Supporting Information

Tuning the bonding dimensions for coordination polymers based on rare earth metal ions

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1. Reagents, measurements and apparatus

The ligand $H_2BIB^{+}\cdot Br^{-}$ was synthesized according to the reference.[1] The other reagents are commercially obtained and directly used without further purification. The Powder X-ray diffraction (PXRD) was recorded on a Bruker D8 (40kV, 40 mA) advanced diffractometer with Cu-Kα radiation (λ=1.5418 Å). IR spectrum was carried out on a NEXUS 870 (Nicolet) infrared spectrometer from 400 to 4000 cm-1 by a KBr pellet. Thermogravimetric (TG) analysis data were collected on a Netzsch STA 409 PC analyzer at a heating rate of 10 °C·min^{-1} under N_2 atmosphere.

2. Synthesis

2.1 $[Eu_2(BIN^{-})_2(H_2O)_8]\cdot 4Cl^{-}\cdot H_2O$ (compound 1, $C_{14}H_{32}Cl_4Eu_2N_4O_{17}$)

$H_2BIB^{+}\cdot Br^{-}$ (0.0530 g, 0.20 mmol), Eu_2O_3 (0.070 g, 0.20 mmol) and a drop of aqueous HCl (6 mol/L) were added to ethanol aqueous solution (V:V=1:1, 3mL), the mixture was transferred into a 12 mL small glass bottle after being dissolved, then heated up to 120 ℃ at the rate of 5 ℃ / min in a stainless steel reactor, and maintained at this temperature for 3 days, then cooled to room temperature at the rate of 3 ℃ / min. The light brown bulk crystals were obtained after filtration and washed by ethanol two times. Yield: 31.2% based on $EuCl_3\cdot 6H_2O$. IR (KBr,cm^{-1}):3363, 1625, 1455, 1401, 1313, 710, 680, 617.

2.2 $[Ho(BIN^{-})(HCOO^{-})(H_2O)_2]\cdot Br^{-}$ (compound 2, $C_8H_{12}BrHoN_2O_8$)

Ho_2O_3 (0.0189 g, 0.05 mmol) and $H_2BIB^{+}\cdot Br^{-}$ (0.0199 g, 0.0750 mmol) were added to 2 mL distilled water and 3 mL N,N-dimethylformamide (DMF), the mixture was transferred to a glass vial and stirred by a glass rod. The glass vial was placed in a polytetrafluoroethylene liner, heated at 180 ° C for 3 days in an autoclave, then cooled to room temperature at a rate of 2 °C / h. Pink flake crystals suitable for X-ray single crystal diffraction were obtained by filtration and washing by ethanol two times. Yield: 32.4% (based on Ho). IR (KBr,cm^{-1}): 3363, 1742, 1625, 1455, 1401, 1346, 1313, 1208，1164, 1103, 1038, 974, 799, 710, 680, 617, 461.

2.3 $[Tb_2(BIN^{-})_3(H_2O)_6]\cdot 3Br^{-}\cdot 5(H_2O)$ (compound 3, $C_{21}H_{43}Br_3N_6O_{23}Tb_2$)

Compound **3** was synthesized applying the similar procedure to compound **2** replacing Ho_2O_3 (0.0189 g, 0.05 mmol) with Tb_2O_3 (0.0183 g, 0.05 mmol). The colorless flake crystals suitable for X-ray single crystal diffraction was finally obtained. Yield: 32.6% (based on Tb). IR (KBr,cm-1): 3363, 1742, 1625, 1455, 1401, 1346, 1313, 1208, 1164, 799, 710, 680, 617, 461.

3. Crystal structure refinement

All crystal data was collected on Bruker D8 venture diffractometer with a CMOS detector using graphite-monochromated Mo-Ka radiation (0.71073 Å). The data were collected and reduced by APEX3 [2] routine, then corrected by SADABS [3] program.The structures were solved by dual space algorithm by SHELXT [4] subprogram and refined by full matrix least square on F^2 by SHELXL [5] subprogram under OLEX2 [6] software package. All the non-hydrogen atoms were refined anisotropically, and all the H atoms were calculated in the theoretical positions. The CCDC reference number of compound **1** to **3** were 2201258 - 2201260, respectively.

