Electronic Supplementary Information

Construction of a family of Ln_3 clusters using multidentate Schiff base and β-diketonate ligands: fluorescent properties, magnetocaloric effect and slow magnetic relaxation

Wen-Min Wang,[a,b*] Yu Gao,[a] Rong-Xin Yue,[a] Na Qiao,[a] Dan-Tong Wang,[a] Ying Shi,[a] Huan Zhang*[c] and Jian-Zhong Cui*[b]

Table S1. The important bond lengths and angles for cluster **1**.

Bond lengths			
Nd(2)-O(6)	2.353(5)	Nd(3)-O(16)	2.276(5)
Nd(2)-O(3)	2.353(5)	Nd(3)-N(4)	2.464(7)
Nd(2)-O(11)	2.257(5)	Nd(3)-O(14)	2.261(6)
Nd(2)-O(5)	2.285(5)	Nd(3)-O(4)	2.386(6)
Nd(2)-O(12)	2.270(5)	Nd(1)-O(6)	2.304(5)
Nd(2)-N(3)	2.491(6)	Nd(1)-O(8)	2.299(5)
Nd(2)-N(6)	2.527(7)	Nd(1)-O(10)	2.260(6)
Nd(2)-O(2)	2.288(5)	Nd(1)-O(9)	2.299(5)
Nd(3)-O(3)	2.316(5)	Nd(1)-O(1)	2.408(6)
Nd(3)-O(13)	2.322(5)	Nd(1)-O(7)	2.272(6)
Nd(3)-O(15)	2.277(6)	Nd(1)-N(1)	2.477(7)
Nd(3)-O(5)	2.330(5)	Nd(1)-O(2)	2.337(5)
Bond angles			
O(3)-Nd(2)-O(6)	161.86(17)	O(16)-Nd(3)-O(4)	85.4(2)
O(11)-Nd(2)-O(6)	84.09(18)	O(14)-Nd(3)-O(3)	86.9(2)
O(11)-Nd(2)-O(3)	79.89(19)	O(14)-Nd(3)-O(13)	72.2(2)
O(11)-Nd(2)-O(5)	107.78(17)	O(14)-Nd(3)-O(15)	73.5(2)
O(11)-Nd(2)-O(12)	75.62(18)	O(14)-Nd(3)-O(5)	139.60(19)
O(11)-Nd(2)-O(2)	152.73(19)	O(14)-Nd(3)-O(16)	143.8(2)
O(5)-Nd(2)-O(6)	125.43(18)	O(14)-Nd(3)-O(4)	76.6(2)
O(5)-Nd(2)-O(3)	68.33(17)	O(6)-Nd(1)-O(1)	162.7(2)
O(5)-Nd(2)-O(2)	87.51(18)	O(6)-Nd(1)-O(2)	68.69(18)

[a] *Department of Chemistry, Taiyuan Normal University, Jinzhong 030619, China*

[b] *Department of Chemistry, Tianjin University, Tianjin 300072, China*

[c] *School of Science, Tianjin University of Science & Technology, Tianjin 300457, China*

**Corresponding Authors E-mail : cuijianzhong@tju.edu.cn, zhanghuan50423@163.com, wangwenmin0506@126.com*

O(12)-Nd(2)-O(6)	81.06(19)	O(8)-Nd(1)-O(6)	87.27(19)
O(12)-Nd(2)-O(3)	86.73(19)	O(8)-Nd(1)-O(9)	143.1(2)
O(12)-Nd(2)-O(5)	153.27(19)	O(8)-Nd(1)-O(1)	96.5(2)
O(12)-Nd(2)-O(2)	100.99(19)	O(8)-Nd(1)-O(2)	73.47(19)
O(2)-Nd(2)-O(6)	68.70(18)	O(10)-Nd(1)-O(6)	83.9(2)
O(2)-Nd(2)-O(3)	127.27(18)	O(10)-Nd(1)-O(8)	143.9(2)
O(3)-Nd(3)-O(13)	86.48(19)	O(10)-Nd(1)-O(9)	72.8(2)
O(3)-Nd(3)-O(5)	68.21(18)	O(10)-Nd(1)-O(1)	83.2(2)
O(3)-Nd(3)-O(4)	161.8(2)	O(10)-Nd(1)-O(7)	72.5(2)
O(13)-Nd(3)-O(5)	74.90(19)	O(10)-Nd(1)-O(2)	133.54(19)
O(13)-Nd(3)-O(4)	95.6(2)	O(9)-Nd(1)-O(6)	104.57(19)
O(15)-Nd(3)-O(3)	87.9(2)	O(9)-Nd(1)-O(1)	82.4(2)
O(15)-Nd(3)-O(13)	145.4(2)	O(9)-Nd(1)-O(2)	78.6(2)
O(15)-Nd(3)-O(5)	133.33(18)	O(7)-Nd(1)-O(6)	88.7(2)
O(15)-Nd(3)-O(4)	80.2(2)	O(7)-Nd(1)-O(8)	72.4(2)
O(5)-Nd(3)-O(4)	129.8(2)	O(7)-Nd(1)-O(9)	141.1(2)
O(16)-Nd(3)-O(3)	104.22(19)	O(7)-Nd(1)-O(1)	76.5(2)
O(16)-Nd(3)-O(13)	141.58(19)	O(7)-Nd(1)-O(2)	139.6(2)
O(16)-Nd(3)-O(15)	72.70(19)	O(2)-Nd(1)-O(1)	128.6(2)
O(16)-Nd(3)-O(5)	75.27(19)		

Table S2. The important bond lengths and angles for cluster **2**.

