Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information

Three novel 1D lanthanide-carboxylate polymeric complexes: syntheses, crystal structures and magnetic analyses

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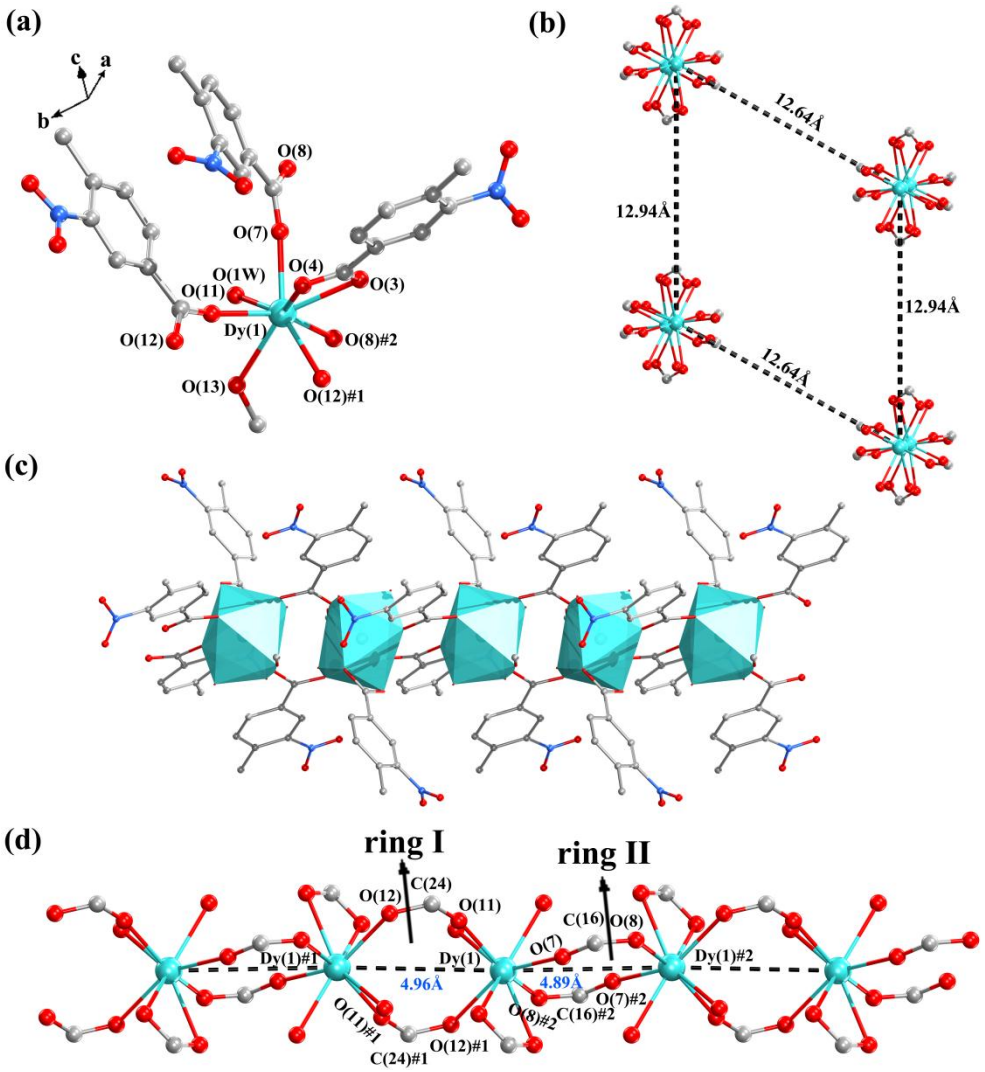

Fig. S1 Crystal structure of complex **3**. (a) View of the coordination environment of the eight-coordinated Dy(III) ion and the numbering scheme of the atoms. Symmetry codes: #1 -x, 1-y, 1-z; #2:1-x, 1-y, 1-z. (b) The rhombic supramolecular topology along *a* axis and the interchain Dy···Dy distances. (c) The polyhedron view of the 1D chain along *c* axis. (d) The two different rings forming from carboxylate bridging resulting to two different intrachain Dy···Dy distances along *c* axis. All hydrogen atoms are omitted for clarity.

