3D Ln-MOFs containing pentanuclear clusters exhibiting magnetic refrigeration and slow magnetic relaxation

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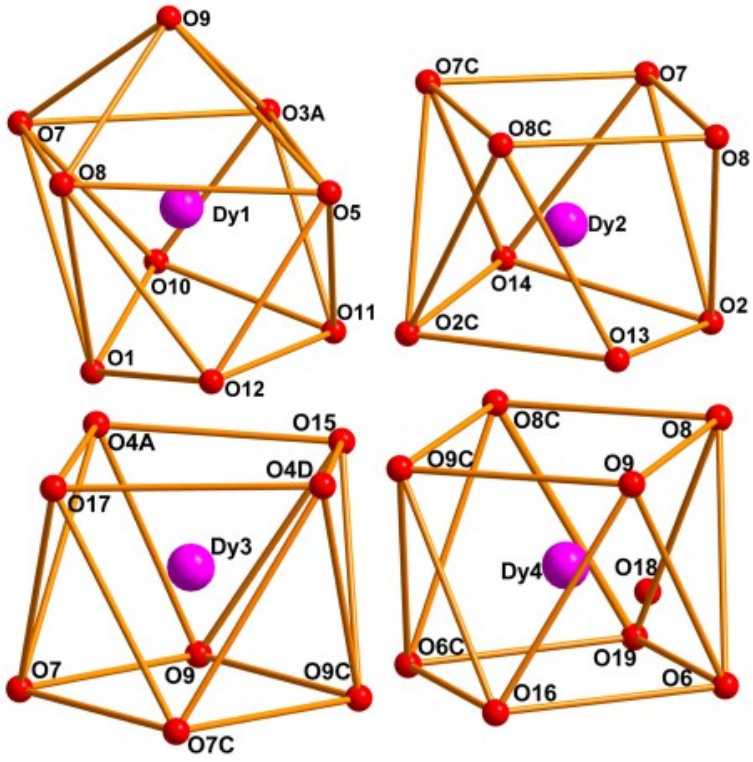

Fig. S1 Mono-capped square antiprismatic geometry for Dy1, and square antiprismatic coordination sphere for Dy2-Dy4.

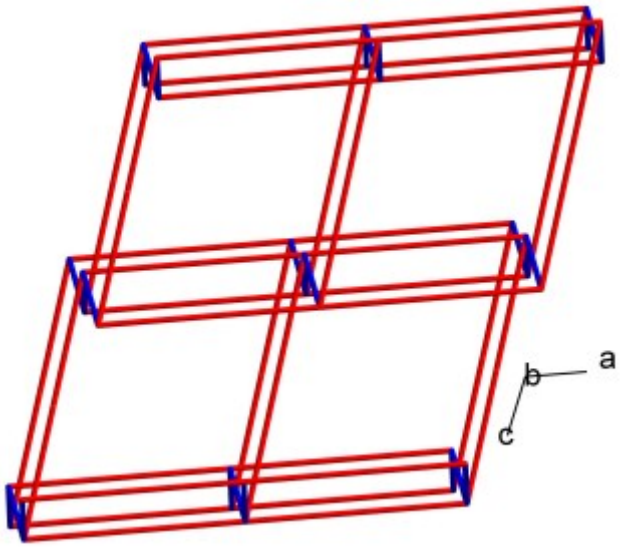

Fig. S2 View of the topological net of **2**.