Bond lengths			
Sm(2)-O(6)	2.415(4)	Sm(1)-O(1)	2.467(5)
Sm(2)-O(14)	2.330(4)	Sm(1)-O(11)	2.341(4)
Sm(2)-O(13)	2.351(4)	Sm(1)-O(15)	2.400(4)
Sm(2)-O(2)	2.378(4)	Sm(1)-N(1)	2.562(5)
Sm(2)-O(3)	2.412(4)	Sm(3)-O(9)	2.330(5)
Sm(2)-O(5)	2.385(4)	Sm(3)-O(3)	2.391(4)
Sm(2)-N(6)	2.583(5)	Sm(3)-O(5)	2.413(4)
Sm(2)-N(3)	2.615(5)	Sm(3)-O(4)	2.491(5)
Sm(1)-O(12)	2.367(5)	Sm(3)-O(10)	2.375(4)
Sm(1)-O(6)	2.389(4)	Sm(3)-O(8)	2.385(4)
Sm(1)-O(16)	2.341(5)	Sm(3)-O(7)	2.341(4)
Sm(1)-O(2)	2.403(4)	Sm(3)-N(4)	2.569(6)
Bond angles			
O(14)-Sm(2)-O(6)	83.04(15)	O(11)-Sm(1)-O(12)	70.69(15)
O(14)-Sm(2)-O(13)	73.04(14)	O(11)-Sm(1)-O(6)	102.32(15)
O(14)-Sm(2)-O(2)	108.04(14)	O(11)-Sm(1)-O(2)	75.93(14)
O(14)-Sm(2)-O(3)	83.41(15)	O(11)-Sm(1)-O(1)	86.21(18)
O(14)-Sm(2)-O(5)	152.84(15)	O(11)-Sm(1)-O(15)	142.64(15)
O(13)-Sm(2)-O(6)	87.20(15)	O(15)-Sm(1)-O(2)	74.16(14)
O(13)-Sm(2)-O(2)	154.87(15)	O(15)-Sm(1)-O(1)	93.39(19)
O(13)-Sm(2)-O(3)	82.19(15)	O(9)-Sm(3)-O(3)	84.24(16)

O(13)-Sm(2)-O(5)	102.94(14)	O(9)-Sm(3)-O(5)	134.66(15)
O(2)-Sm(2)-O(6)	68.33(14)	O(9)-Sm(3)-O(4)	85.00(17)
O(2)-Sm(2)-O(3)	122.92(14)	O(9)-Sm(3)-O(10)	70.94(16)
O(2)-Sm(2)-O(5)	87.03(13)	O(9)-Sm(3)-O(8)	143.59(16)
O(3)-Sm(2)-O(6)	164.76(14)	O(9)-Sm(3)-O(7)	74.69(16)
O(5)-Sm(2)-O(6)	123.97(14)	O(3)-Sm(3)-O(5)	69.31(14)
O(5)-Sm(2)-O(3)	69.44(14)	O(3)-Sm(3)-O(4)	165.53(16)
O(12)-Sm(1)-O(6)	87.19(15)	O(5)-Sm(3)-O(4)	125.10(15)
O(12)-Sm(1)-O(2)	132.87(14)	O(10)-Sm(3)-O(3)	104.31(15)
O(12)-Sm(1)-O(1)	84.54(19)	O(10)-Sm(3)-O(5)	80.53(15)
O(12)-Sm(1)-O(15)	146.53(15)	O(10)-Sm(3)-O(4)	81.17(16)
O(6)-Sm(1)-O(2)	68.36(14)	O(10)-Sm(3)-O(8)	145.38(16)
O(6)-Sm(1)-O(1)	165.45(17)	O(8)-Sm(3)-O(3)	86.40(15)
O(6)-Sm(1)-O(15)	86.93(16)	O(8)-Sm(3)-O(5)	72.59(15)
O(16)-Sm(1)-O(12)	76.34(16)	O(8)-Sm(3)-O(4)	96.63(16)
O(16)-Sm(1)-O(6)	88.40(16)	O(7)-Sm(3)-O(3)	89.47(16)
O(16)-Sm(1)-O(2)	138.51(15)	O(7)-Sm(3)-O(5)	137.93(15)
O(16)-Sm(1)-O(1)	78.03(18)	O(7)-Sm(3)-O(4)	78.36(17)
O(16)-Sm(1)-O(11)	144.58(16)	O(7)-Sm(3)-O(10)	141.17(16)
O(16)-Sm(1)-O(15)	70.59(16)	O(7)-Sm(3)-O(8)	70.10(16)
O(2)-Sm(1)-O(1)	125.68(17)		

Table S3. The important bond lengths and angles for cluster **3**.