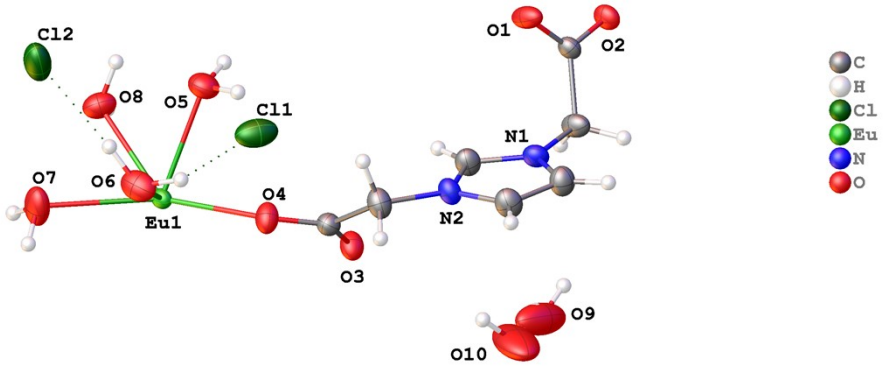

Figure S1. The asymmetric unit of compound **1** with displacement ellipsoids at the 50% probability level. The labels of C and H atoms are omitted for clarity.

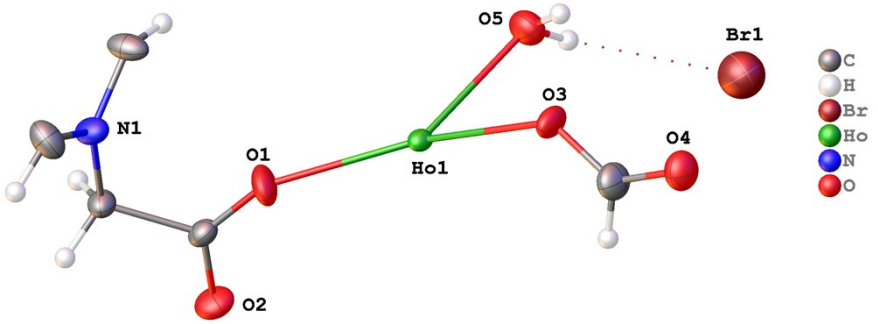

Figure S2. The asymmetric unit of compound **2** with displacement ellipsoids at the 50% probability level. The labels of C and H atoms are omitted for clarity.

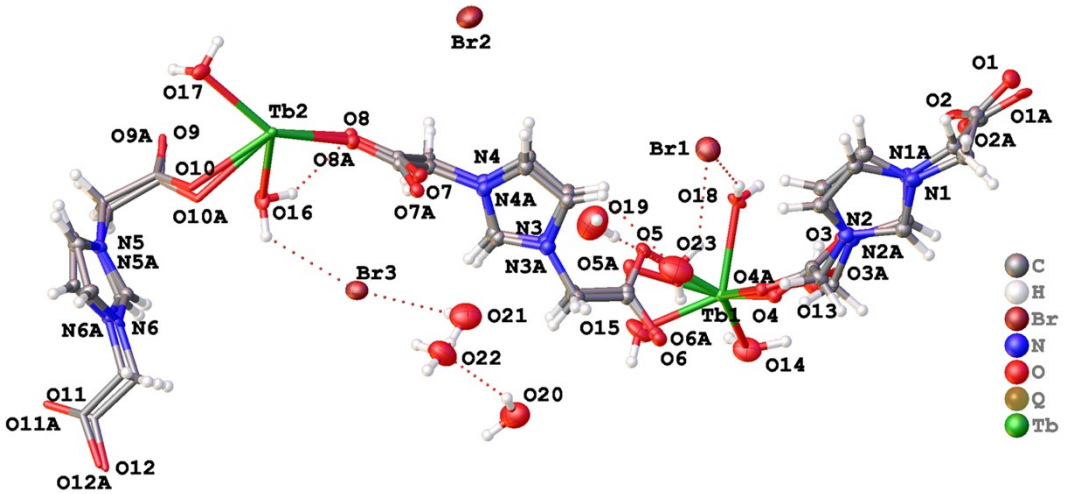

Figure S3. The asymmetric unit of compound **3** with displacement ellipsoids at the 50% probability level. The labels of C and H atoms are omitted for clarity. The ligand BIN^- is disordered in the micro structure.