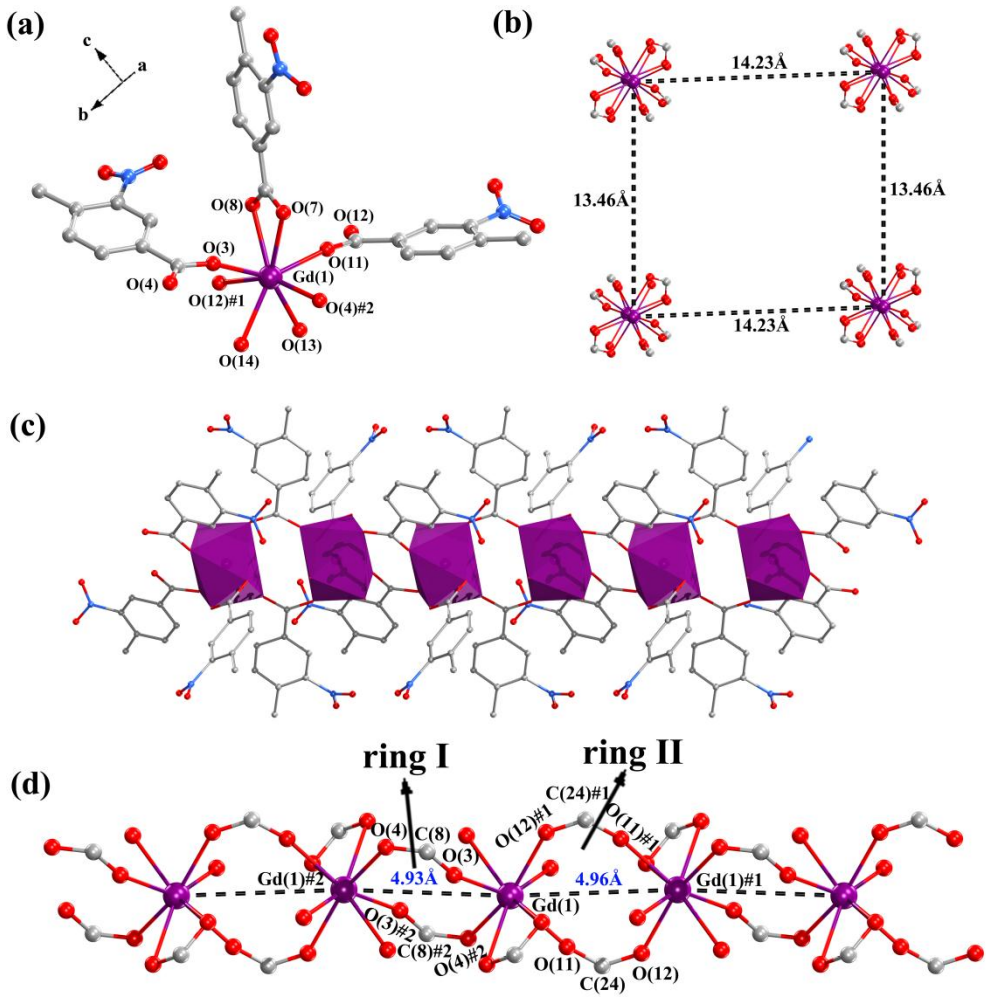

Fig. S2 Crystal structure of complex **2**. (a) View of the coordination environment of the eight-coordinated Gd(III) ion and the numbering scheme of the atoms. Symmetry codes: #1 2-x, 1-y, 1-z; #2: 1-x, 1-y, 1-z. (b) The rhombic supramolecular topology along *a* axis and the interchain Gd···Gd distances. (c) The polyhedron view of the 1D chain along *c* axis. (d) The two different rings forming from carboxylate bridging resulting to two different intrachain Gd···Gd distances along *c* axis. The interstitial 4, 4'-bpy and methanol molecule, and all hydrogen atoms are omitted for clarity.

