

Supporting Information

A New Family 3d-4f Heterometallic Tetrazole-based Coordination Frameworks: *In Situ* Tetrazole Ligand Synthesis, Structure, Luminescence and Magnetic Properties

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Table S1 Selected Bond Distances (Å) and Angles (°) for Compounds **1-3**

Compound 1 ^(a)			
Cu(2)-N(3)	1.872(3)	Cu(2)-N(3)#2	1.872(3)
Eu(1)-O(3)	2.337(3)	Eu(1)-O(1W)#3	2.458(3)
Eu(1)-O(3)#3	2.337(3)	Eu(1)-O(1W)	2.458(3)
Eu(1)-O(4)#4	2.354(3)	Eu(1)-O(2W)#3	2.525(3)
Eu(1)-O(4)#1	2.354(3)	Eu(1)-O(2W)	2.525(3)
N(3)#2-Cu(2)-N(3)	180.000(1)		
O(3)-Eu(1)-O(3)#3	82.12(14)	O(1W)#3-Eu(1)-O(1W)	132.63(13)
O(3)-Eu(1)-O(4)#4	141.15(9)	O(3)-Eu(1)-O(2W)#3	80.73(9)
O(3)#3-Eu(1)-O(4)#4	110.87(10)	O(3)#3-Eu(1)-O(2W)#3	75.16(9)
O(3)-Eu(1)-O(4)#1	110.87(10)	O(4)#4-Eu(1)-O(2W)#3	137.34(9)
O(3)#3-Eu(1)-O(4)#1	141.15(9)	O(4)#1-Eu(1)-O(2W)#3	71.40(9)
O(4)#4-Eu(1)-O(4)#1	82.36(13)	O(1W)#3-Eu(1)-O(2W)#3	68.73(9)
O(3)-Eu(1)-O(1W)#3	146.38(9)	O(1W)-Eu(1)-O(2W)#3	125.80(9)
O(3)#3-Eu(1)-O(1W)#3	76.88(10)	O(3)-Eu(1)-O(2W)	75.16(9)
O(4)#4-Eu(1)-O(1W)#3	71.78(10)	O(3)#3-Eu(1)-O(2W)	80.73(9)
O(4)#1-Eu(1)-O(1W)#3	73.03(9)	O(4)#4-Eu(1)-O(2W)	71.40(9)
O(3)-Eu(1)-O(1W)	76.88(10)	O(4)#1-Eu(1)-O(2W)	137.34(9)
O(3)#3-Eu(1)-O(1W)	146.38(9)	O(1W)#3-Eu(1)-O(2W)	125.80(9)
O(4)#6-Eu(1)-O(1W)	73.03(9)	O(1W)-Eu(1)-O(2W)	68.73(9)
O(4)#4-Eu(1)-O(1W)	71.78(10)	O(2W)#3-Eu(1)-O(2W)	147.89(11)
Compound 2 ^(b)			
Cu(1)-N(2)	1.867(4)	Cu(1)-N(2)#1	1.867(4)
Gd(1)-O(3)	2.330(3)	Gd(1)-O(1W)#2	2.450(3)
Gd(1)-O(3)#2	2.330(3)	Gd(1)-O(1W)	2.450(3)
Gd(1)-O(4)#3	2.340(3)	Gd(1)-O(2W)#2	2.519(3)
Gd(1)-O(4)#4	2.340(3)	Gd(1)-O(2W)	2.519(3)
N(2)#1-Cu(1)-N(2)	180.000(1)		
O(3)#2-Gd(1)-O(3)	82.25(16)	O(1W)#2-Gd(1)-O(1W)	133.04(16)
O(3)#2-Gd(1)-O(4)#3	110.43(11)	O(3)#2-Gd(1)-O(2W)	80.50(11)
O(3)-Gd(1)-O(4)#3	141.23(12)	O(3)-Gd(1)-O(2W)	75.16(11)
O(3)#2-Gd(1)-O(4)#4	141.23(12)	O(4)#3-Gd(1)-O(2W)	71.38(11)
O(3)-Gd(1)-O(4)#4	110.43(11)	O(4)#4-Gd(1)-O(2W)	137.57(11)
O(4)#3-Gd(1)-O(4)#4	82.95(16)	O(1W)#2-Gd(1)-O(2W)	68.68(11)
O(3)#2-Gd(1)-O(1W)#2	146.12(12)	O(1W)-Gd(1)-O(2W)	125.90(11)
O(3)-Gd(1)-O(1W)#2	76.70(11)	O(3)#2-Gd(1)-O(2W)#2	75.16(11)
O(4)#3-Gd(1)-O(1W)#2	73.33(11)	O(3)-Gd(1)-O(2W)#2	80.50(11)
O(4)#4-Gd(1)-O(1W)#2	71.92(12)	O(4)#3-Gd(1)-O(2W)#2	137.57(11)
O(3)#2-Gd(1)-O(1W)	76.70(11)	O(4)#4-Gd(1)-O(2W)#2	71.38(11)
O(3)-Gd(1)-O(1W)	146.12(12)	O(1W)#2-Gd(1)-O(2W)#2	125.90(11)
O(4)#3-Gd(1)-O(1W)	71.92(12)	O(1W)-Gd(1)-O(2W)#2	68.68(11)
O(4)#4-Gd(1)-O(1W)	73.33(11)	O(2W)-Gd(1)-O(2W)#2	147.54(14)
Compound 3 ^(c)			