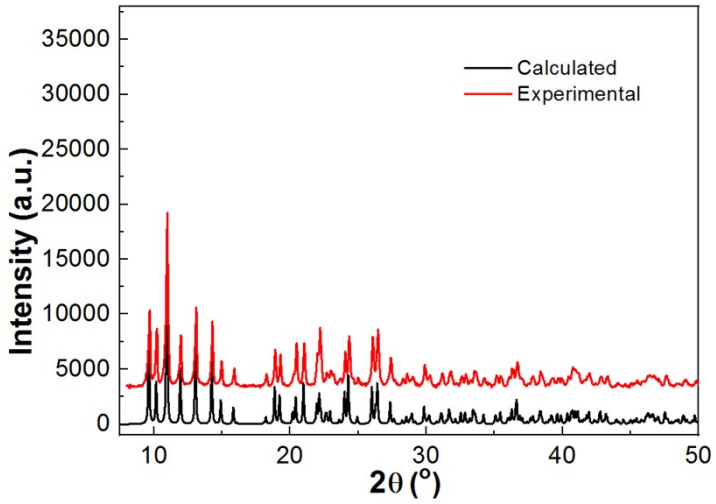

Figure S4. Powder X-ray diffraction (PXRD) patterns of compound **1**.

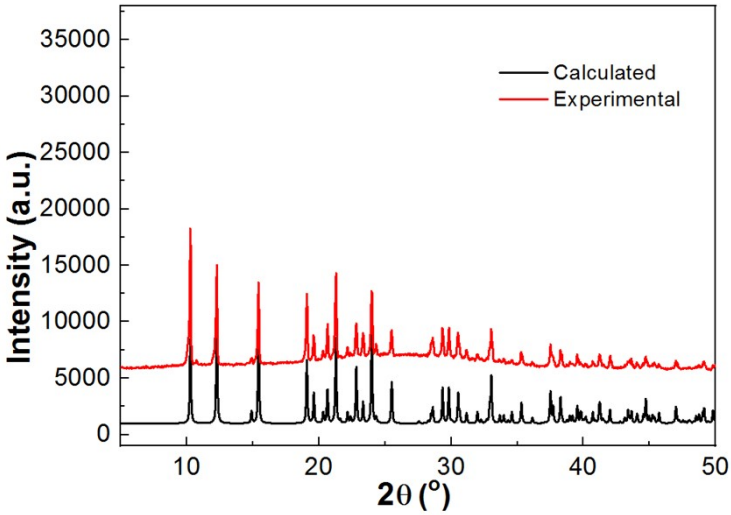

Figure S5. Powder X-ray diffraction (PXRD) patterns of compound **2**.

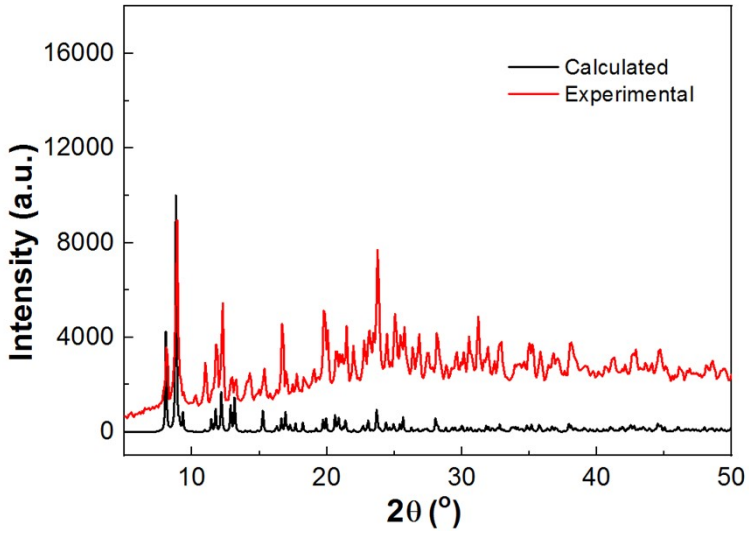

Figure S6. Powder X-ray diffraction (PXRD) patterns of compound **3**.

Table S1. Crystal data and structure refinement for compound **1**.

Item	value	
Empirical formula	C_{14} H_{32} Cl_4 Eu_2 N_4 O_{17}	
Formula weight	974.15	
Temperature	293.0(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 9.1299(5) Å	α= 101.793(1)°.
	b = 9.5805(6) Å	β= 116.073(1)°.
	c = 10.0625(6) Å	γ = 95.318(1)°.
Volume	757.04(8) $Å^3$	
Z	1	
Density (calculated)	2.137 Mg/m^3	
Absorption coefficient	4.534 mm^{-1}	
F(000)	474	
Crystal size	0.22 x 0.21 x 0.2 mm^3	
Theta range for data collection	2.518 to 27.585°.	
Index ranges	-11<=h<=11, -12<=k<=12, -13<=l<=13	
Reflections collected	7416	
Independent reflections	3459 [R(int) = 0.0165]	
Completeness to theta = 25.242°	99.6 %	
Max. and min. transmission	0.4641 and 0.4354	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3459 / 0 / 196	
Goodness-of-fit on F^2	1.048	
Final R indices [I>2sigma(I)]	R1 = 0.0199, wR2 = 0.0465	
R indices (all data)	R1 = 0.0228, wR2 = 0.0474	
Largest diff. peak and hole	0.884 and -0.759 $e.Å^{-3}$	

Table S2. Crystal data and structure refinement for compound **2**.

