Electronic Supplementary Material for CrystEngComm

Electronic Supplementary Information

2-D Coordination Network of Cyclic Amide with Lanthanide Metal Cation and Its Columnar Stacking

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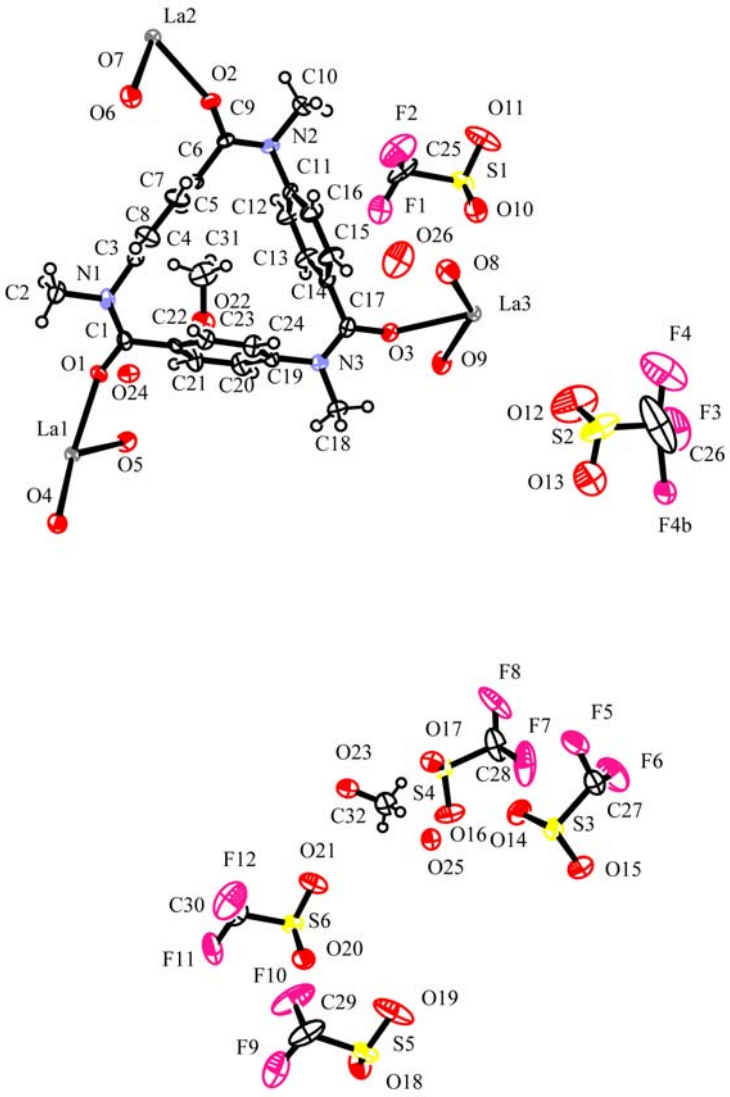


Fig. S1 ORTEP diagram of asymmetric unit in the crystal of **1**-La. The ellipsoids of non–hydrogen atoms are drawn at the 50 % probability level. The positions of hydrogen atoms included in the water and methanol molecules were not calculated. Selected bond lengths (Å) and angles (°): La(1)–O(1) 2.489(4), O(1)–C(1) 1.246(6), C(1)–N(1) 1.345(7), N(1)–C(2) 1.467(7), La(2)–O(2) 2.485(4), O(2)–C(9) 1.237(7), C(9)–N(2) 1.338(7), N(2)–C(10) 1.480(7), La(3)–O(3) 2.484(4), O(3)–C(17) 1.247(6), C(17)–N(3) 1.314(7), N(3)–C(18) 1.469(7), O(1)–La(1)–O(1)$^{\#1}$ 119.834(12), O(2)–La(2)–O(2)$^{\#2}$ 119.823(12), O(3)–La(3)–O(3)$^{\#3}$ 119.811(13), La(1)–O(1)–C(1) 160.0(4), C(22)–C(1)–N(1) 119.0(5), C(1)–N(1)–C(3) 121.1(5), La(2)–O(2)–C(9) 158.9(4), C(6)–C(9)–N(2) 118.5(5), C(9)–N(2)–C(11) 121.4(5), La(3)–O(3)–C(17) 160.2(4), C(14)–C(17)–N(3) 118.8(5), C(17)–N(3)–C(19) 121.0(5). Symmetry transformations used to generate equivalent atoms: #1 –y+1, x–y+2, z. #2 –y+1, x–y+1, z. #3 –x+y, –x+2, z.