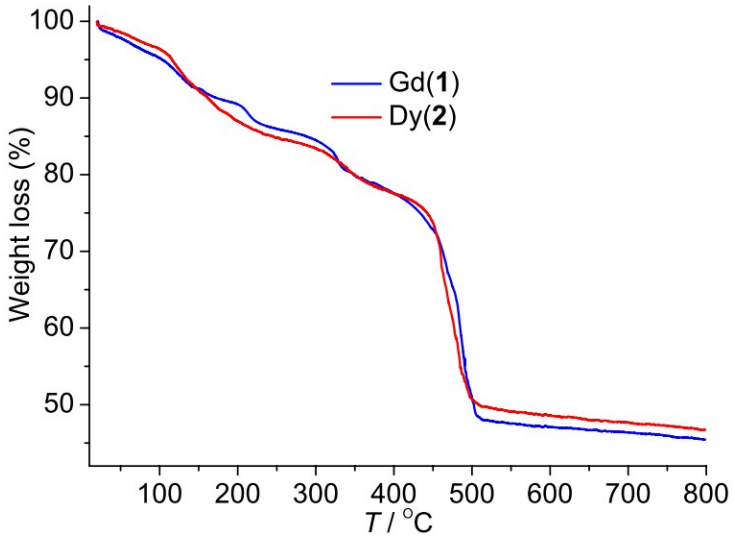

Fig. S3 TGA curves of **1** and **2**.

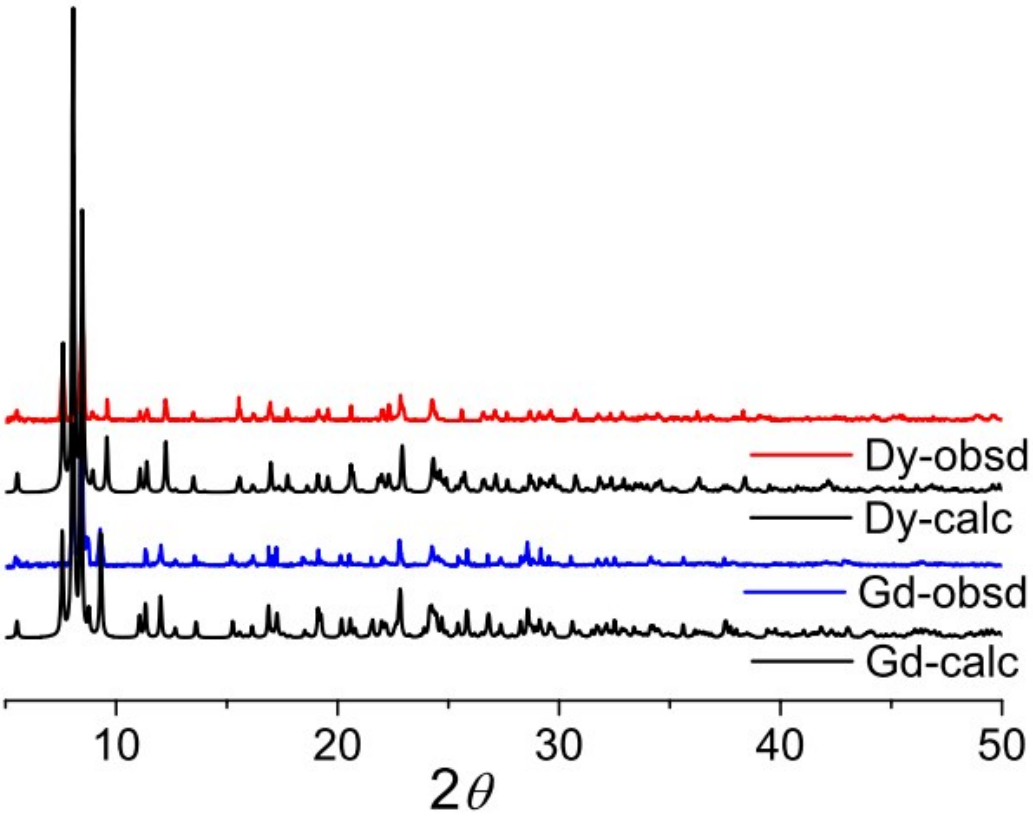

Fig. S4 Comparison of the simulated and experimental XRD patterns of **1** and **2**.