Item	value	
Empirical formula	$C_8 H_{12} Br Ho N_2 O_8$	
Formula weight	509.04	
Temperature	296.1(5) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	*C m c a*	
Unit cell dimensions	a = 17.191(4) Å	α= 90°.
	b = 9.0546(18) Å	β= 90°.
	c = 16.425(4) Å	γ = 90°.
Volume	2556.6(9) $Å^3$	
Z	8	
Density (calculated)	2.645 Mg/m^3	
Absorption coefficient	9.356 mm^{-1}	
F(000)	1920	
Crystal size	0.26 x 0.24 x 0.18 mm^3	
Theta range for data collection	2.829 to 24.988°.	
Index ranges	-20<=h<=20, -10<=k<=8, -19<=l<=19	
Reflections collected	6165	
Independent reflections	1172 [R(int) = 0.0270]	
Completeness to theta = 24.988°	99.6 %	
Max. and min. transmission	0.72 and 0.46	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1172 / 0 / 98	
Goodness-of-fit on F^2	1.112	
Final R indices [I>2sigma(I)]	R1 = 0.0415, wR2 = 0.1256	
R indices (all data)	R1 = 0.0443, wR2 = 0.1272	
Largest diff. peak and hole	1.686 and -3.188 $e.Å^{-3}$	

Table S2. Crystal data and structure refinement for compound **3**.

Item	value	
Empirical formula	C_{21} H_{43} Br_3 N_6 O_{23} Tb_2	
Formula weight	1305.18	
Temperature	296.1(1) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.791(2) Å	α= 87.302(3)°.
	b = 11.185(3) Å	β= 86.119(3)°.
	c = 20.117(5) Å	γ = 78.386(3)°.
Volume	1931.9(8) $Å^3$	
Z	2	
Density (calculated)	2.244 Mg/m^3	
Absorption coefficient	6.826 mm^{-1}	
F(000)	1260	
Crystal size	0.22 x 0.22 x 0.13 mm^3	
Theta range for data collection	2.149 to 27.551°.	
Index ranges	-11<=h<=11, -14<=k<=13, -26<=l<=26	
Reflections collected	18484	
Independent reflections	8690 [R(int) = 0.0525]	
Completeness to theta = 25.242°	98.0 %	
Max. and min. transmission	0.62 and 0.41	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8690 / 2578 / 832	
Goodness-of-fit on F^2	1.129	
Final R indices [I>2sigma(I)]	R1 = 0.0968, wR2 = 0.2422	
R indices (all data)	R1 = 0.1259, wR2 = 0.2500	
Largest diff. peak and hole	4.317 and -3.330 $e.Å^{-3}$	

Table S4. Selected bond lengths [Å] and angles [°] for compound **1**.

Eu(1)-O(1)#2	2.475(2)
Eu(1)-O(2)#2	2.666(2)
Eu(1)-O(2)#3	2.3626(19)
Eu(1)-O(3)#1	2.415(2)
Eu(1)-O(4)	2.379(2)
Eu(1)-O(5)	2.456(2)
Eu(1)-O(6)	2.475(2)
Eu(1)-O(7)	2.463(2)
Eu(1)-O(8)	2.466(2)
O(1)#2-Eu(1)-O(2)#2	50.35(6)
O(1)#2-Eu(1)-O(6)	74.92(8)
O(2)#3-Eu(1)-O(1)#2	122.98(7)
O(2)#3-Eu(1)-O(2)#2	72.67(7)
O(2)#3-Eu(1)-O(3)#1	76.32(7)
O(2)#3-Eu(1)-O(4)	76.07(7)
O(2)#3-Eu(1)-O(5)	77.01(8)
O(2)#3-Eu(1)-O(6)	140.62(8)
O(2)#3-Eu(1)-O(7)	144.85(8)
O(2)#3-Eu(1)-O(8)	81.97(8)
O(3)#1-Eu(1)-O(1)#2	83.31(8)
O(3)#1-Eu(1)-O(2)#2	67.61(7)
O(3)#1-Eu(1)-O(5)	134.67(8)
O(3)#1-Eu(1)-O(6)	143.06(8)
O(3)#1-Eu(1)-O(7)	75.59(8)
O(3)#1-Eu(1)-O(8)	71.04(8)
O(4)-Eu(1)-O(1)#2	80.78(8)
O(4)-Eu(1)-O(2)#2	68.15(7)
O(4)-Eu(1)-O(3)#1	132.94(7)
O(4)-Eu(1)-O(5)	73.06(8)
O(4)-Eu(1)-O(6)	72.81(8)
O(4)-Eu(1)-O(7)	139.08(8)
O(4)-Eu(1)-O(8)	139.86(8)
O(5)-Eu(1)-O(1)#2	141.99(8)
O(5)-Eu(1)-O(2)#2	135.17(7)
O(5)-Eu(1)-O(6)	71.31(8)

