Supporting Information (SI)

Solvothermal Synthesis, Crystal Structure, and Properties of Lanthanide-Organic Frameworks Based on Thiophene - 2, 5 - Dicarboxylic acid

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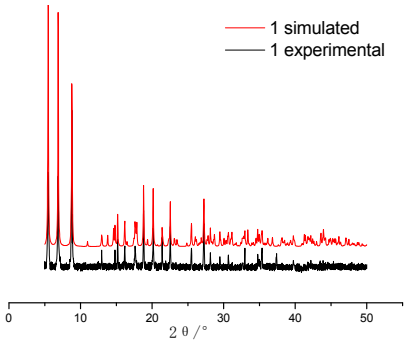

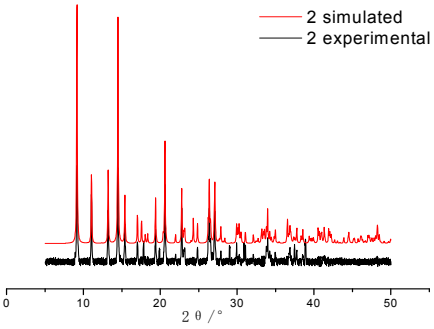

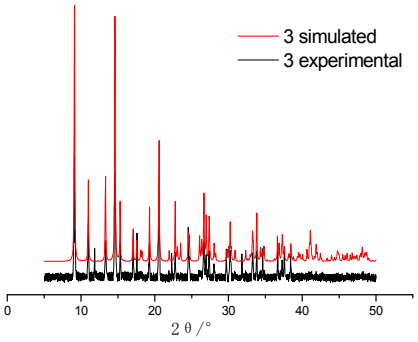

