Supporting Information

Rationally assembled nonanuclear lanthanide clusters: Dy_9 displays slow relaxation of magnetization and Tb_9 serves as luminescent sensor for Fe^{3+}, CrO_4^{2-} and $Cr_2O_7^{2-}$

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Content

1. ^{1}H, ^{13}C NMR and FT-IR spectra of H_2L

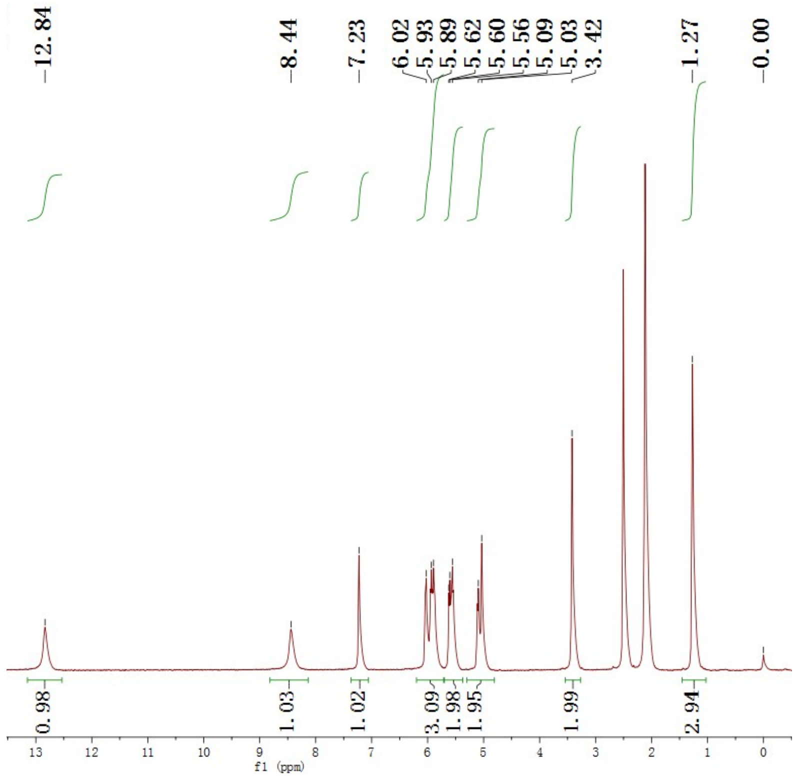


Figure S1. ^{1}H NMR spectrum of H_2L.

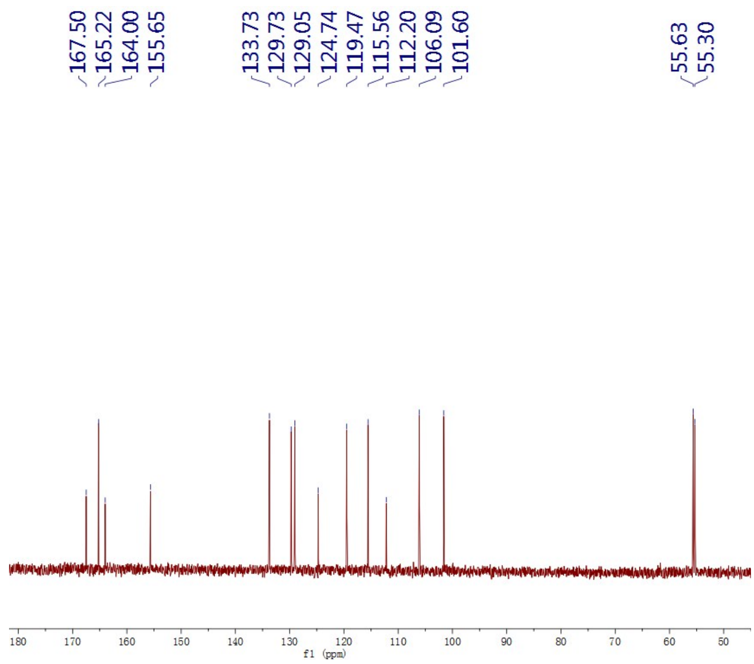


Figure S2. ^{13}C NMR spectrum of H_2L.

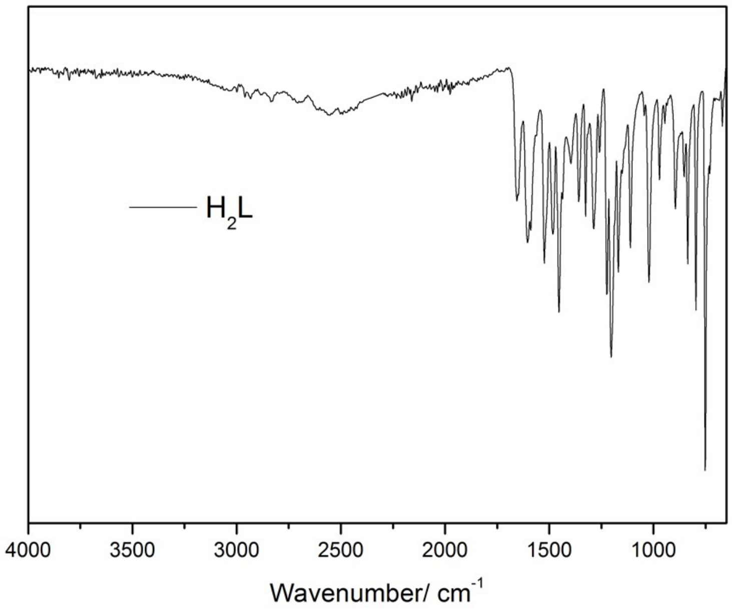


Figure S3. FT-IR spectrum of H_2L.

2. Selected bond length and angles for five complexes

Table S1. Selected bond length (Å) for **1-5**

Atom	Atom	Length/Å	Atom	Atom	Length/Å	Atom	Atom	Length/Å

Atom	Atom	Length/Å	Atom	Atom	Length/Å	Atom	Atom	Length/Å
Complex **1**								
Eu1	Eu2	3.7255(10)	Eu2	O2	2.255(8)	Eu3	O9	2.6139(14)
Eu1	Eu2^{1}	3.7255(10)	Eu2	O3	2.418(10)	Eu3	O11	2.440(8)
Eu1	O7	2.834(15)	Eu2	O7	2.6041(13)	Eu3	O11^{3}	2.374(9)
Eu1	O8	2.448(8)	Eu2	O10^{2}	2.333(8)	Eu3	N1	2.576(11)
Eu1	O8^{2}	2.448(8)	Eu2	O10	2.365(8)	O7	Eu2^{2}	2.6042(12)
Eu1	O8^{1}	2.448(8)	Eu2	O12	2.378(8)	O7	Eu2^{3}	2.6042(12)
Eu1	O8^{3}	2.448(8)	Eu2	O12^{3}	2.439(8)	O7	Eu2^{1}	2.6042(12)
Eu1	O9	2.844(17)	Eu2	N3	2.586(12)	O8	Eu3^{2}	2.339(8)
Eu1	O10^{3}	2.452(8)	Eu3	Eu3^{3}	3.6878(9)	O9	Eu3^{2}	2.6139(13)
Eu1	O10^{1}	2.452(8)	Eu3	Eu3^{2}	3.6879(9)	O9	Eu3^{3}	2.6139(13)
Eu1	O10^{2}	2.452(8)	Eu3	O1	2.261(9)	O9	Eu3^{1}	2.6139(13)
Eu1	O10	2.452(8)	Eu3	O4	2.408(10)	O10	Eu2^{3}	2.333(8)
Eu2	Eu2^{2}	3.6754(9)	Eu3	O8^{3}	2.339(8)	O11	Eu3^{2}	2.374(8)
Eu2	Eu2^{3}	3.6755(9)	Eu3	O8	2.367(8)	O12	Eu2^{2}	2.439(8)

^{1}3/2-X,3/2-Y,+Z; ^{2}+Y,3/2-X,+Z; ^{3}3/2-Y,+X,+Z

Atom	Atom	Length/Å	Atom	Atom	Length/Å	Atom	Atom	Length/Å
Complex **3**								
Tb1	Tb2^{1}	3.6467(5)	Tb2	O1	2.5427(7)	Tb3	O6^{2}	2.394(5)
Tb1	Tb2	3.6466(5)	Tb2	O2	2.262(5)	Tb3	O8	2.226(5)
Tb1	O1	2.784(8)	Tb2	O2^{1}	2.315(5)	Tb3	O10	2.348(7)
Tb1	O2^{2}	2.405(5)	Tb2	O5	2.313(5)	Tb3	N2	2.548(6)
Tb1	O2^{1}	2.405(5)	Tb2	O5^{1}	2.413(5)	O1	Tb2^{2}	2.5427(6)
Tb1	O2^{3}	2.405(5)	Tb2	O7	2.220(5)	O1	Tb2^{1}	2.5427(6)
Tb1	O2	2.406(5)	Tb2	O9	2.353(5)	O1	Tb2^{3}	2.5427(6)
Tb1	O3^{3}	2.408(5)	Tb2	N1	2.551(6)	O2	Tb2^{2}	2.315(5)
Tb1	O3^{1}	2.408(5)	Tb3	Tb3^{2}	3.5779(5)	O3	Tb3^{2}	2.259(5)
Tb1	O3	2.408(5)	Tb3	Tb3^{1}	3.5779(4)	O4	Tb3^{1}	2.5375(8)
Tb1	O3^{2}	2.408(5)	Tb3	O3^{1}	2.259(5)	O4	Tb3^{3}	2.5375(8)
Tb1	O4	2.826(9)	Tb3	O3	2.310(5)	O4	Tb3^{2}	2.5375(8)
Tb2	Tb2^{2}	3.5883(4)	Tb3	O4	2.5374(8)	O5	Tb2^{2}	2.413(5)
Tb2	Tb2^{1}	3.5884(4)	Tb3	O6	2.309(5)	O6	Tb3^{1}	2.394(5)

^{1}3/2-Y,+X,+Z; ^{2}+Y,3/2-X,+Z; ^{3}3/2-X,3/2-Y,+Z

Atom	Atom	Length/Å	Atom	Atom	Length/Å	Atom	Atom	Length/Å
Complex **2**								
Gd1	O1	2.800(16)	Gd2	O9	2.413(11)	O1	Gd2^{1}	2.5881(11)
Gd1	O2^{3}	2.442(9)	Gd2	N3	2.606(12)	O2	Gd1^{2}	2.442(9)
Gd1	O2	2.442(9)	Gd3	Gd1^{1}	3.7096(11)	O2	Gd1^{3}	2.442(9)
Gd1	O2^{2}	2.442(9)	Gd3	Gd1^{2}	3.7096(11)	O2	Gd1^{1}	2.442(9)
Gd1	O2^{1}	2.442(9)	Gd3	Gd1^{3}	3.7096(11)	O2	Gd3^{1}	2.359(9)
Gd1	O3^{2}	2.446(9)	Gd3	O2^{2}	2.359(9)	O3	Gd1^{1}	2.446(9)
Gd1	O3^{3}	2.446(9)	Gd3	O2	2.330(10)	O3	Gd1^{3}	2.446(9)
Gd1	O3	2.446(9)	Gd3	O4	2.5986(16)	O3	Gd1^{2}	2.446(9)
Gd1	O3^{1}	2.446(9)	Gd3	O5	2.369(10)	O3	Gd2^{2}	2.349(9)
Gd2	Gd1^{1}	3.7097(11)	Gd3	O5^{2}	2.428(9)	O4	Gd1^{2}	2.83(2)
Gd2	Gd1^{2}	3.7097(11)	Gd3	O7	2.257(10)	O4	Gd1^{3}	2.83(2)
Gd2	Gd1^{3}	3.7097(11)	Gd3	O10	2.396(11)	O4	Gd1^{1}	2.83(2)
Gd2	O1	2.5881(12)	Gd3	N1	2.584(11)	O4	Gd3^{3}	2.5986(15)
Gd2	O3	2.349(9)	O1	Gd1^{1}	2.800(16)	O4	Gd3^{2}	2.5986(15)
Gd2	O3	2.319(9)	O1	Gd1^{2}	2.800(16)	O4	Gd3^{1}	2.5986(15)
Gd2	O6^{1}	2.428(9)	O1	Gd1^{3}	2.800(16)	O5	Gd3^{1}	2.428(9)
Gd2	O6	2.368(9)	O1	Gd2^{2}	2.5881(11)	O6	Gd2^{2}	2.428(9)
Gd2	O8	2.262(10)	O1	Gd2^{3}	2.5881(11)			

^{1}+Y,3/2-X,+Z; ^{2}3/2-Y,+X,+Z; ^{3}3/2-X,3/2-Y,+Z

Atom	Atom	Length/Å	Atom	Atom	Length/Å	Atom	Atom	Length/Å
Complex **4**								
Dy1	Dy2^{1}	3.6759(6)	Dy2	O1^{1}	2.335(5)	Dy3	O7	2.243(5)
Dy1	Dy2^{2}	3.6759(6)	Dy2	O1	2.300(5)	Dy3	O8	2.246(6)
Dy1	O1	2.421(5)	Dy2	O2	2.5690(8)	Dy3	O9	2.380(6)
Dy1	O1^{2}	2.421(5)	Dy2	O5^{1}	2.423(5)	Dy3	N2	2.570(7)
Dy1	O1^{1}	2.421(5)	Dy2	O5	2.343(5)	O1	Dy2^{3}	2.335(5)
Dy1	O1^{3}	2.421(5)	Dy2	O6	2.243(6)	O2	Dy2^{2}	2.5690(8)
Dy1	O2	2.806(11)	Dy2	O10	2.379(6)	O2	Dy2^{3}	2.5690(8)
Dy1	O3^{3}	2.421(5)	Dy2	N1	2.567(7)	O2	Dy2^{1}	2.5690(8)
Dy1	O3^{2}	2.421(5)	Dy3	Dy3^{3}	3.6135(5)	O3	Dy3^{3}	2.296(5)
Dy1	O3	2.421(5)	Dy3	Dy3^{1}	3.6136(5)	O4	Dy3^{3}	2.5611(8)
Dy1	O3^{1}	2.421(5)	Dy3	O3	2.336(5)	O4	Dy3^{1}	2.5611(8)
Dy1	O4	2.818(11)	Dy3	O3^{1}	2.296(5)	O4	Dy3^{2}	2.5611(8)
Dy2	Dy2^{1}	3.6250(5)	Dy3	O4	2.5611(8)	O5	Dy2^{3}	2.423(5)
Dy2	Dy2^{3}	3.6250(5)	Dy3	O7^{3}	2.408(6)	O7	Dy3^{1}	2.408(5)

^{1}+Y,3/2-X,+Z; ^{2}3/2-X,3/2-Y,+Z; ^{3}3/2-Y,+X,+Z

Atom	Atom	Length/Å	Atom	Atom	Length/Å	Atom	Atom	Length/Å
Complex **5**								
Ho1	Ho1^{1}	3.6083(6)	Ho2	O10	2.822(10)	Ho3	N2	2.555(8)
Ho1	Ho1^{2}	3.6083(6)	Ho2	O11	2.406(6)	O3	Ho3^{1}	2.399(6)
Ho1	O5^{2}	2.244(6)	Ho2	O11^{3}	2.406(6)	O5	Ho1^{1}	2.244(6)
Ho1	O6^{2}	2.331(6)	Ho2	O11^{1}	2.406(6)	O6	Ho1^{1}	2.331(6)
Ho1	O6	2.415(6)	Ho2	O11^{2}	2.406(6)	O9	Ho3^{1}	2.324(6)
Ho1	O7	2.357(7)	Ho2	O12	2.776(11)	O10	Ho3^{2}	2.5510(9)
Ho1	O11	2.333(6)	Ho3	Ho3^{2}	3.5980(6)	O10	Ho3^{1}	2.5511(9)
Ho1	O11^{2}	2.281(6)	Ho3	O2	2.233(6)	O10	Ho3^{3}	2.5510(9)
Ho1	O12	2.5556(8)	Ho3	O3	2.308(6)	O11	Ho1^{1}	2.281(6)
Ho1	N3^{2}	2.545(8)	Ho3	O3^{2}	2.399(6)	O12	Ho1^{1}	2.5556(8)

