

Electronic Supplementary Information (ESI)

Large magnetic entropy changes in three Gd^{III} coordination polymers containing Gd^{III} chains

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Table S1. Selected bond lengths (Å) and angles (°) for **1^a**

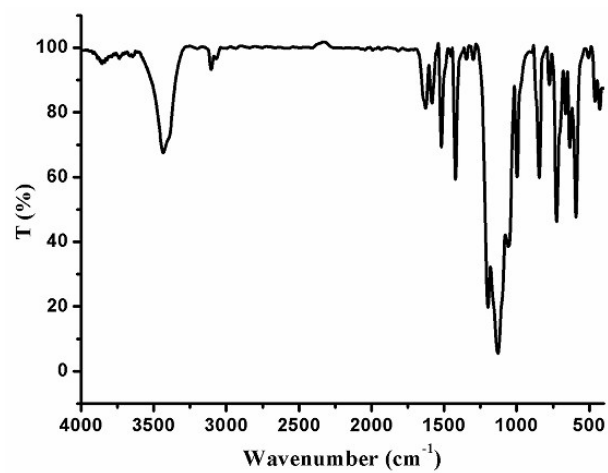
Gd1—O3	2.318(7)	Gd2—O5	2.298(6)
Gd1—O9 ^{#1}	2.339(6)	Gd2—O11 ^{#1}	2.338(6)
Gd1—O7	2.365(6)	Gd2—O4	2.365(6)
Gd1—O2 ^{#1}	2.398(6)	Gd2—O6 ^{#2}	2.398(6)
Gd1—O12	2.452(6)	Gd2—O10 ^{#3}	2.439(6)
Gd1—O1W	2.547(7)	Gd2—N3	2.552(8)
Gd1—N2	2.559(9)	Gd2—O2W	2.557(7)
Gd1—N1	2.607(8)	Gd2—N4	2.573(7)
Gd1—O9	2.917(7)		
O3—Gd1—O9 ^{#1}	75.2(2)	O5—Gd2—O11 ^{#1}	74.3(2)
O3—Gd1—O7	86.4(2)	O5—Gd2—O4	88.2(2)
O9 ^{#1} —Gd1—O7	88.9(2)	O11 ^{#1} —Gd2—O4	88.0(2)
O3—Gd1—O2 ^{#1}	128.9(2)	O5—Gd2—O6 ^{#2}	126.8(2)
O9 ^{#1} —Gd1—O2 ^{#1}	79.1(2)	O11 ^{#1} —Gd2—O6 ^{#2}	79.5(2)
O7—Gd1—O2 ^{#1}	136.5(2)	O4—Gd2—O6 ^{#2}	136.5(2)
O3—Gd1—O12	85.8(2)	O5—Gd2—O10 ^{#3}	84.9(2)
O9 ^{#1} —Gd1—O12	122.4(2)	O11 ^{#1} —Gd2—O10 ^{#3}	122.8(2)
O7—Gd1—O12	144.2(2)	O4—Gd2—O10 ^{#3}	144.9(2)
O2 ^{#1} —Gd1—O12	72.0(2)	O6 ^{#2} —Gd2—O10 ^{#3}	71.7(2)
O3—Gd1—O1W	137.7(2)	O5—Gd2—N3	138.7(3)
O9 ^{#1} —Gd1—O1W	70.4(2)	O11 ^{#1} —Gd2—N3	146.5(2)
O7—Gd1—O1W	69.3(2)	O4—Gd2—N3	88.1(2)
O2 ^{#1} —Gd1—O1W	67.3(2)	O6 ^{#2} —Gd2—N3	80.7(3)
O12—Gd1—O1W	133.6(2)	O10 ^{#3} —Gd2—N3	75.1(2)
O3—Gd1—N2	138.9(3)	O5—Gd2—O2W	138.0(2)
O9 ^{#1} —Gd1—N2	145.0(3)	O11 ^{#1} —Gd2—O2W	70.2(2)
O7—Gd1—N2	86.8(2)	O4—Gd2—O2W	69.0(2)
O2 ^{#1} —Gd1—N2	80.4(3)	O6 ^{#2} —Gd2—O2W	67.5(2)
O12—Gd1—N2	76.6(2)	O10 ^{#3} —Gd2—O2W	133.5(2)
O1W—Gd1—N2	75.6(3)	N3—Gd2—O2W	77.3(2)
O3—Gd1—N1	75.6(2)	O5—Gd2—N4	75.8(2)
O9 ^{#1} —Gd1—N1	145.1(2)	O11 ^{#1} —Gd2—N4	143.5(2)
O7—Gd1—N1	70.4(2)	O4—Gd2—N4	70.5(2)
O2 ^{#1} —Gd1—N1	135.1(2)	O6 ^{#2} —Gd2—N4	136.2(2)
O12—Gd1—N1	73.8(2)	O10 ^{#3} —Gd2—N4	74.4(2)
O1W—Gd1—N1	123.3(2)	N3—Gd2—N4	64.3(3)
N2—Gd1—N1	63.9(3)	O2W—Gd2—N4	124.1(2)
O3—Gd1—O9	66.4(2)	O12—Gd1—O9	51.16(18)
O9 ^{#1} —Gd1—O9	71.6(2)	O1W—Gd1—O9	122.08(19)
O7—Gd1—O9	149.5(2)	N2—Gd1—O9	122.6(2)
O2 ^{#1} —Gd1—O9	63.83(19)	N1—Gd1—O9	113.0(2)