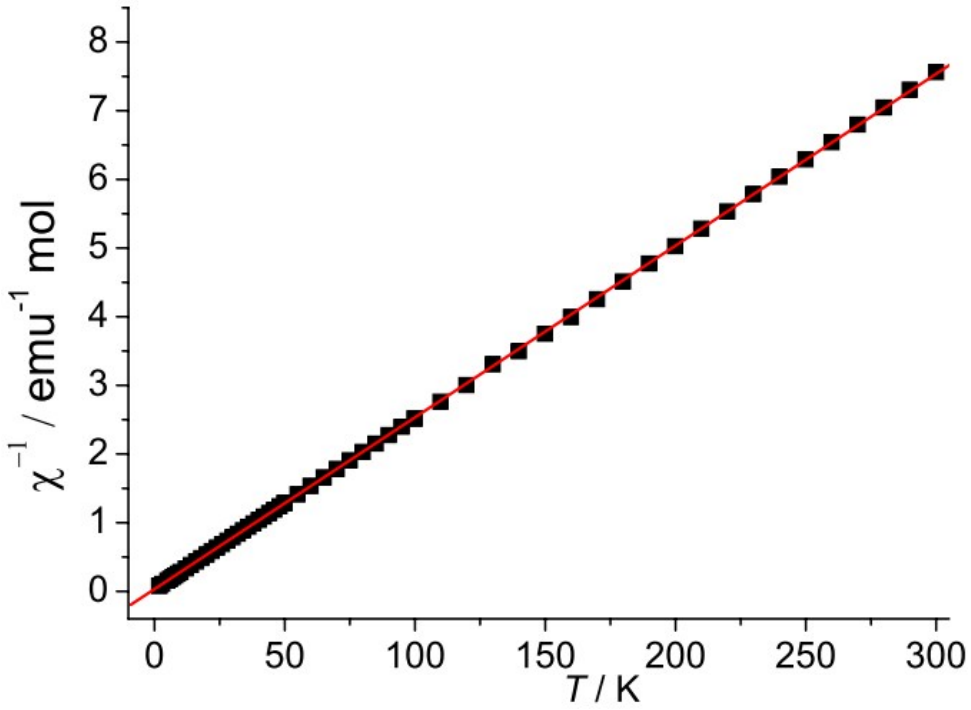

Fig. S5 The 1/χ vs T and Currie-Weiss fit for **1**.

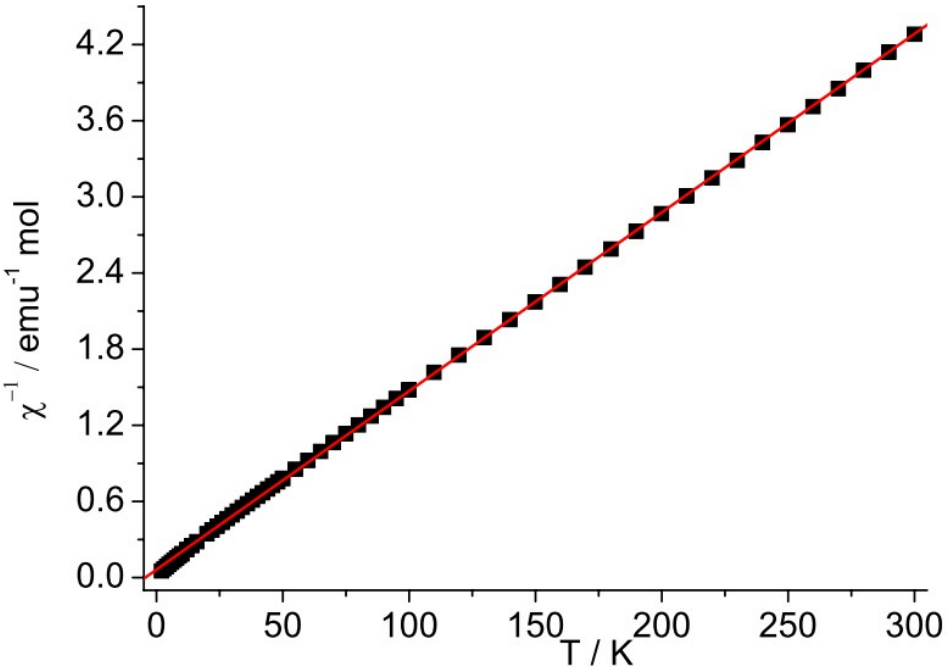

Fig. S6 The 1/χ vs T and theCurrie-Weiss fit for **2**.

