Supplementary Information of

Photoluminescence Enhancement Induced by a Halide Anion Encapsulation in a Series of Novel Lanthanide(III) Coordination Polymers

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Content

Experimental details of anion exchange studies. The pseudohalogen anions exchange experiments by the metal-organic network of compound **1** were undertaken as follows: 15 mg of compound **1**, 2 mL of DMF and 1 mL of aqueous solution containing a pseudohalogen (CN^-, SCN^- or N_3^- with the concentration of 10^{-3} mol/L) or halogen (Br^- or I^- with the concentration of 10^{-1},10^{-3}, 10^{-5} mol/L) ions in a form of sodium salts were placed in the 20 mL vial. The obtained suspension was treated ultrasonically for 30 min and then heated to 90 °C for 72 h. The obtained samples were in a form of a turbid liquid with a pale yellow solid. They were cooled to room temperature and their luminescent spectra were run with the slit width of 5 mm at room temperature on a Hitachi F-7000 spectrophotometer.

Based on the test of IR (Figure SI12), the N_3^- anion main peak 2140-2030cm^{-1}, the CN^- anion main peak 2140-2080cm^{-1} and SCN^- main peak 1900cm^{-1} cannot be observed. This proves that the outside pseudohalogen anions cannot exchange the halogen anions inside. The PXRD test (Figure SI11) demonstrate that the framework of **1** have not affected by the experiment conditions.

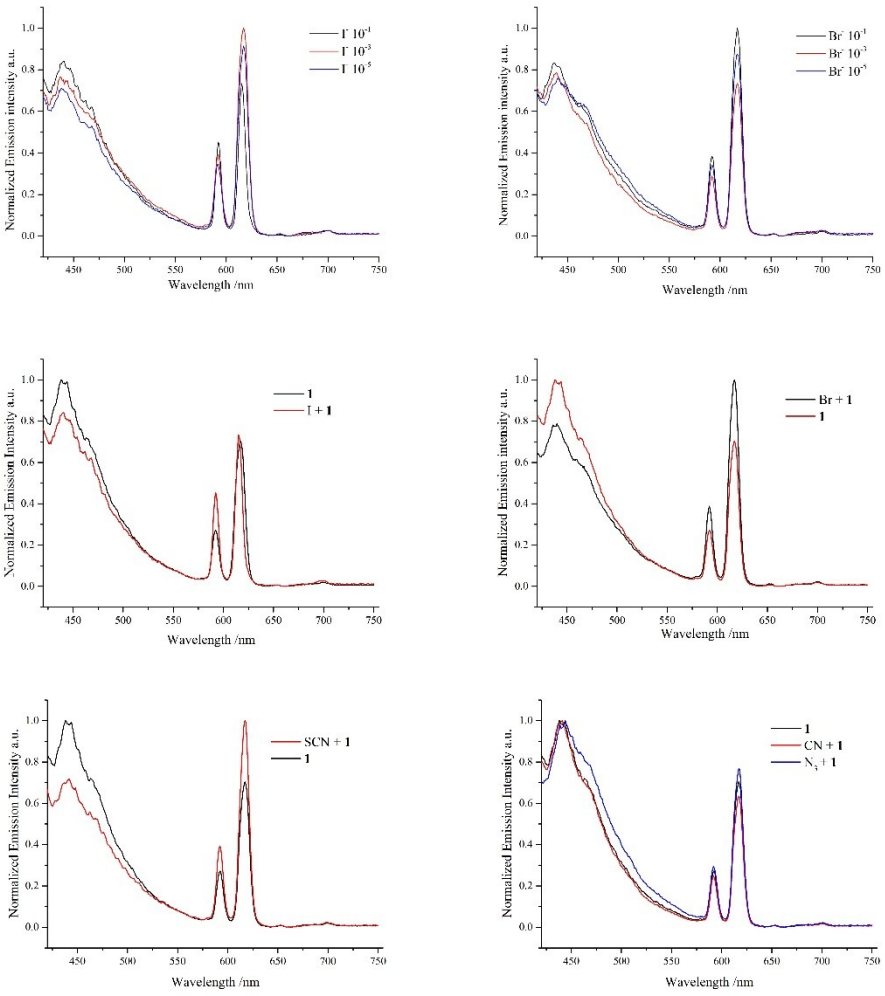

Figure SI1. The emission spectra of **1** before and after anion exchange experiments.

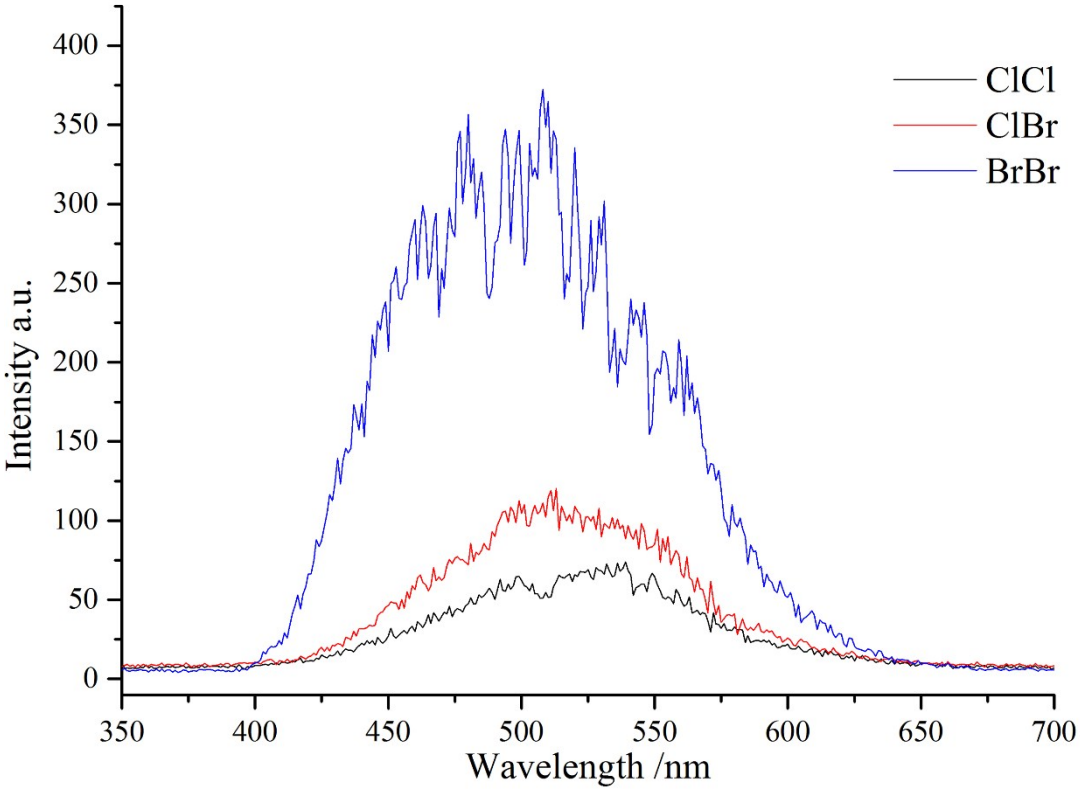

Figure SI2. The phosphorescence spectra of compounds **7-9**.

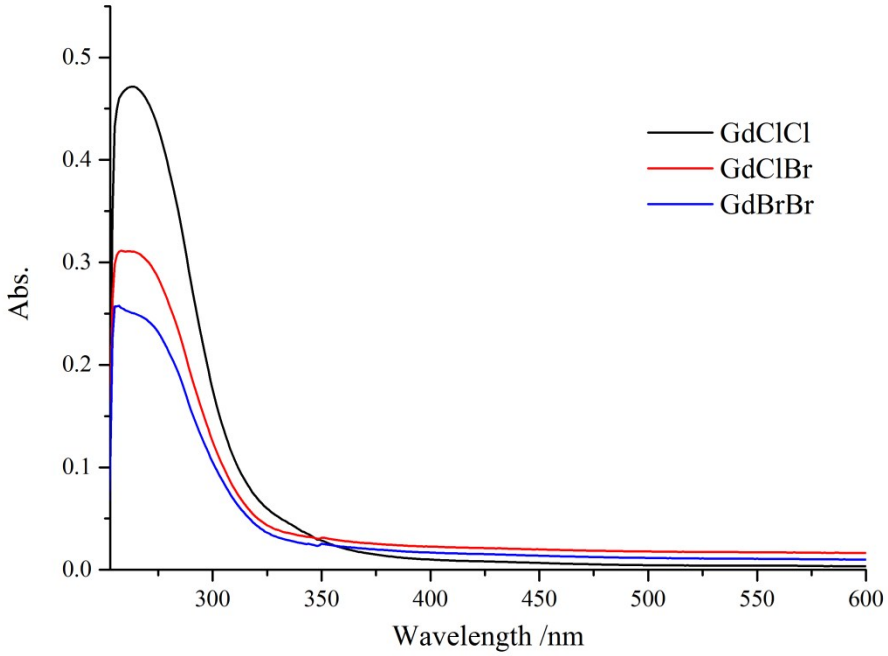

Figure SI3. Absorption spectrum of the complex **7-9** in DMSO solution.