^aSymmetry codes: #1: $-x+1, -y+2, -z+1$; #2: $-x+2, -y+2, -z+1$; #3: $x+1, y, z$.

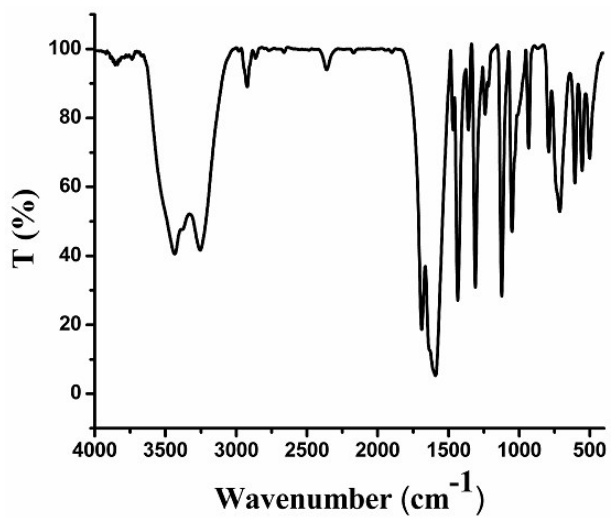
Table S2. Selected bond lengths (Å) and angles (°) for **3^a**

O6—Gd1 ^{#1}	2.379(2)	Gd1—O1	2.465(2)
O6—Gd1 ^{#2}	2.648(2)	Gd1—O4 ^{#3}	2.542(2)
O5—Gd1 ^{#2}	2.422(2)	Gd1—O1W	2.384(2)
O3—Gd1 ^{#3}	2.458(2)	Gd1—O2	2.425(2)
Gd1—O4	2.377(2)		
O4—Gd1—O6 ^{#1}	162.04(8)	O1W—Gd1—O1	78.22(8)
O4—Gd1—O1W	88.30(8)	O5 ^{#4} —Gd1—O1	146.02(8)
O6 ^{#1} —Gd1—O1W	80.04(9)	O2—Gd1—O1	53.22(8)
O4—Gd1—O5 ^{#4}	74.62(8)	O3 ^{#3} —Gd1—O1	129.31(8)
O6 ^{#1} —Gd1—O5 ^{#4}	117.09(8)	O4—Gd1—O4 ^{#3}	66.68(9)
O1W—Gd1—O5 ^{#4}	83.57(9)	O6 ^{#1} —Gd1—O4 ^{#3}	128.21(8)
O4—Gd1—O2	96.78(9)	O1W—Gd1—O4 ^{#3}	149.46(8)
O6 ^{#1} —Gd1—O2	80.03(8)	O5 ^{#4} —Gd1—O4 ^{#3}	73.39(8)
O1W—Gd1—O2	127.74(8)	O2—Gd1—O4 ^{#3}	74.78(8)
O5 ^{#4} —Gd1—O2	147.85(9)	O3 ^{#3} —Gd1—O4 ^{#3}	51.83(7)
O4—Gd1—O3 ^{#3}	117.96(8)	O1—Gd1—O4 ^{#3}	110.42(8)
O6 ^{#1} —Gd1—O3 ^{#3}	78.70(8)	O4—Gd1—O6 ^{#4}	123.01(8)
O1W—Gd1—O3 ^{#3}	143.96(8)	O6 ^{#1} —Gd1—O6 ^{#4}	66.34(9)
O5 ^{#4} —Gd1—O3 ^{#3}	80.68(9)	O1W—Gd1—O6 ^{#4}	72.37(8)
O2—Gd1—O3 ^{#3}	76.27(8)	O5 ^{#4} —Gd1—O6 ^{#4}	50.80(7)
O4—Gd1—O1	76.38(8)	O2—Gd1—O6 ^{#4}	137.59(8)
O6 ^{#1} —Gd1—O1	87.82(8)	O3 ^{#3} —Gd1—O6 ^{#4}	72.53(8)
O4 ^{#3} —Gd1—O6 ^{#4}	105.93(7)	O1—Gd1—O6 ^{#4}	143.45(8)