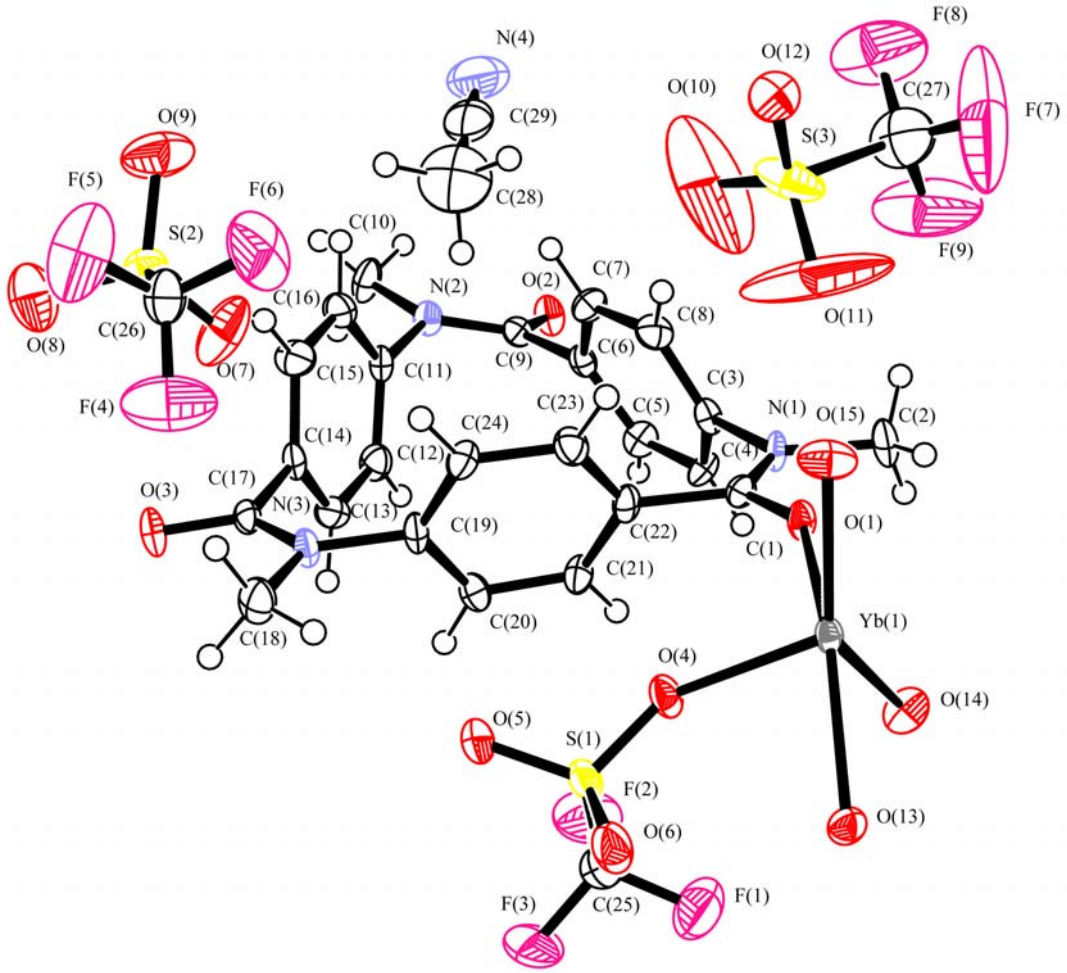
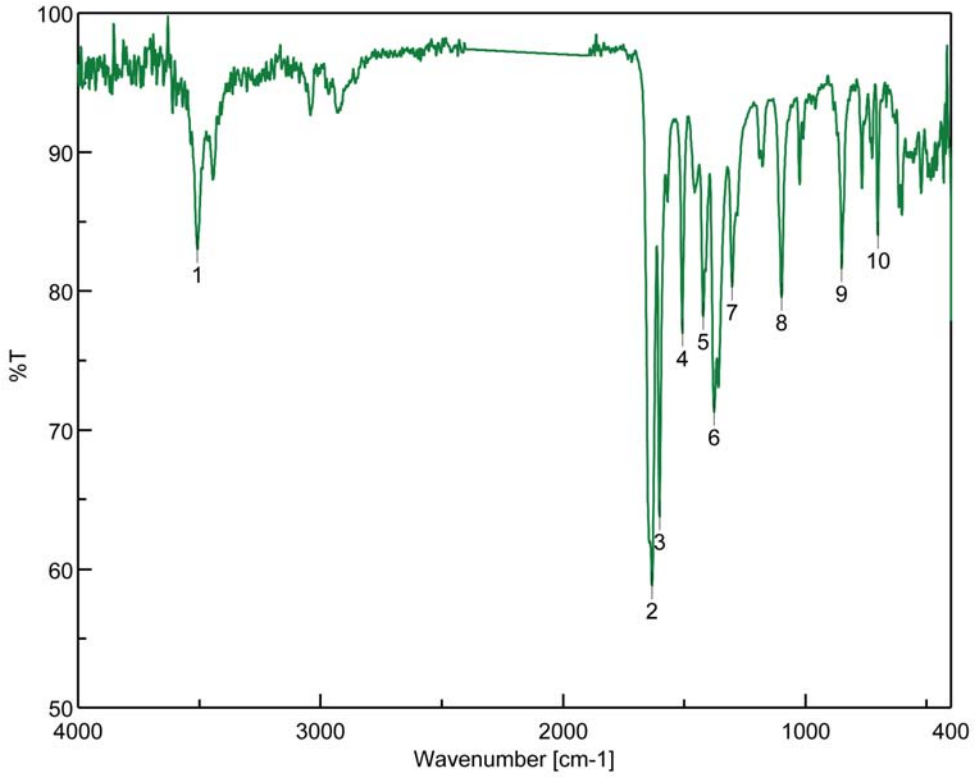
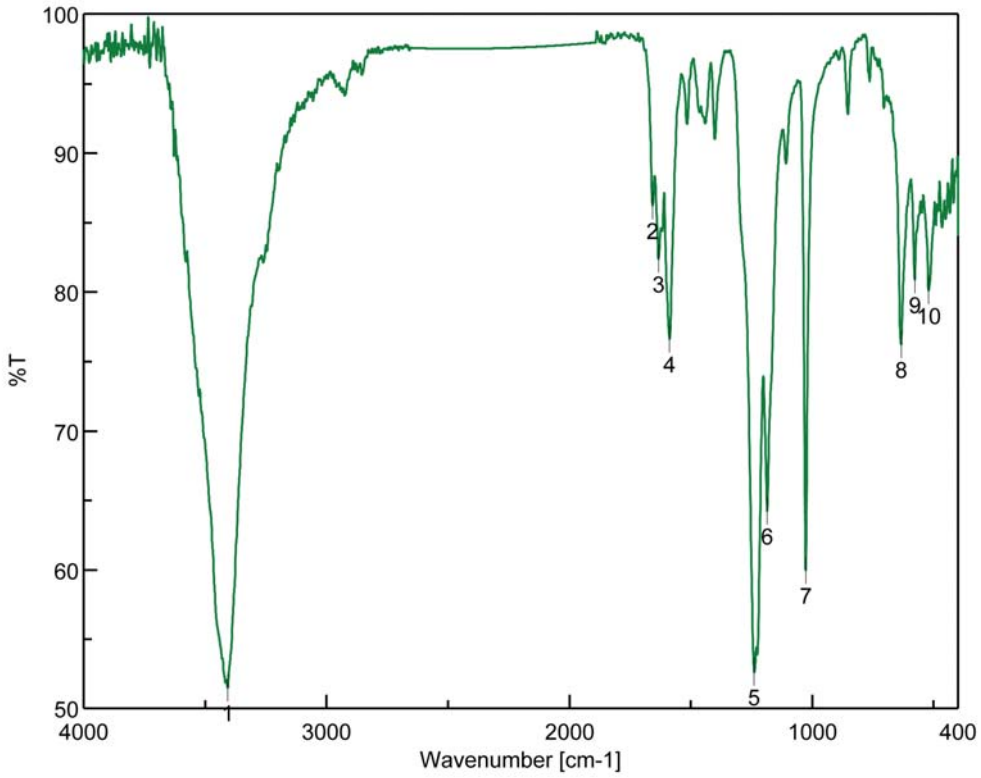