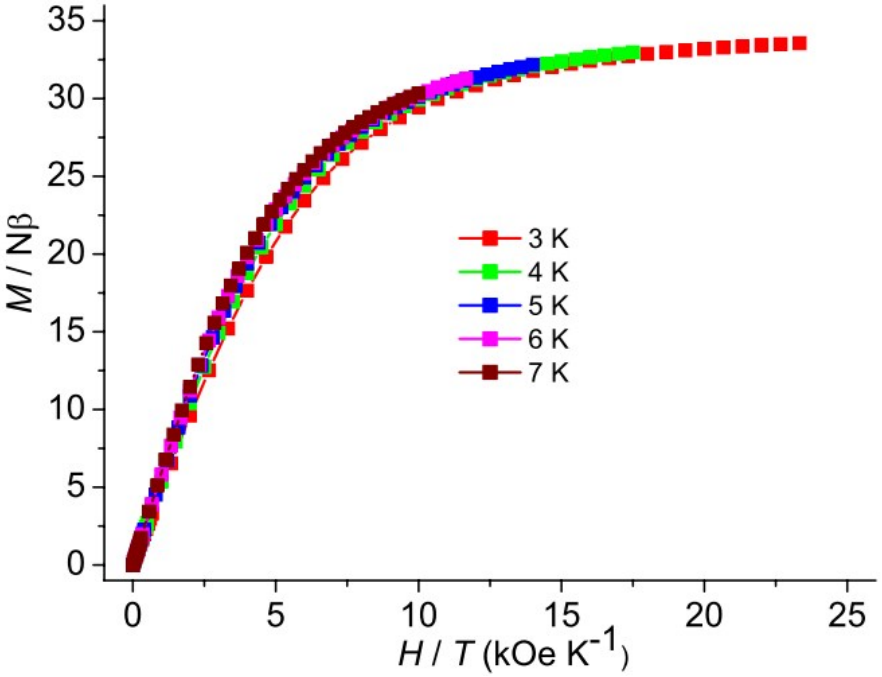

Fig. S7 Reduced magnetization (M vs H/T) plot for **1**.