Atom	Atom	Length/Å	Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ho2	O9[3]	2.426(6)	Ho3	O8	2.361(7)	O12	Ho1[3]	2.5556(8)
Ho2	O9	2.426(6)	Ho3	O9	2.289(6)	O12	Ho1[2]	2.5556(8)
Ho2	O9[2]	2.426(6)	Ho3	O9[2]	2.324(6)	N3	Ho1[1]	2.545(8)
Ho2	O9[1]	2.426(6)	Ho3	O10	2.5510(9)			

[1]1/2-Y,+X,+Z;[2]+Y,1/2-X,+Z;[3]1/2-X,1/2-Y,+Z

Table S2. Selected bond angle (°) for **1-5**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
		Complex **1**									
Eu2	Eu1	Eu2^{1}	88.47(3)	O10	Eu1	O10^{1}	119.6(4)	N3	Eu2	Eu2^{3}	177.7(3)
O7	Eu1	Eu2^{1}	44.235(16)	O10^{3}	Eu1	O10^{2}	119.6(4)	N3	Eu2	O7	133.2(3)
O7	Eu1	Eu2	44.235(16)	O10	Eu1	O10^{3}	75.35(17)	Eu3^{2}	Eu3	Eu1	60.357(9)
O7	Eu1	O9	180.0	O10	Eu1	O10^{2}	75.35(17)	Eu3^{3}	Eu3	Eu1	60.358(9)
O8	Eu1	Eu2	75.90(18)	O10^{1}	Eu1	O10^{2}	75.35(17)	Eu3^{3}	Eu3	Eu3^{2}	90.0
O8^{2}	Eu1	Eu2^{1}	112.26(19)	Eu2^{3}	Eu2	Eu1	60.444(9)	O1	Eu3	Eu1	84.3(2)
O8^{3}	Eu1	Eu2^{1}	109.89(19)	Eu2^{2}	Eu2	Eu1	60.445(9)	O1	Eu3	Eu3^{2}	110.9(2)
O8^{1}	Eu1	Eu2^{1}	75.90(18)	Eu2^{2}	Eu2	Eu2^{3}	90.001(1)	O1	Eu3	Eu3^{3}	122.8(2)
O8^{2}	Eu1	Eu2	109.89(19)	O2	Eu2	Eu1	85.9(2)	O1	Eu3	O4	84.7(3)
O8	Eu1	Eu2^{1}	164.28(18)	O2	Eu2	Eu2^{3}	110.8(2)	O1	Eu3	O8	75.9(3)
O8^{3}	Eu1	Eu2	109.89(19)	O2	Eu2	Eu2^{2}	125.0(3)	O1	Eu3	O8^{3}	85.1(3)
O8^{1}	Eu1	Eu2	164.28(19)	O2	Eu2	O3	84.0(4)	O1	Eu3	O9	133.3(4)
O8^{2}	Eu1	O7	120.11(18)	O2	Eu2	O7	134.6(4)	O1	Eu3	O11^{3}	142.2(3)
O8^{1}	Eu1	O7	120.11(18)	O2	Eu2	O10^{2}	87.1(3)	O1	Eu3	O11	127.0(3)
O8	Eu1	O7	120.11(18)	O2	Eu2	O10	76.2(3)	O1	Eu3	N1	70.9(3)
O8^{3}	Eu1	O7	120.11(18)	O2	Eu2	O12^{3}	125.5(3)	O4	Eu3	Eu1	157.3(3)
O8^{3}	Eu1	O8^{1}	75.42(16)	O2	Eu2	O12	143.2(3)	O4	Eu3	Eu3^{3}	141.3(3)
O8^{1}	Eu1	O8^{2}	75.42(16)	O2	Eu2	N3	71.5(4)	O4	Eu3	Eu3^{2}	105.7(3)
O8	Eu1	O8^{3}	75.42(16)	O3	Eu2	Eu1	159.7(3)	O4	Eu3	O9	134.7(4)
O8	Eu1	O8^{2}	75.42(16)	O3	Eu2	Eu2^{2}	139.0(3)	O4	Eu3	O11	72.4(3)
O8^{3}	Eu1	O8^{2}	119.8(4)	O3	Eu2	Eu2^{3}	107.2(3)	O4	Eu3	N1	73.1(3)
O8	Eu1	O8^{1}	119.8(4)	O3	Eu2	O7	134.7(4)	O8	Eu3	Eu1	40.06(19)
O8^{1}	Eu1	O9	59.89(18)	O3	Eu2	O12^{3}	72.8(3)	O8^{3}	Eu3	Eu1	39.9(2)
O8^{3}	Eu1	O9	59.89(18)	O3	Eu2	N3	73.1(4)	O8	Eu3	Eu3^{3}	96.6(2)
O8	Eu1	O9	59.89(18)	O7	Eu2	Eu1	49.4(4)	O8^{3}	Eu3	Eu3^{3}	38.68(19)
O8^{2}	Eu1	O9	59.89(18)	O7	Eu2	Eu2^{2}	45.12(2)	O8	Eu3	Eu3^{2}	38.14(19)
O8^{2}	Eu1	O10^{3}	142.4(3)	O7	Eu2	Eu2^{3}	45.11(2)	O8^{3}	Eu3	Eu3^{2}	96.7(2)
O8	Eu1	O10^{3}	140.3(3)	O10^{2}	Eu2	Eu1	40.0(2)	O8	Eu3	O4	117.6(3)
O8^{1}	Eu1	O10	142.4(3)	O10	Eu2	Eu1	40.2(2)	O8^{3}	Eu3	O4	157.5(3)
O8^{1}	Eu1	O10^{3}	74.7(3)	O10^{2}	Eu2	Eu2^{2}	38.8(2)	O8^{3}	Eu3	O8	79.0(4)
O8^{3}	Eu1	O10	74.7(3)	O10	Eu2	Eu2^{2}	96.8(2)	O8^{3}	Eu3	O9	64.8(3)
O8^{1}	Eu1	O10^{1}	73.3(3)	O10^{3}	Eu2	Eu2^{3}	96.9(2)	O8	Eu3	O9	64.4(3)
O8	Eu1	O10	73.3(3)	O10	Eu2	Eu2^{3}	38.2(2)	O8	Eu3	O11^{3}	129.9(3)
O8^{2}	Eu1	O10	140.3(3)	O10	Eu2	O3	119.9(4)	O8^{3}	Eu3	O11^{3}	75.7(3)
O8^{3}	Eu1	O10^{2}	142.4(3)	O10^{2}	Eu2	O3	155.9(3)	O8	Eu3	O11	74.0(3)
O8	Eu1	O10^{1}	142.4(3)	O10	Eu2	O7	64.4(3)	O8^{3}	Eu3	O11	129.2(3)

O8^{1}	Eu1	O10^{2}	140.3(3)	O10^{2}	Eu2	O7	64.8(3)	O8	Eu3	N1	143.9(3)
O8^{2}	Eu1	O10^{2}	73.3(3)	O10^{2}	Eu2	O10	79.3(4)	O8^{3}	Eu3	N1	84.5(3)
O8	Eu1	O10^{2}	74.7(3)	O10	Eu2	O12	130.2(3)	O8^{3}	Eu3	C6^{3}	93.1(3)
O9	Eu1	Eu2^{1}	135.765(16)	O10^{2}	Eu2	O12^{3}	129.7(3)	O9	Eu3	Eu1	49.6(4)
O9	Eu1	Eu2	135.765(16)	O10	Eu2	O12^{3}	74.3(3)	O9	Eu3	Eu3^{3}	45.14(3)
O10^{3}	Eu1	Eu2	94.02(19)	O10^{2}	Eu2	O12	76.0(3)	O9	Eu3	Eu3^{2}	45.13(3)
O10^{1}	Eu1	Eu2^{1}	38.5(2)	O10	Eu2	N3	143.7(3)	O11	Eu3	Eu1	98.8(2)
O10^{1}	Eu1	Eu2	93.55(19)	O10^{2}	Eu2	N3	82.9(3)	O11^{3}	Eu3	Eu1	100.1(2)
O10^{2}	Eu1	Eu2	37.7(2)	O12	Eu2	Eu1	100.4(2)	O11	Eu3	Eu3^{2}	39.34(19)
O10^{3}	Eu1	Eu2^{1}	37.7(2)	O12^{3}	Eu2	Eu1	99.2(2)	O11^{3}	Eu3	Eu3^{2}	103.5(2)
O10	Eu1	Eu2	38.5 (2)	O12^{3}	Eu2	Eu2^{2}	103.3(2)	O11^{3}	Eu3	Eu3^{3}	40.7(2)
O10^{1}	Eu1	Eu2^{1}	93.55(19)	O12^{3}	Eu2	Eu2^{3}	39.7(2)	O11	Eu3	Eu3^{3}	103.2(2)
O10^{2}	Eu1	Eu2^{1}	94.02(19)	O12	Eu2	Eu2^{2}	40.9(2)	O11^{3}	Eu3	O4	100.8(3)
O10^{3}	Eu1	O7	59.80(19)	O12	Eu2	Eu2^{3}	103.6(2)	O11	Eu3	O9	64.8(3)
O10^{1}	Eu1	O7	59.80(19)	O12	Eu2	O3	98.2(4)	O11^{3}	Eu3	O9	65.7(3)
O10^{2}	Eu1	O7	59.80(19)	O12	Eu2	O7	66.0(3)	O11^{3}	Eu3	O11	89.7(4)
O10	Eu1	O7	59.80(19)	O12^{3}	Eu2	O7	65.2(3)	O11	Eu3	N1	138.7(3)
O10^{1}	Eu1	O9	120.20(19)	O12	Eu2	O12^{3}	89.5(4)	O11^{3}	Eu3	N1	75.1(3)
O10	Eu1	O9	120.20(19)	O12	Eu2	N3	74.1(3)	N1	Eu3	Eu1	121.3(2)
O10^{2}	Eu1	O9	120.20(19)	O12^{3}	Eu2	N3	139.3(3)	N1	Eu3	Eu3^{2}	177.9(2)
O10^{3}	Eu1	O9	120.20(19)	N3	Eu2	Eu1	120.0(3)	N1	Eu3	Eu3^{3}	89.9(2)
O10	Eu1	O10^{3}	75.35(17)	N3	Eu2	Eu2^{2}	88.4(3)	N1	Eu3	O9	134.6(2)

^{1}3/2-X,3/2-Y,+Z;^{2}+Y,3/2-X,+Z;^{3}3/2-Y,+X,+Z

Complex **2**

O2^{1}	Gd1	O1	119.9(2)	O8	Gd2	Gd1^{1}	86.0(3)	Gd2^{3}	O1	Gd1^{1}	86.9(4)
O2	Gd1	O1	119.9(2)	O8	Gd2	Gd1^{3}	86.0(3)	Gd2^{2}	O1	Gd1^{3}	86.9(4)
O2^{2}	Gd1	O1	119.9(2)	O8	Gd2	O1	134.2(4)	Gd2^{3}	O1	Gd1^{3}	86.9(4)
O2^{3}	Gd1	O1	119.9(2)	O8	Gd2	O3^{1}	76.4(3)	Gd2	O1	Gd1^{2}	86.9(4)
O2	Gd1	O2^{3}	120.1(5)	O8	Gd2	O3	87.3(4)	Gd2	O1	Gd1^{3}	86.9(4)
O2^{2}	Gd1	O2^{1}	120.1(5)	O8	Gd2	O6^{1}	125.6(4)	Gd2^{2}	O1	Gd1	86.9(4)
O2^{2}	Gd1	O2	75.6(2)	O8	Gd2	O6	143.3(4)	Gd2^{2}	O1	Gd1^{2}	86.9(4)
O2^{2}	Gd1	O2^{3}	75.6(2)	O8	Gd2	O9	83.9(4)	Gd2^{1}	O1	Gd1	86.9(4)
O2^{1}	Gd1	O2^{3}	75.6(2)	O8	Gd2	N3	71.3(4)	Gd2^{1}	O1	Gd1^{3}	86.9(4)
O2	Gd1	O2^{1}	75.6(2)	O9	Gd2	Gd1^{3}	159.9(3)	Gd2	O1	Gd1	86.9(4)
O2^{1}	Gd1	O3^{2}	140.1(3)	O9	Gd2	Gd1^{2}	159.9(3)	Gd2^{1}	O1	Gd1^{2}	86.9(4)
O2^{1}	Gd1	O3^{3}	73.2(3)	O9	Gd2	Gd1^{1}	159.9(3)	Gd2^{3}	O1	Gd1^{2}	86.9(4)
O2^{1}	Gd1	O3^{1}	74.8(3)	O9	Gd2	O1	135.3(4)	Gd2^{3}	O1	Gd1	86.9(4)
O2^{3}	Gd1	O3^{2}	73.2(3)	O9	Gd2	O61	72.9(4)	Gd2^{1}	O1	Gd1^{1}	86.9(4)
O2^{2}	Gd1	O3^{1}	140.1(3)	O9	Gd2	N3	72.8(4)	Gd2	O1	Gd1^{1}	86.9(4)