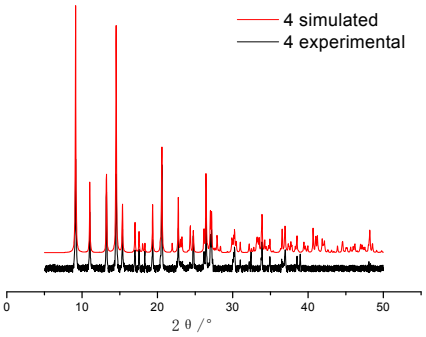

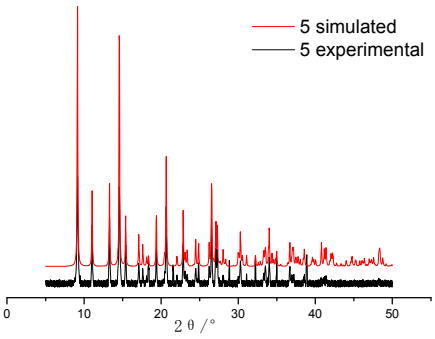

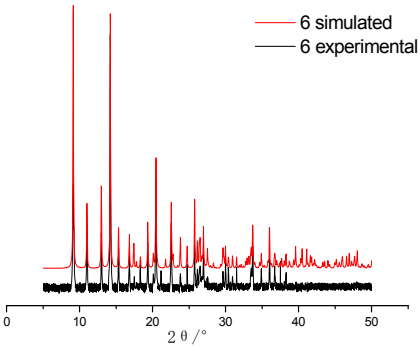

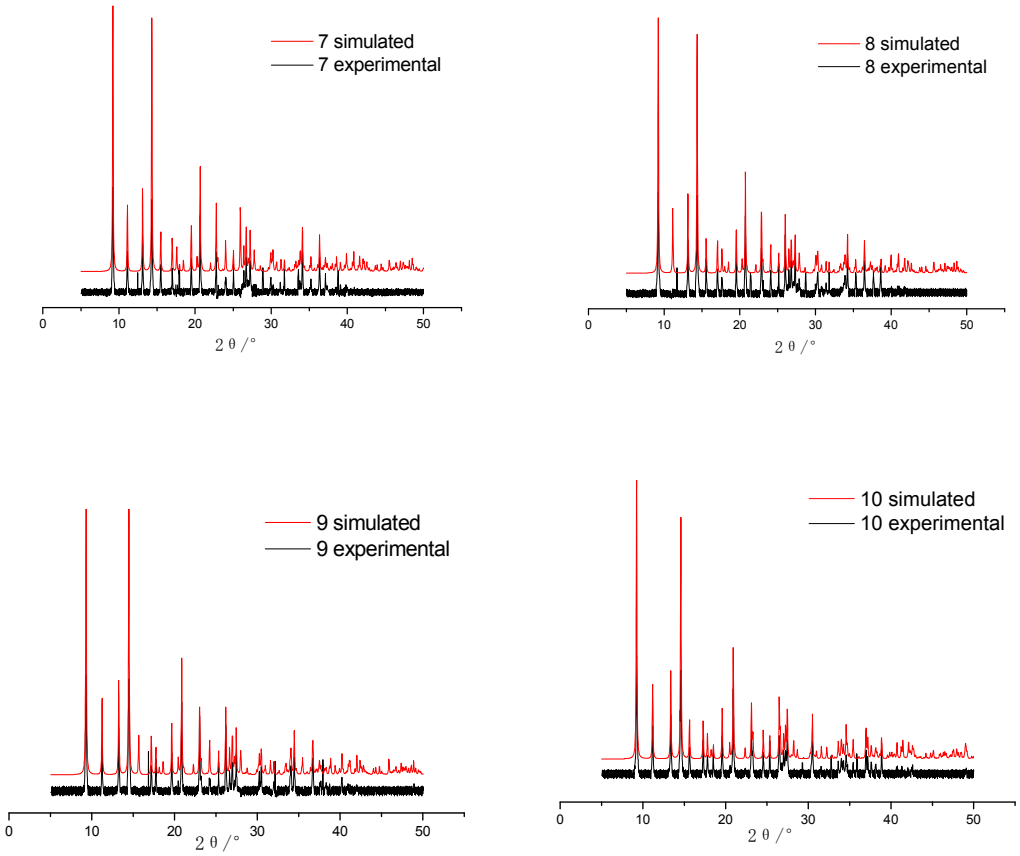

Figure 1 The simulated and experimental PXRD patterns of **1-10**

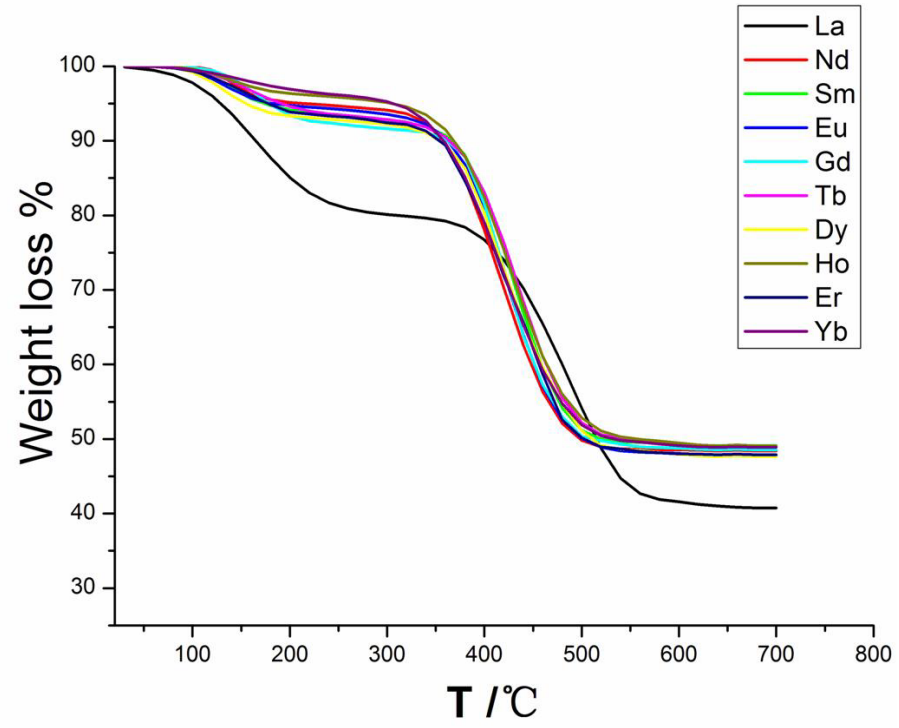

Figure 2. TGA curve of **1-10**.