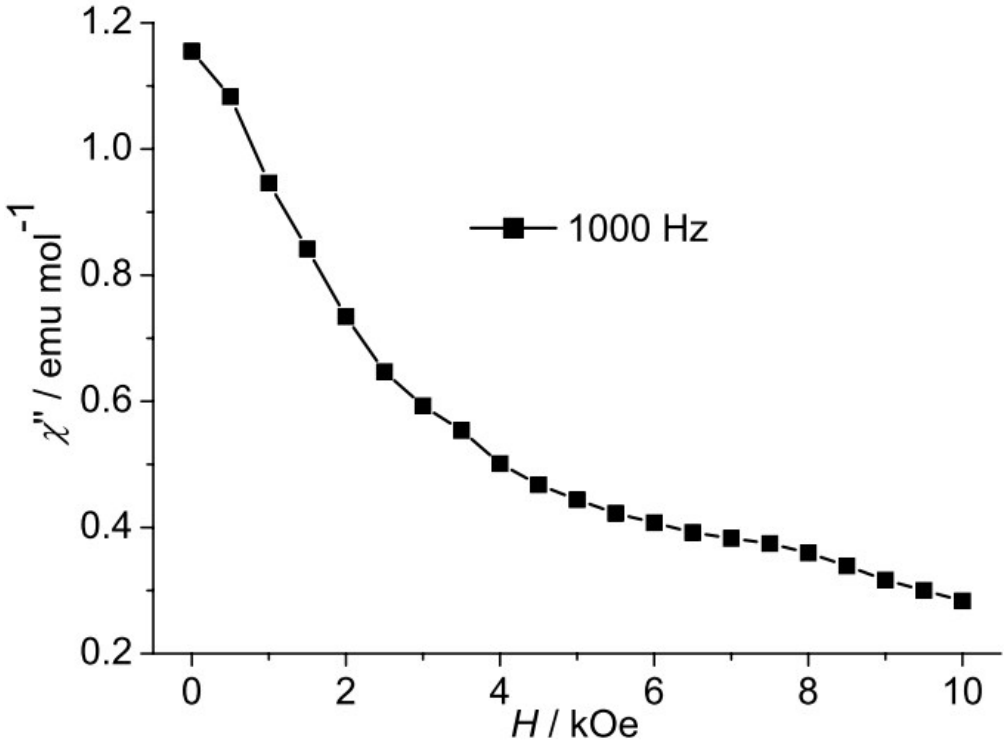

Fig. S8 The out-of-phase (χ'') ac susceptibility for **2** (2 K, f = 1000 Hz) under the applied static field from 0-10kOe.

Table S1 Selected bond lengths (Å) and angles (°) for compound **1**

Gd1-O8	2.343(6)	Gd1-O7	2.366(6)
Gd1-O1	2.369(7)	Gd1-O3A	2.387(14)
Gd1-O5	2.417(7)	Gd1-O9	2.429(6)
Gd1-O10	2.523(7)	Gd1-O11	2.585(15)
Gd1-O12	2.741(10)	Gd1-O11B	2.765(15)
Gd2-O2	2.324(7)	Gd2-O14	2.401(9)
Gd2-O13	2.415(10)	Gd2-O8	2.421(6)
Gd2-O7	2.430(6)	Gd3-O17	2.338(9)
Gd3-O4A	2.375(7)	Gd3-O9	2.407(6)
Gd3-O7	2.442(6)	Gd3-O15	2.504(9
Gd4-O19	2.23(2)	Gd4-O6	2.316(7)
Gd4-O9	2.382(7)	Gd4-O8	2.440(6)
Gd4-O18	2.467(18)	Gd4-O16	2.505(11)
O8- Gd1-O7	70.2(2)	O8- Gd1-O1	85.7(2)
O7- Gd1-O1	84.4(2)	O8- Gd1-O3A	138.9(3)
O7- Gd1-O3A	87.9(4)	O1- Gd1-O3A	127.4(4)
O8- Gd1-O5	87.0(2)	O7- Gd1-O5	141.6(2)
O1- Gd1-O5	125.5(3)	O3A- Gd1-O5	90.2(4)
O8- Gd1-O9	68.8(2)	O7- Gd1-O9	66.1(2)
O1- Gd1-O9	145.9(2)	O3A- Gd1-O9	70.6(3)
O5- Gd1-O9	77.1(2)	O8- Gd1-O10	135.6(2)
O7- Gd1-O10	74.0(2)	O1- Gd1-O10	65.4(3
O3A- Gd1-O10	62.4(4)	O5- Gd1-O10	137.0(3)
O9- Gd1-O10	118.1(2)	O8- Gd1-O11	146.9(4)
O7- Gd1-O11	138.9(4)	O1- Gd1-O11	83.2(4)
O3A- Gd1-O11	69.6(4)	O5- Gd1-O11	74.5(4)
O9- Gd1-O11	130.4(4)	O10- Gd1-O11	65.3(4)
O8- Gd1-O12	72.8(3)	O7- Gd1-O12	130.8(3)
O1- Gd1-O12	61.5(3)	O3A- Gd1-O12	140.7(4)
O5- Gd1-O12	64.8(3)	O9- Gd1-O12	126.3(3)
O10- Gd1-O12	115.5(3)	O11- Gd1-O12	74.5(4)
O8- Gd1-O11B	128.9(3)	O7- Gd1-O11B	142.6(4)
O1- Gd1-O11B	67.9(4)	O3A- Gd1-O11B	89.6(4)
O5- Gd1-O11B	75.7(4)	O9- Gd1-O11B	146.1(4)
O10- Gd1-O11B	71.9(4)	O11- Gd1-O11B	20.1(6)
O12- Gd1-O11B	56.3(4)	O2C- Gd2-O2	106.7(4)
O2C- Gd2-O14	74.9(3)	O2- Gd2-O14	74.9(3)
O2C- Gd2-O13	75.3(3)	O2- Gd2-O13	75.3(3)
O14- Gd2-O13	129.1(4)	O2C- Gd2-O8C	84.7(2)
O2- Gd2-O8C	145.2(2)	O14- Gd2-O8C	139.58(19)

