Supplementary Materials

Series of novel 3D microporous heterometallic 3d-4f coordination frameworks with (5, 6) -connected topology: Synthesis, crystal structure and magnetic properties

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Compound 1			ſ
Eu(1)-O(2)	2.304(4)	Cu(1)-N(3)#2	1.980(4)
Eu(1)-O(3)	2.402(3)	Cu(1)-N(3)	1.980(4)
Eu(1)-O(5)	2.530(4)	Cu(1)-N(5)#3	2.041(4)
Eu(1)-O(6)	2.441(4)	Cu(1)-N(5)#4	2.041(4)
Eu(1)-O(7)	2.470(3)	Cu(1)-O(4)#2	2.411(3)
Eu(1)-O(8)	2.472(4)	Cu(1)-O(4)	2.411(3)
Eu(1)-O(3)#1	2.587(3)	Cu(2)-N(1)	1.967(4)
Eu(1)-O(4)#1	2.546(3)	Cu(2)-N(1)#5	1.967(4)
Eu(1)-O(1W)	2.424(4)	Cu(2)-N(4)#6	2.058(4)
O(2)-Eu(1)-O(3)	79.11(12)	Cu(2)-N(4)#7	2.058(4)
O(2)-Eu(1)-O(1W)	93.54(16)	Cu(2)-O(1)#5	2.412(4)
O(2)-Eu(1)-O(6)	80.36(14)	Cu(2)-O(1)	2.412(4)
O(3)-Eu(1)-O(6)	78.29(12)	N(3)#2-Cu(1)-N(3)	179.999(2)
O(1W)-Eu(1)-O(6)	122.72(14)	N(3)#2-Cu(1)-N(5)#3	90.19(16)
O(2)-Eu(1)-O(7)	124.63(12)	N(3)-Cu(1)-N(5)#3	89.81(16)
O(3)-Eu(1)-O(7)	88.90(12)	N(3)#2-Cu(1)-N(5)#4	89.81(16)
O(1W)-Eu(1)-O(7)	76.97(14)	N(3)-Cu(1)-N(5)#4	90.19(16)
O(6)-Eu(1)-O(7)	149.46(14)	N(5)#3-Cu(1)-N(5)#4	180.0(2)
O(2)-Eu(1)-O(8)	71.90(13)	N(3)#2-Cu(1)-O(4)#2	75.13(14)
O(3)-Eu(1)-O(8)	78.27(13)	N(3)-Cu(1)-O(4)#2	104.87(14)
O(1W)-Eu(1)-O(8)	78.34(15)	N(5)#3-Cu(1)-O(4)#2	88.97(14)
O(6)-Eu(1)-O(8)	146.45(14)	N(5)#4-Cu(1)-O(4)#2	91.03(14)
O(7)-Eu(1)-O(8)	52.73(12)	N(3)#2-Cu(1)-O(4)	104.87(14)
O(2)-Eu(1)-O(5)	79.04(12)	N(3)-Cu(1)-O(4)	75.13(14)
O(3)-Eu(1)-O(5)	128.52(12)	N(5)#3-Cu(1)-O(4)	91.03(14)
O(1W)-Eu(1)-O(5)	70.46(13)	N(5)#4-Cu(1)-O(4)	88.97(14)
O(6)-Eu(1)-O(5)	52.38(12)	O(4)#2-Cu(1)-O(4)	180.0
O(7)-Eu(1)-O(5)	140.99(12)	N(1)-Cu(2)-N(1)#5	180.00
O(8)-Eu(1)-O(5)	135.47(14)	N(1)-Cu(2)-N(4)#6	90.49(17)
O(2)-Eu(1)-O(4)#1	157.05(11)	N(1)#5-Cu(2)-N(4)#6	89.51(17)
O(3)-Eu(1)-O(4)#1	113.70(11)	N(1)-Cu(2)-N(4)#7	89.51(17)
O(1W)-Eu(1)-O(4)#1	81.26(15)	N(1)#5-Cu(2)-N(4)#7	90.49(17)
O(6)-Eu(1)-O(4)#1	83.73(13)	N(4)#6-Cu(2)-N(4)#7	180.00(1)
O(7)-Eu(1)-O(4)#1	76.18(11)	N(1)-Cu(2)-O(1)#5	104.36(15)
O(8)-Eu(1)-O(4)#1	127.91(12)	N(1)#5-Cu(2)-O(1)#5	75.64(14)
O(5)-Eu(1)-O(4)#1	78.16(12)	N(4)#6-Cu(2)-O(1)#5	89.65(15)
O(2)-Eu(1)-O(3)#1	138.43(12)	N(4)#7-Cu(2)-O(1)#5	90.35(15)
O(3)-Eu(1)-O(3)#1	63.25(13)	N(1)-Cu(2)-O(1)	75.64(15)
O(1W)-Eu(1)-O(3)#1	127.99(15)	N(1)#5-Cu(2)-O(1)	104.36(14)
O(6)-Eu(1)-O(3)#1	75.52(12)	N(4)#6-Cu(2)-O(1)	90.35(15)
O(7)-Eu(1)-O(3)#1	73.96(12)	N(4)#7-Cu(2)-O(1)	89.65(15)
O(8)-Eu(1)-O(3)#1	113.91(12)	O(1)#5-Cu(2)-O(1)	180.00