Table 1. Selected bond distances (Å) and angles (deg) for compounds **1-10.**

1			
La(1)-O(1)	2.583(6)	O(8)#4-La(1)-O(9)	73.3(2)
La(1)-O(2)	2.687(6)	O(2)-La(1)-O(9)	122.76(19)
La(1)-O(8)#4	2.594(6)	O(12)-La(1)-O(9)	131.9(2)
La(1)-O(9)	2.689(6)	O(1)-La(1)-O(9)	109.5(2)
La(1)-O(9)#2	2.486(6)	O(8)#4-La(1)-O(9)	73.3(2)
La(1)-O(10)#3	2.501(6)	O(2)-La(1)-O(9)	122.76(19)
La(1)-O(11)	2.686(8)	O(14)-La(2)-O(15)	98.2(3)
La(1)-O(12)	2.586(7)	O(14)-La(2)-O(10)#3	117.3(2)
La(1)-O(13)	2.530(8)	O(15)-La(2)-O(10)#3	142.2(3)
La(2)-O(2)	2.592(6)	O(14)-La(2)-O(2)	149.1(2)
La(2)-O(3)#5	2.675(7)	O(15)-La(2)-O(2)	85.5(3)
La(2)-O(4)#5	2.611(6)	O(10)#3-La(2)-O(2)	70.9(2)
La(2)-O(5)	2.597(8)	O(14)-La(2)-O(5)	81.4(3)
La(2)-O(6)	2.763(8)	O(15)-La(2)-O(5)	109.0(3)
La(2)-O(7)#4	2.601(6)	O(10)#3-La(2)-O(5)	67.0(3)
La(2)-O(10)#3	2.587(6)	O(2)-La(2)-O(5)	126.6(3)
La(2)-O(11)#3	2.617(6)	O(14)-La(2)-O(7)#4	149.5(2)
La(2)-O(14)	2.516(7)	O(15)-La(2)-O(7)#4	76.1(3)
La(2)-O(15)	2.568(9)	O(10)#3-La(2)-O(7)#4	66.8(2)
O(9)#2-La(1)-O(10)#3	77.4(2)	O(2)-La(2)-O(7)#4	61.3(2)
O(9)#2-La(1)-O(13)	84.0(3)	O(5)-La(2)-O(7)#4	72.6(3)
O(10)#3-La(1)-O(13)	139.3(3)	O(14)-La(2)-O(4)#5	82.3(3)
O(9)#2-La(1)-O(11)	133.11(19)	O(15)-La(2)-O(4)#5	110.9(3)
O(10)#3-La(1)-O(11)	129.40(19)	O(10)#3-La(2)-O(4)#5	87.5(2)
O(13)-La(1)-O(11)	89.4(3)	O(2)-La(2)-O(4)#5	67.8(2)
O(9)#2-La(1)-O(12)	73.6(2)	O(5)-La(2)-O(4)#5	138.5(2)
O(10)#3-La(1)-O(12)	70.7(2)	O(7)#4-La(2)-O(4)#5	127.9(2)

O(13)-La(1)-O(12)	69.4(3)	O(14)-La(2)-O(11)#3	68.41(19)
O(11)-La(1)-O(12)	145.2(2)	O(15)-La(2)-O(11)#3	166.6(3)
O(9)#2-La(1)-O(1)	138.9(2)	O(10)#3-La(2)-O(11)#3	50.33(18)
O(10)#3-La(1)-O(1)	102.0(2)	O(2)-La(2)-O(11)#3	106.5(2)
O(13)-La(1)-O(1)	69.9(2)	O(5)-La(2)-O(11)#3	69.0(2)
O(11)-La(1)-O(1)	79.2(2)	O(7)#4-La(2)-O(11)#3	114.76(18)
O(12)-La(1)-O(1)	67.9(2)	O(4)#5-La(2)-O(11)#3	69.5(2)
O(9)#2-La(1)-O(8)#4	72.56(19)	O(14)-La(2)-O(3)#5	70.2(2)
O(10)#3-La(1)-O(8)#4	74.1(2)	O(15)-La(2)-O(3)#5	66.0(3)
O(13)-La(1)-O(8)#4	133.6(2)	O(10)#3-La(2)-O(3)#5	136.1(2)
O(11)-La(1)-O(8)#4	79.3(2)	O(2)-La(2)-O(3)#5	83.7(2)
O(12)-La(1)-O(8)#4	135.3(2)	O(5)-La(2)-O(3)#5	149.6(3)
O(1)-La(1)-O(8)#4	147.66(19)	O(7)#4-La(2)-O(3)#5	130.0(2)
O(9)#2-La(1)-O(2)	148.0(2)	O(4)#5-La(2)-O(3)#5	49.3(2)
O(10)#3-La(1)-O(2)	70.7(2)	O(11)#3-La(2)-O(3)#5	108.5(2)
O(13)-La(1)-O(2)	119.0(2)	O(14)-La(2)-O(6)	70.1(2)
O(11)-La(1)-O(2)	72.97(19)	O(15)-La(2)-O(6)	65.6(3)
O(12)-La(1)-O(2)	93.1(2)	O(10)#3-La(2)-O(6)	113.1(2)
O(1)-La(1)-O(2)	49.9(2)	O(2)-La(2)-O(6)	136.9(2)
O(8)#4-La(1)-O(2)	100.52(19)	O(5)-La(2)-O(6)	47.6(3)
O(9)#2-La(1)-O(9)	85.98(11)	O(7)#4-La(2)-O(6)	80.5(2)
O(10)#3-La(1)-O(9)	146.6(2)	O(4)#5-La(2)-O(6)	150.9(2)
O(13)-La(1)-O(9)	65.4(2)	O(11)#3-La(2)-O(6)	107.1(2)
O(11)-La(1)-O(9)	49.81(17)	O(3)#5-La(2)-O(6)	109.9(2)
O(12)-La(1)-O(9)	131.9(2)	O(14)-La(2)-O(15)	98.2(3)
O(1)-La(1)-O(9)	109.5(2)	O(14)-La(2)-O(10)#3	117.3(2)