Bond lengths			
Gd(2)-O(11)	2.310(7)	Gd(3)-O(5)	2.391(6)
Gd(2)-O(12)	2.308(6)	Gd(3)-O(14)	2.316(7)
Gd(2)-O(3)	2.418(6)	Gd(3)-O(4)	2.464(7)
Gd(2)-O(5)	2.377(6)	Gd(3)-N(4)	2.545(8)
Gd(2)-O(2)	2.369(7)	Gd(1)-O(8)	2.339(7)
Gd(2)-N(6)	2.602(9)	Gd(1)-O(10)	2.355(7)
Gd(2)-O(6)	2.393(6)	Gd(1)-O(2)	2.397(7)
Gd(2)-N(3)	2.597(8)	Gd(1)-O(7)	2.336(7)
Gd(3)-O(16)	2.347(7)	Gd(1)-O(9)	2.304(8)
Gd(3)-O(13)	2.383(7)	Gd(1)-N(1)	2.541(9)
Gd(3)-O(3)	2.339(6)	Gd(1)-O(1)	2.453(8)
Gd(3)-O(15)	2.321(7)	Gd(1)-O(6)	2.360(7)
Bond angles			
O(11)-Gd(2)-O(3)	85.4(2)	O(5)-Gd(3)-O(4)	126.4(2)
O(11)-Gd(2)-O(5)	103.7(2)	O(14)-Gd(3)-O(16)	142.9(3)
O(11)-Gd(2)-O(2)	151.2(2)	O(14)-Gd(3)-O(13)	71.2(2)
O(11)-Gd(2)-O(6)	83.7(2)	O(14)-Gd(3)-O(3)	90.5(2)
O(12)-Gd(2)-O(11)	73.8(2)	O(14)-Gd(3)-O(15)	74.2(3)
O(12)-Gd(2)-O(3)	81.8(2)	O(14)-Gd(3)-O(5)	138.8(2)
O(12)-Gd(2)-O(5)	149.8(2)	O(14)-Gd(3)-O(4)	78.9(2)

O(12)-Gd(2)-O(2)	108.3(2)	O(8)-Gd(1)-O(10)	142.9(2)
O(12)-Gd(2)-O(6)	85.6(2)	O(8)-Gd(1)-O(2)	75.1(2)
O(5)-Gd(2)-O(3)	68.1(2)	O(8)-Gd(1)-O(1)	94.6(3)
O(5)-Gd(2)-O(6)	124.4(2)	O(8)-Gd(1)-O(6)	86.1(2)
O(2)-Gd(2)-O(3)	123.4(2)	O(10)-Gd(1)-O(2)	75.1(2)
O(2)-Gd(2)-O(5)	88.3(2)	O(10)-Gd(1)-O(1)	86.0(3)
O(2)-Gd(2)-O(6)	68.2(2)	O(10)-Gd(1)-O(6)	102.7(3)
O(6)-Gd(2)-O(3)	165.2(2)	O(2)-Gd(1)-O(1)	127.0(3)
O(16)-Gd(3)-O(13)	143.3(2)	O(7)-Gd(1)-O(8)	71.0(3)
O(16)-Gd(3)-O(5)	77.6(2)	O(7)-Gd(1)-O(10)	143.5(2)
O(16)-Gd(3)-O(4)	82.1(3)	O(7)-Gd(1)-O(2)	140.6(2)
O(13)-Gd(3)-O(5)	73.3(2)	O(7)-Gd(1)-O(1)	76.0(3)
O(13)-Gd(3)-O(4)	97.7(2)	O(7)-Gd(1)-O(6)	89.7(3)
O(3)-Gd(3)-O(16)	100.1(2)	O(9)-Gd(1)-O(8)	145.5(2)
O(3)-Gd(3)-O(13)	89.9(2)	O(9)-Gd(1)-O(10)	71.5(2)
O(3)-Gd(3)-O(5)	69.1(2)	O(9)-Gd(1)-O(2)	132.0(2)
O(3)-Gd(3)-O(4)	164.1(2)	O(9)-Gd(1)-O(7)	75.3(3)
O(15)-Gd(3)-O(16)	71.7(2)	O(9)-Gd(1)-O(1)	84.0(3)
O(15)-Gd(3)-O(13)	144.8(2)	O(9)-Gd(1)-O(6)	86.6(2)
O(15)-Gd(3)-O(3)	84.0(2)	O(6)-Gd(1)-O(2)	68.2(2)
O(15)-Gd(3)-O(5)	134.5(2)	O(6)-Gd(1)-O(1)	164.5(3)
O(15)-Gd(3)-O(4)	81.8(3)		

Table S4. The important bond lengths and angles for cluster **4**.

Bond lengths			
Tb(2)-O(10)	2.267(5)	Tb(3)-O(8)	2.378(5)
Tb(2)-O(9)	2.319(4)	Tb(3)-O(5)	2.377(5)
Tb(2)-O(3)	2.391(5)	Tb(3)-N(4)	2.502(6)
Tb(2)-O(2)	2.334(5)	Tb(3)-O(7)	2.312(5)
Tb(2)-O(6)	2.391(5)	Tb(1)-O(11)	2.341(5)
Tb(2)-O(5)	2.338(4)	Tb(1)-O(12)	2.305(5)
Tb(2)-N(3)	2.550(6)	Tb(1)-O(13)	2.356(5)
Tb(2)-N(6)	2.570(6)	Tb(1)-O(2)	2.387(5)
Tb(3)-O(16)	2.342(5)	Tb(1)-O(6)	2.362(5)
Tb(3)-O(3)	2.341(5)	Tb(1)-O(14)	2.305(5)
Tb(3)-O(4)	2.435(5)	Tb(1)-O(1)	2.462(6)
Tb(3)-O(15)	2.326(5)	Tb(1)-N(1)	2.529(7)
Bond angles			
O(10)-Tb(2)-O(9)	74.47(16)	O(5)-Tb(3)-O(8)	73.51(17)
O(10)-Tb(2)-O(3)	82.56(18)	O(7)-Tb(3)-O(16)	75.59(18)
O(10)-Tb(2)-O(2)	152.01(19)	O(7)-Tb(3)-O(3)	87.33(18)
O(10)-Tb(2)-O(6)	83.04(18)	O(7)-Tb(3)-O(4)	78.8(2)
O(10)-Tb(2)-O(5)	106.84(16)	O(7)-Tb(3)-O(15)	145.06(18)
O(9)-Tb(2)-O(3)	86.10(18)	O(7)-Tb(3)-O(8)	72.16(19)