O(5)-Eu(1)-O(7)	109.35(9)
O(5)-Eu(1)-O(8)	69.46(8)
O(6)-Eu(1)-O(2)#2	115.69(7)
O(6)-Eu(1)-C(1)#2	95.22(8)
O(7)-Eu(1)-O(1)#2	73.86(8)
O(7)-Eu(1)-O(2)#2	114.53(8)
O(7)-Eu(1)-O(6)	69.92(9)
O(7)-Eu(1)-O(8)	69.19(8)
O(8)-Eu(1)-O(1)#2	139.02(8)
O(8)-Eu(1)-O(2)#2	135.33(7)
O(8)-Eu(1)-O(6)	107.33(8)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y-2,-z+1 #2 x,y-1,z #3 -x,-y-1,-z+1

#4 x,y+1,z

Table S5. Selected bond lengths [Å] and angles [°] for compound **2**.

Ho(1)-O(1)	2.324(7)
Ho(1)-O(2)#2	2.318(8)
Ho(1)-O(3)	2.357(10)
Ho(1)-O(4)#4	2.350(11)
Ho(1)-O(5)	2.472(7)
O(1)-Ho(1)-O(1)#1	71.8(4)
O(1)#1-Ho(1)-O(3)	144.1(2)
O(1)#1-Ho(1)-O(4)#4	84.1(3)
O(1)-Ho(1)-O(5)	140.0(3)
O(1)-Ho(1)-O(5)#1	73.2(3)
O(1)#1-Ho(1)-O(5)#1	140.0(3)
O(2)#3-Ho(1)-O(1)#1	120.1(3)
O(2)#3-Ho(1)-O(1)	78.7(3)
O(2)#2-Ho(1)-O(1)	120.1(3)
O(2)#2-Ho(1)-O(2)#3	73.0(4)
O(2)#3-Ho(1)-O(3)	80.6(3)
O(2)#2-Ho(1)-O(4)#4	143.0(2)
O(2)#2-Ho(1)-O(5)	70.2(3)
O(2)#2-Ho(1)-O(5)#1	137.0(3)
O(3)-Ho(1)-O(5)#1	72.2(2)
O(4)#4-Ho(1)-O(3)	95.3(4)
O(4)#4-Ho(1)-O(5)	73.6(2)
O(5)-Ho(1)-O(5)#1	128.2(4)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,z #2 -x+1,-y+1,-z+1 #3 x,-y+1,-z+1

#4 -x+1,y+1/2,-z+1/2 #5 x,-y+2,-z+1 #6 x,y-1/2,-z+1/2

Table S6. Selected bond lengths [Å] and angles [°] for compound **3**.

Tb(1)-O(2)#1	2.30(2)
Tb(1)-O(4)	2.472(14)
Tb(1)-O(5)	2.509(17)
Tb(1)-O(6)#2	2.418(16)
Tb(1)-O(13)	2.358(17)
Tb(1)-O(14)	2.481(16)
Tb(1)-O(15)	2.437(16)
Tb(1)-O(18)	2.420(13)
Tb(2)-O(7)#3	2.375(19)
Tb(2)-O(8)	2.397(14)
Tb(2)-O(9)#4	2.387(13)
Tb(2)-O(10)	2.459(13)
Tb(2)-O(12)#5	2.212(14)
Tb(2)-O(16)	2.495(11)
Tb(2)-O(17)	2.447(14)