$O2^{3}$	Gd1	$O3^{1}$	142.6(3)	N3	Gd2	$Gd1^{1}$	120.1(3)	$Gd2^{2}$	O1	$Gd1^{1}$	86.9(4)
O2	Gd1	$O3^{2}$	142.6(3)	N3	Gd2	$Gd1^{3}$	120.1(3)	$Gd2^{1}$	O1	$Gd2^{3}$	89.83(4)
$O2^{2}$	Gd1	$O3^{3}$	142.6(3)	N3	Gd2	$Gd1^{2}$	120.1(3)	$Gd2^{2}$	O1	$Gd2^{3}$	89.83(4)
$O2^{3}$	Gd1	$O3^{3}$	74.8(3)	$Gd1^{3}$	Gd3	$Gd1^{2}$	0.00(3)	$Gd2^{1}$	O1	Gd2	89.83(4)
$O2^{2}$	Gd1	O3	73.2(3)	$O2^{2}$	Gd3	$Gd1^{2}$	40.2(2)	Gd2	O1	$Gd2^{3}$	173.8(7)
O2	Gd1	$O3^{1}$	73.2(3)	O2	Gd3	$Gd1^{2}$	40.1(2)	$Gd2^{2}$	O1	$Gd2^{1}$	173.8(7)
O2	Gd1	O3	74.8(3)	$O2^{2}$	Gd3	$Gd1^{3}$	40.2(2)	$Gd2^{2}$	O1	Gd2	89.83(4)
$O2^{2}$	Gd1	$O3^{2}$	74.8(3)	O2	Gd3	$Gd1^{3}$	40.1(2)	Gd1	O2	$Gd1^{3}$	0.00(5)
$O2^{1}$	Gd1	O3	142.6(3)	$O2^{2}$	Gd3	$Gd1^{1}$	40.2(2)	$Gd1^{3}$	O2	$Gd1^{2}$	0.00(5)
$O2^{3}$	Gd1	O3	140.1(3)	O2	Gd3	$Gd1^{1}$	40.1(2)	Gd1	O2	$Gd1^{2}$	0.00(5)
O2	Gd1	$O3^{3}$	140.1(3)	O2	Gd3	$O2^{2}$	79.3(4)	Gd1	O2	$Gd1^{1}$	0.00(5)
$O3^{3}$	Gd1	O1	59.6(2)	O2	Gd3	O4	65.0(4)	$Gd1^{2}$	O2	$Gd1^{1}$	0.00(5)
O3	Gd1	O1	59.6(2)	$O2^{2}$	Gd3	O4	64.7(4)	$Gd1^{3}$	O2	$Gd1^{1}$	0.00(5)
$O3^{1}$	Gd1	O1	59.6(2)	$O2^{2}$	Gd3	$O5^{2}$	74.1(3)	Gd3	O2	$Gd1^{3}$	102.0(4)
$O3^{2}$	Gd1	O1	59.6(2)	$O2^{2}$	Gd3	O5	130.4(3)	$Gd3^{1}$	O2	Gd1	101.2(3)
$O3^{2}$	Gd1	O3	75.18(19)	O2	Gd3	$O5^{2}$	129.8(3)	$Gd3^{1}$	O2	$Gd1^{1}$	101.2(3)
$O3^{1}$	Gd1	O3	75.18(19)	O2	Gd3	O5	75.8(3)	$Gd3^{1}$	O2	$Gd1^{3}$	101.2(3)
$O3^{3}$	Gd1	O3	119.2(4)	O2	Gd3	O10	156.5(4)	Gd3	O2	Gd1	102.0(4)
$O3^{3}$	Gd1	$O3^{2}$	75.18(19)	$O2^{2}$	Gd3	O10	118.2(4)	Gd3	O2	$Gd1^{2}$	102.0(4)
$O3^{1}$	Gd1	$O3^{2}$	119.2(4)	$O2^{2}$	Gd3	N1	144.2(3)	$Gd3^{1}$	O2	$Gd1^{2}$	101.2(3)
$O3^{3}$	Gd1	$O3^{1}$	75.18(19)	O2	Gd3	N1	84.4(4)	Gd3	O2	$Gd1^{1}$	102.0(4)
$Gd1^{3}$	Gd2	$Gd1^{1}$	0.00(3)	O4	Gd3	$Gd1^{1}$	49.5(4)	Gd3	O2	$Gd3^{1}$	102.9(4)
O1	Gd2	$Gd1^{3}$	48.9(4)	O4	Gd3	$Gd1^{2}$	49.5(4)	Gd2	O3	$Gd1^{2}$	102.2(4)
O1	Gd2	$Gd1^{1}$	48.9(4)	O4	Gd3	$Gd1^{3}$	49.5(4)	$Gd2^{2}$	O3	$Gd1^{1}$	101.3(3)
O1	Gd2	$Gd1^{2}$	48.9(4)	O5	Gd3	$Gd1^{3}$	100.3(2)	$Gd2^{2}$	O3	$Gd1^{3}$	101.3(3)
O1	Gd2	N3	133.3(3)	O5	Gd3	$Gd1^{1}$	100.3(2)	$Gd2^{2}$	O3	$Gd1^{2}$	101.3(3)
O3	Gd2	$Gd1^{2}$	40.1(2)	$O5^{2}$	Gd3	$Gd1^{2}$	99.1(2)	Gd2	O3	$Gd1^{3}$	102.2(4)
$O3^{1}$	Gd2	$Gd1^{1}$	40.3(2)	$O5^{2}$	Gd3	$Gd1^{1}$	99.1(2)	Gd2	O3	Gd1	102.2(4)
O3	Gd2	$Gd1^{3}$	40.1(2)	O5	Gd3	$Gd1^{2}$	100.3(2)	Gd2	O3	$Gd1^{1}$	102.2(4)
O3	Gd2	Gd11	40.1(2)	$O5^{2}$	Gd3	$Gd1^{3}$	99.1(2)	$Gd2^{2}$	O3	Gd1	101.3(3)
$O3^{1}$	Gd2	$Gd1^{3}$	40.3(2)	O5	Gd3	O4	66.0(4)	Gd2	O3	$Gd2^{2}$	103.1(3)
$O3^{1}$	Gd2	$Gd1^{2}$	40.3(2)	$O5^{2}$	Gd3	O4	65.3(4)	$Gd3^{1}$	O4	$Gd1^{1}$	86.1(4)
$O3^{1}$	Gd2	O1	64.1(3)	O5	Gd3	$O5^{2}$	90.2(5)	$Gd3^{3}$	O4	$Gd1^{2}$	86.1(4)
O3	Gd2	O1	64.4(3)	O5	Gd3	O10	100.2(4)	$Gd3^{3}$	O4	$Gd1^{1}$	86.1(4)
O3	Gd2	$O3^{1}$	79.5(4)	O5	Gd3	N1	74.4(3)	$Gd3^{2}$	O4	$Gd1^{1}$	86.1(4)
$O3^{1}$	Gd2	$O6^{1}$	74.3(3)	$O5^{2}$	Gd3	N1	138.2(3)	$Gd3^{1}$	O4	$Gd1^{2}$	86.1(4)
O3	Gd2	O6	76.0(3)	O7	Gd3	$Gd1^{3}$	84.7(2)	Gd3	O4	Gd1	86.1(4)
$O3^{1}$	Gd2	O6	130.3(3)	O7	Gd3	$Gd1^{1}$	84.7(2)	$Gd3^{2}$	O4	Gd1	86.1(4)
O3	Gd2	$O6^{1}$	129.7(3)	O7	Gd3	$Gd1^{2}$	84.7(2)	$Gd3^{3}$	O4	$Gd1^{3}$	86.1(4)
$O3^{1}$	Gd2	O9	120.0(4)	O7	Gd3	$O2^{2}$	75.6(3)	Gd3	O4	$Gd1^{2}$	86.1(4)

O3	Gd2	O9	155.6(4)	O7	Gd3	O2	85.6(4)	Gd3	O4	Gd1^{3}	86.1(4)
O3	Gd2	N3	82.9(4)	O7	Gd3	O4	133.6(5)	Gd3^{2}	O4	Gd1^{2}	86.1(4)
O3^{1}	Gd2	N3	143.7(3)	O7	Gd3	O5^{2}	126.1(4)	Gd3^{1}	O4	Gd1^{3}	86.1(4)
O6^{1}	Gd2	Gd1^{3}	99.3(2)	O7	Gd3	O5	142.5(4)	Gd3^{3}	O4	Gd1	86.1(4)
O6^{1}	Gd2	Gd1^{1}	99.3(2)	O7	Gd3	O10	84.1(4)	Gd3^{1}	O4	Gd1	86.1(4)
O6	Gd2	Gd1^{3}	100.5(2)	O7	Gd3	N1	71.5(4)	Gd3	O4	Gd1^{1}	86.1(4)
O6	Gd2	Gd1^{2}	100.5(2)	O10	Gd3	Gd1^{3}	157.9(3)	Gd3^{2}	O4	Gd1^{3}	86.1(4)
O6^{1}	Gd2	Gd1^{2}	99.3(2)	O10	Gd3	Gd1^{2}	157.9(3)	Gd3^{3}	O4	Gd3^{2}	89.74(6)
O6	Gd2	Gd1^{1}	100.5(2)	O10	Gd3	Gd1^{1}	157.9(3)	Gd3	O4	Gd31	89.74(6)
O6	Gd2	O1	66.4(3)	O10	Gd3	O4	135.1(5)	Gd3^{3}	O4	Gd3	172.2(9)
O6^{1}	Gd2	O1	65.6(3)	O10	Gd3	O5^{2}	72.7(4)	Gd3	O4	Gd3^{2}	89.74(6)
O6	Gd2	O6^{1}	89.3(4)	O10	Gd3	N1	72.3(4)	Gd3^{1}	O4	Gd3^{2}	172.2(9)
O6	Gd2	O9	98.0(4)	N1	Gd3	Gd1^{2}	121.6(3)	Gd3^{3}	O4	Gd3^{1}	89.74(6)
O6	Gd2	N3	74.2(4)	N1	Gd3	Gd1^{3}	121.6(3)	Gd3	O5	Gd3^{1}	99.7(3)
O6^{1}	Gd2	N3	139.2(3)	N1	Gd3	Gd1^{1}	121.6(3)	Gd2	O6	Gd2^{2}	99.3(3)
O8	Gd2	Gd1^{2}	86.0(3)	N1	Gd3	O4	134.4(3)				

^{1}+Y,3/2-X,+Z; ^{3}3/2-X,3/2-Y,+Z; ^{2}3/2-Y,+X,+Z

Complex **3**

Tb2	Tb1	Tb2^{1}	58.946(9)	Tb2^{3}	Tb2	Tb2^{1}	90	O3	Tb3	O10	121.2(2)
O1	Tb1	Tb2	44.091(8)	O1	Tb2	Tb1	49.63(19)	O3^{1}	Tb3	O10	155.5(2)
O1	Tb1	Tb2^{1}	44.092(8)	O1	Tb2	Tb2^{3}	45.122(13)	O3	Tb3	N2	143.89(19)
O1	Tb1	O4	180	O1	Tb2	Tb2^{1}	45.121(12)	O3^{1}	Tb3	N2	83.5(2)
O2^{2}	Tb1	Tb2^{1}	38.52(11)	O1	Tb2	N1	134.34(15)	O4	Tb3	Tb1	50.5(2)
O2^{3}	Tb1	Tb2^{1}	93.68(12)	O2	Tb2	Tb1	40.05(12)	O4	Tb3	Tb3^{3}	45.169(16)
O2^{1}	Tb1	Tb2^{1}	37.23(11)	O2^{1}	Tb2	Tb1	40.33(12)	O4	Tb3	Tb3^{1}	45.171(17)
O2	Tb1	Tb2^{1}	92.88(12)	O2	Tb2	Tb2^{3}	38.90(12)	O4	Tb3	N2	133.94(15)
O2^{3}	Tb1	Tb2	92.88(12)	O2^{1}	Tb2	Tb2^{3}	96.83(12)	O6	Tb3	Tb1	101.09(12)
O2^{1}	Tb1	Tb2	38.53(11)	O2^{1}	Tb2	Tb2^{1}	37.84(12)	O6^{3}	Tb3	Tb1	99.35(11)
O2	Tb1	Tb2	37.22(11)	O2	Tb2	Tb2^{1}	96.99(13)	O6^{3}	Tb3	Tb3^{1}	103.04(12)
O2^{2}	Tb1	Tb2	93.68(12)	O21	Tb2	O1	64.26(18)	O6	Tb3	Tb3^{1}	41.36(12)
O2	Tb1	O1	59.36(12)	O2	Tb2	O1	64.96(19)	O6	Tb3	Tb3^{3}	103.53(13)
O2^{1}	Tb1	O1	59.36(12)	O2	Tb2	O2^{1}	79.5(2)	O6^{3}	Tb3	Tb3^{3}	39.59(11)
O2^{3}	Tb1	O1	59.36(12)	O2	Tb2	O5	76.89(16)	O6	Tb3	O3	130.32(18)
O2^{2}	Tb1	O1	59.36(12)	O2^{1}	Tb2	O5^{1}	73.95(16)	O6^{3}	Tb3	O4	64.53(17)
O2^{1}	Tb1	O2^{3}	118.7(2)	O2	Tb2	O5^{1}	129.48(17)	O6	Tb3	O4	65.69(18)
O2^{2}	Tb1	O2	118.7(2)	O2^{1}	Tb2	O9	118.22(19)	O6	Tb3	O6^{3}	88.9(2)
O2^{1}	Tb1	O2	74.94(11)	O2	Tb2	O9	156.78(18)	O6	Tb3	O10	95.8(2)
O2^{1}	Tb1	O2^{2}	74.95(11)	O2^{1}	Tb2	N1	144.47(18)	O6^{3}	Tb3	N2	139.00(18)
O2^{3}	Tb1	O2^{2}	74.95(11)	O2	Tb2	N1	84.21(19)	O6	Tb3	N2	74.84(19)
O2^{3}	Tb1	O2	74.95(11)	O5^{1}	Tb2	Tb1	99.18(11)	O8	Tb3	Tb1	86.05(13)

O2^{2}	Tb1	O3^{1}	139.67(16)	O5	Tb2	Tb1	101.21(11)	O8	Tb3	Tb3^{3}	109.55(13)
O2^{2}	Tb1	O3	143.55(16)	O5	Tb2	Tb2^{3}	41.66(11)	O8	Tb3	Tb3^{1}	126.66(14)
O2^{2}	Tb1	O3^{3}	76.20(16)	O5^{1}	Tb2	Tb2^{3}	102.98(12)	O8	Tb3	O3	75.68(18)
O2	Tb1	O3^{1}	76.20(16)	O5	Tb2	Tb2^{1}	103.55(12)	O8	Tb3	O3^{1}	88.49(18)
O2^{1}	Tb1	O3^{3}	143.55(16)	O5^{1}	Tb2	Tb2^{1}	39.58(11)	O8	Tb3	O4	135.5(2)
O2^{1}	Tb1	O3^{2}	76.20(16)	O5	Tb2	O1	66.28(17)	O8	Tb3	O6	145.12(18)
O2	Tb1	O3^{2}	143.55(16)	O5^{1}	Tb2	O1	64.91(16)	O8	Tb3	O6^{3}	123.90(18)
O2^{3}	Tb1	O3^{2}	139.67(16)	O5	Tb2	O2^{1}	130.40(17)	O8	Tb^{3}	O10	84.7(2)
O2	Tb1	O3	73.71(17)	O5	Tb2	O5^{1}	88.7(2)	O8	Tb3	N2	72.23(19)
O2^{1}	Tb1	O3^{1}	73.70(17)	O5	Tb2	O9	98.89(19)	O10	Tb3	Tb1	161.19(18)
O2^{3}	Tb1	O3^{3}	73.70(17)	O5	Tb2	N1	74.77(18)	O10	Tb3	Tb3^{1}	137.09(19)
O2^{2}	Tb1	O3^{2}	73.70(17)	O5^{1}	Tb2	N1	138.36(17)	O10	Tb3	Tb3^{3}	107.48(16)
O2	Tb1	O3^{3}	139.67(16)	O7	Tb2	Tb1	85.19(12)	O10	Tb3	O4	132.9(3)
O2^{3}	Tb1	O3^{1}	143.55(16)	O7	Tb2	Tb2^{3}	125.16(13)	O10	Tb3	O6^{3}	72.7(2)
O2^{3}	Tb1	O3	76.20(16)	O7	Tb2	Tb2^{1}	109.84(13)	O10	Tb3	N2	71.9(2)
O2^{1}	Tb1	O3	139.67(16)	O7	Tb2	O1	134.0(2)	N2	Tb3	Tb1	120.39(14)
O2^{3}	Tb1	O4	120.64(12)	O7	Tb2	O2	87.06(18)	N2	Tb3	Tb3^{3}	178.13(14)
O2	Tb1	O4	120.64(12)	O7	Tb2	O2^{1}	75.64(17)	N2	Tb3	Tb3^{1}	89.31(15)
O2^{2}	Tb1	O4	120.64(12)	O7	Tb2	O5	144.43(18)	Tb2^{3}	O1	Tb1	86.28(19)
O2^{1}	Tb1	O4	120.64(12)	O7	Tb2	O5^{1}	125.15(18)	Tb2^{1}	O1	Tb1	86.28(19)
O3^{2}	Tb1	Tb2^{1}	76.89(12)	O7	Tb2	O9	83.54(19)	Tb2	O1	Tb1	86.28(19)
O3^{3}	Tb1	Tb2^{1}	113.76(11)	O7	Tb2	N1	72.15(19)	Tb2^{2}	O1	Tb1	86.28(19)
O3^{1}	Tb1	Tb2^{1}	109.59(12)	O9	Tb2	Tb1	158.08(15)	Tb2^{2}	O1	Tb2^{1}	89.76(2)
O3^{2}	Tb1	Tb2	113.77(12)	O9	Tb2	Tb2^{1}	106.16(13)	Tb2	O1	Tb2^{1}	89.76(2)
O3^{1}	Tb1	Tb2	76.89(12)	O9	Tb2	Tb2^{3}	140.44(15)	Tb2	O1	Tb2^{3}	89.76(2)
O3	Tb1	Tb2	109.59(12)	O9	Tb2	O1	134.7(2)	Tb2	O1	Tb2^{2}	172.6(4)
O3	Tb1	Tb2^{1}	164.81(12)	O9	Tb2	O5^{1}	72.54(17)	Tb2^{2}	O1	Tb2^{3}	89.76(2)
O3^{3}	Tb1	Tb2	164.80(12)	O9	Tb2	N1	72.71(19)	Tb2^{3}	O1	Tb2^{1}	172.6(4)
O3^{1}	Tb1	O1	120.93(12)	N1	Tb2	Tb1	121.19(13)	Tb2	O2	Tb1	102.72(19)
O3^{3}	Tb1	O1	120.93(12)	N1	Tb2	Tb2^{3}	89.71(14)	Tb2^{3}	O2	Tb1	101.14(18)
O3	Tb1	O1	120.93(12)	N1	Tb2	Tb2^{1}	177.69(13)	Tb2	O2	Tb2^{3}	103.26(18)
O3^{2}	Tb1	O1	120.93(12)	Tb3^{3}	Tb3	Tb1	60.650(5)	Tb3	O3	Tb1	101.36(19)
O3^{3}	Tb1	O3^{2}	74.69(11)	Tb3^{1}	Tb3	Tb1	60.651(5)	Tb3^{3}	O3	Tb1	102.9(2)
O3	Tb1	O3^{1}	74.69(11)	Tb3^{1}	Tb3	Tb3^{3}	90.001(1)	Tb3^{3}	O3	Tb3	103.09(19)
O3^{1}	Tb1	O3^{2}	74.69(11)	O3	Tb3	Tb1	40.29(12)	Tb3^{1}	O4	Tb1	85.6(2)
O3^{3}	Tb1	O3^{1}	118.1(2)	O3^{1}	Tb3	Tb1	40.02(13)	Tb3	O4	Tb1	85.6(2)
O3	Tb1	O3^{2}	118.1(2)	O3	Tb3	Tb3^{1}	96.87(13)	Tb3^{3}	O4	Tb1	85.6(2)
O3	Tb1	O3^{3}	74.68(11)	O3^{1}	Tb3	Tb3^{1}	38.96(12)	Tb3^{2}	O4	Tb1	85.6(2)
O3^{2}	Tb1	O4	59.07(12)	O3^{1}	Tb3	Tb3^{3}	97.02(13)	Tb3^{1}	O4	Tb3^{2}	89.66(3)
O3	Tb1	O4	59.07(12)	O3	Tb3	Tb3^{3}	37.96(12)	Tb3	O4	Tb3^{2}	171.2(4)

