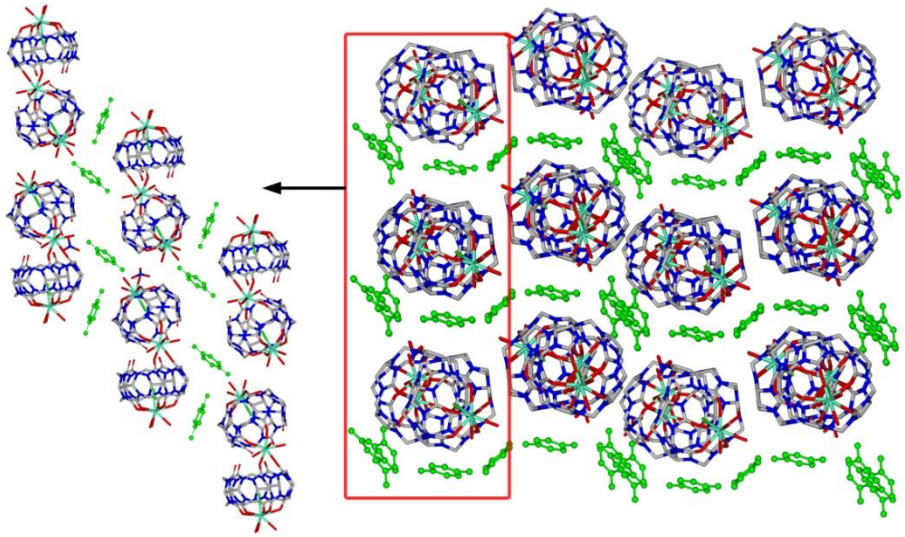
SI-Figure 3. Comparison to the two portal sizes of a Q[5] molecule in the Q[5]-pair found in compounds 3 and 4



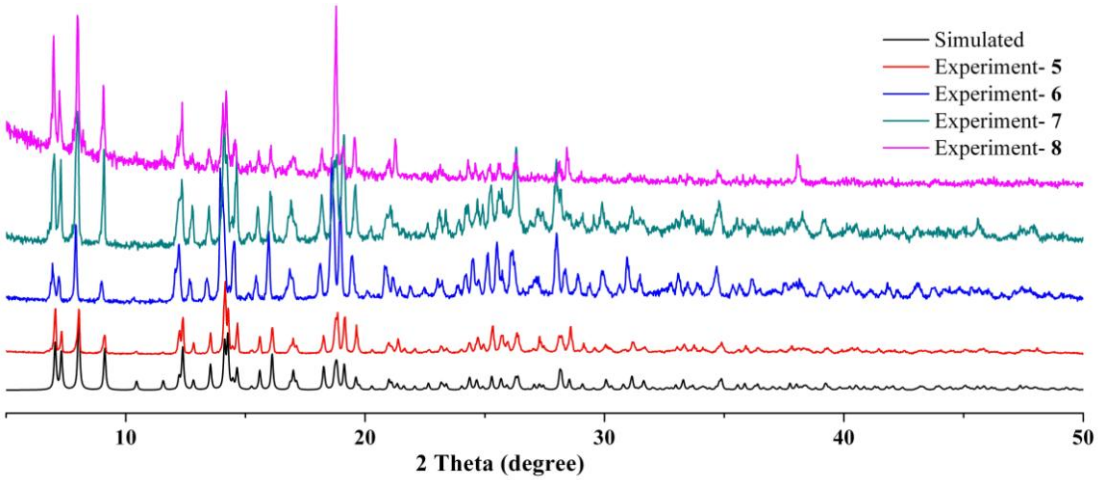
SI-Figure 4 discrete "molecular bowl" and half covered "molecular bowl" of Q[5] molecule with Ln^{3+}



SI-Figure 5 the supramolecular assemblies corresponding to the Q[5]-light lanthanides (Figure3b)