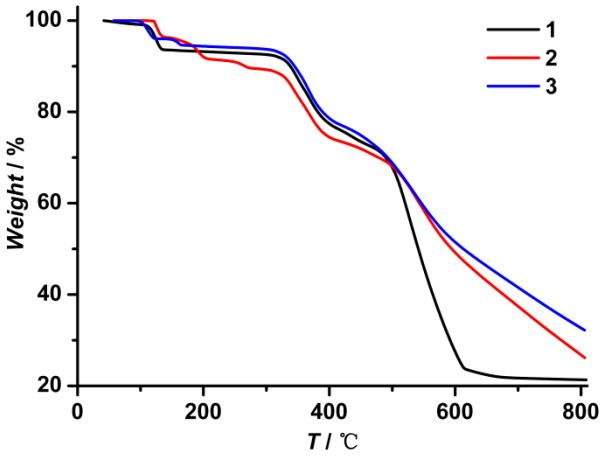

Fig. S3 The TGA curves for complexes **1**-**3**.

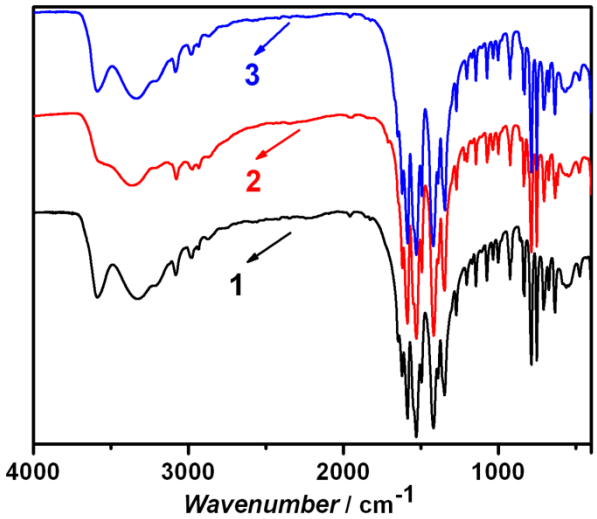

Fig. S4 The IR spectra on KBr pellets for **1**-**3**.

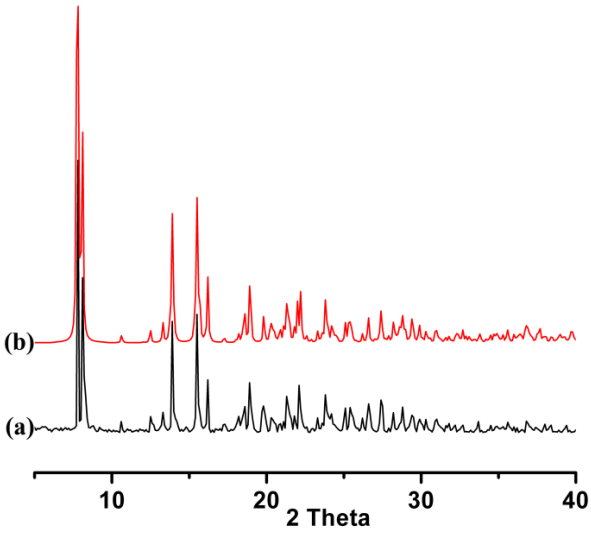

Fig. S5 The Powder X-ray diffraction (PXRD) patterns for complex **1**: (a) the experimental pattern at room temperature; (b) the simulated pattern from single crystal X-ray data.

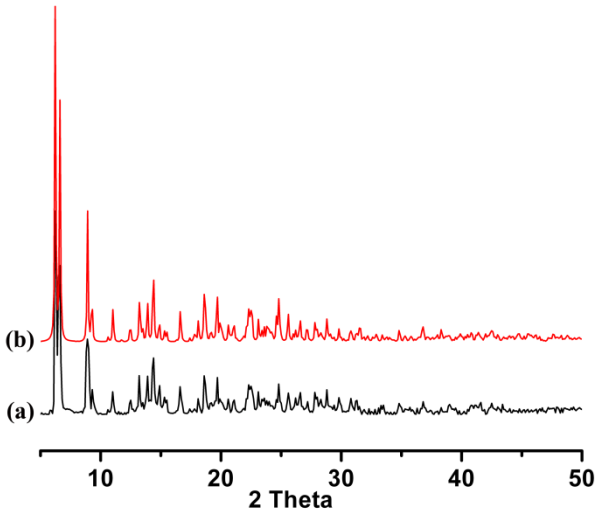

Fig. S6 The PXRD patterns for complex **2**: (a) the experimental pattern at room temperature; (b) the simulated pattern from single crystal X-ray data.