O(9)-Tb(2)-O(2)	103.41(17)	O(7)-Tb(3)-O(5)	138.65(18)
O(9)-Tb(2)-O(6)	82.41(18)	O(11)-Tb(1)-O(13)	144.00(19)
O(9)-Tb(2)-O(5)	153.69(18)	O(11)-Tb(1)-O(2)	73.38(18)
O(2)-Tb(2)-O(3)	125.39(17)	O(11)-Tb(1)-O(6)	86.57(17)
O(2)-Tb(2)-O(6)	69.11(17)	O(11)-Tb(1)-O(1)	96.68(18)
O(2)-Tb(2)-O(5)	87.41(16)	O(12)-Tb(1)-O(11)	70.86(19)
O(6)-Tb(2)-O(3)	163.55(16)	O(12)-Tb(1)-O(13)	141.86(19)
O(5)-Tb(2)-O(3)	68.33(16)	O(12)-Tb(1)-O(2)	139.08(18)
O(5)-Tb(2)-O(6)	123.88(16)	O(12)-Tb(1)-O(6)	89.78(18)
O(16)-Tb(3)-O(4)	81.1(2)	O(12)-Tb(1)-O(14)	74.18(19)
O(16)-Tb(3)-O(8)	147.44(18)	O(12)-Tb(1)-O(1)	76.4(2)
O(16)-Tb(3)-O(5)	132.72(17)	O(13)-Tb(1)-O(2)	78.61(17)
O(3)-Tb(3)-O(16)	87.04(18)	O(13)-Tb(1)-O(6)	103.98(17)
O(3)-Tb(3)-O(4)	163.6(2)	O(13)-Tb(1)-O(1)	82.68(19)
O(3)-Tb(3)-O(8)	87.09(17)	O(2)-Tb(1)-O(1)	127.43(18)
O(3)-Tb(3)-O(5)	68.53(16)	O(6)-Tb(1)-O(2)	68.72(16)
O(15)-Tb(3)-O(16)	71.44(17)	O(6)-Tb(1)-O(1)	163.79(19)
O(15)-Tb(3)-O(3)	102.02(18)	O(14)-Tb(1)-O(11)	143.98(19)
O(15)-Tb(3)-O(4)	85.0(2)	O(14)-Tb(1)-O(13)	71.92(19)
O(15)-Tb(3)-O(8)	141.03(18)	O(14)-Tb(1)-O(2)	133.96(18)
O(15)-Tb(3)-O(5)	74.92(17)	O(14)-Tb(1)-O(6)	84.87(18)
O(8)-Tb(3)-O(4)	96.8(2)	O(14)-Tb(1)-O(1)	83.2(2)
O(5)-Tb(3)-O(4)	127.83(19)		

Table S5. The important bond lengths and angles for cluster **5**.

Bond lengths			
Dy(2)-O(5)	2.331(5)	Dy(3)-O(12)	2.350(5)
Dy(2)-O(2)	2.319(5)	Dy(3)-O(11)	2.300(5)
Dy(2)-O(3)	2.385(5)	Dy(3)-O(4)	2.418(6)
Dy(2)-O(6)	2.383(5)	Dy(3)-N(4)	2.483(7)
Dy(2)-O(9)	2.298(5)	Dy(1)-O(2)	2.372(5)
Dy(2)-O(10)	2.261(5)	Dy(1)-O(6)	2.340(5)
Dy(2)-N(3)	2.538(6)	Dy(1)-O(8)	2.319(5)
Dy(2)-N(6)	2.544(7)	Dy(1)-O(7)	2.287(6)
Dy(3)-O(5)	2.347(5)	Dy(1)-O(13)	2.333(5)
Dy(3)-O(3)	2.318(5)	Dy(1)-O(14)	2.287(6)
Dy(3)-O(16)	2.308(5)	Dy(1)-O(1)	2.455(6)
Dy(3)-O(15)	2.316(5)	Dy(1)-N(1)	2.510(7)
Bond angles			
O(5)-Dy(2)-O(3)	67.59(17)	O(12)-Dy(3)-O(4)	95.3(2)
O(5)-Dy(2)-O(6)	124.50(17)	O(11)-Dy(3)-O(5)	139.23(19)
O(2)-Dy(2)-O(5)	88.11(17)	O(11)-Dy(3)-O(3)	87.69(19)
O(2)-Dy(2)-O(3)	125.77(18)	O(11)-Dy(3)-O(16)	144.04(19)
O(2)-Dy(2)-O(6)	68.89(17)	O(11)-Dy(3)-O(15)	74.65(19)