Fig. S2 ORTEP diagram of asymmetric unit in the crystal of **1**-Yb. The ellipsoids of non–hydrogen atoms are drawn at the 50 % probability level. The positions of hydrogen atoms included in the water molecules were not calculated. Selected bond lengths (Å) and angles (°): Yb(1)–O(1) 2.253(3), Yb(1)–O(2)$^{\#2}$ 2.222(3), Yb(1)–O(3)$^{\#1}$ 2.185(4), O(1)–C(1) 1.245(5), C(1)–N(1) 1.338(6), N(1)–C(2) 1.481(7), O(2)–C(9) 1.246(4), C(9)–N(2) 1.334(5), N(2)–C(10) 1.475(5), O(3)–C(17) 1.246(5), C(17)–N(3) 1.316(5), N(3)–C(18) 1.485(5), O(1)–Yb(1)–O(2)$^{\#2}$ 134.37(11), O(2)$^{\#2}$–Yb(1)–O(3)$^{\#1}$ 92.10(12), O(3)$^{\#1}$–Yb(1)–O(1) 109.51(12), C(22)–C(1)–N(1) 118.1(4), C(1)–N(1)–C(3) 121.2(5), C(6)–C(9)–N(2) 118.7(3), C(9)–N(2)–C(11) 121.2(3), C(14)–C(17)–N(3) 119.0(3), C(17)–N(3)–C(19) 122.7(3). Symmetry transformations used to generate equivalent atoms: #1 x, y, z+1. #2 x, y–1, z+1.