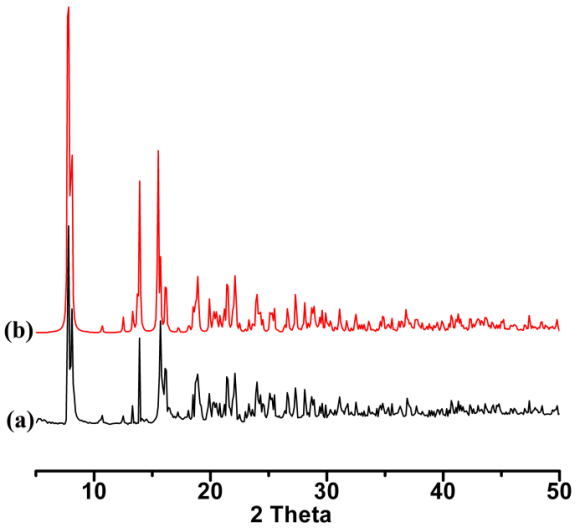

Fig. S7 The PXRD patterns for complex **3**: (a) the experimental pattern at room temperature; (b) the simulated pattern from single crystal X-ray data.

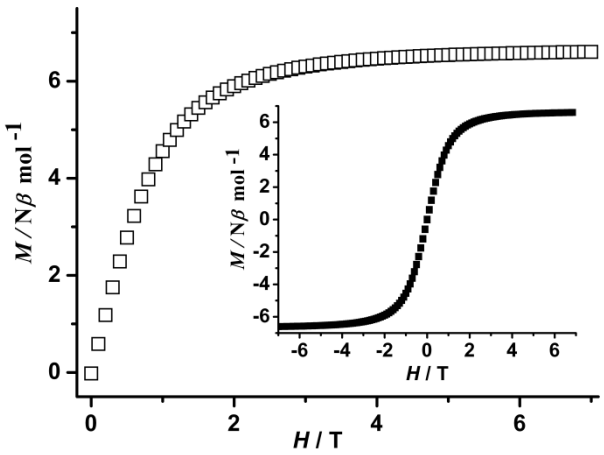

Fig. S8 Field dependence of magnetization at 2.0 K for **1.** Insert: displaying no magnetic hysteresis loop.

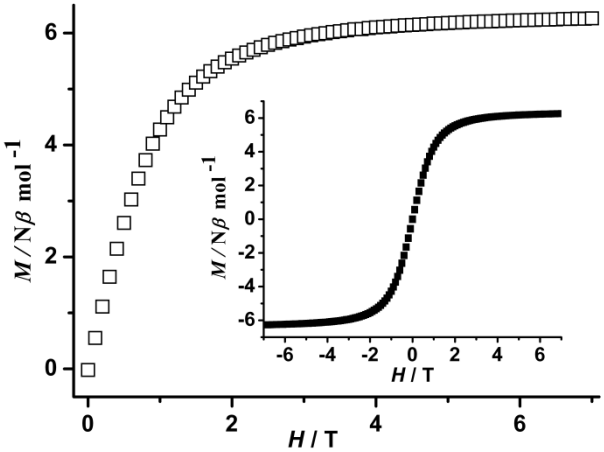

Fig. S9 Field dependence of magnetization at 2.0 K for **2.** Insert: displaying no magnetic hysteresis loop.

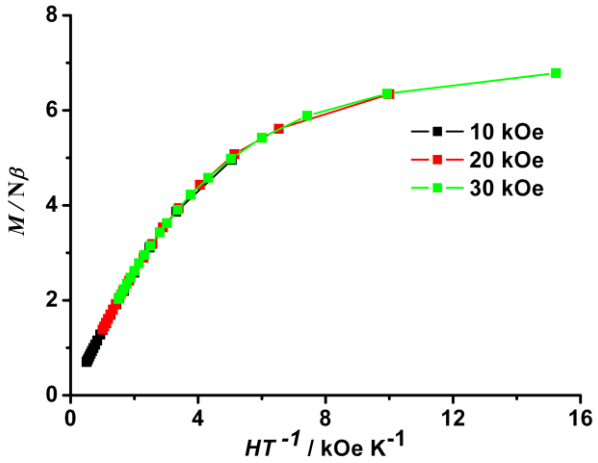

Fig. S10 *M*/Nβ *vs.* HT^{-1} plots measured at various applied magnetic fields for **1**.