2			
Nd(1)-O(1)	2.3230(14)	O(1)-Nd(1)-O(6)#2	72.32(5)
Nd(1)-O(2)#2	2.3294(14)	O(4)#1-Nd(1)-O(6)#2	143.87(5)
Nd(1)-O(3)#3	2.3669(16)	O(2)#2-Nd(1)-O(6)#2	75.84(5)
Nd(1)-O(4)#1	2.3247(13)	O(3)#3-Nd(1)-O(6)#2	75.57(5)
Nd(1)-O(5)	2.4938(18)	O(8)-Nd(1)-O(6)#2	130.17(5)
Nd(1)-O(6)	2.5052(15)	O(1)-Nd(1)-O(5)	85.27(6)
Nd(1)-O(6)#2	2.3923(15)	O(4)#1-Nd(1)-O(5)	77.94(5)
Nd(1)-O(8)	2.3839(14)	O(2)#2-Nd(1)-O(5)	93.37(5)
O(1)-Nd(1)-O(4)#1	141.87(5)	O(3)#3-Nd(1)-O(5)	156.85(5)
O(1)-Nd(1)-O(2)#2	138.58(5)	O(8)-Nd(1)-O(5)	81.41(5)
O(4)#1-Nd(1)-O(2)#2	77.00(5)	O(6)#2-Nd(1)-O(5)	126.91(5)
O(1)-Nd(1)-O(3)#3	98.58(5)	O(1)-Nd(1)-O(6)	72.72(5)
O(4)#1-Nd(1)-O(3)#3	85.36(5)	O(4)#1-Nd(1)-O(6)	118.68(5)
O(2)#2-Nd(1)-O(3)#3	98.42(5)	O(2)#2-Nd(1)-O(6)	74.30(5)
O(1)-Nd(1)-O(8)	70.47(5)	O(3)#3-Nd(1)-O(6)	151.29(5)
O(4)#1-Nd(1)-O(8)	73.30(5)	O(8)-Nd(1)-O(6)	121.46(5)
O(2)#2-Nd(1)-O(8)	150.29(5)	O(6)#2-Nd(1)-O(6)	75.73(6)
O(3)#3-Nd(1)-O(8)	78.47(5)	O(5)-Nd(1)-O(6)	51.54(5)

3			
Sm(1)-O(1)	2.357(2)	O(1)-Sm(1)-O(8)	70.33(9)
Sm(1)-O(2)#1	2.373(2)	O(4)#4-Sm(1)-O(8)	72.58(8)
Sm(1)-O(3)#5	2.379(2)	O(2)#1-Sm(1)-O(8)	151.01(8)
Sm(1)-O(4)#4	2.358(2)	O(3)#5-Sm(1)-O(8)	77.62(8)
Sm(1)-O(5)	2.489(3)	O(6)#1-Sm(1)-O(8)	128.96(9)
Sm(1)-O(6)	2.400(3)	O(1)-Sm(1)-O(5)	82.31(10)
Sm(1)-O(6)#1	2.489(3)	O(4)#4-Sm(1)-O(5)	79.00(9)
Sm(1)-O(8)	2.424(2)	O(2)#1-Sm(1)-O(5)	95.01(9)

O(1)-Sm(1)-O(4)#4	140.21(9)	O(3)#5-Sm(1)-O(5)	156.64(8)
O(1)-Sm(1)-O(2)#1	138.18(8)	O(6)#1-Sm(1)-O(5)	125.33(8)
O(4)#4-Sm(1)-O(2)#1	78.56(8)	O(8)-Sm(1)-O(5)	82.38(8)
O(1)-Sm(1)-O(3)#5	101.90(9)	O(1)-Sm(1)-O(6)	72.33(9)
O(4)#4-Sm(1)-O(3)#5	83.57(9)	O(4)#4-Sm(1)-O(6)	119.05(9)
O(2)#1-Sm(1)-O(3)#5	96.66(9)	O(2)#1-Sm(1)-O(6)	73.63(8)
O(1)-Sm(1)-O(6)#1	72.41(9)	O(3)#5-Sm(1)-O(6)	151.69(8)
O(4)#4-Sm(1)-O(6)#1	145.67(8)	O(6)#1-Sm(1)-O(6)	74.53(9)
O(2)#1-Sm(1)-O(6)#1	75.70(9)	O(8)-Sm(1)-O(6)	123.38(8)
O(3)#5-Sm(1)-O(6)#1	77.32(8)	O(5)-Sm(1)-O(6)	51.57(8)