Table S1 Selected bond distances (Å) and angles (°) for complexes 1-5.

Compound 2			
Tb(1)-O(2)	2.288(3)	Cu(1)-N(3)#2	1.976(4)
Tb(1)-O(3)	2.365(4)	Cu(1)-N(3)	1.976(4)
Tb(1)-O(1W)	2.399(5)	Cu(1)-N(5)#3	2.036(4)
Tb(1)-O(6)	2.409(4)	Cu(1)-N(5)#4	2.036(4)
Tb(1)-O(7)	2.441(3)	Cu(1)-O(4)#2	2.391(3)
Tb(1)-O(8)	2.447(3)	Cu(1)-O(4)	2.391(3)
Tb(1)-O(5)	2.510(3)	Cu(2)-N(1)	1.969(4)
Tb(1)-O(4)#1	2.523(3)	Cu(2)-N(1)#5	1.969(4)
Tb(1)-O(3)#1	2.565(3)	Cu(2)-N(4)#6	2.056(4)
O(2)-Tb(1)-O(3)	80.47(12)	Cu(2)-N(4)#7	2.056(4)
O(2)-Tb(1)-O(1W)	92.90(14)	Cu(2)-O(1)	2.413(4)
O(3)-Tb(1)-O(1W)	156.32(11)	Cu(2)-O(1)#5	2.413(4)
O(2)-Tb(1)-O(6)	79.67(12)	N(3)-Cu(1)-N(3)#2	180.0(2)
O(3)-Tb(1)-O(6)	78.71(12)	N(3)-Cu(1)-N(5)#3	90.00(16)
O(1W)-Tb(1)-O(6)	122.71(13)	N(3)#2-Cu(1)-N(5)#3	90.00(16)
O(2)-Tb(1)-O(7)	125.35(11)	N(3)-Cu(1)-N(5)#4	90.00(16)
O(3)-Tb(1)-O(7)	88.18(12)	N(3)#2-Cu(1)-N(5)#4	90.00(16)
O(1W)-Tb(1)-O(7)	77.12(13)	N(5)#3-Cu(1)-N(5)#4	179.998(1)
O(6)-Tb(1)-O(7)	149.60(13)	N(3)-Cu(1)-O(4)	75.54(14)
O(2)-Tb(1)-O(8)	72.00(12)	N(3)#2-Cu(1)-O(4)	104.25(14)
O(3)-Tb(1)-O(8)	78.31(13)	N(5)#3-Cu(1)-O(4)	90.92(14)
O(1W)-Tb(1)-O(8)	78.02(14)	N(5)#4-Cu(1)-O(4)	89.08(14)
O(6)-Tb(1)-O(8)	145.94(14)	N(3)-Cu(1)-O(4)#2	104.25(14)
O(7)-Tb(1)-O(8)	53.35(12)	N(3)#2-Cu(1)-O(4)#2	75.54(14)
O(2)-Tb(1)-O(5)	78.38(11)	N(5)#3-Cu(1)-O(4)#2	89.08(14)
O(3)-Tb(1)-O(5)	129.71(12)	N(5)#4-Cu(1)-O(4)#2	90.92(14)
O(1W)-Tb(1)-O(5)	69.88(13)	O(4)-Cu(1)-O(4)#2	180.00
O(6)-Tb(1)-O(5)	52.91(13)	N(1)-Cu(2)-N(1)#5	180.00
O(7)-Tb(1)-O(5)	140.45(13)	N(1)-Cu(2)-N(4)#6	89.18(16)
O(8)-Tb(1)-O(5)	134.63(12)	N(1)#5-Cu(2)-N(4)#6	90.82(16)
O(2)-Tb(1)-O(4)#1	156.40(10)	N(1)-Cu(2)-N(4)#7	90.82(16)
O(3)-Tb(1)-O(4)#1	113.91(11)	N(1)#5-Cu(2)-N(4)#7	89.18(16)
O(1W)-Tb(1)-O(4)#1	80.57(13)	N(4)#6-Cu(2)-N(4)#7	180.0
O(6)-Tb(1)-O(4)#1	84.85(12)	N(1)-Cu(2)-O(1)	75.44(15)
O(7)-Tb(1)-O(4)#1	75.53(10)	N(1)#5-Cu(2)-O(1)	104.56(15)
O(8)-Tb(1)-O(4)#1	127.63(12)	N(4)#6-Cu(2)-O(1)	89.80(14)
O(5)-Tb(1)-O(4)#1	78.08(11)	N(4)#7-Cu(2)-O(1)	90.20(14)
O(2)-Tb(1)-O(3)#1	138.94(13)	N(1)-Cu(2)-O(1)#5	104.56(15)
O(3)-Tb(1)-O(3)#1	62.78(13)	N(1)#5-Cu(2)-O(1)#5	75.44(15)
O(1W)-Tb(1)-O(3)#1	128.09(13)	N(4)#6-Cu(2)-O(1)#5	90.20(14)
O6-Tb(1)-(3)#1	75.93(12)	N(4)#7-Cu(2)-O(1)#5	89.80(14)