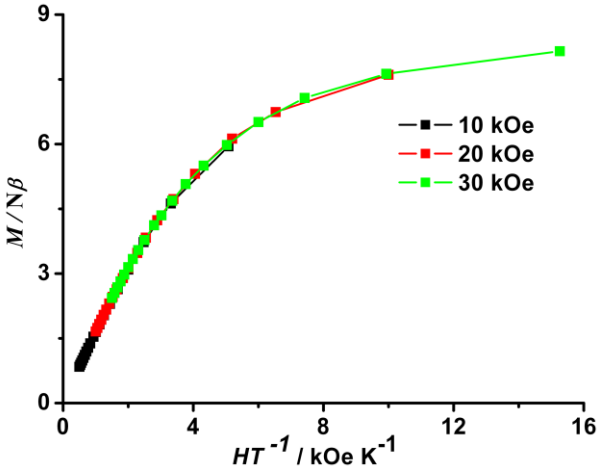

Fig. S11 *M*/Nβ *vs.* HT^{-1} plots measured at various applied magnetic fields for **2.**

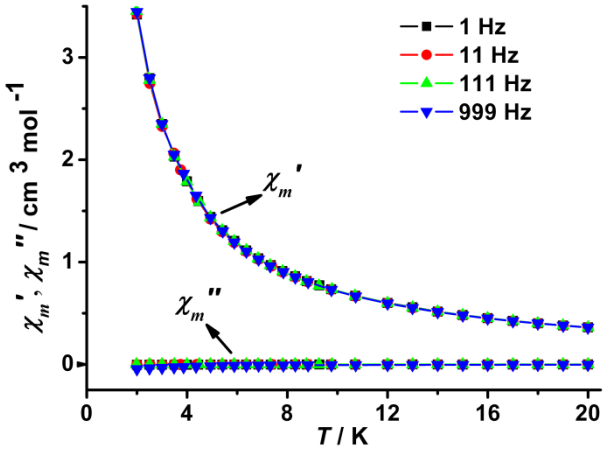

Fig. S12 Temperature dependence of in-phase (χ_m') and out-of-phase (χ_m'') ac susceptibilities of **1** at H_{ac} = 3.5 Oe and H_{dc} = 0.

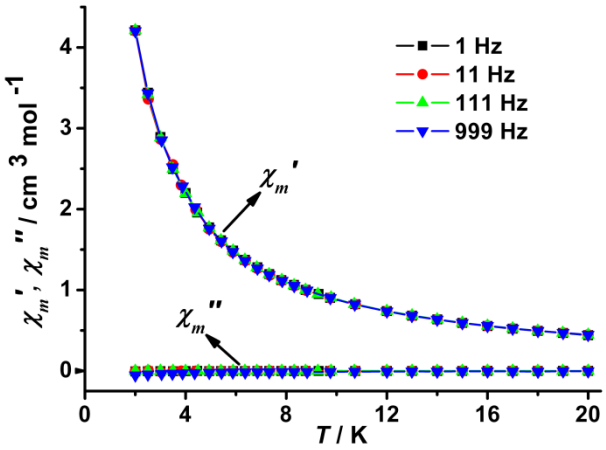

Fig. S13 Temperature dependence of in-phase (χ_m') and out-of-phase (χ_m'') ac susceptibilities of **2** at H_{ac} = 3.5 Oe and H_{dc} = 0.