O(6)-Dy(2)-O(3)	163.47(17)	O(11)-Dy(3)-O(12)	72.1(2)
O(9)-Dy(2)-O(5)	153.35(18)	O(11)-Dy(3)-O(4)	77.0(2)
O(9)-Dy(2)-O(2)	102.71(18)	O(2)-Dy(1)-O(1)	127.82(19)
O(9)-Dy(2)-O(3)	86.59(18)	O(6)-Dy(1)-O(2)	68.72(17)
O(9)-Dy(2)-O(6)	82.13(18)	O(6)-Dy(1)-O(1)	163.4(2)
O(10)-Dy(2)-O(5)	106.58(17)	O(8)-Dy(1)-O(2)	73.61(19)
O(10)-Dy(2)-O(2)	152.13(19)	O(8)-Dy(1)-O(6)	86.89(18)
O(10)-Dy(2)-O(3)	82.06(18)	O(8)-Dy(1)-O(13)	144.1(2)
O(10)-Dy(2)-O(6)	83.33(18)	O(8)-Dy(1)-O(1)	96.37(19)
O(10)-Dy(2)-O(9)	74.76(18)	O(7)-Dy(1)-O(2)	139.21(18)
O(5)-Dy(3)-O(12)	74.28(18)	O(7)-Dy(1)-O(6)	89.93(19)
O(5)-Dy(3)-O(4)	128.8(2)	O(7)-Dy(1)-O(8)	70.8(2)
O(3)-Dy(3)-O(5)	68.45(17)	O(7)-Dy(1)-O(13)	141.9(2)
O(3)-Dy(3)-O(12)	87.64(19)	O(7)-Dy(1)-O(1)	75.9(2)
O(3)-Dy(3)-O(4)	162.6(2)	O(13)-Dy(1)-O(2)	78.46(18)
O(16)-Dy(3)-O(5)	75.40(17)	O(13)-Dy(1)-O(6)	103.68(18)
O(16)-Dy(3)-O(3)	102.23(19)	O(13)-Dy(1)-O(1)	83.18(19)
O(16)-Dy(3)-O(15)	71.58(18)	O(14)-Dy(1)-O(2)	133.65(19)
O(16)-Dy(3)-O(12)	141.81(18)	O(14)-Dy(1)-O(6)	84.30(19)
O(16)-Dy(3)-O(4)	86.0(2)	O(14)-Dy(1)-O(8)	143.8(2)
O(15)-Dy(3)-O(5)	132.90(18)	O(14)-Dy(1)-O(7)	74.1(2)
O(15)-Dy(3)-O(3)	86.74(19)	O(14)-Dy(1)-O(13)	72.1(2)
O(15)-Dy(3)-O(12)	146.45(19)	O(14)-Dy(1)-O(1)	83.5(2)
O(15)-Dy(3)-O(4)	81.4(2)		

Table S6. The important bond lengths and angles for cluster **6**.

Bond lengths			
Ho(2)-O(2)	2.272(4)	Ho(1)-O(9)	2.265(4)
Ho(2)-O(5)	2.279(4)	Ho(1)-O(8)	2.251(5)
Ho(2)-O(13)	2.252(4)	Ho(1)-N(1)	2.456(5)
Ho(2)-O(3)	2.358(4)	Ho(1)-O(6)	2.303(4)
Ho(2)-O(14)	2.258(4)	Ho(3)-O(5)	2.328(4)
Ho(2)-N(3)	2.523(5)	Ho(3)-O(4)	2.402(5)
Ho(2)-N(6)	2.494(5)	Ho(3)-O(15)	2.283(4)
Ho(2)-O(6)	2.346(4)	Ho(3)-O(3)	2.297(4)
Ho(1)-O(2)	2.316(4)	Ho(3)-O(12)	2.252(5)
Ho(1)-O(10)	2.271(4)	Ho(3)-O(11)	2.282(4)
Ho(1)-O(7)	2.313(4)	Ho(3)-O(16)	2.260(4)
Ho(1)-O(1)	2.376(5)	Ho(3)-N(4)	2.479(6)
Bond angles			
O(2)-Ho(2)-O(5)	88.12(14)	O(8)-Ho(1)-O(7)	72.41(16)
O(2)-Ho(2)-O(3)	125.72(15)	O(8)-Ho(1)-O(1)	76.40(18)
O(2)-Ho(2)-O(6)	67.99(14)	O(8)-Ho(1)-O(9)	143.92(16)
O(5)-Ho(2)-O(3)	68.75(14)	O(8)-Ho(1)-O(6)	86.83(16)

O(5)-Ho(2)-O(6)	127.48(15)	O(6)-Ho(1)-O(2)	68.00(15)
O(13)-Ho(2)-O(2)	107.24(14)	O(6)-Ho(1)-O(7)	86.49(15)
O(13)-Ho(2)-O(5)	152.86(15)	O(6)-Ho(1)-O(1)	161.47(17)
O(13)-Ho(2)-O(3)	84.17(15)	O(5)-Ho(3)-O(4)	128.70(16)
O(13)-Ho(2)-O(14)	75.86(15)	O(15)-Ho(3)-O(5)	73.48(15)
O(13)-Ho(2)-O(6)	79.54(15)	O(15)-Ho(3)-O(4)	96.39(16)
O(14)-Ho(2)-O(2)	153.34(16)	O(15)-Ho(3)-O(3)	87.69(15)
O(14)-Ho(2)-O(5)	100.53(15)	O(3)-Ho(3)-O(5)	68.96(14)
O(14)-Ho(2)-O(3)	80.73(15)	O(3)-Ho(3)-O(4)	162.31(17)
O(14)-Ho(2)-O(6)	87.11(15)	O(12)-Ho(3)-O(5)	133.36(15)
O(6)-Ho(2)-O(3)	161.65(14)	O(12)-Ho(3)-O(4)	83.35(17)
O(2)-Ho(1)-O(1)	130.34(16)	O(12)-Ho(3)-O(15)	143.93(16)
O(10)-Ho(1)-O(2)	133.28(15)	O(12)-Ho(3)-O(3)	83.28(16)
O(10)-Ho(1)-O(7)	145.18(16)	O(12)-Ho(3)-O(11)	72.92(16)
O(10)-Ho(1)-O(1)	80.22(18)	O(12)-Ho(3)-O(16)	72.58(16)
O(10)-Ho(1)-O(6)	87.47(16)	O(11)-Ho(3)-O(5)	78.31(16)
O(7)-Ho(1)-O(2)	74.80(15)	O(11)-Ho(3)-O(4)	82.95(16)
O(7)-Ho(1)-O(1)	95.71(18)	O(11)-Ho(3)-O(15)	143.04(16)
O(9)-Ho(1)-O(2)	75.04(15)	O(11)-Ho(3)-O(3)	104.05(15)
O(9)-Ho(1)-O(10)	73.05(15)	O(16)-Ho(3)-O(5)	139.65(16)
O(9)-Ho(1)-O(7)	141.56(16)	O(16)-Ho(3)-O(4)	76.20(18)
O(9)-Ho(1)-O(1)	86.09(17)	O(16)-Ho(3)-O(15)	72.38(16)
O(9)-Ho(1)-O(6)	103.60(15)	O(16)-Ho(3)-O(3)	88.77(16)
O(8)-Ho(1)-O(2)	139.52(16)	O(16)-Ho(3)-O(11)	141.31(17)
O(8)-Ho(1)-O(10)	73.04(16)		