4

Eu(1)-O(1)	2.321(4)	O(1)-Eu(1)-O(6)#1	72.20(16)
Eu(1)-O(2)#1	2.333(4)	O(2)#1-Eu(1)-O(6)#1	75.90(15)
Eu(1)-O(3)#3	2.377(4)	O(4)#2-Eu(1)-O(6)#1	144.53(15)
Eu(1)-O(4)#2	2.334(3)	O(3)#3-Eu(1)-O(6)#1	75.61(14)
Eu(1)-O(5)	2.516(5)	O(8)-Eu(1)-O(6)#1	129.63(14)
Eu(1)-O(6)	2.506(4)	O(1)-Eu(1)-O(6)	72.52(16)
Eu(1)-O(6)#1	2.401(4)	O(2)#1-Eu(1)-O(6)	74.24(15)
Eu(1)-O(8)	2.390(4)	O(4)#2-Eu(1)-O(6)	118.21(14)
O(1)-Eu(1)-O(2)#1	138.32(15)	O(3)#3-Eu(1)-O(6)	151.48(14)
O(1)-Eu(1)-O(4)#2	141.51(15)	O(8)-Eu(1)-O(6)	121.80(15)
O(2)#1-Eu(1)-O(4)#2	77.37(14)	O(6)#1-Eu(1)-O(6)	75.88(15)
O(1)-Eu(1)-O(3)#3	99.35(16)	O(1)-Eu(1)-O(5)	84.66(16)
O(2)#1-Eu(1)-O(3)#3	97.94(15)	O(2)#1-Eu(1)-O(5)	93.74(16)
O(4)#2-Eu(1)-O(3)#3	85.50(14)	O(4)#2-Eu(1)-O(5)	77.71(15)
O(1)-Eu(1)-O(8)	70.56(15)	O(3)#3-Eu(1)-O(5)	156.93(13)
O(2)#1-Eu(1)-O(8)	150.53(14)	O(8)-Eu(1)-O(5)	81.76(14)
O(4)#2-Eu(1)-O(8)	73.20(14)	O(6)#1-Eu(1)-O(5)	126.78(14)

O(3)#3-Eu(1)-O(8)	78.28(15)	O(6)-Eu(1)-O(5)	51.33(13)

5

Gd(1)-O(1)	2.334(3)	O(1)-Gd(1)-O(8)	73.23(11)
Gd(1)-O(2)#2	2.349(3)	O(4)#1-Gd(1)-O(8)	70.38(12)
Gd(1)-O(3)#3	2.357(3)	O(2)#2-Gd(1)-O(8)	77.68(12)
Gd(1)-O(2)#3	2.359(4)	O(3)#3-Gd(1)-O(8)	150.40(11)
Gd(1)-O(5)	2.459(4)	O(6)#4-Gd(1)-O(8)	129.77(11)
Gd(1)-O(6)	2.373(3)	O(1)-Gd(1)-O(5)	78.93(12)
Gd(1)-O(6)#4	2.457(5)	O(4)#1-Gd(1)-O(5)	83.56(13)
Gd(1)-O(8)	2.409(3)	O(2)#2-Gd(1)-O(5)	156.45(11)
O(1)-Gd(1)-O(4)#1	141.35(12)	O(3)#3-Gd(1)-O(5)	94.23(12)
O(1)-Gd(1)-O(2)#2	83.87(11)	O(6)#4-Gd(1)-O(5)	125.88(11)
O(4)#1-Gd(1)-O(2)#2	100.49(12)	O(8)-Gd(1)-O(5)	82.00(11)
O(1)-Gd(1)-O(3)#3	77.24(11)	O(1)-Gd(1)-O(6)	119.46(11)
O(4)#1-Gd(1)-O(3)#3	138.65(12)	O(4)#1-Gd(1)-O(6)	72.31(12)
O(2)#2-Gd(1)-O(3)#3	97.55(12)	O(2)#2-Gd(1)-O(6)	151.35(10)
O(1)-Gd(1)-O(6)#4	144.26(11)	O(3)#3-Gd(1)-O(6)	74.07(12)
O(4)#1-Gd(1)-O(6)#4	72.60(12)	O(6)#4-Gd(1)-O(6)	74.41(12)
O(2)#2-Gd(1)-O(6)#4	76.98(11)	O(8)-Gd(1)-O(6)	122.82(11)
O(3)#3-Gd(1)-O(6)#4	75.75(12)	O(5)-Gd(1)-O(6)	51.99(10)