O3^{3}	Tb1	O4	59.07(12)	O3^{1}	Tb3	O3	79.5(2)	Tb3^{1}	O4	Tb3^{3}	171.2(4)
O3^{1}	Tb1	O4	59.07(12)	O3	Tb3	O4	64.8(2)	Tb3^{3}	O4	Tb3^{2}	89.66(3)
O4	Tb1	Tb2	135.909(8)	O3^{1}	Tb3	O4	65.5(2)	Tb3	O4	Tb3^{1}	89.66(3)
O4	Tb1	Tb2^{1}	135.908(8)	O3	Tb3	O6^{3}	74.04(16)	Tb3	O4	Tb3^{3}	89.66(3)
Tb2^{3}	Tb2	Tb1	60.528(5)	O3^{1}	Tb3	O6^{3}	129.59(18)	Tb2	O5	Tb2^{3}	98.77(16)
Tb2^{1}	Tb2	Tb1	60.528(5)	O3^{1}	Tb3	O6	76.64(17)	Tb3	O6	Tb3^{1}	99.04(17)

^{1}3/2-Y,+X,+Z;^{2}3/2-X,3/2-Y,+Z;^{3}+Y,3/2-X,+Z

Complex **4**

Dy2^{1}	Dy1	Dy2^{2}	59.084(11)	Dy2^{1}	Dy2	Dy2^{3}	89.998(1)	O3	Dy3	O7	130.38(19)
O1	Dy1	Dy2^{2}	94.01(13)	O1	Dy2	Dy1	40.07(13)	O3^{1}	Dy3	O9	155.8(2)
O1^{3}	Dy1	Dy2^{2}	38.54(13)	O1^{1}	Dy2	Dy1	40.25(13)	O3	Dy3	O9	120.5(2)
O1^{2}	Dy1	Dy2^{1}	38.54(12)	O1^{1}	Dy2	Dy2^{1}	38.19(12)	O3^{1}	Dy3	N2	83.3(2)
O1^{1}	Dy1	Dy2^{2}	93.48(12)	O1	Dy2	Dy2^{1}	96.99(13)	O3	Dy3	N2	143.4(2)
O1	Dy1	Dy2^{1}	93.48(12)	O1	Dy2	Dy2^{3}	38.89(13)	O4	Dy3	Dy1	49.9(2)
O1^{1}	Dy1	Dy2^{1}	37.69(12)	O1^{1}	Dy2	Dy2^{3}	96.88(13)	O4	Dy3	Dy3^{1}	45.133(18)
O1^{2}	Dy1	Dy2^{2}	37.69(12)	O1	Dy2	O1^{1}	79.4(2)	O4	Dy3	Dy3^{3}	45.134(18)
O1^{3}	Dy1	Dy2^{1}	94.01(13)	O1	Dy2	O2	65.0(2)	O4	Dy3	N2	133.89(16)
O1^{2}	Dy1	O1^{1}	75.33(11)	O1^{1}	Dy2	O2	64.6(2)	O7	Dy3	Dy1	100.77(13)
O1	Dy1	O1^{1}	75.33(11)	O1	Dy2	O5^{1}	129.54(19)	O7^{3}	Dy3	Dy1	99.48(13)
O1	Dy1	O1^{2}	119.6(2)	O11	Dy2	O5^{1}	74.35(18)	O7	Dy3	Dy3^{3}	103.44(14)
O1	Dy1	O1^{3}	75.33(11)	O1	Dy2	O5	76.55(19)	O7	Dy3	Dy3^{1}	41.15(13)
O1^{1}	Dy1	O1^{3}	119.6(2)	O11	Dy2	O5	130.37(19)	O7^{3}	Dy3	Dy3^{3}	39.83(13)
O1^{2}	Dy1	O1^{3}	75.33(11)	O11	Dy2	O10	117.9(2)	O7^{3}	Dy3	Dy3^{1}	103.07(14)
O1^{2}	Dy1	O2	59.78(12)	O1	Dy2	O10	156.9(2)	O7	Dy3	O4	65.8(2)
O1	Dy1	O2	59.78(12)	O1	Dy2	N1	84.4(2)	O7^{3}	Dy3	O4	65.0(2)
O1^{1}	Dy1	O2	59.78(12)	O1^{1}	Dy2	N1	144.2(2)	O7	Dy3	O7^{3}	88.8(3)
O1^{3}	Dy1	O2	59.78(12)	O2	Dy2	Dy1	49.6(2)	O7	Dy3	O9	96.8(2)
O1^{2}	Dy1	O3^{3}	142.95(18)	O2	Dy2	Dy2^{1}	45.127(17)	O7	Dy3	N2	74.9(2)
O1^{1}	Dy1	O3^{3}	139.86(17)	O2	Dy2	Dy2^{3}	45.126(17)	O7^{3}	Dy3	N2	139.0(2)
O1	Dy1	O3^{3}	73.17(17)	O5^{1}	Dy2	Dy1	99.17(13)	O8	Dy3	Dy1	85.73(15)
O1^{3}	Dy1	O3^{2}	73.16(17)	O5	Dy2	Dy1	100.79(13)	O8	Dy3	Dy3^{1}	125.68(16)
O1^{1}	Dy1	O3^{2}	142.95(18)	O5	Dy2	Dy2^{1}	103.46(14)	O8	Dy3	Dy3^{3}	110.04(15)
O1	Dy1	O3	75.17(18)	O5^{1}	Dy2	Dy2^{3}	103.01(13)	O8	Dy3	O3^{1}	87.4(2)
O1^{2}	Dy1	O3	139.86(17)	O5	Dy2	Dy2^{3}	41.31(13)	O8	Dy3	O3	75.55(19)
O1^{3}	Dy1	O3^{3}	75.17(18)	O5^{1}	Dy2	Dy2^{1}	39.66(13)	O8	Dy3	O4	134.7(3)
O1	Dy1	O3^{2}	139.86(17)	O5	Dy2	O2	66.0(2)	O8	Dy3	O7	144.4(2)
O1	Dy1	O3^{1}	142.95(18)	O5^{1}	Dy2	O2	64.9(2)	O8	Dy3	O7^{3}	124.9(2)
O1^{1}	Dy1	O3	73.16(17)	O5	Dy2	O5^{1}	88.8(3)	O8	Dy3	O9	84.9(2)
O1^{2}	Dy1	O3^{1}	73.16(17)	O5	Dy2	O10	99.7(2)	O8	Dy3	N2	71.7(2)
O1^{3}	Dy1	O3	142.95(18)	O5	Dy2	N1	74.9(2)	O9	Dy3	Dy1	160.49(18)

O1^{1}	Dy1	O3^{1}	75.17(18)	O5^{1}	Dy2	N1	138.2(2)	O9	Dy3	Dy3^{1}	137.84(19)
O1^{3}	Dy1	O3^{1}	139.86(18)	O6	Dy2	Dy1	85.00(14)	O9	Dy3	Dy3^{3}	107.10(17)
O1^{2}	Dy1	O3^{2}	75.17(18)	O6	Dy2	Dy2^{1}	110.35(15)	O9	Dy3	O4	133.6(3)
O1	Dy1	O4	120.22(12)	O6	Dy2	Dy2^{3}	124.35(15)	O9	Dy3	O7^{3}	72.3(2)
O1^{3}	Dy1	O4	120.22(12)	O6	Dy2	O1^{1}	75.61(19)	O9	Dy3	N2	72.5(2)
O1^{2}	Dy1	O4	120.22(12)	O6	Dy2	O1	86.3(2)	N2	Dy3	Dy1	120.27(15)
O1^{1}	Dy1	O4	120.22(12)	O6	Dy2	O2	133.9(3)	N2	Dy3	Dy3^{3}	178.22(15)
O2	Dy1	Dy2^{1}	44.211(10)	O6	Dy2	O5	143.7(2)	N2	Dy3	Dy3^{1}	89.19(16)
O2	Dy1	Dy2^{2}	44.211(9)	O6	Dy2	O5^{1}	126.0(2)	Dy2^{3}	O1	Dy1	101.2(2)
O2	Dy1	O4	180	O6	Dy2	O10	83.7(2)	Dy2	O1	Dy1	102.2(2)
O3^{1}	Dy1	Dy2^{1}	76.17(12)	O6	Dy2	N1	71.6(2)	Dy2	O1	Dy2^{3}	102.9(2)
O3^{1}	Dy1	Dy2^{2}	109.66(12)	O10	Dy2	Dy1	157.67(17)	Dy2	O2	Dy1	86.2(2)
O3^{3}	Dy1	Dy2^{2}	112.82(12)	O10	Dy2	Dy2^{1}	106.05(16)	Dy2^{3}	O2	Dy1	86.2(2)
O3^{2}	Dy1	Dy2^{1}	112.82(12)	O10	Dy2	Dy2^{3}	140.95(17)	Dy2^{2}	O2	Dy1	86.2(2)
O3^{2}	Dy1	Dy2^{2}	76.17(12)	O10	Dy2	O2	134.8(3)	Dy2^{1}	O2	Dy1	86.2(2)
O3	Dy1	Dy2^{1}	109.66(12)	O10	Dy2	O5^{1}	72.5(2)	Dy2^{2}	O2	Dy2	172.3(5)
O3^{3}	Dy1	Dy2^{1}	164.44(12)	O10	Dy2	N1	72.7(2)	Dy2^{3}	O2	Dy2	89.75(3)
O3	Dy1	Dy2^{2}	164.44(12)	N1	Dy2	Dy1	121.41(15)	Dy2^{1}	O2	Dy2	89.74(3)
O3^{2}	Dy1	O2	120.34(12)	N1	Dy2	Dy2^{1}	177.62(15)	Dy2^{3}	O2	Dy2^{1}	172.3(5)
O3^{3}	Dy1	O2	120.34(12)	N1	Dy2	Dy2^{3}	89.86(15)	Dy2^{3}	O2	Dy2^{2}	89.74(3)
O3	Dy1	O2	120.34(12)	N1	Dy2	O2	134.46(15)	Dy2^{1}	O2	Dy2^{2}	89.74(3)
O3^{1}	Dy1	O2	120.34(12)	Dy3^{3}	Dy3	Dy1	60.569(6)	Dy3	O3	Dy1	101.2(2)
O3	Dy1	O3^{1}	75.21(11)	Dy3^{1}	Dy3	Dy1	60.569(6)	Dy3^{3}	O3	Dy1	102.4(2)
O3	Dy1	O3^{3}	75.21(11)	Dy3^{3}	Dy3	Dy3^{1}	90	Dy3^{3}	O3	Dy3	102.6(2)
O3^{1}	Dy1	O3^{2}	75.21(11)	O3	Dy3	Dy1	40.24(13)	Dy3^{1}	O4	Dy1	86.1(2)
O3^{3}	Dy1	O3^{1}	119.3(2)	O3^{1}	Dy3	Dy1	40.03(14)	Dy3^{3}	O4	Dy1	86.1(2)
O3^{3}	Dy1	O3^{2}	75.21(11)	O3	Dy3	Dy3^{1}	96.95(13)	Dy3	O4	Dy1	86.1(2)
O3	Dy1	O3^{2}	119.3(2)	O3	Dy3	Dy3^{3}	38.32(12)	Dy3^{2}	O4	Dy1	86.1(2)
O3^{1}	Dy1	O4	59.66(12)	O3^{1}	Dy3	Dy3^{1}	39.12(13)	Dy3^{3}	O4	Dy3^{2}	89.73(3)
O3	Dy1	O4	59.66(12)	O3^{1}	Dy3	Dy3^{3}	97.08(13)	Dy3	O4	Dy3^{2}	172.2(5)
O3^{2}	Dy1	O4	59.66(12)	O3^{1}	Dy3	O3	79.3(3)	Dy3^{1}	O4	Dy3^{2}	89.73(3)
O3^{3}	Dy1	O4	59.66(12)	O3	Dy3	O4	64.7(2)	Dy3^{1}	O4	Dy3^{3}	172.2(5)
O4	Dy1	Dy2^{2}	135.789(9)	O3^{1}	Dy3	O4	65.3(2)	Dy3	O4	Dy3^{1}	89.74(3)
O4	Dy1	Dy2^{1}	135.789(10)	O3	Dy3	O7^{3}	74.61(18)	Dy3	O4	Dy3^{3}	89.73(3)
Dy2^{1}	Dy2	Dy1	60.457(6)	O3^{1}	Dy3	O7^{3}	129.86(19)	Dy2	O5	Dy2^{3}	99.03(19)
Dy2^{3}	Dy2	Dy1	60.457(6)	O3^{1}	Dy3	O7	76.60(19)	Dy3	O7	Dy3^{1}	99.02(19)

^{1}3/2-Y,+X,+Z;^{2}+Y,3/2-X,+Z;^{3}3/2-X,3/2-Y,+Z

Complex **5**

Ho1^{1}	Ho1	Ho1^{2}	90	O9^{3}	Ho2	O10	59.75(15)	O8	Ho3	O32	72.8(2)
O5^{2}	Ho1	Ho1^{2}	124.59(17)	O9^{1}	Ho2	O12	120.25(15)	O8	Ho3	O10	132.8(3)
O5^{2}	Ho1	Ho1^{1}	109.88(16)	O9^{2}	Ho2	O12	120.25(15)	O8	Ho3	N2	72.0(3)
O5^{2}	Ho1	O6^{2}	144.4(2)	O9	Ho2	O12	120.25(15)	O9	Ho3	Ho32	97.45(15)