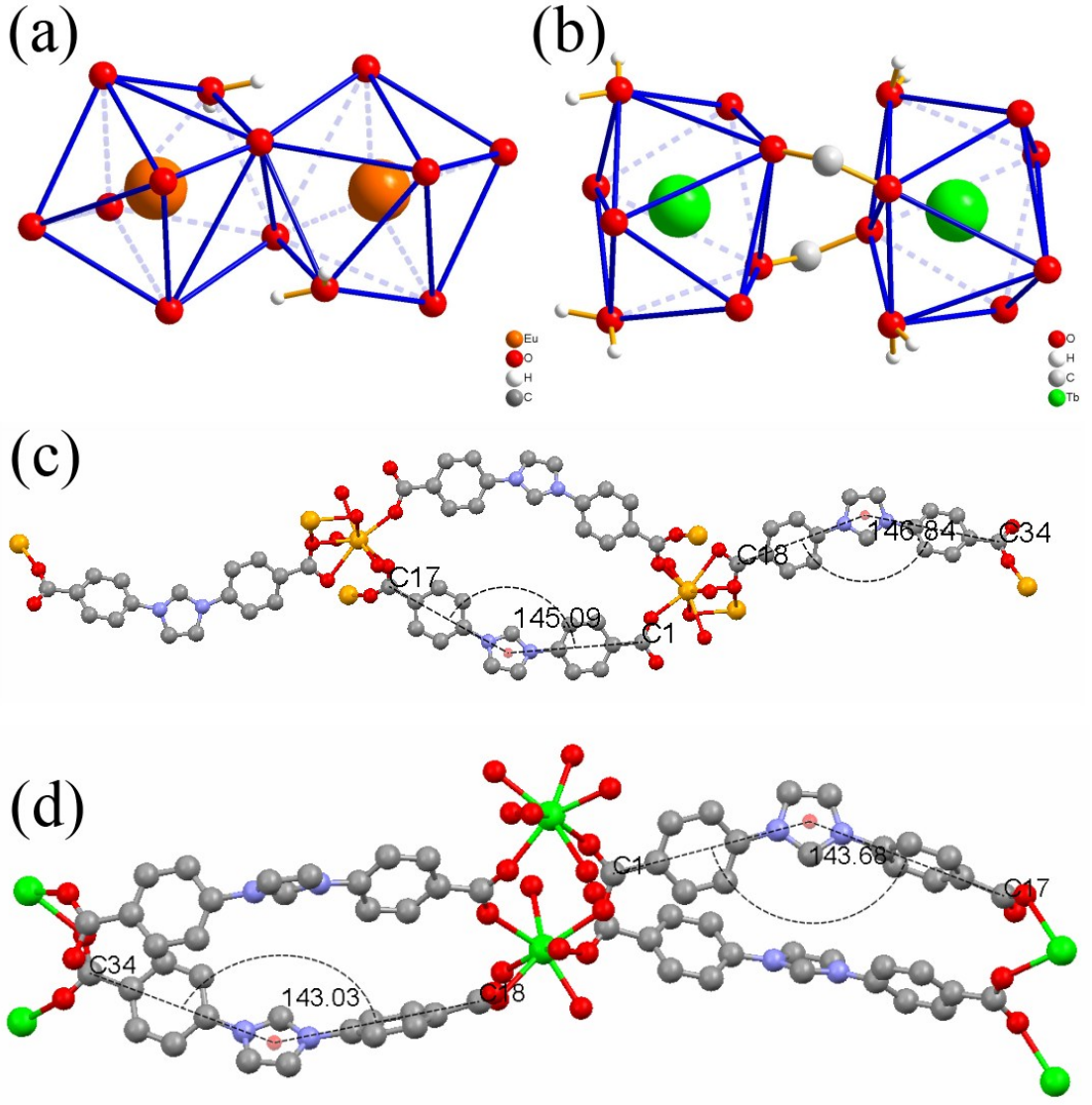

Figure SI4. (a) The coordination geometry of the Eu_2 unit in **1**. (b) The coordination geometry of Tb centres in **6.** (c) The angle data of Bcpi in **1.** (d) The angle data of Bcpi in **6**.

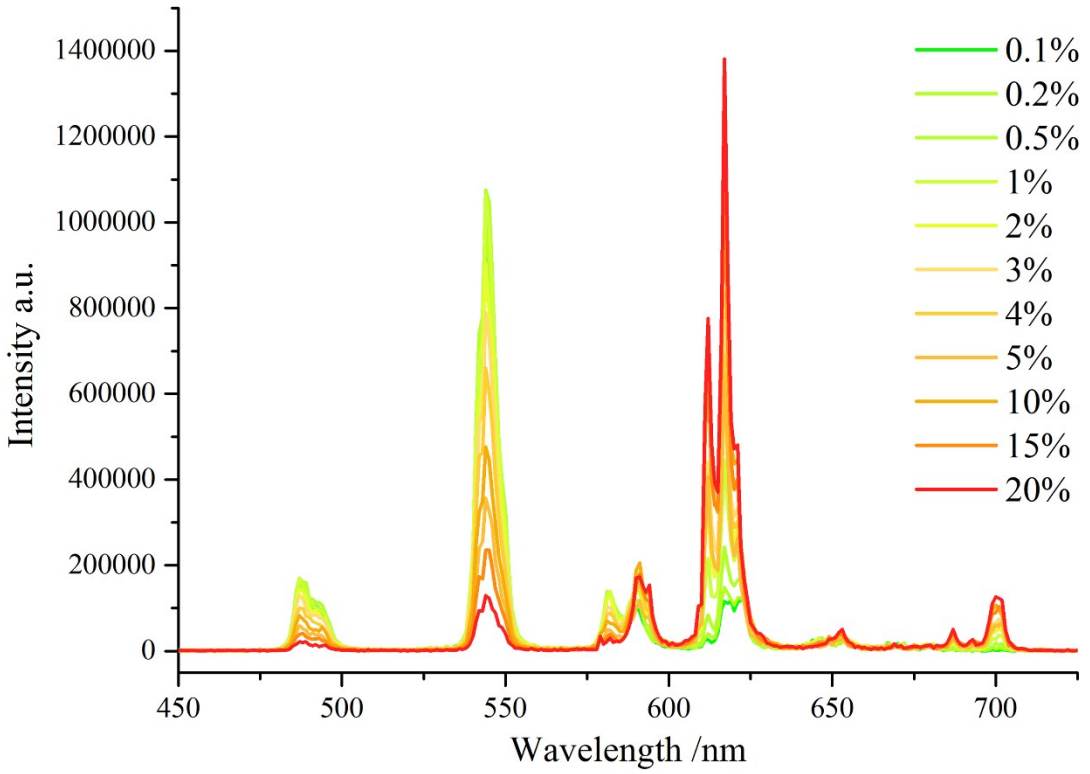

Figure SI5. The emission spectra of compounds $\{[Tb_{1-x}Eu_x(Bcpi)_2(H_2O)]Cl\cdot(H_2O)\}_n$ (**10**) with a different content of Eu/Tb. The content of $TbCl_3$ was initially fixed and calculated as 100%.

Table SI1. The molar ratio of the starting Tb/Eu salt and that in $\{[Tb_{1-x}Eu_x(Bcpi)_2(H_2O)]Cl\cdot(H_2O)\}_n$ (**10**) calculated by ICP analysis.

Sample	The molar ratio of the starting Tb/Eu salt	the Tb/Eu ratios calculated by ICP analysis
$Tb_{0.999}Eu_{0.001}Bcpi$	1:0.001	1:0.0009
$Tb_{0.998}Eu_{0.002}Bcpi$	1:0.002	1:0.0018
$Tb_{0.995}Eu_{0.005}Bcpi$	1:0.005	1:0.0052
$Tb_{0.99}Eu_{0.01}Bcpi$	1:0.01	1:0.0091
$Tb_{0.98}Eu_{0.02}Bcpi$	1:0.02	1:0.0192
$Tb_{0.97}Eu_{0.03}Bcpi$	1:0.03	1:0.0309
$Tb_{0.95}Eu_{0.05}Bcpi$	1:0.05	1:0.0494
$Tb_{0.90}Eu_{0.10}Bcpi$	1:0.10	1:0.0974
$Tb_{0.85}Eu_{0.15}Bcpi$	1:0.15	1:0.1449
$Tb_{0.80}Eu_{0.20}Bcpi$	1:0.20	1:0.2046

Table SI2. The I_{tot}/I_{MD} calculation for compound **1**.

Integral ranges	Transitions	Integral intensities	Integral ratio	I_{tot}/I_{MD}
577-581 nm	J = 0	26453	0.005912331	169.138
583-603 nm	J = 1	456161.5	0.101953573	9.808386
605-638 nm	J = 2	3020533.5	0.675099019	1.481264
647-657 nm	J = 3	106550.5	0.023814382	41.99143
666-715 nm	J = 4	772770.1	0.17271662	5.789831
Total integration		4474208.1		

Table SI3. The I_{tot}/I_{MD} calculation for compound **2**.

Integral ranges	Transitions	Integral intensities	Integral ratio	I_{tot}/I_{MD}
577-581 nm	J = 0	25527.5	0.002639086	378.9190677
583-603 nm	J = 1	931377.5	0.096287741	10.38553809
605-638 nm	J = 2	6689843	0.691609867	1.445901869
647-657 nm	J = 3	204966	0.021189811	47.1924929
666-715 nm	J = 4	1682659.5	0.173956835	5.748552515
Total integration		9672856.5		

Table SI4. The I_{tot}/I_{MD} calculation for compound **3**.

Integral ranges	Transitions	Integral intensities	Integral ratio	Itot/IMD
577-581 nm	J = 0	42597.5	0.003862225	258.9181
583-603 nm	J = 1	1221860	0.110783468	9.026618
605-638 nm	J = 2	7155164.5	0.648743665	1.541441
647-657 nm	J = 3	193771	0.017568808	56.91906
666-715 nm	J = 4	2260561.5	0.204960341	4.878993
577-715		11029263		

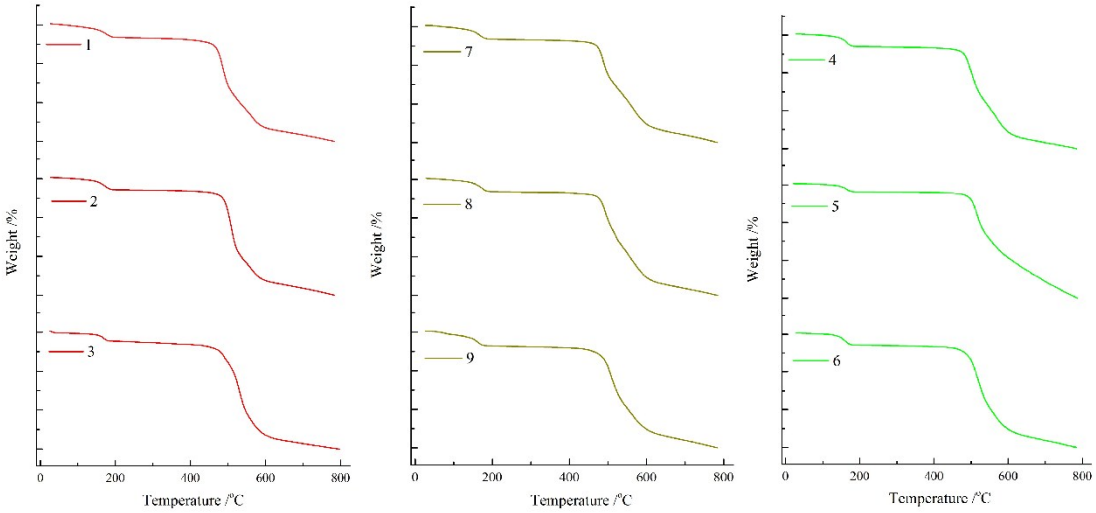

Figure SI6. The TG curves of coordination polymers **1–9**: Eu-CP (a), Tb-CPs (b) and Gd-CPs (c).