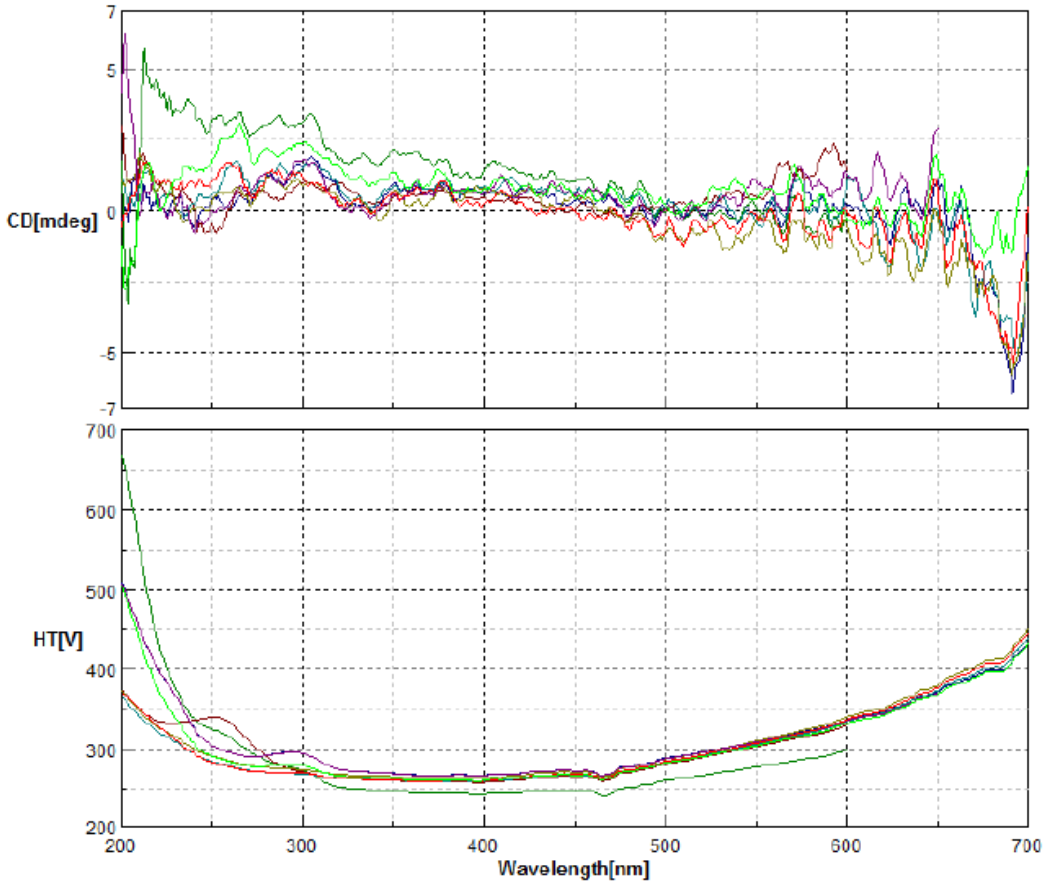


SI-Figure 6 the supramolecular assemblies corresponding to the Q[5]- moderately heavy lanthanides (Figure3c)



SI-Figure 7 Powder X-ray diffraction (PXRD) of Complexes 5-8 and a comparison with simulation show that the sample produced is phase pure.

It is well known that the solid-state circular dichroism (CD) spectroscopy is the most effective method to calculate the enantionmeric excess values. However, investigation using solid-state CD spectroscopy in a KBr pellet showed that every single crystal of complexs 5-8 were CD-silent[1]. The result suggests the sample in present case had undergone spontaneous resolution with an enantiomeric excess value of 50%. It should be noted that the enantiomeric excess value of compound 5-8 are stochastic and variable.



SI-Figure 7 the solid-state circular dichroism (CD) spectroscopy of complexs 5-8

Reference: 1. K. Chen, Y.-F. Hu, X. Xiao, S.-F. Xue, Z. Tao, Y.-Q. Zhang, Q.-J. Zhu and J.-X. Liu, RSC Adv. 2012, **2**, 3217.