O5^{2}	Ho1	O6	125.8(2)	O9^{3}	Ho2	O12	120.25(15)	O92	Ho3	Ho32	38.39(15)
O5^{2}	Ho1	O7	84.0(2)	O11	Ho2	O9^{1}	143.5(2)	O9	Ho3	O3	76.3(2)
O5^{2}	Ho1	O11^{2}	86.3(2)	O11	Ho2	O9^{3}	139.4(2)	O92	Ho3	O32	73.9(2)
O5^{2}	Ho1	O1^{1}	75.4(2)	O11	Ho2	O9^{2}	72.9(2)	O9	Ho3	O32	129.8(2)
O5^{2}	Ho1	O1^{2}	133.1(3)	O11^{1}	Ho2	O9^{1}	75.6(2)	O9	Ho3	O8	155.0(2)
O5^{2}	Ho1	N3^{2}	72.1(2)	O11^{2}	Ho2	O9^{3}	72.9(2)	O92	Ho3	O8	121.1(2)
O6	Ho1	Ho1^{1}	39.65(13)	O11^{2}	Ho2	O9^{1}	139.4(2)	O9	Ho3	O92	80.0(3)
O6^{2}	Ho1	Ho1^{2}	41.38(14)	O11^{2}	Ho2	O9^{2}	75.6(2)	O92	Ho3	O10	65.3(2)
O6	Ho1	Ho1^{2}	102.75(15)	O11^{3}	Ho2	O9^{1}	72.9(2)	O9	Ho3	O10	65.8(2)
O6^{2}	Ho1	Ho1^{1}	103.22(15)	O11^{3}	Ho2	O9^{2}	143.5(2)	O92	Ho3	N2	143.4(2)
O6^{2}	Ho1	O6	88.3(3)	O11	Ho2	O9	75.6(2)	O9	Ho3	N2	83.1(2)
O6^{2}	Ho1	O7	99.3(2)	O11^{3}	Ho2	O9^{3}	75.6(2)	O10	Ho3	Ho32	45.154(17)
O6^{2}	Ho1	O1^{1}	130.0(2)	O11^{1}	Ho2	O9	72.9(2)	O10	Ho3	N2	134.00(19)
O6	Ho1	O1^{2}	65.1(2)	O11^{1}	Ho2	O9^{2}	139.4(2)	N2	Ho3	Ho32	178.20(16)
O6^{2}	Ho1	O1^{2}	66.2(2)	O11^{2}	Ho2	O9	143.5(2)	C12	O1	C15	118.1(9)
O6^{2}	Ho1	N3^{2}	75.1(2)	O11^{3}	Ho2	O9	139.4(2)	C14	O2	Ho3	143.9(6)
O6	Ho1	N3^{2}	138.5(2)	O11^{1}	Ho2	O9^{3}	143.5(2)	Ho3	O3	Ho31	99.7(2)
O7	Ho1	Ho1^{2}	140.61(18)	O11^{3}	Ho2	O10	120.41(16)	C1	O3	Ho31	134.9(5)
O7	Ho1	Ho1^{1}	106.06(16)	O11^{2}	Ho2	O10	120.41(16)	C1	O3	Ho3	121.3(5)
O7	Ho1	O6	72.6(2)	O11	Ho2	O10	120.41(16)	C17	O4	C16	116.9(8)
O7	Ho1	O12	135.1(3)	O11^{1}	Ho2	O10	120.41(16)	C21	O5	Ho11	140.4(6)
O7	Ho1	N3^{2}	73.1(2)	O11	Ho2	O11^{1}	75.15(15)	Ho11	O6	Ho1	99.0(2)
O11^{2}	Ho1	Ho1^{2}	39.08(16)	O11	Ho2	O11^{2}	75.15(15)	Ho3	O9	Ho2	101.9(2)
O11	Ho1	Ho1^{2}	96.67(17)	O11^{1}	Ho2	O11^{2}	119.2(3)	Ho3^{1}	O9	Ho2	100.9(2)
O11^{2}	Ho1	Ho1^{1}	96.82(17)	O11	Ho2	O11^{3}	119.2(3)	Ho3	O9	Ho3^{1}	102.5(2)
O11	Ho1	Ho1^{1}	38.04(16)	O11^{1}	Ho2	O11^{3}	75.15(15)	Ho3^{2}	O10	Ho2	85.8(2)
O11	Ho1	O6	74.3(2)	O11^{2}	Ho2	O11^{3}	75.15(15)	Ho3^{1}	O10	Ho2	85.8(2)
O11^{2}	Ho1	O6	129.3(2)	O11^{2}	Ho2	O12	59.59(16)	Ho3^{3}	O10	Ho2	85.8(2)
O11^{2}	Ho1	O6^{2}	77.0(2)	O11^{1}	Ho2	O12	59.59(16)	Ho3	O10	Ho2	85.8(2)
O11	Ho1	O7	118.3(2)	O11	Ho2	O12	59.59(16)	Ho3^{1}	O10	Ho3	89.69(3)
O11^{2}	Ho1	O7	157.0(2)	O11^{3}	Ho2	O12	59.59(16)	Ho3^{1}	O10	Ho3^{2}	171.6(5)
O11^{2}	Ho1	O11	79.0(3)	O12	Ho2	O10	180	Ho3^{2}	O10	Ho3	89.69(3)
O11^{2}	Ho1	O12	64.6(2)	O2	Ho3	Ho3^{2}	109.85(16)	Ho3^{1}	O10	Ho3^{3}	89.69(3)
O11	Ho1	O12	63.9(2)	O2	Ho3	O3^{2}	124.0(2)	Ho3^{2}	O10	Ho3^{3}	89.69(3)
O11^{2}	Ho1	N3^{2}	84.1(2)	O2	Ho3	O3	144.8(2)	Ho3	O10	Ho3^{3}	171.6(5)
O11	Ho1	N3^{2}	144.1(2)	O2	Ho3	O8	85.1(3)	Ho1^{1}	O11	Ho1	102.9(2)
O12	Ho1	Ho1^{1}	45.093(14)	O2	Ho3	O9	88.2(2)	Ho1^{1}	O11	Ho2	102.8(3)
O12	Ho1	Ho1^{2}	45.093(15)	O2	Ho3	O9^{2}	75.4(2)	Ho1	O11	Ho2	101.3(2)
N3^{2}	Ho1	Ho1^{2}	89.52(18)	O2	Ho3	O10	135.4(3)	Ho1^{2}	O12	Ho1^{3}	89.81(3)
N3^{2}	Ho1	Ho1^{1}	177.86(16)	O2	Ho3	N2	71.9(2)	Ho1^{1}	O12	Ho1	89.81(3)
N3^{2}	Ho1	O12	134.23(18)	O3^{2}	Ho3	Ho3^{2}	39.22(14)	Ho1^{2}	O12	Ho1	89.81(3)
O9^{3}	Ho2	O9^{1}	75.30(14)	O3	Ho3	Ho3^{2}	103.50(16)	Ho1	O12	Ho1^{3}	173.5(5)
O9^{2}	Ho2	O9^{1}	119.5(3)	O3	Ho3	O3^{2}	89.3(3)	Ho1^{2}	O12	Ho1^{1}	173.5(5)
O9^{3}	Ho2	O9	119.5(3)	O3	Ho3	O8	95.7(3)	Ho1^{1}	O12	Ho1^{3}	89.81(3)

O9^{1}	Ho2	O9	75.30(14)	O3	Ho3	O9^{2}	130.7(2)	Ho1^{2}	O12	Ho2	86.7(2)
O9^{3}	Ho2	O9^{2}	75.30(14)	O3^{2}	Ho3	O10	64.5(2)	Ho1	O12	Ho2	86.7(2)
O9^{2}	Ho2	O9	75.30(14)	O3	Ho3	O10	65.7(2)	Ho1^{1}	O12	Ho2	86.7(2)
O9	Ho2	O10	59.75(15)	O3	Ho3	N2	74.9(2)	Ho1^{3}	O12	Ho2	86.7(2)
O9^{1}	Ho2	O10	59.75(15)	O3^{2}	Ho3	N2	139.4(2)				
O9^{2}	Ho2	O10	59.75(15)	O8	Ho3	Ho3+	107.45(19)				

^{1}1/2-Y,+X,+Z;^{2}+Y,1/2-X,+Z;^{3}1/2-X,1/2-Y,+Z

3. IR spectra of five complexes

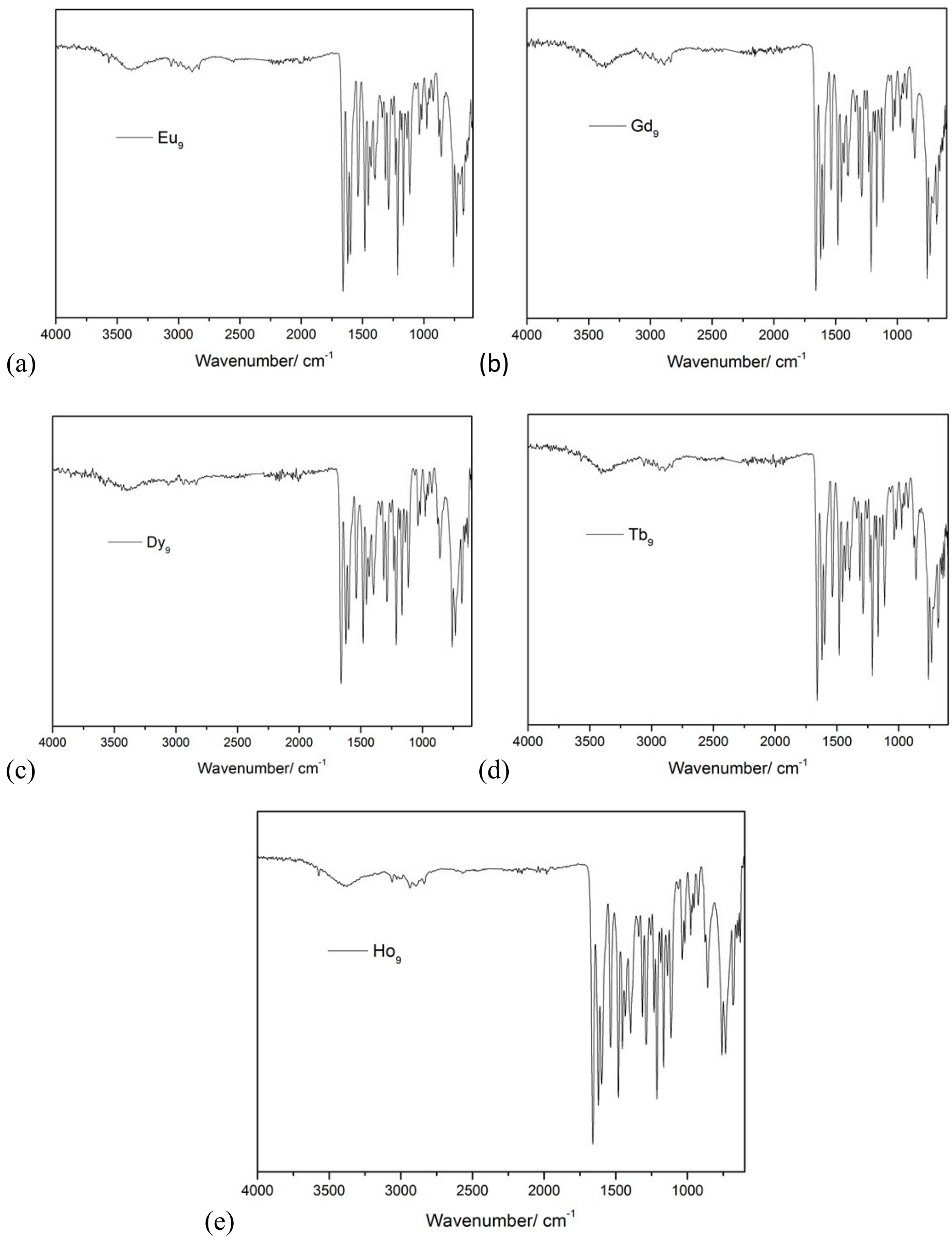


Figure S4. IR spectra of **1**[H_3O]·H_2O(a), **2**[H_3O]·4H_2O(b), **3**[H_3O]·3H_2O(c), **4**[H_3O]·6H_2O(d) and **5**[H_3O]·2H_2O(e).

4. PXRD patterns of five complexes

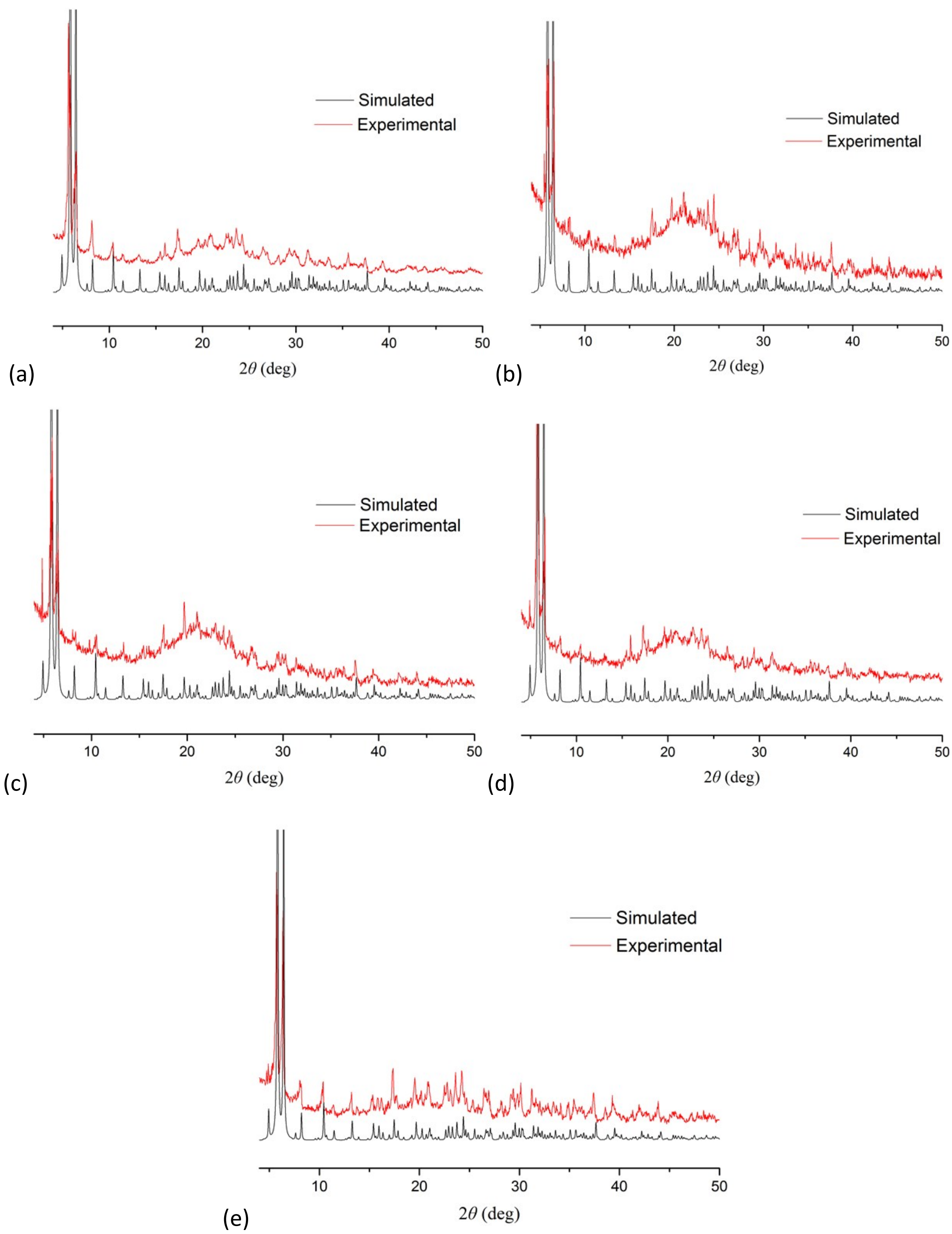


Figure S5. PXRD patterns of **1**$[H_3O]\cdot H_2O$(a), **2**$[H_3O]\cdot 4H_2O$(b), **3**$[H_3O]\cdot 3H_2O$(c), **4**$[H_3O]\cdot 6H_2O$(d) and **5**$[H_3O]\cdot 2H_2O$(e).