O13- Gd2-O8C	76.1(3)	O2C- Gd2-O8	145.2(2)
O2- Gd2-O8	84.7(2)	O14- Gd2-O8	139.58(19)
O13- Gd2-O8	76.1(3)	O8C- Gd2-O8	69.5(3)
O2C- Gd2-O7	144.5(2)	O2- Gd2-O7	83.9(2)
O14- Gd2-O7	75.5(3)	O13- Gd2-O7	139.7(2)
O8C- Gd2-O7	106.0(2)	O8- Gd2-O7	67.8(2)
O2C- Gd2-O7C	83.9(2)	O2- Gd2-O7C	144.5(2)
O14- Gd2-O7C	75.5(3)	O13- Gd2-O7C	139.7(2)
O8C- Gd2-O7C	67.8(2)	O8- Gd2-O7C	106.0(2)
O7- Gd2-O7C	70.0(3)	O17- Gd3-O4A	80.3(3)
O17- Gd3-O4D	80.3(3)	O4A- Gd3-O4D	113.5(4)
O17- Gd3-O9C	139.67(18)	O4A- Gd3-O9C	139.3(2)
O4D- Gd3-O9C	76.2(3)	O17- Gd3-O9	139.67(18)
O4A- Gd3-O9	76.2(3)	O4D- Gd3-O9	139.3(2)
O17- Gd3-O7C	80.6(3)	O4A- Gd3-O7C	150.5(2)
O9C- Gd3-O7C	73.2(3)	O4D- Gd3-O7C	85.1(2)
O9C- Gd3-O7C	65.3(2)	O9- Gd3-O7C	105.2(2)
O17- Gd3-O7	80.6(3)	O4A- Gd3-O7	85.1(2)
O4D- Gd3-O7	150.5(2)	O9C- Gd3-O7	105.2(2)
O7C- Gd3-O7	69.7(3)	O9- Gd3-O7	65.3(2)
O4A- Gd3-O15	69.9(2)	O17- Gd3-O15	123.4(4)
O4D- Gd3-O15	69.9(2)	O9- Gd3-O15	77.9(3)
O7- Gd3-O15	139.61(19)	O9C- Gd3-O15	77.9(3)
O7C- Gd3-O15	139.61(19)	O19- Gd4-O6C	70.2(4)
O19- Gd4-O6	70.2(4)	O6C- Gd4-O6	111.9(4)
O19- Gd4-O9	142.87(16)	O9- Gd4-O6C	141.7(3)
O6- Gd4-O9	77.7(2)	O19- Gd4-O9C	142.87(16)
O6C- Gd4-O9C	77.7(2)	O6- Gd4-O9C	141.7(3)
O9- Gd4-O9C	74.1(3)	O19- Gd4-O8	90.4(5)
O6C- Gd4-O8	146.9(3)	O6- Gd4-O8	84.3(2)
O9- Gd4-O8	68.0(2)	O9C-Gd4-O8	107.9(2)
O19- Gd4-O8C	90.4(5)	O6C-Gd4-O8C	84.3(2)
O6- Gd4-O8C	146.9(3)	O9- Gd4-O8C	107.9(2)
O9C- Gd4-O8C	68.0(2)	O8- Gd4-O8C	68.9(3)
O19- Gd4-O18	20.4(6)	O6C- Gd4-O18	80.6(3)
O6- Gd4-O18	80.6(3)	O9- Gd4-O18	137.3(3)
O9C- Gd4-O18	137.3(2)	O8- Gd4-O18	73.6(4)
O8C- Gd4-O18	73.6(4)	O19- Gd4-O16	109.3(7)
O6C- Gd4-O16	72.0(3)	O6- Gd4-O16	72.0(3)
O9- Gd4-O16	76.7(3)	O9C- Gd4-O16	76.7(3)
O8- Gd4-O16	140.93(19)	O8C- Gd4-O16	140.93(19)
O18- Gd4-O16	129.7(5)	O6- Gd4-O16	

Symmetry codes: A x, y, z-1, B -x+1/2, -y+1/2, -z+1, C x, -y+1, z, D x, -y+1, z-1.