Table S7. The important bond lengths and angles for cluster **7**.

Bond lengths			
Er(2)-O(3)	2.384(5)	Er(1)-O(7)	2.272(5)
Er(2)-O(11)	2.280(5)	Er(1)-O(10)	2.291(5)
Er(2)-O(12)	2.289(5)	Er(1)-N(1)	2.475(6)
Er(2)-O(2)	2.302(5)	Er(1)-O(1)	2.388(5)
Er(2)-O(6)	2.368(5)	Er(3)-O(3)	2.322(5)
Er(2)-O(5)	2.303(5)	Er(3)-O(14)	2.276(5)
Er(2)-N(6)	2.516(6)	Er(3)-O(13)	2.317(5)
Er(2)-N(3)	2.538(6)	Er(3)-O(4)	2.418(5)
Er(1)-O(9)	2.301(5)	Er(3)-O(15)	2.319(5)
Er(1)-O(8)	2.344(5)	Er(3)-O(16)	2.285(5)
Er(1)-O(2)	2.337(5)	Er(3)-N(4)	2.503(7)
Er(1)-O(6)	2.316(5)	Er(3)-O(5)	2.345(5)
Bond angles			
O(11)-Er(2)-O(3)	84.37(17)	O(7)-Er(1)-O(10)	143.54(19)
O(11)-Er(2)-O(12)	75.24(17)	O(7)-Er(1)-O(1)	76.4(2)

O(11)-Er(2)-O(2)	107.96(16)	O(10)-Er(1)-O(9)	72.35(18)
O(11)-Er(2)-O(6)	79.61(17)	O(10)-Er(1)-O(8)	142.51(17)
O(11)-Er(2)-O(5)	153.29(17)	O(10)-Er(1)-O(2)	75.28(17)
O(12)-Er(2)-O(3)	80.74(18)	O(10)-Er(1)-O(6)	103.09(18)
O(12)-Er(2)-O(2)	153.91(18)	O(10)-Er(1)-O(1)	86.4(2)
O(12)-Er(2)-O(6)	87.73(18)	O(3)-Er(3)-O(4)	162.87(19)
O(12)-Er(2)-O(5)	100.22(17)	O(3)-Er(3)-O(5)	69.30(17)
O(2)-Er(2)-O(3)	125.10(17)	O(14)-Er(3)-O(3)	83.22(19)
O(2)-Er(2)-O(6)	67.98(16)	O(14)-Er(3)-O(13)	72.79(19)
O(2)-Er(2)-O(5)	87.79(17)	O(14)-Er(3)-O(4)	83.7(2)
O(6)-Er(2)-O(3)	162.22(17)	O(14)-Er(3)-O(15)	143.89(19)
O(5)-Er(2)-O(3)	68.93(17)	O(14)-Er(3)-O(16)	72.80(19)
O(5)-Er(2)-O(6)	126.91(17)	O(14)-Er(3)-O(5)	133.86(18)
O(9)-Er(1)-O(8)	144.92(18)	O(13)-Er(3)-O(3)	103.75(18)
O(9)-Er(1)-O(2)	133.32(17)	O(13)-Er(3)-O(4)	82.8(2)
O(9)-Er(1)-O(6)	87.34(19)	O(13)-Er(3)-O(15)	143.17(19)
O(9)-Er(1)-O(1)	81.1(2)	O(13)-Er(3)-O(5)	78.55(18)
O(8)-Er(1)-O(1)	94.9(2)	O(15)-Er(3)-O(3)	88.26(18)
O(2)-Er(1)-O(8)	75.20(17)	O(15)-Er(3)-O(4)	95.82(19)
O(2)-Er(1)-O(1)	129.34(19)	O(15)-Er(3)-O(5)	73.40(18)
O(6)-Er(1)-O(8)	86.82(18)	O(16)-Er(3)-O(3)	88.70(19)
O(6)-Er(1)-O(2)	68.29(17)	O(16)-Er(3)-O(13)	141.54(19)
O(6)-Er(1)-O(1)	162.13(19)	O(16)-Er(3)-O(4)	76.8(2)
O(7)-Er(1)-O(9)	73.36(19)	O(16)-Er(3)-O(15)	71.98(19)
O(7)-Er(1)-O(8)	71.84(19)	O(16)-Er(3)-O(5)	139.22(18)
O(7)-Er(1)-O(2)	139.74(19)	O(5)-Er(3)-O(4)	127.80(18)
O(7)-Er(1)-O(6)	87.27(19)		

Table S8 The Dy^{III} geometry analysis by SHAPE 2.0 for cluster **5**.