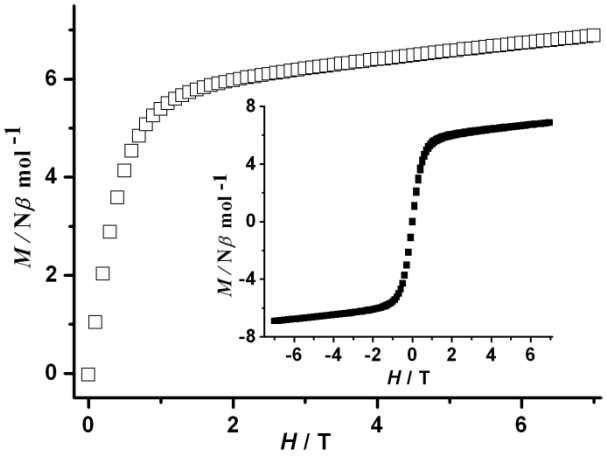

Fig. S14 Field dependence of magnetization at 2.0 K for **3**. Insert: displaying no magnetic hysteresis loop.

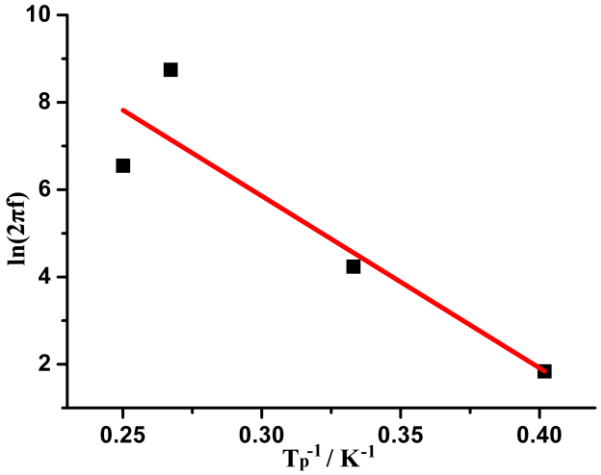

Fig. S15 The plot of ln(2π*f*) versus 1/T_P under a dc field of 5000 Oe for **3.** The red solid line is the best fitting by the Arrhenius law.

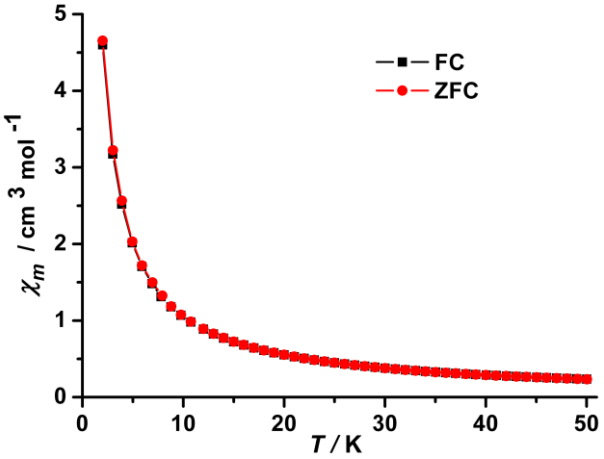

Fig. S16 Plots of zero-field-cooled (ZFC) and field-cooled (FC) susceptibilities versus *T* at the applied field of 50 Oe for complex **3**.

Table 1. Crystallographic data and structure refinement summary for complexes **1-3**.

	1	**2**	**3**
formula	C25H24GdN3O14	C35H34GdN5O15	C25H24DyN3O14
fw	747.72	921.92	752.97
space group	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$
crystal system	Triclinic	Triclinic	Triclinic
***a*/Å**	9.8217(4)	9.8528(6)	9.798(3)
***b*/Å**	12.9436(7)	13.4639(8)	12.935(4)
***c*/Å**	13.4474(8)	14.2272(10)	13.396(4)
***α*/°**	118.50(6)	92.229(5)	118.378(3)
***β*/°**	97.59(4)	90.403(5)	97.249(4)
***γ*/°**	99.98(4)	96.000(5)	99.837(4)
V/Å^3	1433.33(13)	1875.5(2)	1429.1(7)
Z	2	2	2
calculated density (g.cm^{-3})	1.733	1.633	1.750
Absorption coefficient (μ,mm^{-1})	2.388	1.846	2.689
F(000)	742	926	746
crystal size (mm)	0.34 x 0.32 x 0.29	0.32 x 0.28 x 0.21	0.29 x 0.27 x 0.25
θ range (deg)	3.17 to 26.75	3.02 to 27.00	1.78 to 26.75
unique reflns (R_{int})	6093 (0.0369)	7952 (0.0465)	6079 (0.0297)
***R1*,[a] *wR2*[b]($I > 2\sigma(I)$)**	0.0356, 0.0796	0.0509, 0.1019	0.0389, 0.1012
***R1*,[a] *wR2*[b](all data)**	0.0415, 0.0869	0.0677, 0.1122	0.0435, 0.1055
GOF on F^2	1.011	1.028	1.049