5. The Curie-Weiss law fits of four complexes.

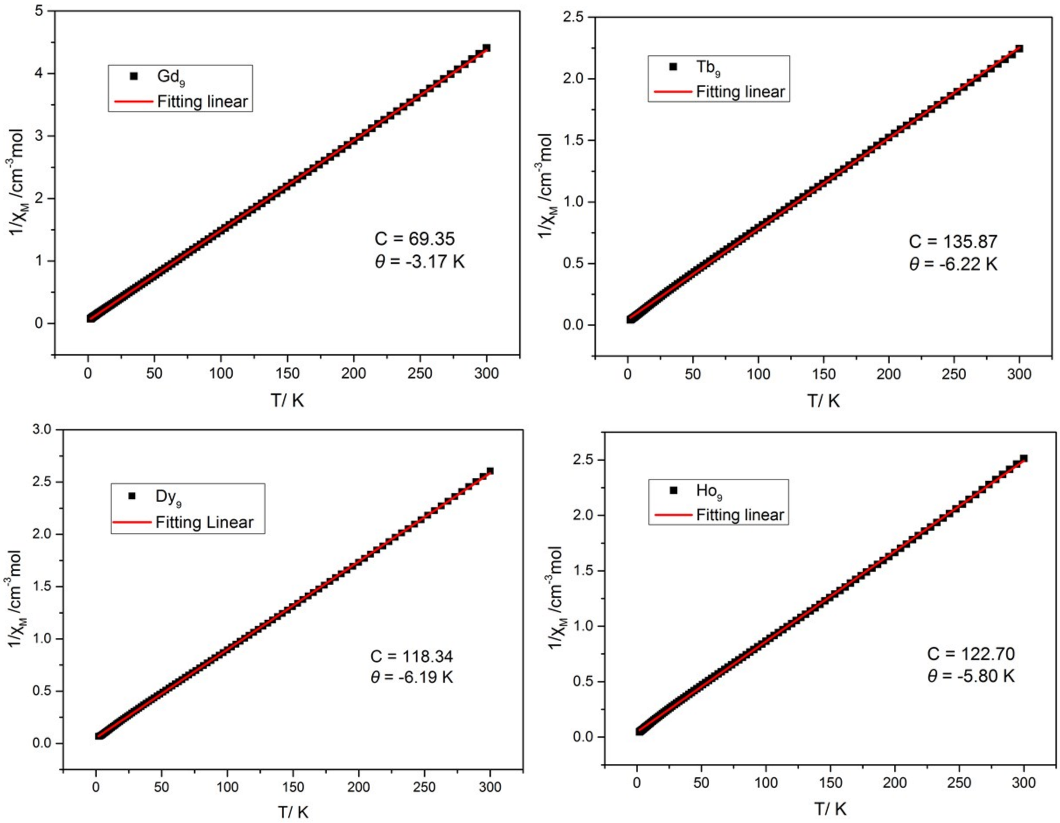


Figure S6. Plot of $1/\chi_M$ versus T for **2**$[H_3O]\cdot 4H_2O$, **3**$[H_3O]\cdot 3H_2O$, **4**$[H_3O]\cdot 6H_2O$ and **5**$[H_3O]\cdot 2H_2O$ and the linear fits represent the Curie-Weiss law fit at 1 kOe field.

6. Magnetic field dependence of out-of-phase (χ'') susceptibilities for 4[H_3O]·6H_2O.

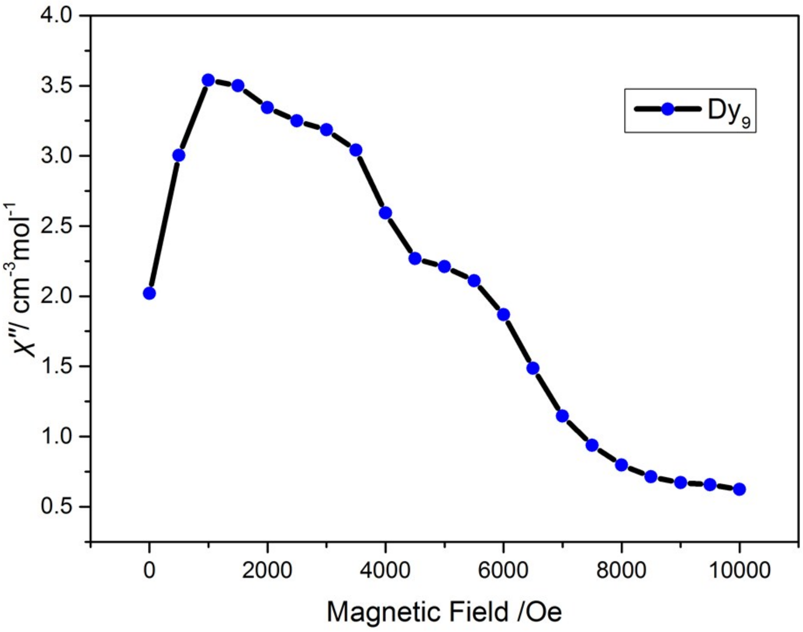


Figure S7. Magnetic field dependence of out-of-phase (χ'') susceptibilities for **4**[H_3O]·6H_2O in the range 0 to 10000 Oe dc field (The temperature at 2 K and the susceptibilities at 1000 Hz frequencies).

7. Temperature dependence of the in-phase (χ') and out-of-phase (χ'') susceptibilities for 4[H_3O]·6H_2O under 1000 Oe dc field

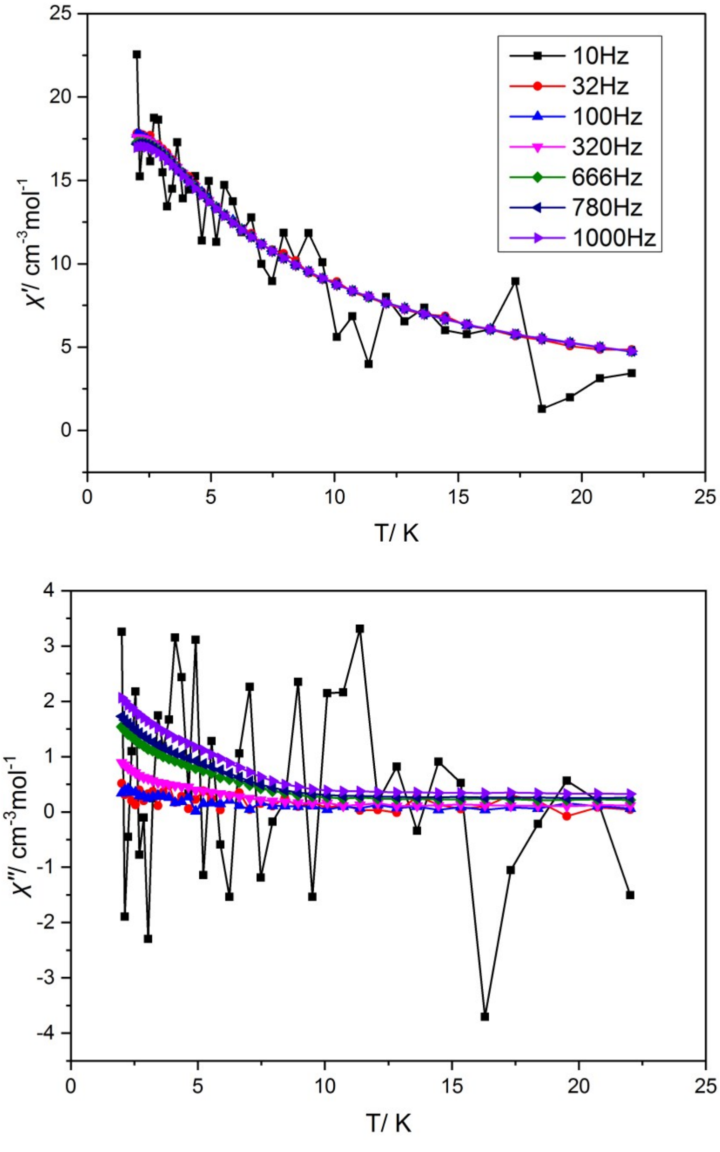
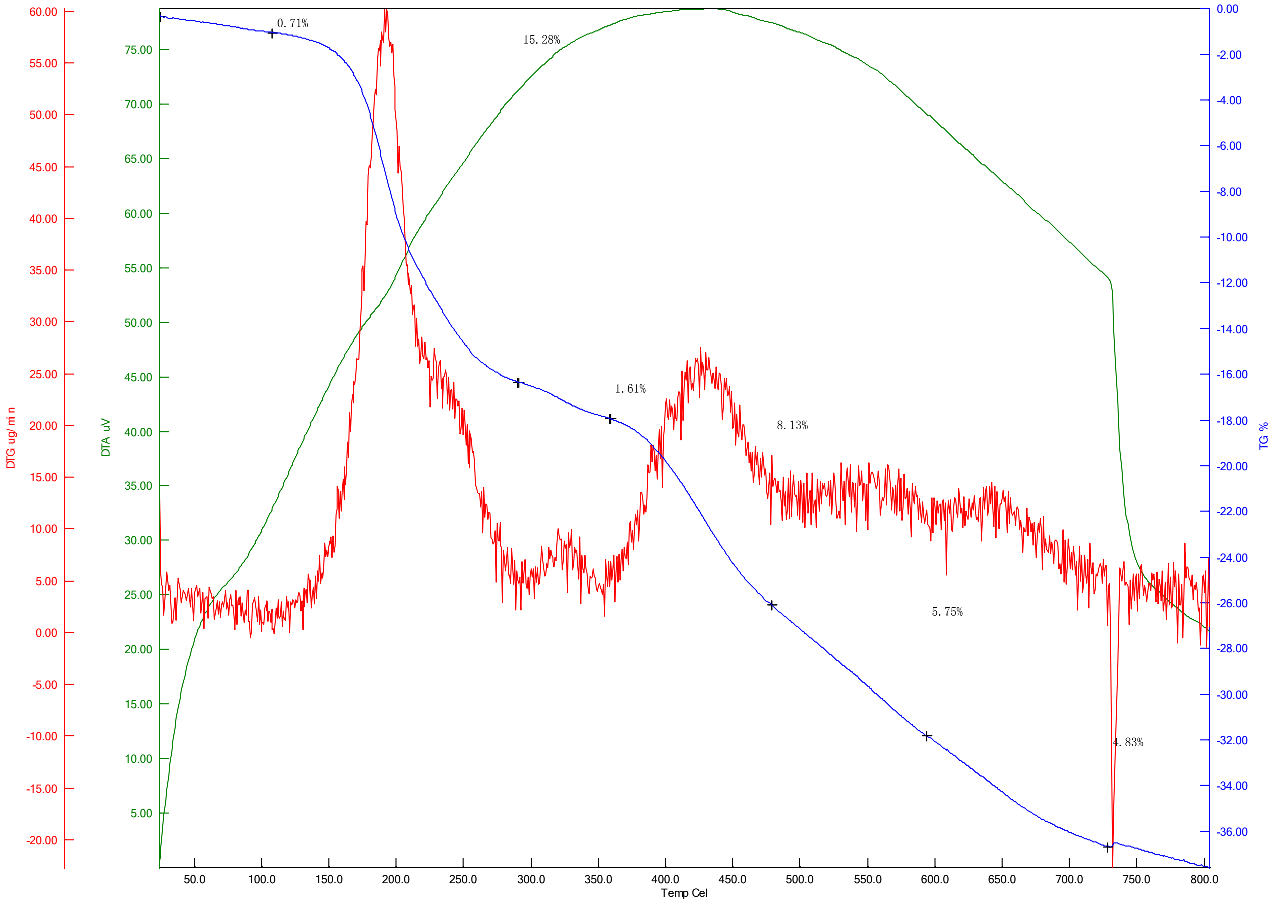


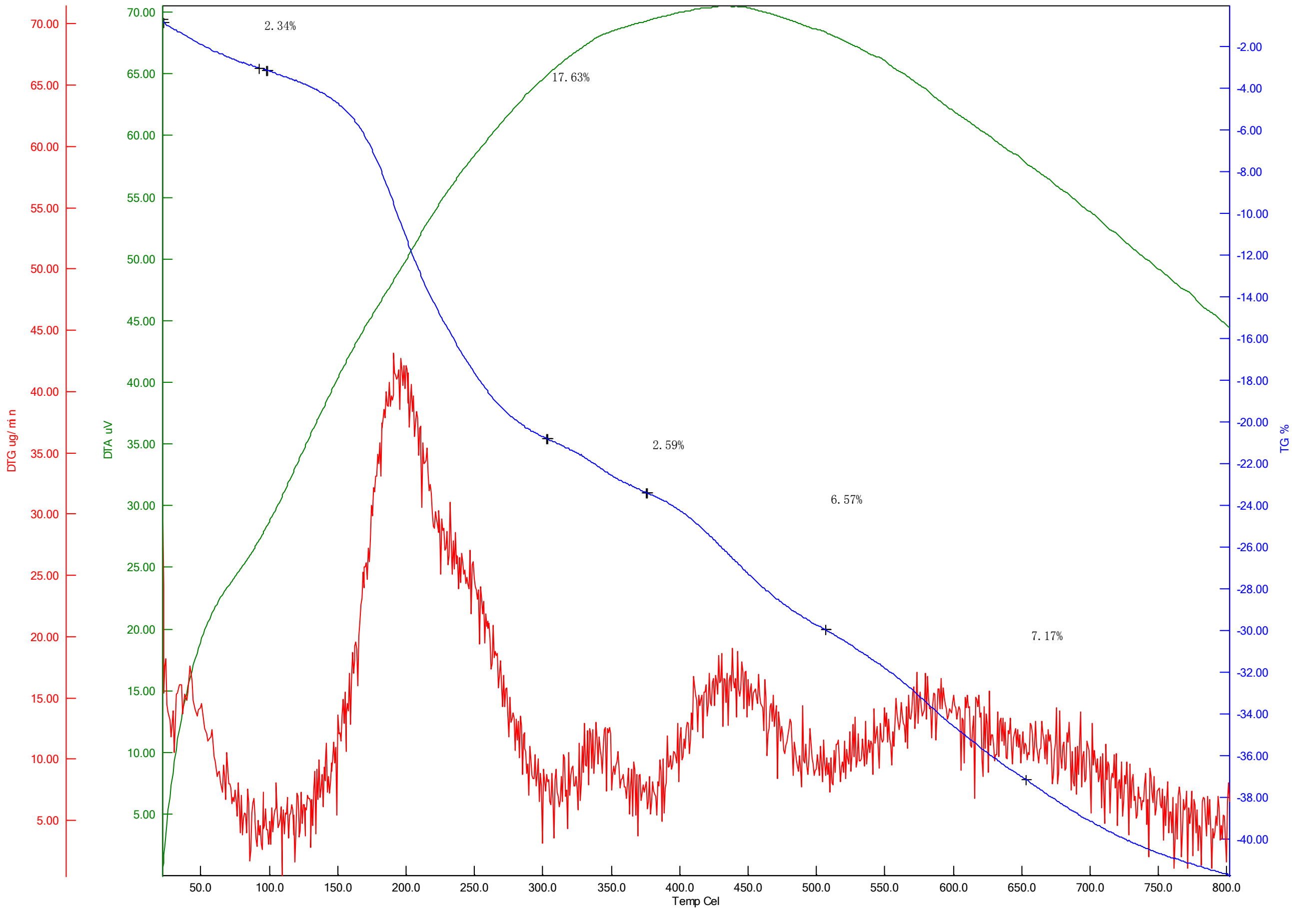
Figure S8. Temperature dependence of the in-phase χ′(left) and out-of-phase χ″(right) susceptibilities for **4**[H_3O]·6H_2O in the range 2 to 22 K. The susceptibilities at 10 Hz, 32 Hz, 100 Hz 320 Hz, 666 Hz, 780 Hz, 1000 Hz frequencies under 1000 Oe dc field.