6

Tb(1)-O(1)	2.326(3)	O(1)-Tb(1)-O(8)	75.40(10)
Tb(1)-O(2)#1	2.329(3)	O(2)#1-Tb(1)-O(8)	77.49(11)
Tb(1)-O(3)#2	2.359(3)	O(3)#2-Tb(1)-O(8)	151.16(10)
Tb(1)-O(4)#3	2.361(3)	O(4)#3-Tb(1)-O(8)	69.69(10)
Tb(1)-O(5)	2.465(3)	O(6)#4-Tb(1)-O(8)	132.73(10)

Tb(1)-O(6)	2.513(3)	O(1)-Tb(1)-O(5)	78.28(10)
Tb(1)-O(6)#1	2.374(3)	O(2)#1-Tb(1)-O(5)	155.02(10)
Tb(1)-O(8)	2.417(3)	O(3)#2-Tb(1)-O(5)	92.01(11)
O(1)-Tb(1)-O(2)#1	84.98(10)	O(4)#3-Tb(1)-O(5)	89.29(12)
O(1)-Tb(1)-O(3)#2	75.82(10)	O(6)#4-Tb(1)-O(5)	125.85(10)
O(2)#1-Tb(1)-O(3)#2	101.79(11)	O(8)-Tb(1)-O(5)	80.40(11)
O(1)-Tb(1)-O(4)#3	144.44(10)	O(1)-Tb(1)-O(6)	120.96(10)
O(2)#1-Tb(1)-O(4)#3	93.80(11)	O(2)#1-Tb(1)-O(6)	151.06(10)
O(3)#2-Tb(1)-O(4)#3	138.47(10)	O(3)#2-Tb(1)-O(6)	75.30(10)
O(1)-Tb(1)-O(6)#4	141.30(10)	O(4)#3-Tb(1)-O(6)	72.74(10)
O(2)#1-Tb(1)-O(6)#4	78.42(10)	O(6)#4-Tb(1)-O(6)	73.11(12)
O(3)#2-Tb(1)-O(6)#4	73.78(11)	O(8)-Tb(1)-O(6)	118.96(11)
O(4)#3-Tb(1)-O(6)#4	72.06(11)	O(5)-Tb(1)-O(6)	52.75(9)

7			
Dy(1)-O(1)	2.290(5)	O(2)#1-Dy(1)-O(8)	77.9(2)
Dy(1)-O(2)#2	2.289(5)	O(1)-Dy(1)-O(8)	75.07(19)
Dy(1)-O(3)#3	2.327(5)	O(4)#2-Dy(1)-O(8)	69.9(2)
Dy(1)-O(4)#2	2.326(6)	O(3)#3-Dy(1)-O(8)	150.6(2)
Dy(1)-O(5)	2.433(6)	O(6)#4-Dy(1)-O(8)	132.96(19)
Dy(1)-O(6)	2.477(5)	O(2)#1-Dy(1)-O(5)	154.85(18)
Dy(1)-O(6)#4	2.343(5)	O(1)-Dy(1)-O(5)	78.3(2)
Dy(1)-O(8)	2.381(5)	O(4)#2-Dy(1)-O(5)	89.0(2)
O(2)#1-Dy(1)-O(1)	84.7(2)	O(3)#3-Dy(1)-O(5)	92.1(2)
O(2)#1-Dy(1)-O(4)#2	94.3(2)	O(6)#4-Dy(1)-O(5)	126.28(18)
O(1)-Dy(1)-O(4)#2	144.4(2)	O(8)-Dy(1)-O(5)	79.9(2)
O(2)#1-Dy(1)-O(3)#3	101.6(2)	O(2)#1-Dy(1)-O(6)	151.18(18)
O(1)-Dy(1)-O(3)#3	75.65(19)	O(1)-Dy(1)-O(6)	121.1(2)
O(4)#2-Dy(1)-O(3)#3	138.6(2)	O(4)#2-Dy(1)-O(6)	72.4(2)

O(2)#1-Dy(1)-O(6)#4	78.18(19)	O(3)#3-Dy(1)-O(6)	75.6(2)
O(1)-Dy(1)-O(6)#4	141.1(2)	O(6)#4-Dy(1)-O(6)	73.4(2)
O(4)#2-Dy(1)-O(6)#4	72.2(2)	O(8)-Dy(1)-O(6)	118.7(2)
O(3)#3-Dy(1)-O(6)#4	74.1(2)	O(5)-Dy(1)-O(6)	52.85(17)