O(7)-Tb(1)-O(3)#1	73.68(11)	O(1)-Cu(2)-O(1)#5	180.00(1)			
O(8)-Tb(1)-O(3)#1	114.35(11)	O(4)#1-Tb(1)-O(3)#1	51.14(11)			
O(5)-Tb(1)-O(3)#1	100.62(10)					
Compound 3						
Gd(1)-O(7)	2.296(6)	Cu(1)-N(3)#2	1.995(7)			
Gd(1)-O(15)	2.374(6)	Cu(1)-N(3)#3	1.995(7)			
Gd(1)-O(3)	2.424(6)	Cu(1)-N(5)#4	2.045(7)			
Gd(1)-O(1W)	2.415(7)	Cu(1)-N(5)	2.045(7)			
Gd(1)-O(2)	2.457(6)	Cu(1)-O(30)#2	2.405(6)			
Gd(1)-O(1)	2.455(7)	Cu(1)-O(30)#3	2.405(6)			
Gd(1)-O(4)	2.513(6)	Cu(2)-N(1)#5	1.965(7)			
Gd(1)-O(30)#1	2.533(6)	Cu(2)-N(1)#6	1.965(7)			
Gd(1)-O(15)#1	2.585(6)	Cu(2)-N(4)#7	2.053(7)			
O(7)-Gd(1)-O(15)	79.6(2)	Cu(2)-N(4)	2.053(7)			
O(7)-Gd(1)-O(3)	80.2(2)	Cu(2)-O(12)#5	2.402(7)			
O(15)-Gd(1)-O(3)	78.6(2)	Cu(2)-O(12)#6	2.402(7)			
O(7)-Gd(1)-O(1W)	93.5(3)	N(3)#2-Cu(1)-N(3)#3	180.00(4)			
O(15)-Gd(1)-O(1W)	156.1(2)	N(3)#2-Cu(1)-N(5)#4	89.0(3)			
O(3)-Gd(1)-O(1W)	123.2(2)	N(3)#3-Cu(1)-N(5)#4	91.0(3)			
O(7)-Gd(1)-O(2)	124.8(2)	N(3)#2-Cu(1)-N(5)	91.0(3)			
O(15)-Gd(1)-O(2)	88.3(2)	N(3)#3-Cu(1)-N(5)	89.0(3)			
O(3)-Gd(1)-O(2)	149.4(2)	N(5)#4-Cu(1)-N(5)	179.999(1)			
O(1W)-Gd(1)-O(2)	76.8(2)	N(3)#2-Cu(1)-O(30)#2	75.00(2)			
O(7)-Gd(1)-O(1)	71.9(2)	N(3)#3-Cu(1)-O(30)#2	105.00(2)			
O(15)-Gd(1)-O(1)	78.2(2)	N(5)#4-Cu(1)-O(30)#2	91.20(2)			
O(3)-Gd(1)-O(1)	146.3(2)	N(5)-Cu(1)-O(30)#2	88.80(2)			
O(1W)-Gd(1)-O(1)	77.9(3)	N(3)#2-Cu(1)-O(30)#3	105.00(2)			
O(2)-Gd(1)-O(1)	52.9(2)	N(3)#3-Cu(1)-O(30)#3	75.00(2)			
O(7)-Gd(1)-O(4)	78.9(2)	N(5)#4-Cu(1)-O(30)#3	88.80(2)			
O(15)-Gd(1)-O(4)	129.3(2)	N(5)-Cu(1)-O(30)#3	91.20(2)			
O(3)-Gd(1)-O(4)	52.8(2)	O(30)#2-Cu(1)-O(30)#3	180.0			
O(1W)-Gd(1)-O(4)	70.5(2)	N(1)#5-Cu(2)-N(1)#6	180.0(3)			
O(2)-Gd(1)-O(4)	140.9(2)	N(1)#5-Cu(2)-N(4)#7	89.5(3)			
O(1)-Gd(1)-O(4)	135.0(2)	N(1)#6-Cu(2)-N(4)#7	90.5(3)			
O(7)-Gd(1)-O(30)#1	156.8(2)	N(1)#5-Cu(2)-N(4)	90.5(3)			
O(15)-Gd(1)-O(30)#1	114.02(19)	N(1)#6-Cu(2)-N(4)	89.5(3)			
O(3)-Gd(1)-O(30)#1	84.2(2)	N(4)#7-Cu(2)-N(4)	179.999(2)			
O(1W)-Gd(1)-O(30)#1	80.7(2)	N(1)#5-Cu(2)-O(12)#5	75.4(3)			
O(2)-Gd(1)-O(30)#1	76.0(2)	N(1)#6-Cu(2)-O(12)#5	104.6(3)			
O(1)-Gd(1)-O(30)#1	127.7(2)	N(4)#7-Cu(2)-O(12)#5	89.8(3)			
O(4)-Gd(1)-O(30)#1	78.0(2)	N(4)-Cu(2)-O(12)#5	90.2(3)			
O(7)-Gd(1)-O(15)#1	138.2(2)	N(1)#5-Cu(2)-O(12)#6	104.6(3)			
O(15)-Gd(1)-O(15)#1	62.9(2)	N(1)#6-Cu(2)-O(12)#6	75.4(3)			
O(3)-Gd(1)-O(15)#1	75.2(2)	N(4)#7-Cu(2)-O(12)#6	90.2(3)			