8. TG curves for five complexes

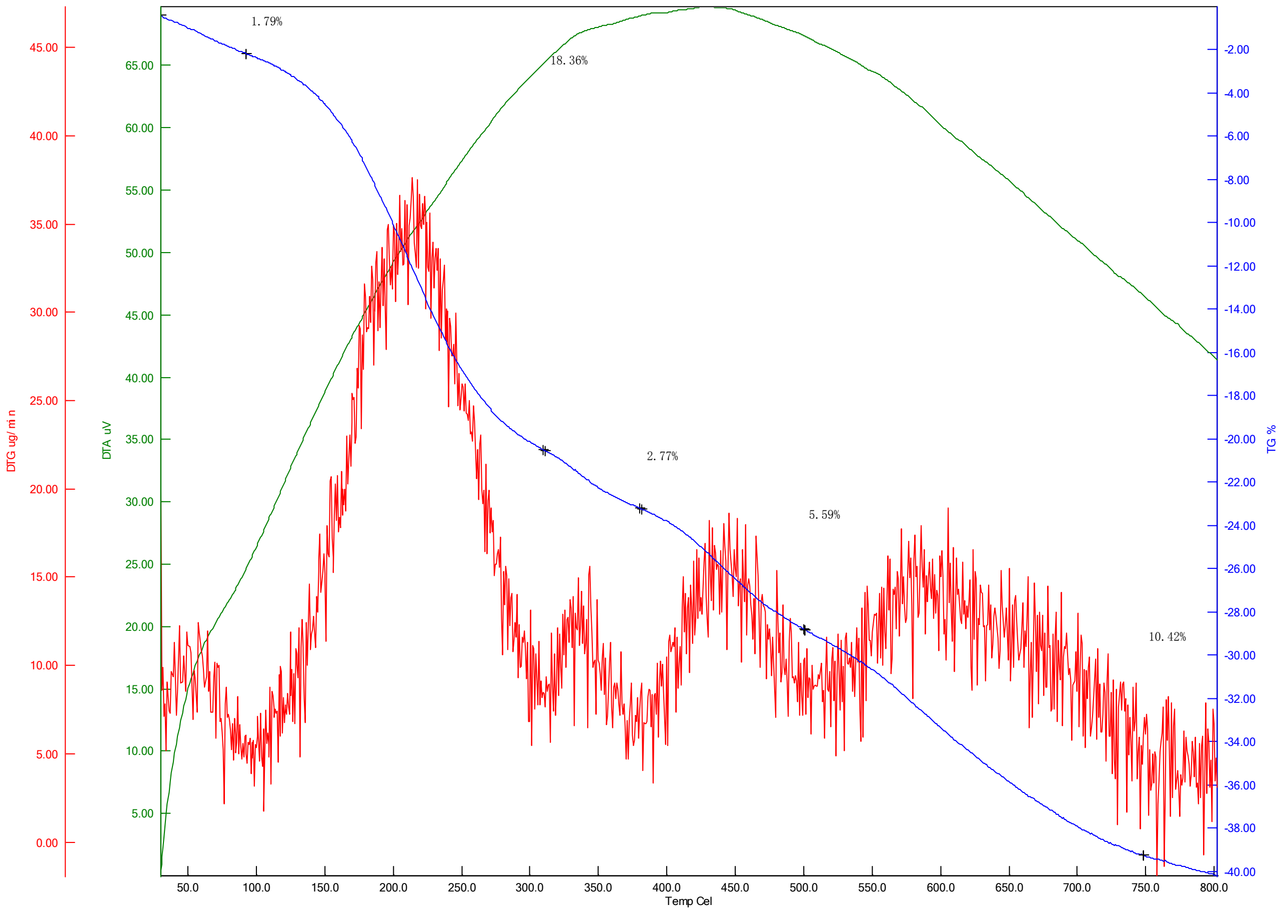
(a)



(b)



(c)



DTG ug/min
DTA uV
TG %
Temp Cel
1.79%
18.36%
2.77%
5.59%
10.42%
45.00
40.00
35.00
30.00
25.00
20.00
15.00
10.00
5.00
0.00
65.00
60.00
55.00
50.00
45.00
40.00
35.00
30.00
25.00
20.00
15.00
10.00
5.00
-2.00
-4.00
-6.00
-8.00
-10.00
-12.00
-14.00
-16.00
-18.00
-20.00
-22.00
-24.00
-26.00
-28.00
-30.00
-32.00
-34.00
-36.00
-38.00
-40.00
50.0
100.0
150.0
200.0
250.0
300.0
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450.0
500.0
550.0
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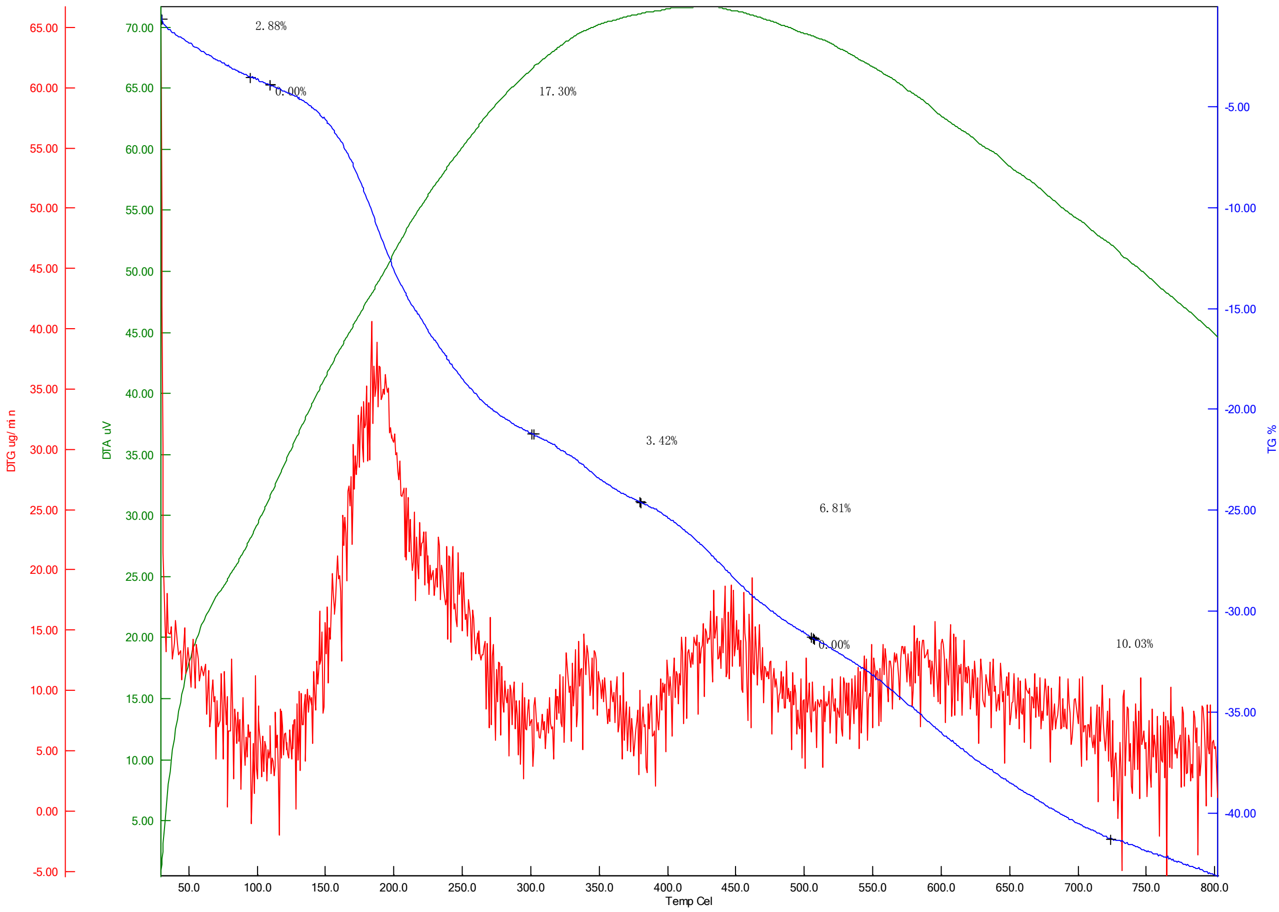
650.0
700.0
750.0
800.0

(d)



(e)

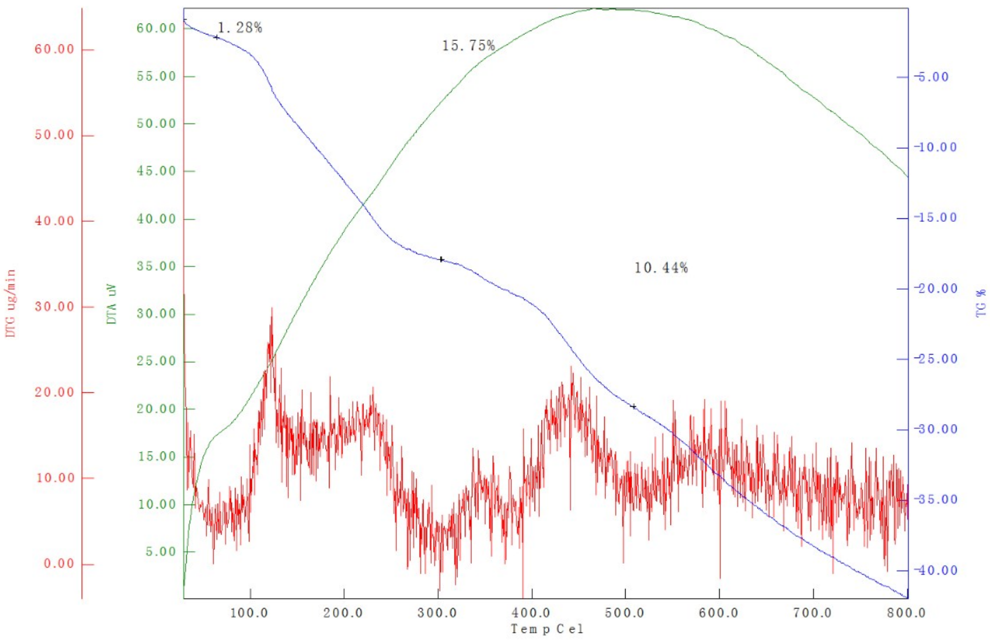


Figure S9. The TG curves of complex **1**[H_3O]·H_2O(a), **2**[H_3O]·4H_2O(b), **3**[H_3O]·3H_2O(c), **4**[H_3O]·6H_2O(d) and **5**[H_3O]·2H_2O(e).

9. The solid-state excitation and emission spectra of H_2L ligand.

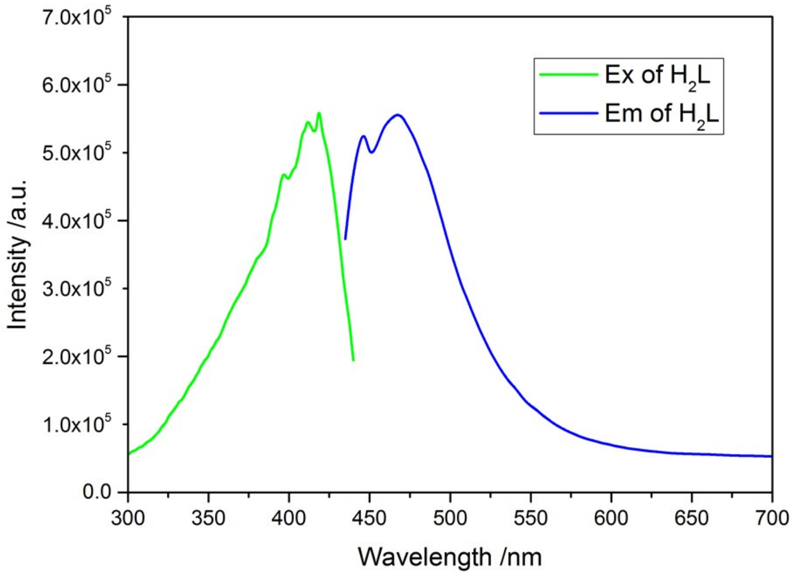


Figure S10. The excitation and emission spectra of H_2L ligand

10. PXRD patterns for investigating the stability of complex 3[H_3O]·3H_2O

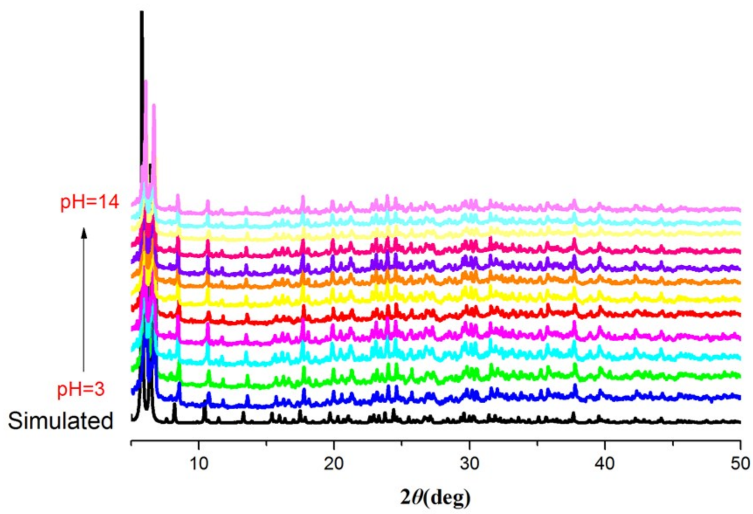


Figure S11. PXRD patterns for the simulated and measured of **3**[H_3O]·3H_2O after soaked in water solutions with different pH values in the range of 3-14 for two days.

11. The Stern-Volmer curve and linear curve of *I* versus ion/anion concentration for 3$[H_3O]\cdot 3H_2O$ among Fe^{3+}, CrO_4^{2-} and $Cr_2O_7^{2-}$

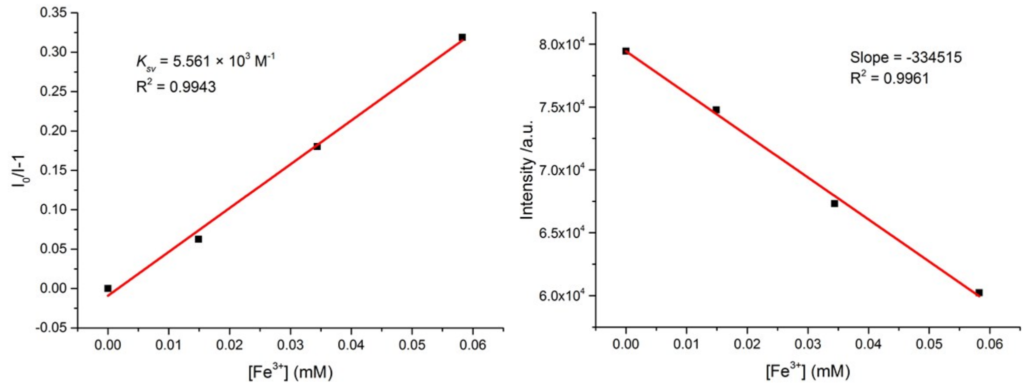


Figure S12. Stern-Volmer plot of I_0/I-1 versus low Fe^{3+} concentration in the aqueous suspension of **3**$[H_3O]\cdot 3H_2O$ (left).Linear region of fluorescence intensity for the suspensions of **3**$[H_3O]\cdot 3H_2O$ in water upon incremental addition of Fe^{3+} solutions (right).