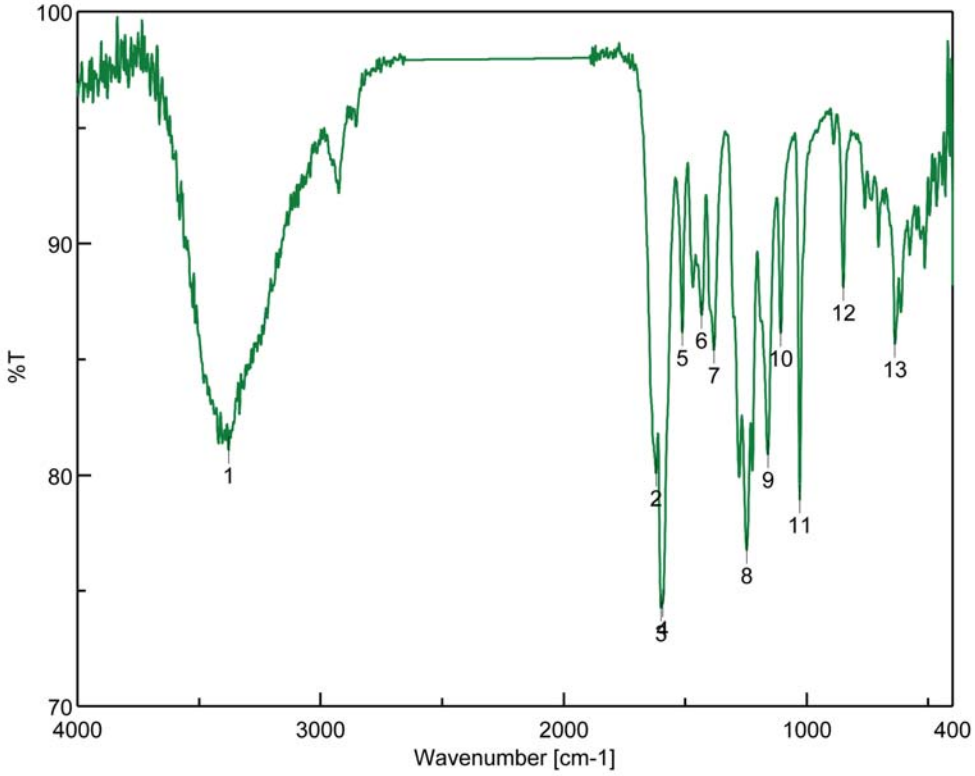
No.	cm^{-1}	%T	No.	cm^{-1}	%T
1	3507.88	82.9828	2	1633.41	58.8259
3	1602.56	63.8032	4	1508.06	76.9477
5	1422.24	78.1575	6	1376.93	71.275
7	1302.68	80.2796	8	1099.23	79.5606
9	850.454	81.6222	10	701.962	84.0191

Fig. S3 Solid-state IR spectrum of ligand **1** with ATR method.



No.	cm^{-1}	%T	No.	cm^{-1}	%T
1	3406.64	51.4996	2	1657.52	86.1978
3	1633.41	82.3524	4	1587.13	76.6163
5	1239.04	52.6362	6	1186.01	64.2419
7	1026.91	59.9545	8	634.466	76.2217
9	578.54	80.8866	10	520.686	80.0935

Fig. S4 Solid-state IR spectrum of complex **1**-La with ATR method.



No.	cm^{-1}	%T	No.	cm^{-1}	%T
1	3378.67	81.0816	2	1619.91	80.088
3	1599.66	74.2541	4	1592.91	74.4541
5	1511.92	86.1586	6	1432.85	86.8998
7	1381.75	85.4027	8	1247.72	76.7546
9	1159.97	80.8808	10	1106.94	86.1259
11	1028.84	78.9324	12	849.49	88.1071
13	637.358	85.6657			

Fig. S5 Solid-state IR spectrum of cpmplex **1**-Yb with ATR method.