O(1W)-Gd(1)-O(15)#1	128.2(2)	N(4)-Cu(2)-O(12)#6	89.8(3)			
O(2)-Gd(1)-O(15)#1	74.2(2)	O(12)#5-Cu(2)-O(12)#6	179.999(2)			
O(1)-Gd(1)-O(15)#1	114.3(2)	O(30)#1-Gd(1)-O(15)#1	51.16(18)			
O(4)-Gd(1)-O(15)#1	110.3(2)					
Compound 4						
$D_{v}(1) = O(2)$	2.2/1(11)	$C_{u}(1) N(3) #2$	1.000(12)			
Dy(1) - O(2) Dy(1) - O(3)	2.241(11) 2 3/10(10)	Cu(1) - N(3) = 0	1.990(12) 1.000(12)			
Dy(1) - O(1W)	2.349(10) 2 358(15)	Cu(1)-N(5)	2.056(11)			
Dy(1) - O(6)	2.330(13) 2.304(13)	Cu(1) - N(5) #4	2.050(11) 2.056(11)			
Dy(1) - O(0)	2.374(13)	Cu(1) - N(3) # 2	2.030(11) 2.378(10)			
Dy(1) - O(7) Dy(1) - O(8)	2.410(11) 2.435(11)	$Cu(1)-O(4)\pi 2$	2.378(10) 2 378(10)			
Dy(1) - O(8)	2.433(11) 2.500(10)	Cu(1) - O(4)	2.378(10) 1.071(14)			
Dy(1) - O(3)	2.500(10) 2.546(0)	Cu(2) - N(1)	1.971(14) 1.971(14)			
Dy(1) - O(3) # 1 Dy(1) - O(4) # 1	2.540(7)	Cu(2) - N(1) # 5	1.971(14) 2.056(12)			
$Dy(1) - O(4)\pi 1$ O(2) Dy(1) O(2)	2.327(10)	Cu(2) - N(4) # 7	2.030(12)			
O(2)-Dy(1)-O(3) O(2) Dy(1) $O(1W)$	00.0(4)	Cu(2) - N(4) # 7 Cu(2) - O(1) # 5	2.030(12)			
O(2)-Dy(1)-O(1W) O(2) Dy(1) $O(1W)$	92.3(3)	Cu(2) - O(1) # 3	2.424(12)			
O(3)-Dy(1)-O(1W)	130.5(3)	U(2)+U(1) $V(2)+2$ $C_{12}(1)$ $V(2)$	2.424(12)			
O(2)-Dy(1)-O(0) O(2) Dy(1) O(6)	79.0(4) 78.0(4)	N(3)#2-Cu(1)-N(3) N(2)#2-Cu(1)-N(5)#3	179.999(2)			
O(3)-Dy(1)-O(0)	10.9(4)	N(3)#2-Cu(1)-N(3)#3 N(2) Cu(1) N(5)#2	90.7(3)			
O(1W) - Dy(1) - O(0)	122.4(4)	N(3)-Cu(1)-N(3)=3	89.3(3)			