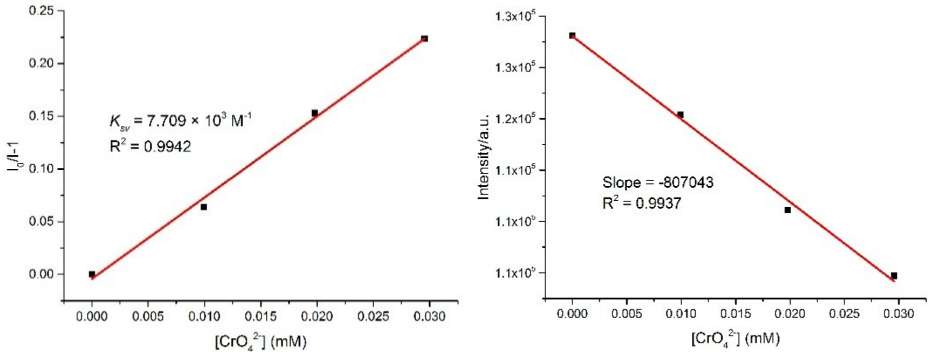


Figure S13. (a) Stern-Volmer plot of I_0/I-1 versus low CrO_4^{2-} concentration in the aqueous suspension of **3**$[H_3O]\cdot 3H_2O$. (b) Linear region of fluorescence intensity for the suspensions of **3**$[H_3O]\cdot 3H_2O$ in water upon incremental addition of CrO_4^{2-} solutions.

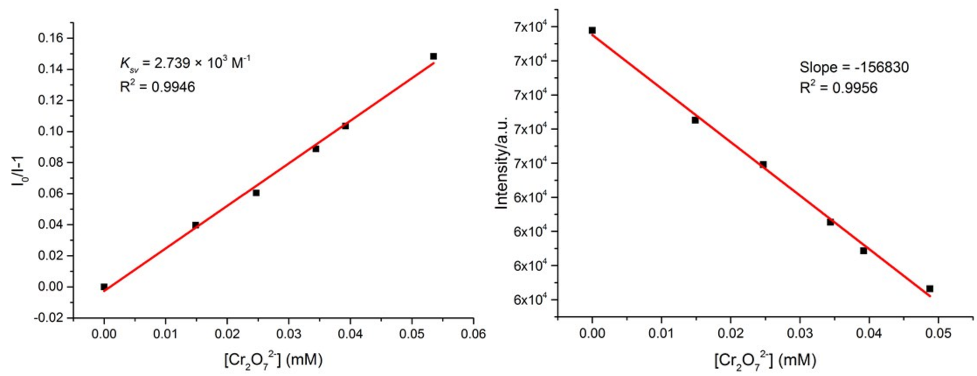
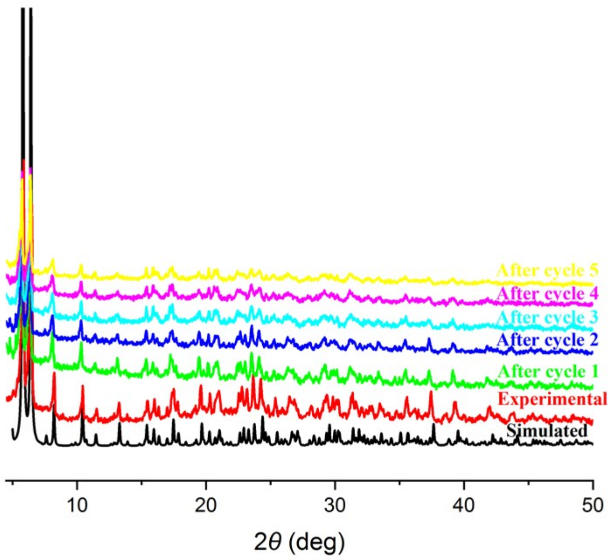


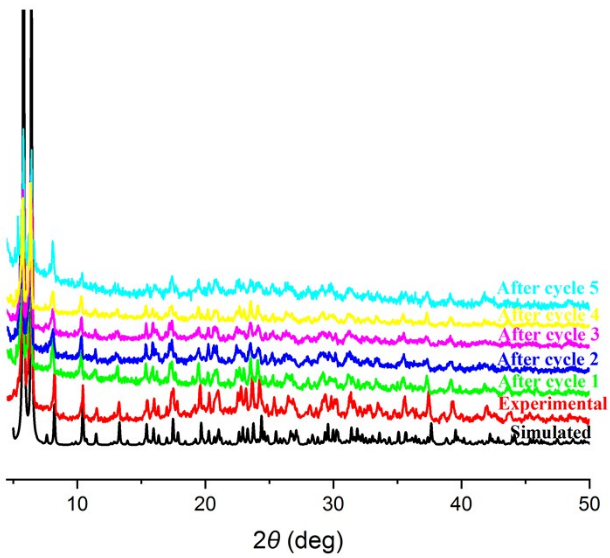
Figure S14. (a) Stern-Volmer plot of I_0/I-1 versus low $Cr_2O_7^{2-}$ concentration in the aqueous suspension of **3**$[H_3O]\cdot 3H_2O$. (b) Linear region of fluorescence intensity for the suspensions of **3**$[H_3O]\cdot 3H_2O$ in water upon incremental addition of $Cr_2O_7^{2-}$ solutions.

12. Simulated and experimental PXRD patterns of 3[H_3O]·3H_2O after detecting Fe^{3+}, CrO_4^{2-} and $Cr_2O_7^{2-}$

(a)



(b)



(c)

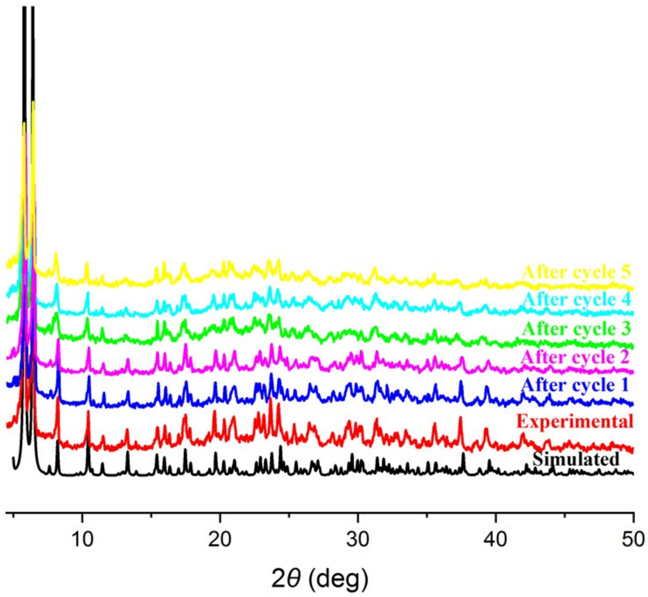


Figure S15. Simulated and experimental PXRD patterns of **3**[H_3O]·3H_2O after detecting Fe^{3+} (a), CrO_4^{2-} (b) and $Cr_2O_7^{2-}$ (c).

13. A comparison of PXRD patterns for the simulated, experimental and measured of 3[H_3O]·3H_2O after the detection of Fe^{3+}, CrO_4^{2-} and $Cr_2O_7^{2-}$

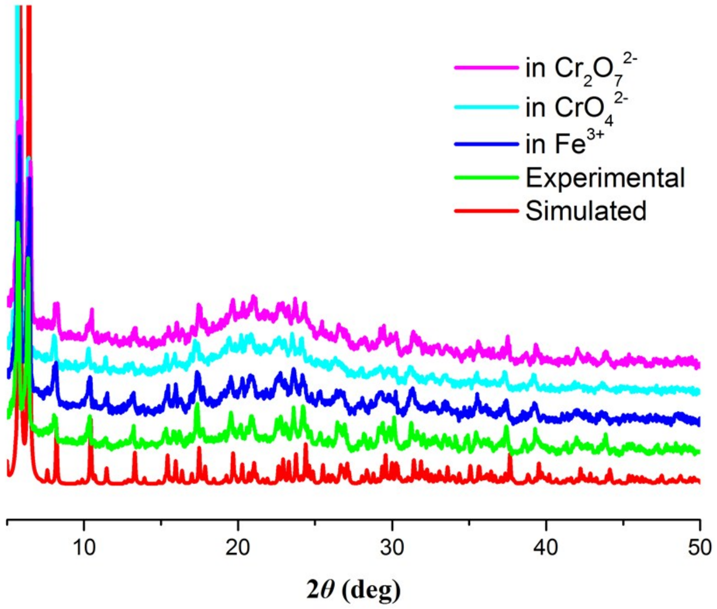


Figure S16. PXRD patterns for simulated, experimental and measured of **3**[H_3O]·3H_2O after the detection of Fe^{3+}, CrO_4^{2-} and $Cr_2O_7^{2-}$.

14. The XPS of 3[H_3O]·3H_2O before and after detection of Fe^{3+}

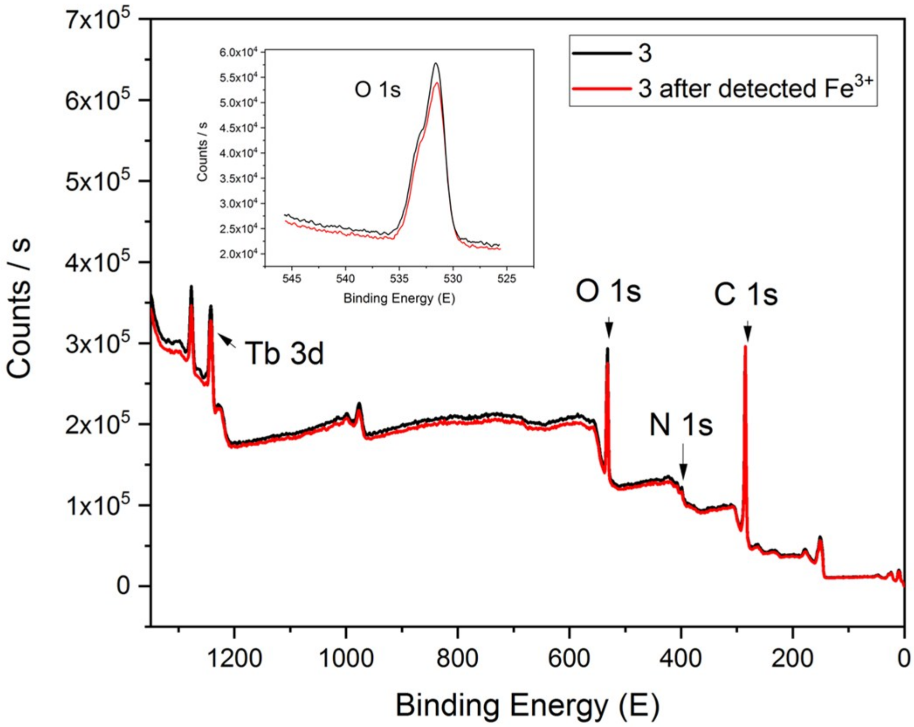
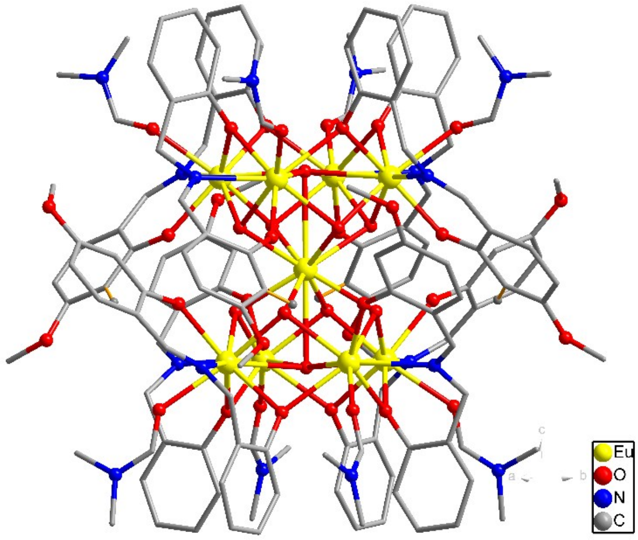


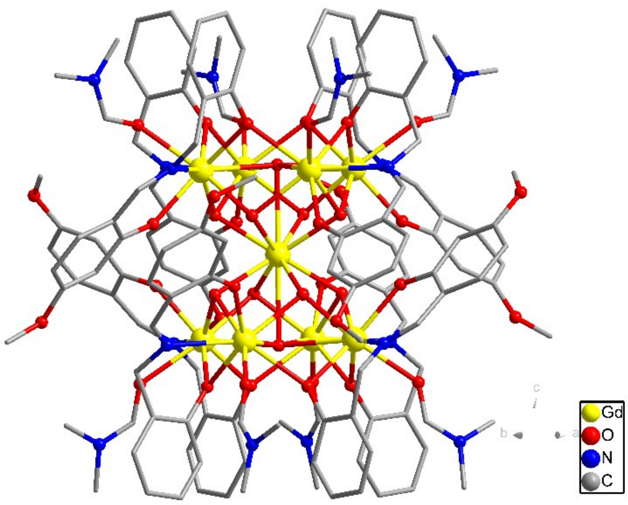
Figure S17. The XPS for **3**[H_3O]·3H_2O before and after the detection of Fe^{3+}.

15. Molecular structures of anionic units of complexes 1[H_3O]·H_2O, 2[H_3O]·4H_2O, 3[H_3O]·3H_2O and 5[H_3O]·2H_2O

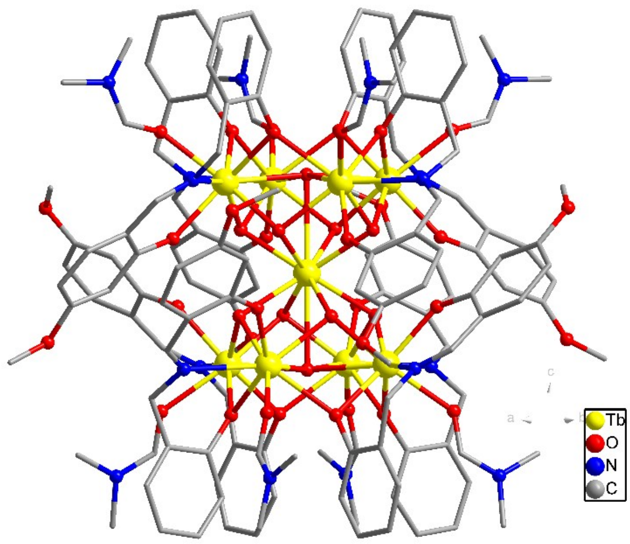
(a)



(b)



(c)



(d)

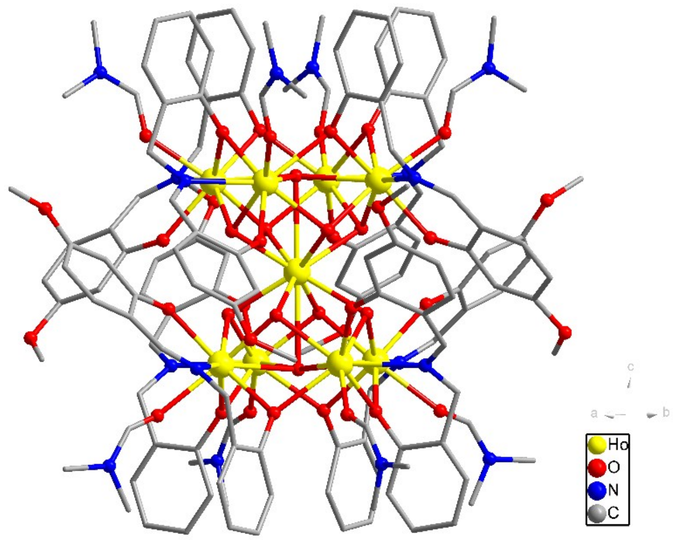


Figure S18. The Molecular structures of anionic units of complexes **1**$[H_3O]\cdot H_2O$ (a), **2**$[H_3O]\cdot 4H_2O$ (b), **3**$[H_3O]\cdot 3H_2O$ (c) and **5**$[H_3O]\cdot 2H_2O$ (d). Hydrogen atoms are omitted for clarity.