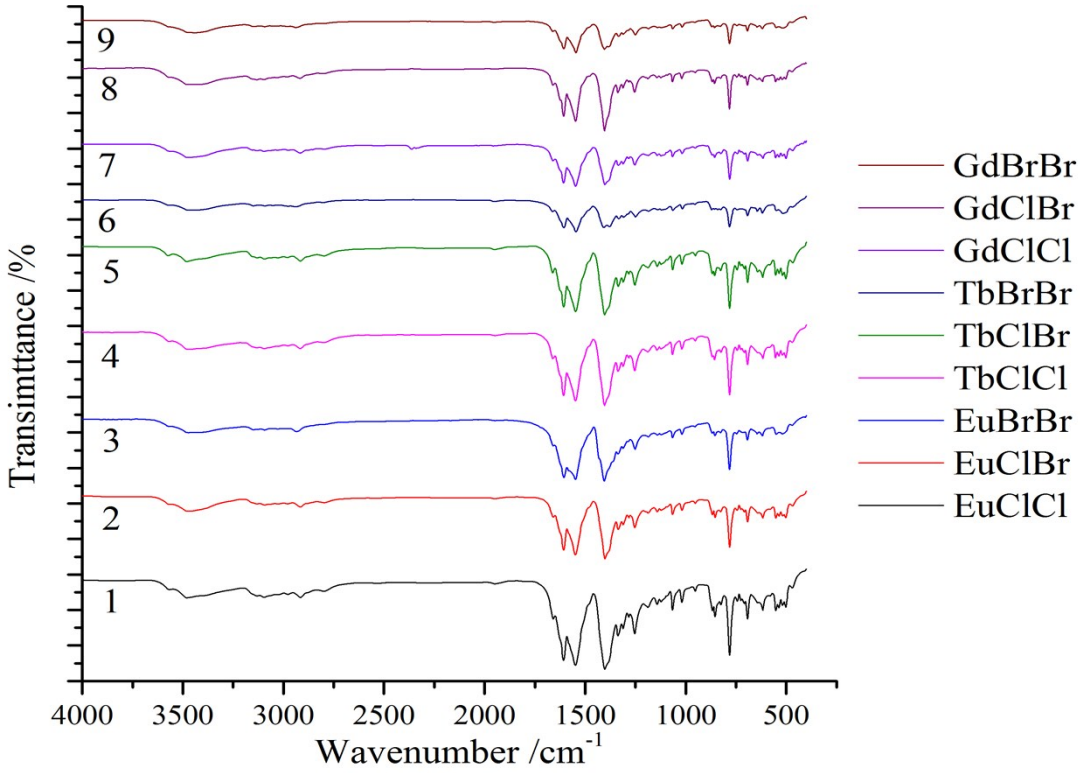

Figure SI7. The IR spectra of compounds **1–9**.

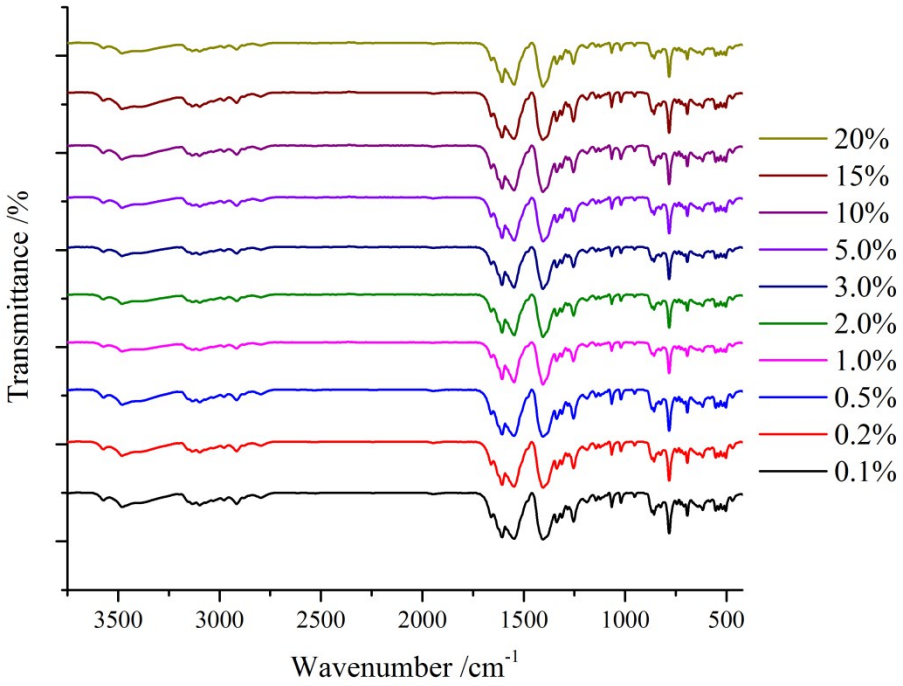

Figure SI8. The IR spectra of compounds **10**.

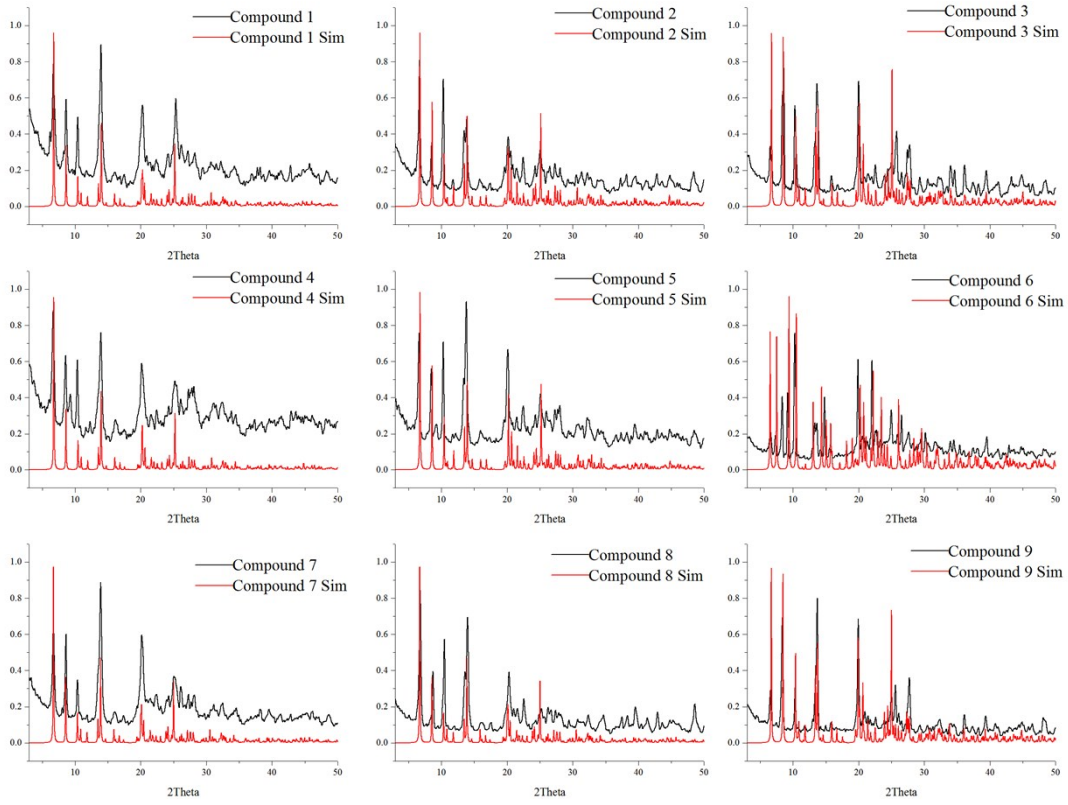

Figure SI9. Powder-XRD analysis of compounds **1-9**. Experimental (black lines), calculated (red lines).