O(2)-Dy(1)-O(7)	125.0(4)	N(3)#2-Cu(1)-N(3)#4	89.3(5)			
O(3)-Dy(1)-O(7)	87.1(4)	N(3)-Cu(1)-N(3)#4	90.7(5)			
O(1W) - Dy(1) - O(7)	78.3(4) 140.5(4)	N(3)#3-Cu(1)-N(3)#4 N(3)#2 Cr(1) O(4)#2	180.0(7)			
O(6)-Dy(1)-O(7)	149.5(4)	N(3)#2-Cu(1)-O(4)#2	75.5(4)			
O(2)-Dy(1)-O(8)	/1./(4)	N(3)-Cu(1)-O(4)#2	104.5(4)			
O(3)-Dy(1)-O(8)	/8.4(4)	N(5)#3-Cu(1)-O(4)#2	89.4(4)			
O(6)-Dy(1)-O(8)	145.3(4)	N(5)#4-Cu(1)-O(4)#2	90.6(4)			
O(7)-Dy(1)-O(8)	53.9(4)	N(3)#2-Cu(1)-O(4)	104.5(4)			
O(2)-Dy(1)-O(5)	78.6(4)	N(3)-Cu(1)-O(4)	75.5(4)			
O(3)-Dy(1)-O(5)	130.3(4)	N(5)#3-Cu(1)-O(4)	90.6(4)			
O(1W)-Dy(1)-O(5)	69.4(4)	N(5)#4-Cu(1)-O(4)	89.4(4)			
O(1W)-Dy(1)-O(8)	77.9(4)	O(4)#2-Cu(1)-O(4)	179.999(1)			
O(6)-Dy(1)-O(5)	53.0(4)	N(1)-Cu(2)-N(1)#5	179.999(1)			
O(7)-Dy(1)-O(5)	140.8(4)	N(1)-Cu(2)-N(4)#6	88.7(5)			
O(8)-Dy(1)-O(5)	134.2(4)	N(1)#5-Cu(2)-N(4)#6	91.3(5)			
O(2)-Dy(1)-O(3)#1	138.3(4)	N(1)-Cu(2)-N(4)#7	91.3(5)			
O(3)-Dy(1)-O(3)#1	62.1(4)	N(1)#5-Cu(2)-N(4)#7	88.7(5)			
O(1W)-Dy(1)-O(3)#1	129.1(4)	N(4)#6-Cu(2)-N(4)#7	179.999(1)			
O(6)-Dy(1)-O(3)#1	76.0(4)	N(1)-Cu(2)-O(1)#5	105.8(5)			
O(7)-Dy(1)-O(3)#1	73.5(4)	N(1)#5-Cu(2)-O(1)#5	74.2(5)			
O(8)-Dy(1)-O(3)#1	115.0(3)	N(4)#6-Cu(2)-O(1)#5	90.9(5)			
O(5)-Dy(1)-O(3)#1	110.4(3)	N(4)#7-Cu(2)-O(1)#5 89.1(5)				
O(2)-Dy(1)-O(4)#1	156.0(3)	N(1)-Cu(2)-O(1)	74.2(5)			
O(3)-Dy(1)-O(4)#1	114.2(3)	N(1)#5-Cu(2)-O(1)	105.8(5)			