Cluster 5	***D*$_{4d}$SAPR**	***D*$_{2d}$TDD**	***C*$_{2v}$JBTPR**	***C*$_{2v}$BTPR**	***D*$_{2d}$JSD**
$Dy1^{III}$	4.365	1.006	3.035	3.0163	3.010
$Dy2^{III}$	4.357	0.975	2.858	2.437	2.987
$Dy3^{III}$	4.128	0.736	2.875	2.763	2.857

SAPR-8 = Square antiprism; **TDD-8** = Triangular dodecahedron; **JBTPR-8** = Biaugmented trigonal prism J50; **BTPR-8** = Biaugmented trigonal prism; **JSD-8** = Snub diphenoid J84

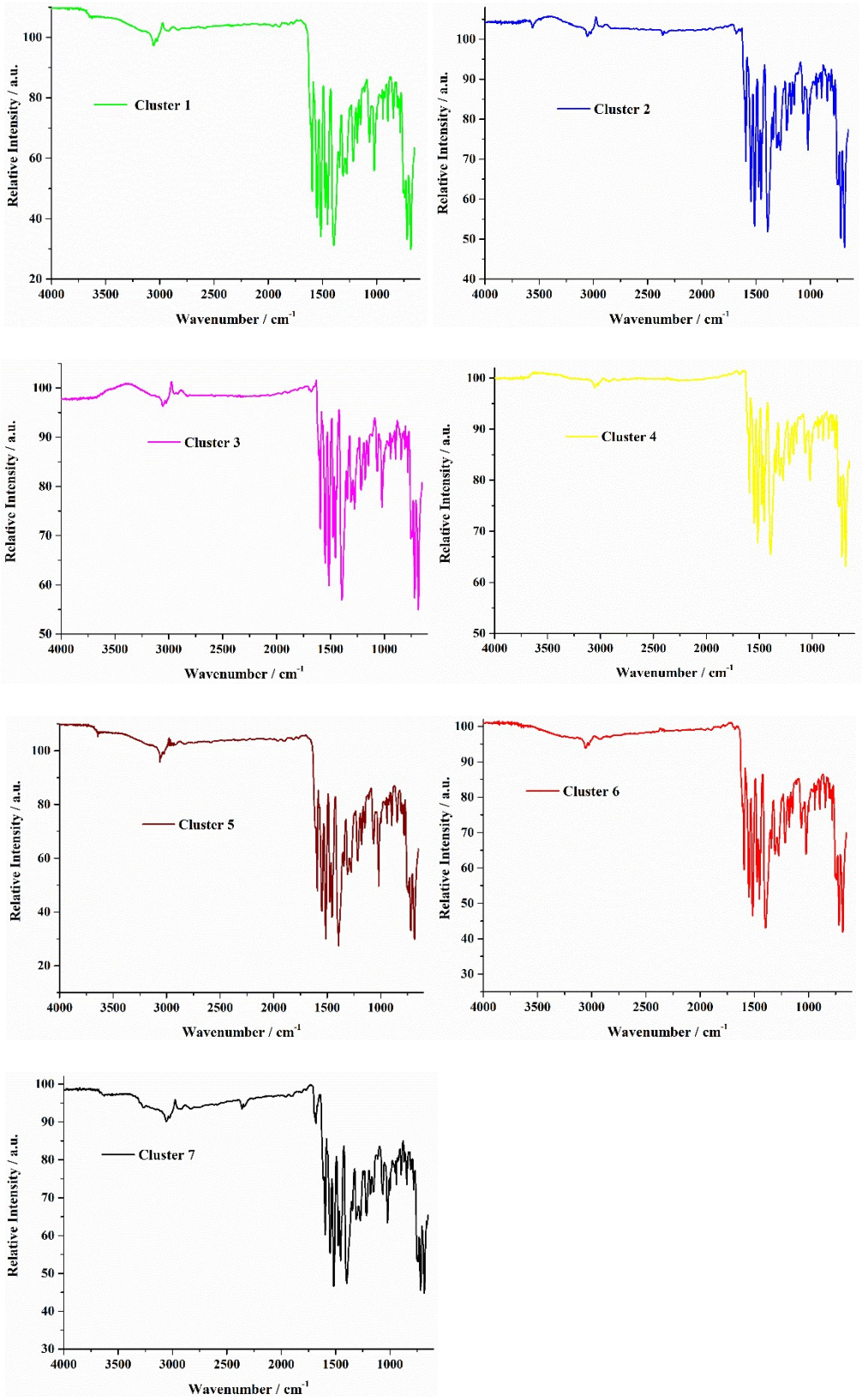

Fig. S1 The IR spectra of clusters **1**-**7**.

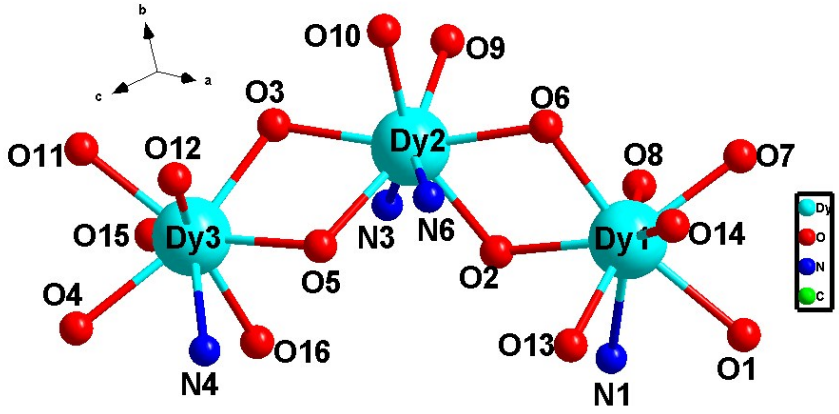

Fig. S2 The coordinate atom labels of central Dy(III) ions in cluster **5**.