$^{a}R = \sum||F_o| - |F_c|| \sum|F_c|$. $^{b}wR_2 = \left[\sum w(|F_o| - |F_c|)^2 / \sum w(F_o^2)\right]^{1/2}$, $w = 1/\sigma(F_o)^2$.

Table 2. Selected bond lengths (Å) and angles (deg) for **1.**

Bond lengths [Å]			
Gd(1)-O(11)	2.227(7)	Gd(1)-O(3)	2.485(3)
Gd(1)-O(7)	2.317(3)	Gd(1)-O(13)	2.487(3)
Gd(1)-O(8)#2	2.329(3)	Gd(1)-O(4)	2.490(3)
Gd(1)-O(12)#1	2.361(8)	Gd(1)-O(1W)	2.446(3)
Angles [deg]			
O(11)-Gd(1)-O(7)	90.68(19)	O(8)#2-Gd(1)-O(4)	128.02(11)
O(11)-Gd(1)-O(8)#2	151.3(2)	O(8)#2-Gd(1)-O(12)#1	75.78(18)
O(11)-Gd(1)-O(4)	78.0(2)	O(8)#2-Gd(1)-O(1W)	78.56(13)
O(11)-Gd(1)-O(13)	70.4(2)	O(8)#2-Gd(1)-O(13)	82.25(13)
O(11)-Gd(1)-O(12)#1	103.6(2)	O(12)#1-Gd(1)-O(13)	73.7(3)
O(11)-Gd(1)-O(3)	129.3(2)	O(12)#1-Gd(1)-O(1W)	137.7(3)
O(11)-Gd(1)-O(1W)	84.0(2)	O(12)#1-Gd(1)-O(4)	76.2(2)
O(7)-Gd(1)-O(3)	71.40(10)	O(12)#1-Gd(1)-O(3)	76.6(2)
O(7)-Gd(1)-O(4)	77.96(10)	O(1W)-Gd(1)-O(3)	130.07(10)
O(7)-Gd(1)-O(13)	139.28(12)	O(1W)-Gd(1)-O(13)	69.89(12)

O(7)-Gd(1)-O(8)#2	105.31(10)	O(1W)-Gd(1)-O(4)	145.10(12)
O(7)-Gd(1)-O(12)#1	147.0(3)	O(3)-Gd(1)-O(4)	52.41(9)
O(7)-Gd(1)-O(1W)	72.57(12)	O(3)-Gd(1)-O(13)	147.91(12)
O(8)#2-Gd(1)-O(3)	78.90(11)	O(4)-Gd(1)-O(13)	128.98(10)

Symmetry transformations used to generate equivalent atoms: #1 -x,-y+1,-z+1, #2 -x+1,-y+1,-z+1

Table 3. Selected bond lengths (Å) and angles (deg) for **2**.