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Ho(1)-O(1)	2.287(5)	O(2)#1-Ho(1)-O(8)	77.92(18)
Ho(1)-O(1)#2	2.279(5)	O(1)-Ho(1)-O(8)	74.89(18)
Ho(1)-O(3)#3	2.320(5)	O(4)#2-Ho(1)-O(8)	69.84(18)
Ho(1)-O(4)#2	2.303(5)	O(3)#3-Ho(1)-O(8)	150.47(18)
Ho(1)-O(5)	2.418(5)	O(6)#4-Ho(1)-O(8)	133.09(19)
Ho(1)-O(6)	2.468(5)	O(2)#1-Ho(1)-O(5)	155.14(16)
Ho(1)-O(6)#4	2.330(5)	O(1)-Ho(1)-O(5)	78.52(18)
Ho(1)-O(8)	2.374(5)	O(4)#2-Ho(1)-O(5)	89.1(2)
O(2)#1-Ho(1)-O(1)	84.60(18)	O(3)#3-Ho(1)-O(5)	92.29(19)
O(2)#1-Ho(1)-O(4)#2	94.2(2)	O(6)#4-Ho(1)-O(5)	125.91(16)
O(1)-Ho(1)-O(4)#2	144.12(18)	O(8)-Ho(1)-O(5)	80.13(18)
O(2)#1-Ho(1)-O(3)#3	101.11(19)	O(2)#1-Ho(1)-O(6)	150.70(17)
O(1)-Ho(1)-O(3)#3	75.64(17)	O(1)-Ho(1)-O(6)	121.48(18)
O(4)#2-Ho(1)-O(3)#3	139.03(18)	O(4)#2-Ho(1)-O(6)	72.70(19)
O(2)#1-Ho(1)-O(6)#4	78.28(17)	O(3)#3-Ho(1)-O(6)	75.65(18)
O(1)-Ho(1)-O(6)#4	141.25(18)	O(6)#4-Ho(1)-O(6)	72.82(19)
O(4)#2-Ho(1)-O(6)#4	72.3(2)	O(8)-Ho(1)-O(6)	119.23(18)
O(3)#3-Ho(1)-O(6)#4	74.0(2)	O(5)-Ho(1)-O(6)	53.11(16)

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Er(1)-O(1)	2.280(4)	O(2)#1-Er(1)-O(8)	77.65(18)
Er(1)-O(2)#1	2.272(5)	O(1)-Er(1)-O(8)	74.95(16)
Er(1)-O(3)#3	2.309(5)	O(4)#2-Er(1)-O(8)	69.76(17)

Er(1)-O(4)#2	2.302(5)	O(3)#3-Er(1)-O(8)	150.19(16)
Er(1)-O(5)	2.401(5)	O(6)#4-Er(1)-O(8)	133.10(16)
Er(1)-O(6)	2.459(5)	O(2)#1-Er(1)-O(5)	154.79(16)
Er(1)-O(6)#4	2.340(5)	O(1)-Er(1)-O(5)	78.63(17)
Er(1)-O(8)	2.373(5)	O(4)#2-Er(1)-O(5)	88.90(19)
O(2)#1-Er(1)-O(1)	84.54(17)	O(3)#3-Er(1)-O(5)	92.38(18)
O(2)#1-Er(1)-O(4)#2	94.00(18)	O(6)#4-Er(1)-O(5)	126.06(16)
O(1)-Er(1)-O(4)#2	144.11(17)	O(8)-Er(1)-O(5)	79.92(17)
O(2)#1-Er(1)-O(3)#3	101.41(18)	O(2)#1-Er(1)-O(6)	150.86(16)
O(1)-Er(1)-O(3)#3	75.31(16)	O(1)-Er(1)-O(6)	121.42(16)
O(4)#2-Er(1)-O(3)#3	139.36(17)	O(4)#2-Er(1)-O(6)	72.90(17)
O(2)#1-Er(1)-O(6)#4	78.39(17)	O(3)#3-Er(1)-O(6)	75.62(17)
O(1)-Er(1)-O(6)#4	141.11(17)	O(6)#4-Er(1)-O(6)	72.88(19)
O(4)#2-Er(1)-O(6)#4	72.40(18)	O(8)-Er(1)-O(6)	119.34(17)
O(3)#3-Er(1)-O(6)#4	74.25(17)	O(5)-Er(1)-O(6)	53.21(15)