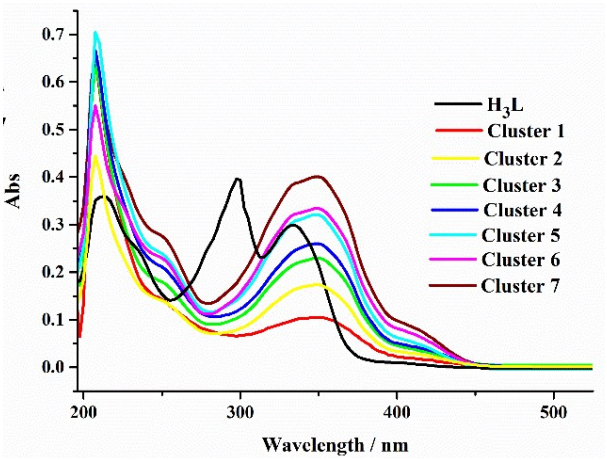

Fig. S3 The UV-vis spectra of clusters **1** -**7** and H_3L ligand were performed at room temperature in ethanol solution.

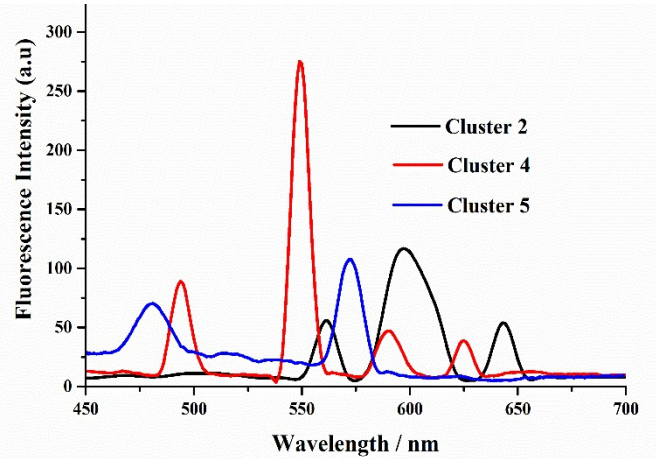

Fig. S4 The solid-state luminescence spectra of clusters **2**, **4** and **5** at room temperature.

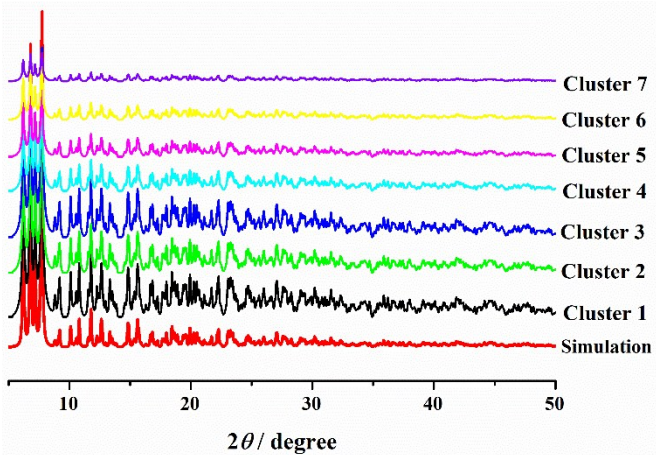

Fig. S5 PXRD patterns for clusters **1**-**7**.

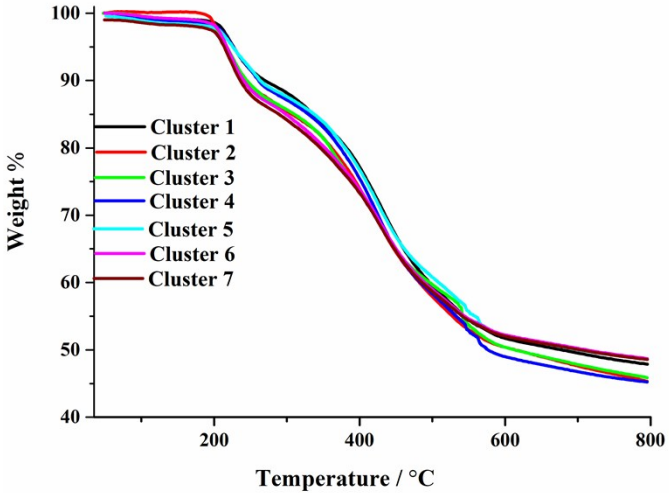

Fig. S6 The TGA curves of clusters **1**-**7**.

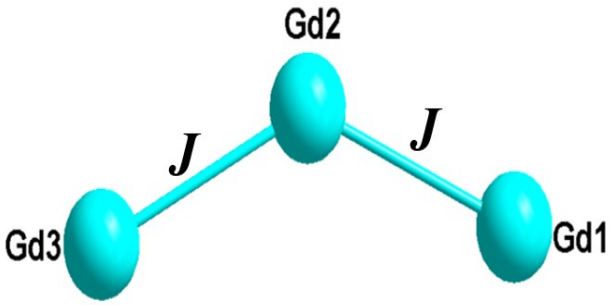

Fig. S7 The magetic coupling model of Gd(III) ions in cluster **3**.