Bond lengths [Å]			
Gd(1)-O(11)	2.308(4)	Gd(1)-O(8)	2.490(4)
Gd(1)-O(12)#1	2.332(3)	Gd(1)-O(7)	2.539(4)
Gd(1)-O(3)	2.338(4)	Gd(1)-O(13)	2.424(4)
Gd(1)-O(4)#2	2.371(3)	Gd(1)-O(14)	2.451(4)
Angles [deg]			
O(11)-Gd(1)-O(12)#1	105.94(14)	O(3)-Gd(1)-O(8)	76.88(13)
O(11)-Gd(1)-O(3)	145.39(15)	O(3)-Gd(1)-O(14)	74.14(15)
O(11)-Gd(1)-O(4)#2	83.83(13)	O(3)-Gd(1)-O(4)#2	101.94(13)
O(11)-Gd(1)-O(13)	72.46(16)	O(3)-Gd(1)-O(13)	141.67(15)
O(11)-Gd(1)-O(14)	139.96(16)	O(4)#2-Gd(1)-O(8)	127.73(12)
O(11)-Gd(1)-O(8)	72.97(14)	O(4)#2-Gd(1)-O(7)	78.05(13)
O(11)-Gd(1)-O(7)	77.74(14)	O(4)#2-Gd(1)-O(13)	84.25(14)
O(12)#1-Gd(1)-O(13)	78.89(15)	O(4)#2-Gd(1)-O(14)	79.43(13)
O(12)#1-Gd(1)-O(3)	82.18(13)	O(13)-Gd(1)-O(8)	128.70(12)
O(12)#1-Gd(1)-O(4)#2	156.70(14)	O(13)-Gd(1)-O(7)	146.70(15)
O(12)#1-Gd(1)-O(14)	79.73(13)	O(13)-Gd(1)-O(14)	69.88(15)
O(12)#1-Gd(1)-O(8)	75.57(12)	O(14)-Gd(1)-O(7)	132.42(13)
O(12)#1-Gd(1)-O(7)	124.30(13)	O(14)-Gd(1)-O(8)	144.01(14)
O(3)-Gd(1)-O(7)	70.37(13)	O(8)-Gd(1)-O(7)	51.86(11)

Symmetry transformations used to generate equivalent atoms: #1 -x+2,-y+1,-z+1, #2 -x+1,-y+1,-z+1,

Table 4. Selected bond lengths (Å) and angles (deg) for **3**.

Bond lengths [Å]			
Dy(1)-O(11)	2.204(6)	Dy(1)-O(12)#1	2.338(7)
Dy(1)-O(1W)	2.413(4)	Dy(1)-O(3)	2.466(3)
Dy(1)-O(7)	2.286(3)	Dy(1)-O(4)	2.469(3)
Dy(1)-O(8)#2	2.302(3)	Dy(1)-O(13)	2.470(4)
Angles [deg]			
O(11)-Dy(1)-O(13)	70.5(2)	O(8)#2-Dy(1)-O(1W)	78.67(15)
O(11)-Dy(1)-O(7)	91.5(2)	O(8)#2-Dy(1)-O(3)	78.35(13)
O(11)-Dy(1)-O(8)#2	151.3(2)	O(8)#2-Dy(1)-O(4)	128.40(14)
O(11)-Dy(1)-O(12)#1	103.0(2)	O(8)#2-Dy(1)-O(13)	82.21(15)
O(11)-Dy(1)-O(1W)	83.8(2)	O(12)#1-Dy(1)-O(13)	73.8(2)
O(11)-Dy(1)-O(3)	130.0(2)	O(12)#1-Dy(1)-O(1W)	138.6(2)

O(11)-Dy(1)-O(4)	77.8(2)	O(12)#1-Dy(1)-O(3)	76.2(2)
O(7)-Dy(1)-O(4)	78.03(13)	O(12)#1-Dy(1)-O(4)	75.9(2)
O(7)-Dy(1)-O(1W)	72.15(14)	O(1W)-Dy(1)-O(13)	70.27(14)
O(7)-Dy(1)-O(8)#2	104.35(13)	O(1W)-Dy(1)-O(4)	144.36(15)
O(7)-Dy(1)-O(12)#1	146.5(2)	O(1W)-Dy(1)-O(3)	129.89(12)
O (7)-Dy(1)-O(3)	71.40(13)	O(3)-Dy(1)-O(4)	53.06(10)
O(7)-Dy(1)-O(13)	139.65(15)	O(3)-Dy(1)-O(13)	147.26(15)
O(8)#2-Dy(1)-O(12)#1	76.8(2)	O(4)-Dy(1)-O(13)	129.05(12)

Symmetry transformations used to generate equivalent atoms: #1 -x,-y+1,-z+1, #2 -x+1,-y+1,-z+1

CCDC 891155 (**1**), 892519 (**2**), 891154 (**3**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge via www.ccdc.can.ac.uk/conts/retrieving.html.