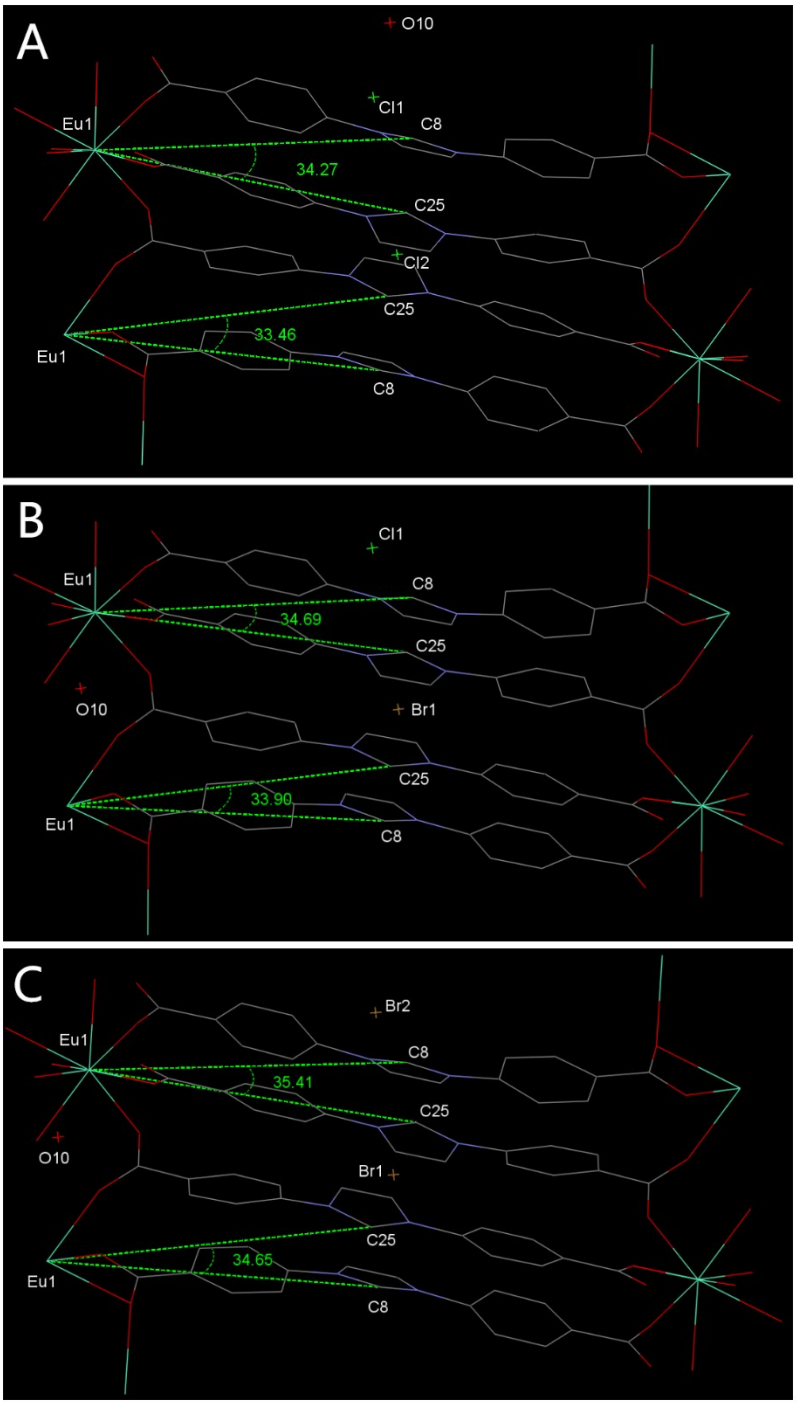

Figure SI10. The angle $\angle C_8Eu_1C_{25}$ of compound **1-3.**

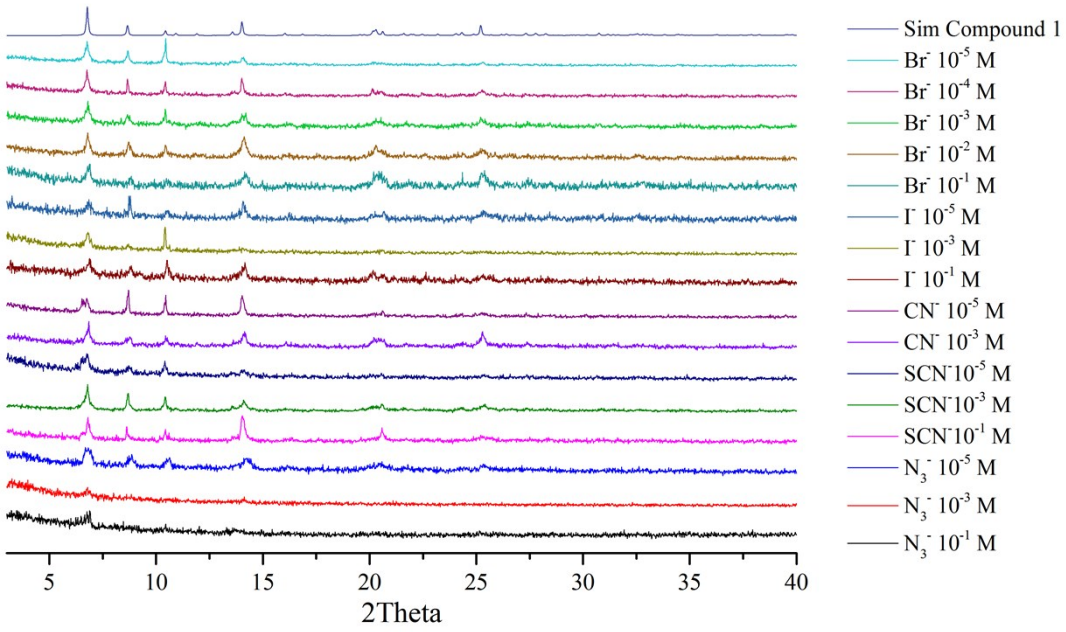

Figure SI11. PXRD spectrum of **1** in anions exchange experiment.

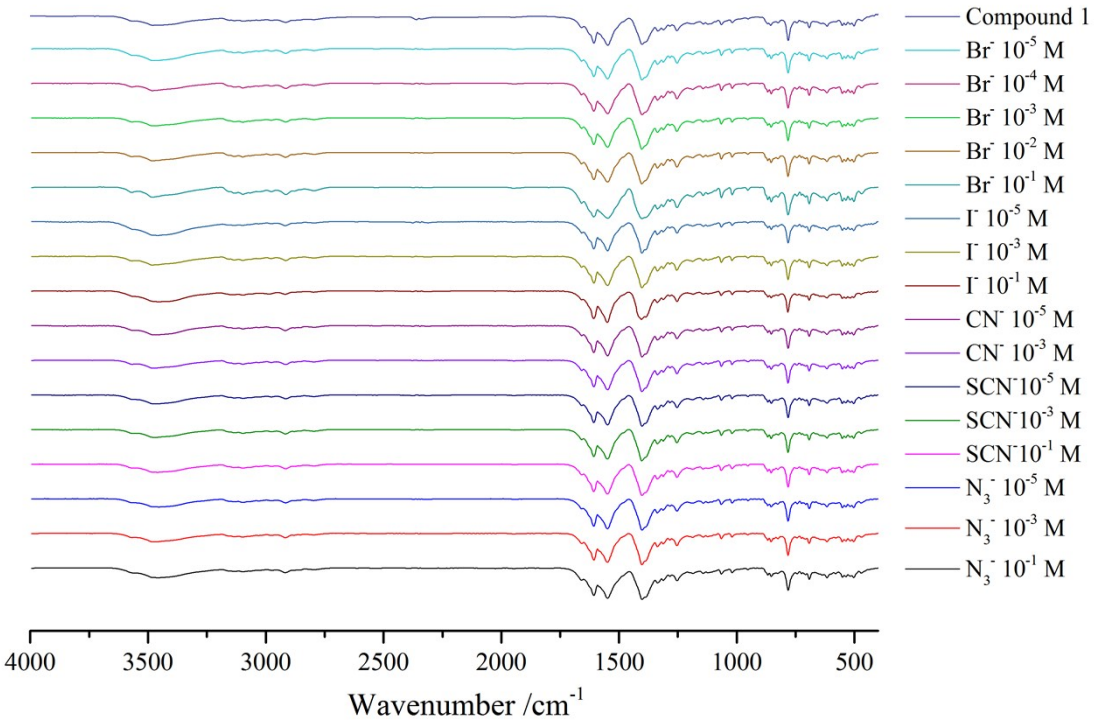

Figure SI12. IR spectrum of 1 in anions exchange experiment.

Table SI5. The selected bond length (Å) and bond angle (deg) data for compound **1–9**.

Compound 1

Eu1—Eu1^{i}	4.0431 (13)	O9—Eu1—Eu1^{i}	71.2 (2)
Eu1—O9	2.500 (8)	O9—Eu1—O7^{iii}	70.9 (3)
Eu1—O5	2.262 (9)	O9—Eu1—C34^{ii}	99.5 (3)
Eu1—O7^{ii}	2.483 (8)	O9—Eu1—O8^{ii}	122.7 (3)
Eu1—O7^{iii}	2.516 (8)	O5—Eu1—Eu1^{i}	82.0 (2)
Eu1—C34^{ii}	2.859 (14)	O5—Eu1—O9	140.2 (3)
Eu1—O1	2.355 (9)	O5—Eu1—O7^{iii}	70.2 (3)
Eu1—O2^{iv}	2.324 (9)	O5—Eu1—O7^{ii}	96.7 (3)
Eu1—O3^{v}	2.328 (9)	O5—Eu1—C34^{ii}	91.2 (3)
Eu1—O8^{ii}	2.572 (9)	O5—Eu1—O1	77.4 (3)
		O5—Eu1—O2^{iv}	146.0 (3)
		O5—Eu1—O3^{v}	95.8 (3)
		O5—Eu1—O8^{ii}	79.6 (3)
		O7^{ii}—Eu1—Eu1^{i}	36.29 (19)
		O7^{iii}—Eu1—Eu1^{i}	35.75 (19)
		O7^{ii}—Eu1—O9	78.9 (3)
		O7^{ii}—Eu1—O7^{iii}	72.0 (3)
		O7^{ii}—Eu1—C34^{ii}	26.3 (3)
		O7^{iii}—Eu1—C34^{ii}	94.1 (4)
		O7^{ii}—Eu1—O8^{ii}	51.7 (3)
		O7^{iii}—Eu1—O8^{ii}	111.1 (3)
		C34^{ii}—Eu1—Eu1^{i}	59.6 (3)
		O1—Eu1—Eu1^{i}	156.7 (2)
		O1—Eu1—O9	132.0 (3)
		O1—Eu1—O7^{ii}	136.2 (3)
		O1—Eu1—O7^{iii}	139.9 (3)
		O1—Eu1—C34^{ii}	109.8 (4)
		O1—Eu1—O8^{ii}	84.8 (3)
		O2^{iv}—Eu1—Eu1^{i}	112.7 (2)
		O2^{iv}—Eu1—O9	73.2 (3)
		O2^{iv}—Eu1—O7^{ii}	82.2 (3)
		O2^{iv}—Eu1—O7^{iii}	139.0 (3)
		O2^{iv}—Eu1—C34^{ii}	72.8 (3)
		O2^{iv}—Eu1—O1	80.2 (3)
		O2^{iv}—Eu1—O3^{v}	103.2 (3)
		O2^{iv}—Eu1—O8^{ii}	73.2 (3)
		O3^{v}—Eu1—Eu1^{i}	116.9 (2)
		O3^{v}—Eu1—O9	72.1 (3)
		O3^{v}—Eu1—O7^{ii}	147.2 (3)
		O3^{v}—Eu1—O7^{iii}	84.1 (3)
		O3^{v}—Eu1—C34^{ii}	171.6 (3)
		O3^{v}—Eu1—O1	76.2 (3)
		O3^{v}—Eu1—O8^{ii}	161.0 (3)
		O8^{ii}—Eu1—Eu1^{i}	81.0 (2)
		O8^{ii}—Eu1—C34^{ii}	25.8 (3)

Symmetry codes: (i) −*x*, −*y*−1, −*z*−1; (ii) *x*+1, *y*, *z*+1; (iii) −*x*−1, −*y*−1, −*z*−2; (iv) −*x*−1, −*y*−1, −*z*−1; (v) −*x*−2, −*y*−1, −*z*−2; (vi) *x*−1, *y*, *z*−1