Cu(2)-N(2)	1.871(3)	Cu(2)-N(2)#1	1.871(3)
Tb(1)-O(4)	2.311(3)	Tb(1)-O(3)#2	2.327(3)
Tb(1)-O(1W)	2.442(3)	Tb(1)-O(3)#4	2.327(3)
Tb(1)-O(2W)	2.508(3)	Tb(1)-O(1W)#3	2.442(3)
Tb(1)-O(4)#3	2.311(3)	Tb(1)-O(2W)#3	2.508(3)
N(2)-Cu(2)-N(2)#1	180.0(2)		
O(4)#3-Tb(1)-O(4)	82.38(14)	O(1W)#3-Tb(1)-O(1W)	132.92(14)
O(4)#3-Tb(1)-O(3)#2	141.45(10)	O(4)#3-Tb(1)-O(2W)	80.34(9)
O(4)-Tb(1)-O(3)#2	110.29(10)	O(4)-Tb(1)-O(2W)	75.32(9)
O(4)#3-Tb(1)-O(3)#4	110.29(10)	O(3)#2-Tb(1)-O(2W)	137.50(10)
O(4)-Tb(1)-O(3)#4	141.45(10)	O(3)#4-Tb(1)-O(2W)	71.50(9)
O(3)#2-Tb(1)-O(3)#4	82.81(13)	O(1W)#3-Tb(1)-O(2W)	125.99(9)
O(4)#3-Tb(1)-O(1W)#3	76.80(10)	O(1W)-Tb(1)-O(2W)	68.65(9)
O(4)-Tb(1)-O(1W)#3	146.04(10)	O(4)#3-Tb(1)-O(2W)#3	75.32(9)
O(3)#2-Tb(1)-O(1W)#3	73.28(10)	O(4)-Tb(1)-O(2W)#3	80.34(9)
O(3)#4-Tb(1)-O(1W)#3	71.85(10)	O(3)#2-Tb(1)-O(2W)#3	71.50(9)
O(4)#3-Tb(1)-O(1W)	146.04(10)	O(3)#4-Tb(1)-O(2W)#3	137.50(10)
O(4)-Tb(1)-O(1W)	76.80(10)	O(1W)#3-Tb(1)-O(2W)#3	68.65(9)
O(3)#2-Tb(1)-O(1W)	71.85(10)	O(1W)-Tb(1)-O(2W)#3	125.99(9)
O(3)#4-Tb(1)-O(1W)	73.28(10)	O(2W)-Tb(1)-O(2W)#3	147.49(12)

- (a) #1: $-x, -y+1, -z$; #2: $-x+1/2, -y+1/2, -z+2$; #3: $-x, y, -z+1/2$; #4: $x, -y+1, z+1/2$;
- (b) #1: $-x+1/2, -y+1/2, -z+2$; #2: $-x, y, -z+1/2$; #3: $x, -y+1, z+1/2$; #4: $-x, -y+1, -z$;
- (c) #1: $-x+1/2, -y+1/2, -z-1$; #2: $-x+1, -y+1, -z+1$; #3: $-x+1, y, -z+1/2$; #4: $x, -y+1, z-1/2$.