O(1)#5-Cu(2)-O(1)	179.999(1)	N(4)#6-Cu(2)-O(1)	89.1(5)	
		N(4)#7-Cu(2)-O(1)	90.9(5)	
Compound 5				
Ho(1)-O(2)	2.270(4)	Cu(1)-N(3)	1.985(4)	
Ho(1)-O(3)	2.337(4)	Cu(1)-N(3)#2	1.985(4)	
Ho(1)-O(1W)	2.370(5)	Cu(1)-N(5)#3	2.032(4	
Ho(1)-O(6)	2.390(4)	Cu(1)-N(5)#4	2.032(4)	
Ho(1)-O(7)	2.420(3)	Cu(1)-O(4)	2.393(4)	
Ho(1)-O(8)	2.426(4)	Cu(1)-O(4)#2	2.393(4)	
Ho(1)-O(5)	2.489(3)	Cu(2)-N(1)	1.973(4)	
Ho(1)-O(4)#1	2.498(3)	Cu(2)-N(1)#5	1.973(4)	
Ho(1)-O(3)#1	2.548(4)	Cu(2)-N(4)#6	2.048(4)	
O(2)-Ho(1)-O(3)	80.57(13)	Cu(2)-N(4)#7	2.048(4)	
O(2)-Ho(1)-O(1W)	92.85(15)	Cu(2)-O(1)#5	2.408(4)	
O(3)-Ho(1)-O(1W)	156.03(12)	Cu(2)-O(1)	2.408(4)	
O(2)-Ho(1)-O(6)	79.73(13)	N(3)#2-Cu(1)-N(3)	180.0(2)	
O(3)-Ho(1)-O(6)	79.04(13)	N(3)#2-Cu(1)-N(5)#3	89.71(17)	
O(1W)-Ho(1)-O(6)	122.71(14)	N(3)-Cu(1)-N(5)#3	90.29(17)	
O(2)-Ho(1)-O(7)	125.56(12)	N(3)#2-Cu(1)-N(5)#4	90.29(17)	
O(3)-Ho(1)-O(7)	88.12(13)	N(3)-Cu(1)-N(5)#4	89.71(17)	
O(1W)-Ho(1)-O(7)	76.96(14)	N(5)#3-Cu(1)-N(5)#4	180.000(1)	
O(6)-Ho(1)-O(7)	149.52(13)	N(3)#2-Cu(1)-O(4)	104.30(14)	
O(2)-Ho(1)-O(8)	71.91(12)	N(3)-Cu(1)-O(4)	75.70(15)	
O(3)-Ho(1)-O(8)	78.26(13)	N(5)#3-Cu(1)-O(4)	89.25(15)	
O(1W)-Ho(1)-O(8)	77.94(14)	N(5)#4-Cu(1)-O(4)	90.75(14)	
O(6)-Ho(1)-O(8)	146.04(15)	N(3)#2-Cu(1)-O(4)#2	75.69(14)	
O(7)-Ho(1)-O(8)	53.65(13)	N(3)-Cu(1)-O(4)#2	104.31(14)	
O(2)-Ho(1)-O(5)	78.35(12)	N(5)#3-Cu(1)-O(4)#2	90.75(15)	
O(3)-Ho(1)-O(5)	130.26(13)	N(5)#4-Cu(1)-O(4)#2	89.25(15)	
O(1W)-Ho(1)-O(5)	69.62(14)	O(4)-Cu(1)-O(4)#2	180.0	
O(6)-Ho(1)-O(5)	53.17(14)	N(1)-Cu(2)-N(1)#5	180.0(2)	
O(7)-Ho(1)-O(5)	140.00(14)	N(1)-Cu(2)-N(4)#6	90.70(17)	
O(8)-Ho(1)-O(5)	134.19(13)	N(1)#5-Cu(2)-N(4)#6	89.30(17)	
O(2)-Ho(1)-O(4)#1	155.73(11)	N(1)-Cu(2)-N(4)#7	89.30(17)	
O(3)-Ho(1)-O(4)#1	114.50(12)	N(1)#5-Cu(2)-N(4)#7	90.70(17)	
O(1W)-Ho(1)-O(4)#1	80.22(13)	N(4)#6-Cu(2)-N(4)#7	180.0	
O(6)-Ho(1)-O(4)#1	84.53(12)	N(1)-Cu(2)-O(1)#5	104.31(16)	
O(7)-Ho(1)-O(4)#1	75.79(11)	N(1)#5-Cu(2)-O(1)#5	75.69(16)	
O(8)-Ho(1)-O(4)#1	128.05(12)	N(4)#6-Cu(2)-O(1)#5	89.56(15)	
O(5)-Ho(1)-O(4)#1	77.43(11)	N(4)#7-Cu(2)-O(1)#5	90.44(15)	
O(2)-Ho(1)-O(3)#1	138.97(14)	N(1)-Cu(2)-O(1)	75.68(16)	
O(3)-Ho(1)-O(3)#1	62.85(14)	N(1)#5-Cu(2)-O(1)	104.32(16)	
O(1W)-Ho(1)-O(3)#1	128.10(14)	N(4)#6-Cu(2)-O(1)	90.44(15)	
O(6)-Ho(1)-O(3)#1	75.82(12)	N(4)#7-Cu(2)-O(1)	89.56(15)	