Compound 2

Eu1—Eu1^{i}	4.0539	O1—Eu1—Eu1^{i}	155.71 (19)
Eu1—O1	2.361 (6)	O1—Eu1—O9	132.6 (2)
Eu1—O2^{ii}	2.330 (6)	O1—Eu1—O8^{iv}	84.1 (2)
Eu1—O5	2.279 (6)	O1—Eu1—C34^{iv}	109.1 (2)
Eu1—O9	2.504 (6)	O1—Eu1—O7^{v}	139.7 (2)
Eu1—O3^{iii}	2.323 (6)	O1—Eu1—O7^{iv}	135.5 (2)
Eu1—O8^{iv}	2.557 (6)	O2^{ii}—Eu1—Eu1^{i}	112.45 (14)
Eu1—C34^{iv}	2.878 (8)	O2^{ii}—Eu1—O1	80.7 (2)
Eu1—O7^{v}	2.517 (6)	O2^{ii}—Eu1—O9	73.2 (2)
Eu1—O7^{iv}	2.491 (6)	O2^{ii}—Eu1—O8^{iv}	73.2 (2)
		O2^{ii}—Eu1—C34^{iv}	72.3 (2)
		O2^{ii}—Eu1—O7^{v}	138.9 (2)
		O2^{ii}—Eu1—O7^{iv}	82.0 (2)
		O5—Eu1—Eu1^{i}	81.58 (16)
		O5—Eu1—O1	77.1 (2)
		O5—Eu1—O2^{ii}	146.3 (2)
		O5—Eu1—O9	139.9 (2)
		O5—Eu1—O3^{iii}	95.6 (2)
		O5—Eu1—O8^{iv}	79.6 (2)
		O5—Eu1—C34^{iv}	91.4 (2)
		O5—Eu1—O7^{v}	69.7 (2)
		O5—Eu1—O7^{iv}	96.5 (2)
		O9—Eu1—Eu1^{i}	71.70 (15)
		O9—Eu1—O8^{iv}	123.1 (2)
		O9—Eu1—C34^{iv}	99.8 (2)
		O9—Eu1—O7^{v}	71.2 (2)
		O3^{iii}—Eu1—Eu1^{i}	116.57 (15)
		O3^{iii}—Eu1—O1	77.3 (2)
		O3^{iii}—Eu1—O2^{ii}	104.0 (2)
		O3^{iii}—Eu1—O9	71.7 (2)
		O3^{iii}—Eu1—O8^{iv}	161.4 (2)
		O3^{iii}—Eu1—C34^{iv}	171.5 (2)
		O3^{iii}—Eu1—O7^{v}	83.7 (2)
		O3^{iii}—Eu1—O7^{iv}	146.9 (2)
		O8^{iv}—Eu1—Eu1^{i}	80.67 (14)
		O8^{iv}—Eu1—C34^{iv}	25.7 (2)
		C34^{iv}—Eu1—Eu1^{i}	59.68 (18)
		O7^{iv}—Eu1—Eu1^{i}	36.16 (13)
		O7^{v}—Eu1—Eu1^{i}	35.74 (13)
		O7^{iv}—Eu1—O9	79.4 (2)
		O7^{iv}—Eu1—O8^{iv}	51.57 (19)
		O7^{v}—Eu1—O8^{iv}	110.7 (2)
		O7^{v}—Eu1—C34^{iv}	94.2 (2)
		O7^{iv}—Eu1—C34^{iv}	26.4 (2)
		O7^{iv}—Eu1—O7^{v}	71.9 (2)

Symmetry codes: (i) −*x*, −*y*−1, −*z*−1; (ii) −*x*+1, −*y*−1, −*z*−1; (iii) −*x*+2, −*y*−1, −*z*; (iv) *x*−1, *y*, *z*−1; (v) −*x*+1, −*y*−1, −*z*; (vi) *x*+1, *y*, *z*+1.

Compound 3

Eu3—Eu3^{i}	4.0442 (10)	O1—Eu3—Eu3^{i}	156.13 (15)
Eu3—O1	2.358 (5)	O1—Eu3—O9	132.32 (19)
Eu3—O9	2.495 (5)	O1—Eu3—O7^{v}	134.80 (19)
Eu3—O3^{ii}	2.311 (6)	O1—Eu3—O7^{iv}	140.4 (2)
Eu3—O2^{iii}	2.327 (6)	O1—Eu3—O8^{v}	83.4 (2)
Eu3—O5	2.260 (6)	O1—Eu3—C34^{v}	108.3 (2)
Eu3—O7^{iv}	2.508 (5)	O9—Eu3—Eu3^{i}	71.55 (12)
Eu3—O7^{v}	2.504 (5)	O9—Eu3—O7^{v}	79.30 (18)
Eu3—O8^{v}	2.557 (6)	O9—Eu3—O7^{iv}	71.04 (18)
Eu3—C34^{v}	2.883 (9)	O9—Eu3—O8^{v}	123.18 (19)
		O9—Eu3—C34^{v}	99.7 (2)
		O3^{ii}—Eu3—Eu3^{i}	117.09 (14)
		O3^{ii}—Eu3—O1	77.4 (2)
		O3^{ii}—Eu3—O9	71.91 (19)
		O3^{ii}—Eu3—O2^{iii}	103.0 (2)
		O3^{ii}—Eu3—O7^{v}	147.42 (18)
		O3^{ii}—Eu3—O7^{iv}	83.86 (19)
		O3^{ii}—Eu3—O8^{v}	160.81 (19)
		O3^{ii}—Eu3—C34^{v}	171.5 (2)
		O2^{iii}—Eu3—Eu3^{i}	112.11 (13)
		O2^{iii}—Eu3—O1	80.3 (2)
		O2^{iii}—Eu3—O9	72.39 (19)
		O2^{iii}—Eu3—O7^{v}	81.90 (19)
		O2^{iii}—Eu3—O7^{iv}	138.37 (18)
		O2^{iii}—Eu3—O8^{v}	73.8 (2)
		O2^{iii}—Eu3—C34^{v}	72.4 (2)
		O5—Eu3—Eu3^{i}	82.03 (13)
		O5—Eu3—O1	77.6 (2)
		O5—Eu3—O9	139.6 (2)
		O5—Eu3—O3^{ii}	95.1 (2)
		O5—Eu3—O2^{iii}	147.5 (2)
		O5—Eu3—O7^{iv}	69.6 (2)
		O5—Eu3—O7^{v}	97.2 (2)
		O5—Eu3—O8^{v}	80.2 (2)
		O5—Eu3—C34^{v}	92.3 (2)
		O7^{v}—Eu3—Eu3^{i}	36.25 (12)
		O7^{iv}—Eu3—Eu3^{i}	36.18 (12)
		O7^{v}—Eu3—O7^{iv}	72.4 (2)
		O7^{iv}—Eu3—O8^{v}	111.35 (18)
		O7^{v}—Eu3—O8^{v}	51.69 (17)
		O7^{v}—Eu3—C34^{v}	26.46 (19)
		O7^{iv}—Eu3—C34^{v}	94.9 (2)
		O8^{v}—Eu3—Eu3^{i}	80.91 (13)
		O8^{v}—Eu3—C34^{v}	25.8 (2)
		C34^{v}—Eu3—Eu3^{i}	59.88 (18)

Symmetry codes: (i) −*x*+2, −*y*−1, −*z*; (ii) −*x*, −*y*−1, −*z*−1; (iii) −*x*+1, −*y*−1, −*z*; (iv) −*x*+1, −*y*−1, −*z*−1; (v) *x*+1, *y*, *z*+1; (vi) *x*−1, *y*, *z*−1.

Compound 4

Tb1—O9	2.465 (4)	O9—Tb1—O7^{i}	71.30 (13)
Tb1—O7^{i}	2.506 (4)	O9—Tb1—O8^{ii}	123.54 (13)
Tb1—O7^{ii}	2.454 (4)	O9—Tb1—C34^{ii}	99.69 (15)
Tb1—O1	2.331 (4)	O7^{ii}—Tb1—O9	79.12 (13)
Tb1—O8^{ii}	2.540 (4)	O7^{ii}—Tb1—O7^{i}	71.42 (14)
Tb1—O5	2.239 (4)	O7^{i}—Tb1—O8^{ii}	110.89 (13)
Tb1—C34^{ii}	2.852 (6)	O7^{ii}—Tb1—O8^{ii}	52.41 (12)
Tb1—O3^{iii}	2.287 (4)	O7^{ii}—Tb1—C34^{ii}	26.65 (13)
Tb1—O2^{iv}	2.305 (4)	O7^{i}—Tb1—C34^{ii}	93.96 (15)
		O1—Tb1—O9	132.63 (14)
		O1—Tb1—O7^{i}	139.94 (13)
		O1—Tb1—O7^{ii}	135.56 (14)
		O1—Tb1—O8^{ii}	83.38 (14)
		O1—Tb1—C34^{ii}	108.93 (16)
		O8^{ii}—Tb1—C34^{ii}	26.36 (14)
		O5—Tb1—O9	139.96 (15)
		O5—Tb1—O7^{ii}	96.85 (14)
		O5—Tb1—O7^{i}	69.74 (14)
		O5—Tb1—O1	76.89 (15)
		O5—Tb1—O8^{ii}	79.63 (15)
		O5—Tb1—C34^{ii}	91.86 (16)
		O5—Tb1—O3^{iii}	94.77 (15)
		O5—Tb1—O2^{iv}	146.37 (15)
		O3^{iii}—Tb1—O9	72.58 (14)
		O3^{iii}—Tb1—O7^{i}	84.54 (13)
		O3^{iii}—Tb1—O7^{ii}	147.56 (13)
		O3^{iii}—Tb1—O1	76.64 (15)
		O3^{iii}—Tb1—O8^{ii}	160.00 (13)
		O3^{iii}—Tb1—C34^{ii}	172.21 (15)
		O3^{iii}—Tb1—O2^{iv}	103.48 (15)
		O2^{iv}—Tb1—O9	73.23 (14)
		O2^{iv}—Tb1—O7^{i}	139.19 (13)
		O2^{iv}—Tb1—O7^{ii}	82.71 (14)
		O2^{iv}—Tb1—O1	80.15 (14)
		O2^{iv}—Tb1—O8^{ii}	73.57 (15)
		O2^{iv}—Tb1—C34^{ii}	72.75 (15)

Symmetry codes: (i) −*x*, −*y*−1, −*z*−1; (ii) *x*+1, *y*, *z*+1; (iii) −*x*−1, −*y*−1, −*z*−1; (iv) −*x*, −*y*−1, −*z*; (v) *x*−1, *y*, *z*−1.