O(2)#1-Tb(1)-O(4)	144.2(7)
O(2)#1-Tb(1)-O(5)	87.4(7)
O(2)#1-Tb(1)-O(6)#2	138.3(6)
O(2)#1-Tb(1)-O(13)	86.8(7)
O(2)#1-Tb(1)-O(14)	72.3(7)
O(2)#1-Tb(1)-O(15)	71.6(7)
O(2)#1-Tb(1)-O(18)	71.8(6)
O(2A)#1-Tb(1)-O(5A)	75.0(18)
O(4)-Tb(1)-O(5)	92.0(7)
O(4)-Tb(1)-O(14)	122.5(6)
O(5A)-Tb(1)-O(14)	128(2)
O(6)#2-Tb(1)-O(4)	73.8(6)
O(6)#2-Tb(1)-O(5)	113.5(6)
O(6)#2-Tb(1)-O(14)	69.8(5)
O(6)#2-Tb(1)-O(15)	81.5(6)
O(6)#2-Tb(1)-O(18)	149.0(5)
O(13)-Tb(1)-O(4)	71.9(6)
O(13)-Tb(1)-O(5)	141.7(7)
O(13)-Tb(1)-O(6)#2	95.5(6)
O(13)-Tb(1)-O(14)	69.1(6)

O(13)-Tb(1)-O(15)	140.9(6)
O(13)-Tb(1)-O(18)	75.8(6)
O(14)-Tb(1)-O(5)	143.1(7)
O(15)-Tb(1)-O(4)	141.3(6)
O(15)-Tb(1)-O(5)	71.0(7)
O(15)-Tb(1)-O(14)	73.4(6)
O(18)-Tb(1)-O(4)	75.2(5)
O(18)-Tb(1)-O(5)	66.4(6)
O(18)-Tb(1)-O(14)	130.4(5)
O(18)-Tb(1)-O(15)	124.0(6)
O(7)#3-Tb(2)-O(8)	130.1(7)
O(7)#3-Tb(2)-O(9)#4	140.0(6)
O(7)#3-Tb(2)-O(10)	74.7(7)
O(7)#3-Tb(2)-O(16)	133.9(6)
O(7)#3-Tb(2)-O(17)	68.6(6)
O(7A)#3-Tb(2)-O(16)	143(2)
O(7A)#3-Tb(2)-O(17)	64(2)
O(8)-Tb(2)-O(10)	137.7(12)
O(8)-Tb(2)-O(16)	68.2(11)
O(8)-Tb(2)-O(17)	143.1(8)
O(8A)-Tb(2)-O(16)	68(5)
O(8A)-Tb(2)-O(17)	147(3)
O(9)#4-Tb(2)-O(8)	75.6(6)
O(9)#4-Tb(2)-O(10)	107.8(5)
O(9)#4-Tb(2)-O(16)	80.5(5)
O(9)#4-Tb(2)-O(17)	74.1(5)
O(9A)#4-Tb(2)-O(16)	75.6(3)
O(9A)#4-Tb(2)-O(17)	77.8(3)
O(10)-Tb(2)-O(16)	70.9(6)
O(10A)-Tb(2)-O(16)	58.8(16)
O(12)#5-Tb(2)-O(7)#3	70.5(6)
O(12)#5-Tb(2)-O(8)	78.5(7)
O(12)#5-Tb(2)-O(9)#4	149.2(6)
O(12)#5-Tb(2)-O(10)	81.0(5)
O(12)#5-Tb(2)-O(16)	74.6(5)
O(12)#5-Tb(2)-O(17)	135.7(5)
O(12A)#5-Tb(2)-O(16)	74.4(3)
O(12A)#5-Tb(2)-O(17)	138.0(3)

O(17)-Tb(2)-O(10)	72.7(6)
O(17)-Tb(2)-O(16)	125.8(5)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z+1 #2 -x,-y+1,-z+1 #3 -x+1,-y+1,-z+2
#4 -x+2,-y+1,-z+2 #5 -x+1,-y+2,-z+2 #6 x,y+1,z

Table S7. Selected hydrogen-bond parameters for compound **1**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(5)-H(5B)...Cl(2)#5	0.96	2.60	3.086(3)	111.3
O(6)-H(6A)...Cl(1)	0.96	2.28	3.193(3)	158.1
O(6)-H(6B)...Cl(2)	0.96	2.23	3.183(3)	173.6
O(7)-H(7A)...O(9)#6	0.96	2.38	3.210(3)	144.4
O(7)-H(7A)...O(10)#6	0.96	2.32	3.06(3)	133.3
O(7)-H(7B)...Cl(2)#7	0.96	2.19	3.074(3)	153.3
O(8)-H(8A)...Cl(1)#8	0.96	2.16	3.089(3)	162.2
O(8)-H(8B)...Cl(1)#5	0.96	2.19	3.129(3)	165.1
C(3)-H(3)...Cl(2)#9	0.93	2.90	3.487(3)	122.5
C(4)-H(4)...O(1)#10	0.93	2.54	3.370(4)	148.0
C(4)-H(4)...O(6)#11	0.93	2.67	3.352(4)	130.3
O(9)-H(9B)...N(1)#12	0.96	2.58	3.267(2)	128.2
O(10)-H(10A)...N(2)	0.96	2.66	3.44(2)	137.8
O(10)-H(10B)...O(10)#12	0.96	1.06	1.97(4)	155.1