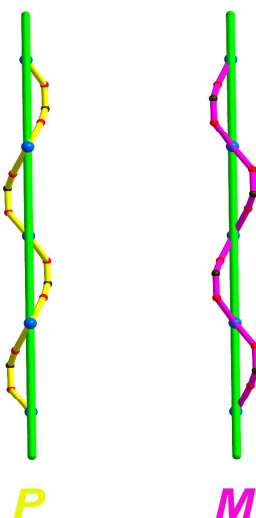


Figure S1. The double-strand *meso*-helical chain: *P* helical chain (left), *M* helical chain (right).

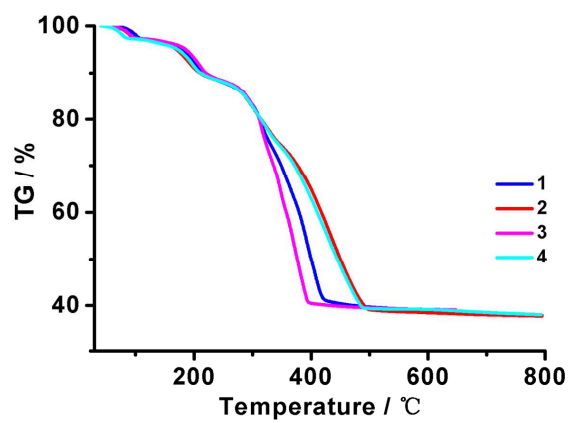


Figure S2. The TGA curves of compounds **1** (blue), **2** (red), **3** (magenta), **4** (cyan).

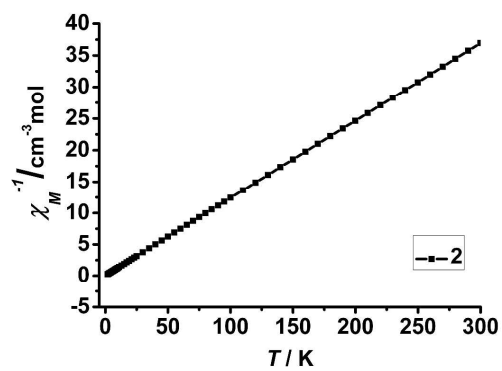


Figure S3. χ_M^{-1} vs T plots for compound **2**.

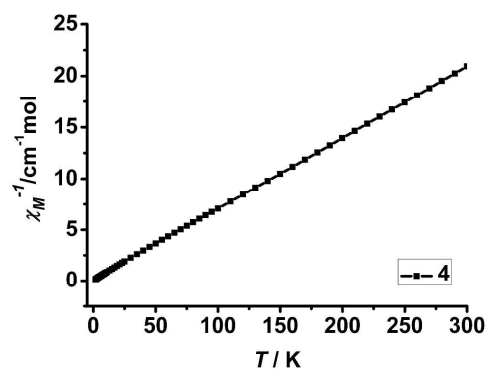


Figure S4. χ_M^{-1} vs T plots for compound **4**.

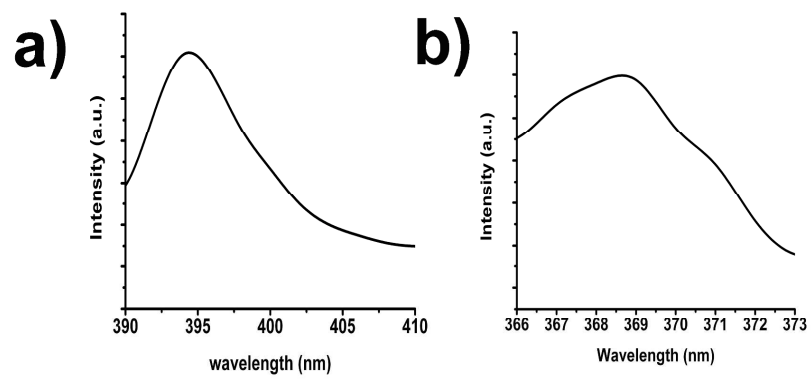


Figure S5. Solid state excitation spectra of **1** (a) and **3** (b) at room temperature.