Compound 5

Tb1—O7^{i}	2.502 (5)	O7^{iii}—Tb1—O7^{i}	71.63 (16)
Tb1—O7^{iii}	2.462 (4)	O7^{i}—Tb1—C34^{iii}	94.38 (16)
Tb1—C34^{iii}	2.857 (6)	O7^{iii}—Tb1—C34^{iii}	26.88 (16)
Tb1—O8^{iii}	2.548 (5)	O7^{i}—Tb1—O8^{iii}	111.00 (15)
Tb1—O2^{iv}	2.307 (4)	O7^{iii}—Tb1—O8^{iii}	52.28 (14)
Tb1—O3^{v}	2.293 (4)	O7^{iii}—Tb1—O9	79.42 (14)
Tb1—O9	2.466 (4)	O5—Tb1—O7^{iii}	96.90 (15)
		O5—Tb1—O7^{i}	69.58 (16)
		O5—Tb1—C34^{iii}	91.95 (18)
		O5—Tb1—O8^{iii}	79.86 (18)
		O5—Tb1—O1	77.08 (18)
		O5—Tb1—O2^{iv}	146.83 (18)
		O5—Tb1—O3^{v}	94.38 (17)
		O5—Tb1—O9	139.70 (17)
		O8^{iii}—Tb1—C34^{iii}	26.00 (16)
		O1—Tb1—O7^{iii}	134.99 (16)
		O1—Tb1—O7^{i}	140.20 (16)
		O1—Tb1—C34^{iii}	108.12 (18)
		O1—Tb1—O8^{iii}	82.96 (16)
		O1—Tb1—O9	132.68 (17)
		O2^{iv}—Tb1—O7^{iii}	82.63 (15)
		O2^{iv}—Tb1—O7^{i}	139.01 (15)
		O2^{iv}—Tb1—C34^{iii}	72.70 (18)
		O2^{iv}—Tb1—O8^{iii}	73.72 (17)
		O2^{iv}—Tb1—O1	80.07 (17)
		O2^{iv}—Tb1—O9	73.07 (16)
		O3^{v}—Tb1—O7^{iii}	147.66 (15)
		O3^{v}—Tb1—O7^{i}	84.25 (15)
		O3^{v}—Tb1—C34^{iii}	172.59 (17)
		O3^{v}—Tb1—O8^{iii}	160.05 (15)
		O3^{v}—Tb1—O1	77.12 (17)
		O3^{v}—Tb1—O2^{iv}	103.63 (17)
		O3^{v}—Tb1—O9	72.48 (15)
		O9—Tb1—O7^{i}	71.26 (15)
		O9—Tb1—C34^{iii}	100.18 (16)
		O9—Tb1—O8^{iii}	123.73 (15)

Symmetry codes: (i) −*x*, −*y*, −*z*; (ii) *x*−1, *y*, *z*−1; (iii) *x*+1, *y*, *z*+1; (iv) −*x*, −*y*, −*z*+1; (v) −*x*−1, −*y*, −*z*.

Compound 6

Tb2—O3^{i}	2.360 (3)	O3—Tb2—O3^{i}	110.81 (17)
Tb2—O3	2.360 (3)	O3—Tb2—O7	71.83 (12)
Tb2—O6^{ii}	2.281 (3)	O3^{i}—Tb2—O7	140.34 (11)
Tb2—O6^{iii}	2.281 (3)	O3—Tb2—O7^{i}	140.34 (11)
Tb2—O7^{i}	2.467 (3)	O3^{i}—Tb2—O7^{i}	71.82 (12)
Tb2—O7	2.467 (3)	O3^{i}—Tb2—O10^{i}	69.78 (15)
Tb2—O10	2.429 (4)	O3^{i}—Tb2—O10	78.55 (14)
Tb2—O10^{i}	2.429 (4)	O3—Tb2—O10^{i}	78.55 (13)
Tb1—O1	2.449 (3)	O3—Tb2—O10	69.78 (15)
Tb1—O1^{iv}	2.449 (3)	O6^{ii}—Tb2—O3^{i}	89.67 (12)
Tb1—O4^{v}	2.296 (4)	O6^{iii}—Tb2—O3	89.67 (12)
Tb1—O4^{vi}	2.296 (3)	O6^{ii}—Tb2—O3	141.81 (13)
Tb1—O5	2.377 (3)	O6^{iii}—Tb2—O3^{i}	141.81 (13)
Tb1—O5^{iv}	2.377 (3)	O6^{iii}—Tb2—O6^{ii}	93.21 (17)
Tb1—O9^{iv}	2.450 (4)	O6^{iii}—Tb2—O7^{i}	72.06 (12)
Tb1—O9	2.450 (4)	O6^{ii}—Tb2—O7	72.06 (12)
		O6^{iii}—Tb2—O7	75.75 (12)
		O6^{ii}—Tb2—O7^{i}	75.75 (12)
		O6^{ii}—Tb2—O10^{i}	79.08 (14)
		O6^{iii}—Tb2—O10^{i}	147.97 (16)
		O6^{ii}—Tb2—O10	147.97 (16)
		O6^{iii}—Tb2—O10	79.08 (14)
		O7—Tb2—O7^{i}	132.43 (17)
		O10—Tb2—O7	133.68 (14)
		O10^{i}—Tb2—O7	72.29 (15)
		O10^{i}—Tb2—O7^{i}	133.68 (14)
		O10—Tb2—O7^{i}	72.29 (15)
		O10^{i}—Tb2—O10	122.7 (2)
		O1—Tb1—O1^{iv}	131.58 (15)
		O1^{iv}—Tb1—O9	132.05 (12)
		O1—Tb1—O9	73.68 (13)
		O1—Tb1—O9^{iv}	132.05 (12)
		O1^{iv}—Tb1—O9^{iv}	73.68 (13)
		O4^{v}—Tb1—O1^{iv}	74.39 (11)
		O4^{vi}—Tb1—O1	74.39 (11)
		O4^{vi}—Tb1—O1^{iv}	73.75 (12)
		O4^{v}—Tb1—O1	73.75 (12)
		O4^{v}—Tb1—O4^{vi}	95.98 (18)
		O4^{vi}—Tb1—O5^{iv}	89.99 (12)
		O4^{vi}—Tb1—O5	142.43 (12)
		O4^{v}—Tb1—O5	89.99 (12)
		O4^{v}—Tb1—O5^{iv}	142.44 (12)
		O4^{vi}—Tb1—O9	78.06 (13)
		O4^{v}—Tb1—O9	147.30 (13)
		O4^{v}—Tb1—O9^{iv}	78.06 (13)
		O4^{vi}—Tb1—O9^{iv}	147.30 (13)
		O5—Tb1—O1	71.83 (11)
		O5^{iv}—Tb1—O1	142.89 (12)
		O5—Tb1—O1^{iv}	142.89 (12)
		O5^{iv}—Tb1—O1^{iv}	71.83 (11)
		O5—Tb1—O5^{iv}	107.39 (16)
		O5^{iv}—Tb1—O9	70.19 (13)
		O5^{iv}—Tb1—O9^{iv}	77.14 (13)
		O5—Tb1—O9^{iv}	70.19 (13)
		O5—Tb1—O9	77.14 (13)
		O9^{iv}—Tb1—O9	123.40 (19)

Symmetry codes: (i) −*x*+1, *y*, −*z*+3/2; (ii) *x*+1/2, −*y*+1/2, *z*+1/2; (iii) −*x*+1/2, −*y*+1/2, −*z*+1; (iv) −*x*, *y*, −*z*+1/2; (v) −*x*+1/2, −*y*+3/2, −*z*+1; (vi) *x*−1/2, −*y*+3/2, *z*−1/2.

Compound 7

Gd1—O3^{i}	2.290 (6)	O1—Gd1—Gd1^{iii}	155.80 (18)	Gd1—Gd1^{i}	4.0059 (7)	O5—Gd1—Gd1^{i}	81.24 (14)
Gd1—O2^{ii}	2.322 (6)	O1—Gd1—O9	132.1 (2)	Gd1—O5	2.258 (5)	O5—Gd1—O9	139.6 (2)
Gd1—Gd1^{iii}	4.0062 (8)	O1—Gd1—O7^{iv}	139.5 (2)	Gd1—O9	2.488 (5)	O5—Gd1—O7^{ii}	96.10 (18)
Gd1—O9	2.483 (6)	O1—Gd1—O7^{v}	135.6 (2)	Gd1—O7^{ii}	2.464 (5)	O5—Gd1—O7^{iii}	69.47 (19)
Gd1—O7^{iv}	2.490 (6)	O1—Gd1—O8^{v}	83.5 (2)	Gd1—O7^{iii}	2.487 (5)	O5—Gd1—O8^{ii}	79.5 (2)
Gd1—O7^{v}	2.464 (6)	O1—Gd1—C34^{v}	109.1 (2)	Gd1—O8^{ii}	2.575 (5)	O5—Gd1—O1	76.9 (2)
Gd1—O8^{v}	2.553 (7)	O3^{i}—Gd1—O1	76.2 (2)	Gd1—O1	2.339 (5)	O5—Gd1—O3^{iv}	94.80 (19)
Gd1—O5	2.248 (6)	O3^{i}—Gd1—O2^{ii}	103.8 (2)	Gd1—O3^{iv}	2.304 (5)	O5—Gd1—O2^{v}	147.0 (2)
Gd1—C34^{v}	2.863 (9)	O3^{i}—Gd1—Gd1^{iii}	117.03 (15)	Gd1—O2^{v}	2.323 (5)	O5—Gd1—C34^{ii}	91.8 (2)
		O3^{i}—Gd1—O9	72.3 (2)	Gd1—C34^{ii}	2.874 (8)	O9—Gd1—Gd1^{i}	72.15 (12)
		O3^{i}—Gd1—O7^{iv}	83.8 (2)			O9—Gd1—O8^{ii}	123.97 (17)
		O3^{i}—Gd1—O7^{v}	148.0 (2)			O9—Gd1—C34^{ii}	100.14 (19)
		O3^{i}—Gd1—O8^{v}	159.7 (2)			O7^{ii}—Gd1—Gd1^{i}	36.19 (12)
		O3^{i}—Gd1—C34^{v}	172.7 (2)			O7^{iii}—Gd1—Gd1^{i}	35.81 (11)
		O2^{ii}—Gd1—O1	80.8 (2)			O7^{ii}—Gd1—O9	80.07 (17)
		O2^{ii}—Gd1—Gd1^{iii}	112.77 (15)			O7^{iii}—Gd1—O9	71.17 (17)
		O2^{ii}—Gd1—O9	72.9 (2)			O7^{ii}—Gd1—O7^{iii}	72.01 (19)
		O2^{ii}—Gd1—O7^{v}	82.5 (2)			O7^{iii}—Gd1—O8^{ii}	111.23 (17)
		O2^{ii}—Gd1—O7^{iv}	138.8 (2)			O7^{ii}—Gd1—O8^{ii}	51.90 (16)
		O2^{ii}—Gd1—O8^{v}	73.5 (2)			O7^{iii}—Gd1—C34^{ii}	94.6 (2)
		O2^{ii}—Gd1—C34^{v}	72.7 (2)			O7^{ii}—Gd1—C34^{ii}	26.38 (19)
		O9—Gd1—Gd1^{iii}	72.04 (15)			O8^{ii}—Gd1—Gd1^{i}	81.10 (12)
		O9—Gd1—O7^{iv}	71.1 (2)			O8^{ii}—Gd1—C34^{ii}	26.23 (18)
		O9—Gd1—O8^{v}	124.0 (2)			O1—Gd1—Gd1^{i}	155.15 (14)
		O9—Gd1—C34^{v}	100.4 (2)			O1—Gd1—O9	132.68 (18)
		O7^{iv}—Gd1—Gd1^{iii}	35.81 (13)			O1—Gd1—O7^{ii}	135.12 (18)
		O7^{v}—Gd1—Gd1^{iii}	36.26 (13)			O1—Gd1—O7^{iii}	139.41 (18)
		O7^{v}—Gd1—O9	80.0 (2)			O1—Gd1—O8^{ii}	83.39 (18)
		O7^{v}—Gd1—O7^{iv}	72.1 (2)			O1—Gd1—C34^{ii}	108.8 (2)
		O7^{iv}—Gd1—O8^{v}	111.8 (2)			O3^{iv}—Gd1—Gd1^{i}	117.44 (13)
		O7^{v}—Gd1—O8^{v}	52.3 (2)			O3^{iv}—Gd1—O9	72.41 (17)
		O7^{v}—Gd1—C34^{v}	26.6 (2)			O3^{iv}—Gd1—O7^{iii}	84.22 (18)
		O7^{iv}—Gd1—C34^{v}	94.7 (2)			O3^{iv}—Gd1—O7^{ii}	148.28 (17)
		O8^{v}—Gd1—Gd1^{iii}	81.64 (14)			O3^{iv}—Gd1—O8^{ii}	159.81 (18)
		O8^{v}—Gd1—C34^{v}	26.3 (2)			O3^{iv}—Gd1—O1	76.44 (19)
		O5—Gd1—O1	77.0 (2)			O3^{iv}—Gd1—O2^{v}	103.97 (19)
		O5—Gd1—O3^{i}	94.8 (2)			O3^{iv}—Gd1—C34^{ii}	172.4 (2)
		O5—Gd1—O2^{ii}	146.6 (2)			O2^{v}—Gd1—Gd1^{i}	112.34 (13)
		O5—Gd1—Gd1^{iii}	81.58 (16)			O2^{v}—Gd1—O9	72.86 (18)
		O5—Gd1—O9	140.0 (2)			O2^{v}—Gd1—O7^{iii}	138.49 (17)
		O5—Gd1—O7^{v}	96.3 (2)			O2^{v}—Gd1—O7^{ii}	82.07 (18)
		O5—Gd1—O7^{iv}	69.9 (2)			O2^{v}—Gd1—O8^{ii}	73.52 (18)
		O5—Gd1—O8^{v}	79.5 (2)			O2^{v}—Gd1—O1	81.34 (19)
		O5—Gd1—C34^{v}	91.4 (2)			O2^{v}—Gd1—C34^{ii}	72.0 (2)
		C34^{v}—Gd1—Gd1^{iii}	60.05 (17)			C34^{ii}—Gd1—Gd1^{i}	59.92 (16)