	O(7)-Ho(1)-O(3)#1	73.72(12)	O(1)#5-Cu(2) - O(1)	180.0
	O(8)-Ho(1)-O(3)#1	114.67	(12)	O(4)#1-Ho(1	O(4)#1-Ho(1)-O(3)#1	
	O(5)-Ho(1)-O(3)#1	1 110.71(11				
Symmetry codes for 1 : #1 -x+1,-y,-z+2		-z+2	#2 -x	+2,-y,-z+2	#3 -x+2,-y-1	,-z+2
#4 x,y+1,z			#5 -x+2,-y,-z+1		#6 -x+1,-y+1,-z+1	
#7 x+1,y-1,z		Z	#8 x-1,y+1,z		#9 x,y-1,z	
Symmetry codes for 2 : #1 -x+1,-y,-z+		-z+2	#2 -x+2,-y,-z+2		#3 -x+2,-y-1,-z+2	
	#4 x,y+1,z		#5 -x-	+2,-y,-z+1	#6 x+1,y-1,z	
	#7 -x+1,-y+	1,-z+1	#8 x-	1,y+1,z	#9 x,y-1,z	
Symmetry codes for 3 :#1 -x+1,-y+2,-z+2		2,-z+2	#2 x,y-1,z		#3 -x+2,-y+1,-z+2	
	#4 -x+2,-y,-	z+2	#5 -:	x+1,-y+3,-z+1	#6 x-1,y+1	,Z
	#7 -x,-y+4,-	z+1	#8 x	+1,y-1,z	#9 x,y+1,z	
Symmet	ry codes for 4 : #1 -x+1,-y,	-z+2	#2 -x	+2,-y,-z+2	#3 -x+2,-y-1	l,-z+2
	#4 x,y+1,z		#5 -2	x+2,-y,-z+1	#6 x+1,y-1,z	
	#7 -x+1,-y+	1,-z+1	#8 x	-1,y+1,z	#9 x,y-1,z	
Symmet	ry codes for 5 : #1 -x+1,-y,	-z+2	#2 -	x+2,-y,-z+2	#3 x,y+1,z	
	#4 -x+2,-y-	l,-z+2	#5 -	-x+2,-y,-z+1	#6 -x+1,-y+	-1,-z+1
	#7 x+1,y-1,	Z	#8 :	x-1,y+1,z	#9 x,y-1,z	



Figure S1. PXRD patterns (a) simulated based on the X-ray single-crystal diffraction data of 1, (b) for as-synthesized 1, (c) for as-synthesized 2, (d) for as-synthesized 3, (e) for as-synthesized 4, and (f) for as-synthesized 5.



Figure S2. TG curve of complexes 1-5.



Figure S3. IR spectra of compound 1.



Figure S5. IR spectra of compound 3.



Figure S7. IR spectra of compound 5.