Table S2 Selected bond lengths (Å) and angles (°) for compound **2**

Dy1-O8	2.305(5)	Dy1-O7	2.341(6)
Dy1-O1	2.325(7)	Dy1-O3A	2.348(14)
Dy1-O5	2.363(6)	Dy1-O9	2.384(6)
Dy1-O10	2.495(10)	Dy1-O11	2.573(17)
Dy1-O12	2.742(11)	Dy2-O14	2.375(9)
Dy2-O2	2.310(6)	Dy2-O8	2.396(6)
Dy2-O13	2.374(10)	Dy2-O7	2.395(6)
Dy3-O4A	2.367(7)	Dy3-O17	2.318(8)
Dy3-O7	2.409(6)	Dy3-O9	2.379(6)
Dy3-O15	2.456(9)	Dy4-O6	2.305(6)
Dy4-O19	2.26(2)	Dy4-O8	2.410(6)
Dy4-O9	2.358(6)	Dy4-O16	2.447(11)
Dy4-O18	2.451(17)		
O8- Dy1-O1	88.2(2)	O8- Dy1-O7	70.5(2)
O7- Dy1-O1	85.1(2)	O8- Dy1-O3A	142.6(4)
O7- Dy1-O3A	85.3(3)	O1- Dy1-O3A	118.5(4)
O8- Dy1-O5	88.6(2)	O7- Dy1-O5	144.7(2)
O1- Dy1-O5	123.4(3)	O3A- Dy1-O5	96.2(4)
O8- Dy1-O9	69.1(2)	O7- Dy1-O9	67.22(19)
O1- Dy1-O9	148.5(2)	O3A- Dy1-O9	75.5(4)
O5- Dy1-O9	79.0(2)	O8- Dy1-O10	133.3(3)
O7- Dy1-O10	60.9(4)	O1- Dy1-O10	72.6(3)
O3A- Dy1-O10	58.3(5)	O5- Dy1-O10	137.0(3)
O9- Dy1-O10	120.0(3)	O8- Dy1-O11	143.9(3)
O7- Dy1-O11	137.6(4)	O1- Dy1-O11	75.5(4)
O3A- Dy1-O11	72.1(4)	O5- Dy1-O11	74.8(4)
O9- Dy1-O11	135.3(4)	O10- Dy1-O11	65.0(5)
O8- Dy1-O12	72.6(3)	O7- Dy1-O12	130.4(3)
O1- Dy1-O12	61.7(3)	O3A- Dy1-O12	141.8(4)
O5- Dy1-O12	63.5(3)	O9- Dy1-O12	126.1(3)
O10- Dy1-O12	113.8(4)	O11- Dy1-O12	71.3(4)
O8- Dy1-O11B	129.4(3)	O7- Dy1-O11B	143.6(4)
O1- Dy1-O11B	67.8(4)	O3A- Dy1-O11B	86.8(4)
O5- Dy1-O11B	71.5(4)	O9- Dy1-O11B	143.6(4)
O10- Dy1-O11B	73.0(5)	O11- Dy1-O11B	14.7(5)
O12- Dy1-O11B	56.8(4)	O2C- Dy2-O2	112.3(4)
O2C- Dy2-O14	75.7(2)	O2- Dy2-O14	75.7(2)
O2C- Dy2-O13	75.7(2)	O2- Dy2-O13	75.7(2)
O14- Dy2-O13	127.4(4)	O2C- Dy2-O8C	82.0(2)
O2- Dy2-O8C	143.8(2)	O14- Dy2-O8C	140.29(17)
O13- Dy2-O8C	76.3(3)	O2C- Dy2-O8	143.8(2)
O2- Dy2-O8	82.0(2)	O14- Dy2-O8	140.29(17)