Symmetry codes: (i) −*x*+2, −*y*+1, −*z*+1; (ii) −*x*+3, −*y*+1, −*z*+2; (iii) −*x*+4, −*y*+1, −*z*+2; (iv) −*x*+3, −*y*+1, −*z*+1; (v) *x*+1, *y*, *z*+1; (vi) *x*−1, *y*, *z*−1.

Symmetry codes: (i) −*x*−2, −*y*, −*z*−2; (ii) *x*−1, *y*, *z*−1; (iii) −*x*−1, −*y*, −*z*−1; (iv) −*x*, −*y*, −*z*−1; (v) −*x*−1, −*y*, −*z*−2; (vi) *x*+1, *y*, *z*+1.

Compound 9

Gd1—O8^{iii}	2.559 (6)	O8^{iii}—Gd1—C34^{iii}	25.9 (2)
Gd1—O7^{ii}	2.514 (6)	O8^{iii}—Gd1—Gd1^{iv}	80.77 (14)
Gd1—O7^{iii}	2.484 (6)	O7^{iii}—Gd1—O8^{iii}	51.82 (19)
Gd1—C34^{iii}	2.876 (9)	O7^{ii}—Gd1—O8^{iii}	110.63 (19)
Gd1—Gd2^{iv}	4.050 (6)	O7^{iii}—Gd1—O7^{ii}	71.7 (2)
Gd1—O1	2.344 (7)	O7^{iii}—Gd1—C34^{iii}	26.6 (2)
Gd1—O9	2.502 (6)	O7^{ii}—Gd1—C34^{iii}	94.3 (2)
Gd1—O2^{v}	2.327 (6)	O7^{ii}—Gd1—Gd1^{iv}	35.63 (13)
Gd1—O3^{vi}	2.316 (6)	O7^{iii}—Gd1—Gd1^{iv}	36.12 (13)
		O7^{iii}—Gd1—O9	79.1 (2)
		O5—Gd1—O8^{iii}	80.0 (2)
		O5—Gd1—O7^{iii}	97.4 (2)
		O5—Gd1—O7^{ii}	69.9 (2)
		O5—Gd1—C34^{iii}	92.5 (3)
		O5—Gd1—Gd1^{iv}	82.25 (15)
		O5—Gd1—O1	76.9 (2)
		O5—Gd1—O9	139.8 (2)
		O5—Gd1—O2^{v}	147.1 (2)
		O5—Gd1—O3^{vi}	94.7 (2)
		C34^{iii}—Gd1—Gd1^{iv}	59.84 (19)
		O1—Gd1—O8^{iii}	83.4 (2)
		O1—Gd1—O7^{ii}	140.37 (19)
		O1—Gd1—O7^{iii}	134.9 (2)
		O1—Gd1—C34^{iii}	108.3 (3)
		O1—Gd1—Gd1^{iv}	155.64 (17)
		O1—Gd1—O9	132.9 (2)
		O9—Gd1—O8^{iii}	123.3 (2)
		O9—Gd1—O7^{ii}	71.05 (19)
		O9—Gd1—C34^{iii}	99.6 (2)
		O9—Gd1—Gd1^{iv}	71.48 (15)
		O2^{v}—Gd1—O8^{iii}	73.9 (2)
		O2^{v}—Gd1—O7^{ii}	138.44 (19)
		O2^{v}—Gd1—O7^{iii}	82.1 (2)
		O2^{v}—Gd1—C34^{iii}	72.4 (2)
		O2^{v}—Gd1—Gd1^{iv}	112.34 (17)
		O2^{v}—Gd1—O1	80.5 (2)
		O2^{v}—Gd1—O9	72.7 (2)
		O3^{vi}—Gd1—O8^{iii}	160.5 (2)
		O3^{vi}—Gd1—O7^{iii}	147.7 (2)
		O3^{vi}—Gd1—O7^{ii}	84.6 (2)
		O3^{vi}—Gd1—C34^{iii}	171.9 (2)
		O3^{vi}—Gd1—Gd1^{iv}	117.36 (15)
		O3^{vi}—Gd1—O1	77.1 (2)
		O3^{vi}—Gd1—O9	72.4 (2)
		O3^{vi}—Gd1—O2^{v}	103.2 (2)

Symmetry codes: (i) $x-1, y, z-1$; (ii) $-x+1, -y+1, -z+1$; (iii) $x+1, y, z+1$; (iv) $-x+2, -y+1, -z+2$; (v) $-x+1, -y+1, -z+2$; (vi) $-x, -y+1, -z+1$.

Table SI6. The hydrogen bond data for compound **1–9**.

Compound **1**:

Donor --- H....Acceptor	D – H (Å)	H...A (Å)	D...A (Å)	D - H...A (degree)	Equivalent Position Code
O(9) --H(9A) ..O(5)	0.88	2.30	3.157(13)	163	-x,-1-y,-1-z
O(9) --H(9A) ..O(6)	0.88	2.22	2.906(14)	134	-x,-1-y,-1-z
O(9) --H(9B) ..O(4)	0.88	1.91	2.722(12)	153	-2-x,-1-y,-2-z
O(10) --H(10B) ..O(2)	0.85	2.02	2.826(16)	159	x,-1/2-y,-1/2+z
C(6) --H(6) ..Cl(1)	0.93	2.61	3.533(14)	174	
C(9) --H(9) ..O(4)	0.93	2.47	3.141(18)	129	1+x,-1/2-y,1/2+z
C(21) --H(21) ..O(10)	0.93	2.46	3.317(19)	154	
C(25) --H(25) ..Cl(2)	0.93	2.32	3.204(13)	159	
C(26) --H(26) ..O(4)	0.93	2.34	3.259(17)	169	1+x,-1/2-y,1/2+z
C(27) --H(27) ..O(6)	0.93	2.26	3.136(19)	157	-1+x,-1/2-y,-1/2+z

Compound **2**:

Donor --- H....Acceptor	D – H (Å)	H...A (Å)	D...A (Å)	D - H...A (degree)	Equivalent Position Code
O(9) --H(9A) ..O(5)	0.87	2.33	3.177(10)	165	-x,-1-y,-1-z
O(9) --H(9A) ..O(6)	0.87	2.21	2.900(10)	136	-x,-1-y,-1-z
O(9) --H(9B) ..O(4)	0.87	1.91	2.689(9)	148	2-x,-1-y,-z
O(10) --H(10A) ..O(2)	0.85	2.40	2.838(12)	113	
O(10) --H(10B) ..O(2)	0.85	2.02	2.826(16)	105	
O(10) --H(10B) ..O(8)	0.85	2.16	2.955(13)	156	-1+x,y,-1+z
C(6) --H(6) ..Br(1)	0.93	2.61	3.539(9)	175	
C(9) --H(9) ..O(4)	0.93	2.44	3.132(12)	131	-1+x,-1/2-y,-1/2+z
C(16) --H(16) ..Br(1)	0.93	2.92	3.845(10)	176	
C(21) --H(21) ..O(10)	0.93	2.45	3.314(15)	154	x,-1/2-y,1/2+z
C(25) --H(25) ..Cl(1)	0.93	2.28	3.178(10)	162	
C(26) --H(26) ..O(4)	0.93	2.38	3.296(12)	167	-1+x,-1/2-y,-1/2+z
C(27) --H(27) ..O(6)	0.93	2.29	3.173(13)	157	1+x,-1/2-y,1/2+z

Compound **3**:

Donor --- H....Acceptor	D – H (Å)	H...A (Å)	D...A (Å)	D - H...A (degree)	Equivalent Position Code
O(9) --H(9A) ..O(5)	0.88	2.39	3.189(8)	151	2-x,-1-y,-z
O(9) --H(9A) ..O(6)	0.88	2.25	2.880(8)	128	2-x,-1-y,-z
O(9) --H(9B) ..O(3)	0.88	2.51	2.825(7)	102	-x,-1-y,-1-z
O(9) --H(9B) ..O(4)	0.88	1.86	2.710(8)	161	-x,-1-y,-1-z
O(10) --H(10A) ..O(2)	0.85	2.48	2.842(10)	107	
O(10) --H(10B) ..O(8)	0.85	2.59	2.960(11)	108	1+x,y,1+z
C(6) --H(6) ..Br(1)	0.93	2.65	3.581(8)	176	
C(9) --H(9) ..O(4)	0.93	2.42	3.129(11)	133	1+x,-1/2-y,1/2+z
C(15) --H(15) ..O(3)	0.93	2.43	2.753(10)	100	
C(21) --H(21) ..O(10)	0.93	2.50	3.356(12)	154	x,-1/2-y,-1/2+z
C(25) --H(25) ..Br(2)	0.93	2.43	3.309(9)	158	
C(26) --H(26) ..O(4)	0.93	2.37	3.275(11)	164	1+x,-1/2-y,1/2+z
C(27) --H(27) ..O(6)	0.93	2.29	3.147(11)	153	-1+x,-1/2-y,-1/2+z
C(32) --H(32) ..O(7)	0.93	2.51	2.819(10)	100	

Compound **4**:

Donor --- H....Acceptor	D – H (Å)	H...A (Å)	D...A (Å)	D - H...A (degree)	Equivalent Position Code
O(9) --H(9A) ..O(5)	0.87	2.32	3.168(6)	164	1-x,-1-y,-z
O(9) --H(9A) ..O(6)	0.87	2.20	2.883(6)	135	1-x,-1-y,-z
O(9) --H(9B) ..O(4)	0.87	1.89	2.690(5)	152	-1-x,-1-y,-1-z
O(10) --H(10A) ..O(8)	0.85	2.10	2.936(8)	167	1+x,-1/2-y,1/2+z
O(10) --H(10B) ..O(2)	0.85	2.18	2.835(8)	133	x,-1/2-y,-1/2+z
C(6) --H(6) ..Cl(1)	0.93	2.57	3.496(7)	175	
C(9) --H(9) ..O(4)	0.93	2.45	3.145(8)	132	1+x,-1/2-y,1/2+z
C(15) --H(15) ..O(3)	0.93	2.43	2.745(7)	100	
C(21) --H(21) ..O(10)	0.93	2.44	3.305(9)	155	
C(25) --H(25) ..Cl(2)	0.93	2.29	3.181(7)	161	
C(26) --H(26) ..O(4)	0.93	2.36	3.272(8)	167	1+x,-1/2-y,1/2+z
C(27) --H(27) ..O(6)	0.93	2.30	3.180(8)	157	-1+x,-1/2-y,-1/2+z

Compound **5**:

Donor --- H....Acceptor	D – H (Å)	H...A (Å)	D...A (Å)	D - H...A (degree)	Equivalent Position Code
O(9) --H(9A) ..O(5)	0.87	2.33	3.177(7)	163	1-x,-y,1-z
O(9) --H(9A) ..O(6)	0.87	2.18	2.886(7)	138	1-x,-y,1-z
O(9) --H(9B) ..O(4)	0.87	1.94	2.689(9)	142	-1-x,-y,-z
O(10) --H(10A) ..O(8)	0.85	2.20	2.952(9)	148	1+x,1/2-y,1/2+z
O(10) --H(10B) ..O(2)	0.85	2.11	2.832(8)	143	x,1/2-y,-1/2+z
C(6) --H(6) ..Br(1)	0.93	2.61	3.542(7)	176	
C(9) --H(9) ..O(4)	0.93	2.44	3.140(9)	132	1+x,1/2-y,1/2+z
C(15) --H(15) ..O(3)	0.93	2.44	2.757(8)	100	
C(16) --H(16) ..Br(1)	0.93	2.90	3.831(7)	177	
C(21) --H(21) ..O(10)	0.93	2.45	3.316(10)	155	
C(25) --H(25) ..Cl(1)	0.93	2.29	3.184(7)	162	
C(26) --H(26) ..O(4)	0.93	2.36	3.273(9)	168	1+x,1/2-y,1/2+z
C(27) --H(27) ..O(6)	0.93	2.30	3.176(9)	156	-1+x,1/2-y,-1/2+z

Compound **6:**

Donor --- H....Acceptor	D – H (Å)	H...A (Å)	D...A (Å)	D - H...A (degree)	Equivalent Position Code
O(9) --H(9A) ..O(6)	0.87	2.48	3.124(5)	131	
O(9) --H(9A) ..O(7)	0.87	2.15	2.964(6)	155	-1/2+x,1/2-y,-1/2+z
O(9) --H(9B) ..O(2)	0.73(5)	2.02(5)	2.724(5)	165(6)	
O(10) --H(10A) ..O(8)	0.74(5)	2.01(5)	2.721(6)	160(6)	1-x,y,3/2-z
O(10) --H(10B) ..O(1)	0.74(6)	2.14(6)	2.876(6)	179(10)	1/2-x,3/2-y,1-z
C(8) --H(8) ..Br(1)	0.93	2.78	3.645(5)	155	
C(10) --H(10) ..O(8)	0.93	2.47	3.275(7)	145	1/2-x,1/2+y,3/2-z
C(16) --H(16) ..Br(1)	0.93	2.87	3.702(5)	150	
C(23) --H(23) ..Br(1)	0.93	2.91	3.617(5)	133	
C(25) --H(25) ..Br(1)	0.93	2.77	3.682(5)	168	
C(27) --H(27) ..O(8)	0.93	2.51	3.399(6)	160	1/2-x,-1/2+y,3/2-z

Compound **7:**

Donor --- H....Acceptor	D – H (Å)	H...A (Å)	D...A (Å)	D - H...A (degree)	Equivalent Position Code
O(9) --H(9A) ..O(5)	0.89	2.30	3.154(10)	161	4-x,1-y,2-z
O(9) --H(9A) ..O(6)	0.89	2.20	2.898(10)	135	4-x,1-y,2-z
O(9) --H(9B) ..O(4)	0.89	1.87	2.689(8)	153	2-x,1-y,1-z
O(10) --H(10B) ..O(2)	0.85	2.50	2.807(10)	102	x,3/2-y,-1/2+z
C(3) --H(3) ..O(9)	0.93	2.60	3.347(11)	138	3-x,1-y,2-z
C(6) --H(6) ..Cl(1)	0.93	2.57	3.492(9)	174	
C(9) --H(9) ..O(4)	0.93	2.47	3.141(18)	129	1+x,3/2-y,1/2+z
C(12) --H(12) ..O(10)	0.93	2.58	3.473(12)	161	-1+x,y,z
C(15) --H(15) ..O(3)	0.93	2.43	2.752(10)	100	
C(21) --H(21) ..O(10)	0.93	2.46	3.317(19)	152	
C(25) --H(25) ..Cl(2)	0.93	2.31	3.197(10)	161	
C(26) --H(26) ..O(4)	0.93	2.33	3.246(12)	167	1+x,3/2-y,1/2+z
C(27) --H(27) ..O(6)	0.93	2.25	3.129(13)	157	-1+x,3/2-y,-1/2+z

Compound **8:**

Donor --- H....Acceptor	D – H (Å)	H...A (Å)	D...A (Å)	D - H...A (degree)	Equivalent Position Code
O(9) --H(9A) ..O(5)	0.88	2.30	3.149(8)	161	-2-x,-y,-2-z
O(9) --H(9A) ..O(6)	0.88	2.18	2.905(8)	139	-2-x,-y,-2-z
O(9) --H(9B) ..O(4)	0.88	1.95	2.688(7)	141	-x,-y,-1-z
O(10) --H(10A) ..O(8)	0.85	2.49	2.948(9)	115	-1+x,y,-1+z
O(10) --H(10B) ..O(2)	0.85	2.39	2.810(8)	111	
O(10) --H(10B) ..O(9)	0.85	2.54	3.383(9)	172	-1-x,-y,-2-z
C(6) --H(6) ..Br(1)	0.93	2.61	3.539(7)	176	
C(9) --H(9) ..O(4)	0.93	2.42	3.107(10)	131	-1+x,1/2-y,-1/2+z
C(15) --H(15) ..O(3)	0.93	2.43	2.753(9)	100	
C(16) --H(16) ..Br(1)	0.93	2.91	3.843(8)	177	
C(21) --H(21) ..O(10)	0.93	2.42	3.281(10)	154	x,1/2-y,1/2+z
C(25) --H(25) ..Cl(1)	0.93	2.28	3.185(9)	162	
C(26) --H(26) ..O(4)	0.93	2.36	3.280(10)	168	-1+x,1/2-y,-1/2+z
C(27) --H(27) ..O(6)	0.93	2.24	3.120(11)	158	1+x,1/2-y,1/2+z

Compound **9**:

Donor --- H....Acceptor	D – H (Å)	H...A (Å)	D...A (Å)	D - H...A (degree)	Equivalent Position Code
O(9) --H(9A) ..O(5)	0.86	2.36	3.199(10)	165	2-x,1-y,2-z
O(9) --H(9A) ..O(6)	0.86	2.20	2.885(10)	136	2-x,1-y,2-z
O(9) --H(9B) ..O(4)	0.86	1.95	2.715(9)	146	-x,1-y,1-z
O(10) --H(10A) ..O(2)	0.85	2.37	2.864(11)	118	x,3/2-y,-1/2+z
O(10) --H(10A) ..O(8)	0.85	2.25	2.971(12)	143	1+x,3/2-y,1/2+z
O(10) --H(10B) ..O(2)	0.85	2.58	2.864(11)	100	x,3/2-y,-1/2+z
C(6) --H(6) ..Br(1)	0.93	2.67	3.594(11)	177	
C(9) --H(9) ..O(4)	1.02(8)	2.44(9)	3.163(13)	128(6)	1+x,3/2-y,1/2+z
C(15) --H(15) ..O(3)	0.93	2.44	2.767(10)	100	
C(21) --H(21) ..O(10)	0.93	2.50	3.361(14)	155	
C(24) --H(24) ..O(5)	0.93	2.52	2.830(11)	100	
C(25) --H(25) ..Br(2)	0.93	2.44	3.326(11)	159	
C(26) --H(26) ..O(4)	0.93	2.38	3.287(12)	165	1+x,3/2-y,1/2+z
C(27) --H(27) ..O(6)	0.93	2.31	3.170(13)	154	-1+x,3/2-y,-1/2+z