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Yb(1)-O(1)	2.2984(17)	O(4)#5-Yb(1)-O(8)	69.76(7)
Yb(1)-O(2)#1	2.311(2)	O(1)-Yb(1)-O(8)	74.12(6)
Yb(1)-O(3)#2	2.3024(18)	O(3)#2-Yb(1)-O(8)	150.03(6)
Yb(1)-O(4)#3	2.2794(17)	O(2)#6-Yb(1)-O(8)	78.13(7)
Yb(1)-O(5)	2.434(2)	O(6)#4-Yb(1)-O(8)	130.29(7)
Yb(1)-O(6)	2.4674(19)	O(4)#5-Yb(1)-O(5)	86.37(7)
Yb(1)-O(6)#4	2.3426(19)	O(1)-Yb(1)-O(5)	77.55(7)
Yb(1)-O(8)	2.3428(18)	O(3)#2-Yb(1)-O(5)	93.99(7)
O(4)#5-Yb(1)-O(1)	142.31(7)	O(2)#6-Yb(1)-O(5)	155.98(6)
O(4)#5-Yb(1)-O(3)#2	139.75(7)	O(6)#4-Yb(1)-O(5)	127.20(6)
O(1)-Yb(1)-O(3)#2	75.94(6)	O(8)-Yb(1)-O(5)	80.82(7)
O(4)#5-Yb(1)-O(2)#6	97.00(7)	O(4)#5-Yb(1)-O(6)	73.67(7)

O(1)-Yb(1)-O(2)#6	85.64(7)	O(1)-Yb(1)-O(6)	119.58(7)
O(3)#2-Yb(1)-O(2)#6	98.47(7)	O(3)#2-Yb(1)-O(6)	74.32(6)
O(4)#5-Yb(1)-O(6)#4	72.18(7)	O(2)#6-Yb(1)-O(6)	149.74(7)
O(1)-Yb(1)-O(6)#4	143.49(6)	O(6)#4-Yb(1)-O(6)	73.72(8)
O(3)#2-Yb(1)-O(6)#4	75.91(7)	O(8)-Yb(1)-O(6)	122.55(7)
O(2)#6-Yb(1)-O(6)#4	76.02(7)	O(5)-Yb(1)-O(6)	53.87(6)

Symmetry transformations used to generate equivalent atoms: For **1**. #1 x,y-1,z; #2 -x+1, y+1/2, -z+1; #3-x+2, y-1/2, -z; #4-x+2, y+1/2, -z+1; #5 x, y+1, z ; #6 -x+1, y-1/2, -z+1; #7 -x+2, y+1/2, -z ; For **2**. #1 x-1, y ,z-1; #2 -x+2, -y+2, -z+2; #3 x-1, -y+3/2, z-1/2; #4 x+1, y, z+1; For **3**. #1 x+1, y, z+1; #2 -x+2, -y+2, -z+2; #3 x+1, -y+3/2, z+1/2; #4 x-1, -y+3/2, z-1/2; #5 x-1, y, z-1; For **4**. #1-x+1, -y+2, -z+1; #2 x, -y+3/2, z+1/2; #3 x-1, -y+3/2, z-1/2; #4 x,-y+3/2, z-1/2; For **5**. #1 x+1, y, z+1; #2 x+1, -y+3/2, z+1/2; #3 -x+2, -y+2, -z+2; #4 x-1, -y+3/2, z-1/2;For **6**. #1 x-1, y, z-1; #2 x-1, -y+1/2, z-1/2 ; #3 -x+1, -y, -z+1 ; #4 x+1, y, z+1; For **7**. #1 -x+2, -y+1, -z+2; #2 x, -y+1/2, z-1/2; #3 x+1, -y+1/2, z+1/2; #4 -x+1, y+1/2, -z+3/2; For **8**. #1 x-1, -y+1/2, z-1/2; #2 x-1, y, z-1; #3 -x, -y, -z ; #4 x+1, -y+1/2, z+1/2; For **9**. #1 x, -y+1/2, z-1/2; #2 x-1, y, z-1; #3 -x+1, -y, -z+1 ; #4 -x,-y,-z ; For **10**. #1 x-1, y, z-1; #2 x, -y+1/2, z-1/2 ; #3 -x+2, -y, -z+1; #4 -x+1, -y, -z; #5 x, -y+1/2, z+1/2.

Eq. 1:

$$\chi_{\mathrm{M}} = \frac{2Ng^2\beta^2}{kT} \times \frac{140e^{56J/kT} + 91e^{42J/kT} + 55e^{30J/kT} + 30e^{20J/kT} + 14e^{12J/kT} + 5e^{6J/kT} + e^{2J/kT}}{15e^{56J/kT} + 13e^{42J/kT} + 11e^{30J/kT} + 9e^{20J/kT} + 7e^{12J/kT} + 5e^{6J/kT} + 3e^{2J/kT} + 1}$$