O13- Dy2-O8	76.3(3)	O8C- Dy2-O8	69.4(3)
O2C- Dy2-O7	144.2(2)	O2- Dy2-O7	81.6(2)
O14- Dy2-O7	76.4(2)	O13- Dy2-O7	139.9(2)
O8C- Dy2-O7	106.4(2)	O8- Dy2-O7	68.05(19)
O2C- Dy2-O7C	81.6(2)	O2- Dy2-O7C	144.2(2)
O14- Dy2-O7C	76.4(2)	O13- Dy2-O7C	139.9(2)
O8C- Dy2-O7C	68.05(19)	O8- Dy2-O7C	106.4(2)
O7- Dy2-O7C	70.4(3)	O17- Dy3-O4A	79.9(2)
O17- Dy3-O4D	79.9(2)	O4A- Dy3-O4D	114.6(4)
O17- Dy3-O9C	140.15(16)	O4A- Dy3-O9C	139.2(2)
O4D- Dy3-O9C	76.0(2)	O17- Dy3-O9	140.15(16)
O4A- Dy3-O9	76.0(2)	O4D- Dy3-O9	139.2(2)
O17- Dy3-O7C	80.3(2)	O4A- Dy3-O7C	149.6(2)
O9C- Dy3-O7C	66.22(19)	O4D- Dy3-O7C	84.1(2)
O9C- Dy3-O9	72.9(3)	O9- Dy3-O7C	106.1(2)
O17- Dy3-O7	80.3(2)	O4A- Dy3-O7	84.1(2)
O4D- Dy3-O7	149.6(2)	O9C- Dy3-O7	106.1(2)
O7C- Dy3-O7	69.9(3)	O9- Dy3-O7	66.22(19)
O4A- Dy3-O15	69.9(2)	O17- Dy3-O15	121.5(4)
O4D- Dy3-O15	69.9(2)	O9- Dy3-O15	78.7(2)
O7- Dy3-O15	140.52(18)	O9C- Dy3-O15	78.7(2)
O7C- Dy3-O15	140.52(18)	O19- Dy4-O6C	74.0(3)
O19- Dy4-O6	74.0(3)	O6C- Dy4-O6	114.2(3)
O19- Dy4-O9	141.8(2)	O9- Dy4-O6C	142.3(2)
O6- Dy 4-O9	77.6(2)	O19- Dy4-O9C	141.8(2)
O6C- Dy4-O9C	77.6(2)	O6- Dy4-O9C	142.3(2)
O9- Dy4-O9C	73.6(3)	O19- Dy4-O8	83.6(5)
O6C- Dy4-O8	145.8(2)	O6- Dy4-O8	82.9(2)
O9- Dy4-O8	67.82(19)	O9C- Dy4-O8	107.51(19)
O19- Dy4-O8C	83.6(5)	O6C- Dy4-O8C	82.9(2)
O6- Dy4-O8C	145.8(2)	O9- Dy4-O8C	107.51(19)
O9C- Dy4-O8C	67.82(19)	O8- Dy4-O8C	69.0(3)
O19- Dy4-O18	13.9(6)	O6C- Dy4-O18	81.1(3)
O6- Dy4-O18	81.1(3)	O9- Dy4-O18	136.5(2)
O9C- Dy4-O18	136.5(2)	O8- Dy4-O18	72.3(3)
O8C- Dy4-O18	72.3(3)	O19- Dy4-O16	116.5(6)
O6C- Dy4-O16	72.8(2)	O6- Dy4-O16	72.8(2)
O9- Dy4-O16	77.7(3)	O9C- Dy4-O16	77.7(3)
O8- Dy4-O16	141.32(18)	O8C- Dy4-O16	141.32(18)
O18- Dy4-O16	130.4(5)		

Symmetry codes: A x, y, z-1, B -x+1/2, -y+1/2, -z+1, C x, -y+1, z, D x, -y+1, z-1.