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y-2,-z+1 #2 x,y-1,z #3 -x,-y-1,-z+1

#4 x,y+1,z #5 -x-1,-y-2,-z #6 x,y-1,z-1 #7 -x-1,-y-3,-z

#8 x+1,y,z #9 x,y+1,z+1 #10 -x-1,-y-1,-z+1

#11 -x-1,-y-2,-z+1 #12 -x,-y-1,-z+2

Table S8. Selected hydrogen-bond parameters for compound **2**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(5)-H(5A)...Br(1)	0.86	2.55	3.275(8)	142.3
O(5)-H(5B)...O(3)	0.86	2.37	2.847(10)	115.3
C(3)-H(3)...O(4)#4	0.93	2.92	3.408(13)	114.6
C(3)-H(3)...O(4)#7	0.93	2.92	3.408(13)	114.6
C(4)-H(4)...O(1)#8	0.93	2.57	3.327(14)	138.5
C(4)-H(4)...O(2)#9	0.93	2.88	3.473(14)	123.1
C(4)-H(4)...O(5)#10	0.93	2.61	3.471(14)	154.4
C(5)-H(5)...O(2)#3	0.93	2.69	3.158(16)	112.1

C(5)-H(5)...O(2)#2	0.93	2.69	3.158(16)	112.1
C(5)-H(5)...O(3)#11	0.93	2.68	3.398(19)	135.0

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,z #2 -x+1,-y+1,-z+1 #3 x,-y+1,-z+1

#4 -x+1,y+1/2,-z+1/2 #5 x,-y+2,-z+1 #6 x,y-1/2,-z+1/2

#7 -x+1,-y+3/2,z+1/2 #8 -x+3/2,-y+3/2,-z+1 #9 -x+3/2,y+1/2,z

#10 x+1/2,-y+3/2,-z+1 #11 -x+1,y-1/2,-z+1/2

Table S9. Selected hydrogen-bond parameters for compound **3**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(13)-H(13A)...O(3)	0.86	2.35	2.81(2)	113.7
O(13)-H(13A)...O(3A)	0.86	1.50	2.09(4)	121.8
O(14)-H(14B)...O(1)#1	0.91	2.62	3.35(3)	137.9
O(14)-H(14B)...Br(3)#7	0.91	2.68	3.309(16)	127.2
O(15)-H(15A)...O(4)#2	0.87	1.90	2.76(2)	174.5
O(15)-H(15A)...O(4A)#2	0.87	1.91	2.77(6)	171.2
O(15)-H(15B)...O(1)#1	0.87	2.04	2.64(3)	125.5
O(15)-H(15B)...O(1A)#1	0.87	2.23	2.71(6)	114.7
O(16)-H(16A)...O(8)	0.85	2.21	2.74(4)	120.6
O(16)-H(16A)...O(8A)	0.85	2.21	2.73(17)	119.9
O(16)-H(16A)...O(19)#8	0.85	2.72	3.38(3)	135.8
O(16)-H(16B)...Br(3)	0.91	2.75	3.348(14)	124.7
O(17)-H(17A)...O(9)	0.86	2.49	2.97(2)	115.7
O(17)-H(17A)...O(9A)	0.86	2.30	2.803(14)	117.4
O(17)-H(17A)...O(16)#4	0.86	2.12	2.786(19)	133.6
O(17)-H(17A)...O(19)#3	0.86	2.28	2.80(3)	119.5
O(17)-H(17B)...O(11)#9	0.86	2.37	2.90(2)	119.9
O(17)-H(17B)...O(11A)#9	0.86	2.48	3.01(5)	120.3
O(17)-H(17B)...O(22)#3	0.86	2.48	3.27(2)	153.2
O(18)-H(18B)...O(3)#1	0.88	2.11	2.82(2)	136.7
C(5)-H(5)...O(18)#10	0.93	2.39	3.10(2)	133.3
C(3)-H(3)...O(20)#9	0.93	3.01	3.45(3)	110.8
C(2)-H(2A)...O(3)#11	0.97	2.40	3.29(3)	151.6
C(2A)-H(2AA)...O(3A)#11	0.97	2.70	3.38(8)	127.4
C(5A)-H(5A)...O(2A)#11	0.93	2.44	3.15(9)	132.6

C(5A)-H(5A)...O(18)#10	0.93	2.77	3.27(7)	114.7
C(6A)-H(6AA)...O(15)#2	0.97	2.83	3.41(5)	119.8
C(6A)-H(6AB)...O(1A)#11	0.97	2.25	3.04(9)	137.7
C(6A)-H(6AB)...O(2A)#11	0.97	2.40	3.28(9)	149.8
C(6A)-H(6AB)...O(5A)#10	0.97	2.73	3.30(6)	118.2
C(9)-H(9A)...O(1)#12	0.97	2.40	3.32(4)	157.7
C(9)-H(9B)...O(14)#2	0.97	2.58	3.33(3)	133.9
C(9)-H(9B)...O(23)	0.97	2.97	3.43(4)	110.5
C(9A)-H(9AB)...O(14)#2	0.97	2.31	3.07(7)	135.3
C(9A)-H(9AB)...O(23)	0.97	2.69	3.25(11)	117.2
C(10A)-H(10A)...O(23)	0.93	2.78	3.44(7)	128.7
C(12)-H(12)...O(1)#12	0.93	2.62	3.34(3)	134.4
C(13)-H(13D)...O(19)#8	0.97	2.58	3.08(3)	112.4
C(13)-H(13D)...O(23)#8	0.97	2.52	3.19(3)	125.8
C(13A)-H(13F)...O(23)#8	0.97	2.68	3.29(7)	121.6
C(16)-H(16C)...O(11)#13	0.97	2.65	3.41(4)	135.1
C(16)-H(16C)...O(22)#8	0.97	2.63	3.19(3)	116.7
C(16)-H(16D)...O(8)#4	0.97	2.86	3.43(3)	118.9
C(16)-H(16D)...O(19)#3	0.97	2.46	3.14(3)	126.3
C(16A)-H(16E)...O(11A)#13	0.97	2.15	2.69(7)	113.2
C(16A)-H(16E)...O(22)#8	0.97	2.06	2.75(8)	126.2
C(19)-H(19)...O(22)#8	0.93	2.66	3.38(3)	135.5
C(19A)-H(19A)...O(22)#8	0.93	2.80	3.39(5)	122.2
O(19)-H(19B)...O(8)#10	0.85	2.11	2.94(3)	165.8
O(19)-H(19B)...O(8A)#10	0.85	2.24	3.06(11)	162.8
O(19)-H(19B)...O(9)#3	0.85	2.81	3.33(3)	120.8
O(19)-H(19B)...O(9A)#3	0.85	2.66	3.18(2)	120.2
O(19)-H(19B)...O(16)#10	0.85	2.95	3.38(3)	113.6
O(19)-H(19C)...O(23)	0.83	2.00	2.82(3)	168.6
O(20)-H(20E)...Br(1)#6	0.85	2.50	3.27(2)	150.9
O(20)-H(20F)...O(22)	0.91	2.58	3.42(3)	154.4
O(21)-H(21A)...Br(3)	0.85	2.69	3.43(2)	146.4
O(21)-H(21B)...O(20)	0.85	2.45	2.87(3)	110.8
O(21)-H(21B)...O(22)	0.85	2.97	3.50(3)	122.8
O(22)-H(22A)...O(11)#5	0.85	2.26	2.96(2)	139.9
O(22)-H(22A)...O(11A)#5	0.85	2.23	2.88(4)	133.3
O(22)-H(22B)...N(5A)#10	0.85	2.83	3.50(5)	136.5
O(23)-H(23A)...O(4)	0.95	2.96	3.50(3)	117.4

O(23)-H(23A)...O(4A)	0.95	2.61	3.12(5)	114.6
O(23)-H(23B)...Br(1)	0.86	2.54	3.29(2)	145.3

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z+1 #2 -x,-y+1,-z+1 #3 -x+1,-y+1,-z+2

#4 -x+2,-y+1,-z+2 #5 -x+1,-y+2,-z+2 #6 x,y+1,z

#7 -x+1,-y+1,-z+1 #8 x+1,y,z #9 x,y-1,z #10 x-1,y,z

#11 -x-1,-y,-z+1 #12 x+1,y+1,z #13 -x+2,-y+2,-z+2

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