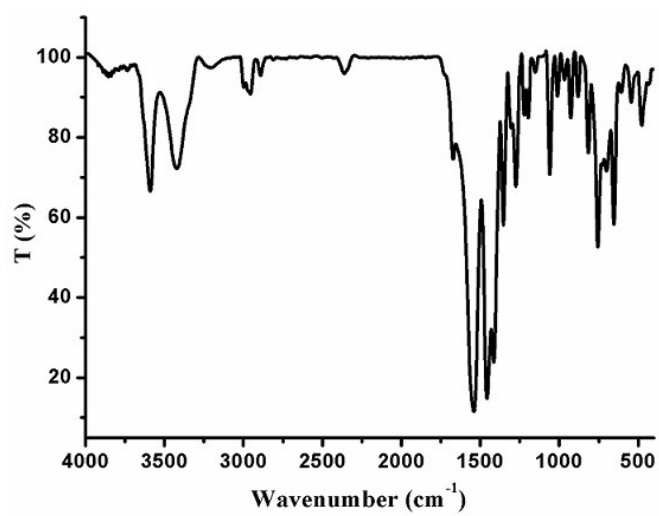
^aSymmetry codes: #1: $-x+1/2, -y+3/2, -z+1$; #2: $x-1/2, y-1/2, z$; #3: $-x, -y+2, -z+1$; #4: $x+1/2, y+1/2, z$.



(a)

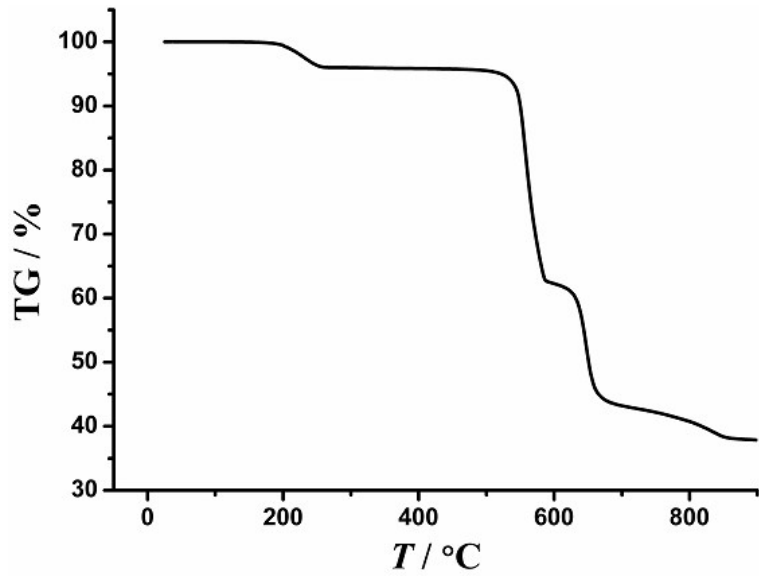


(b)

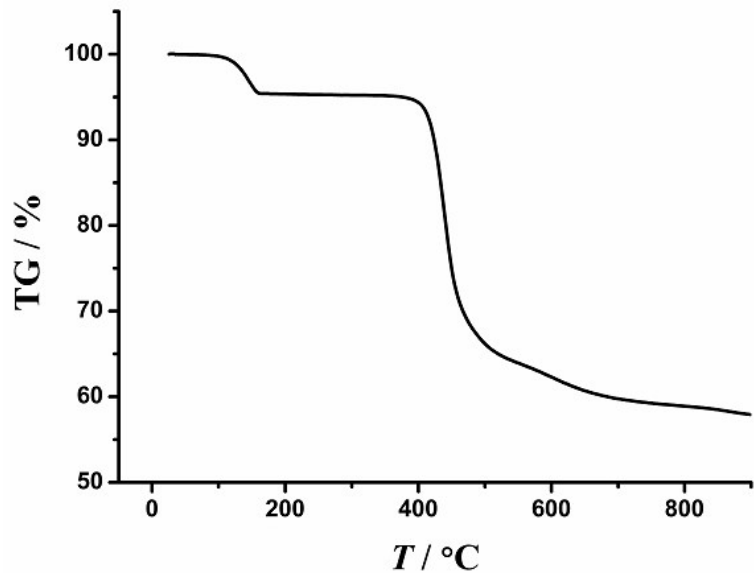


(c)

Fig. S1. The IR spectra of **1** (a), **2** (b) and **3** (c).

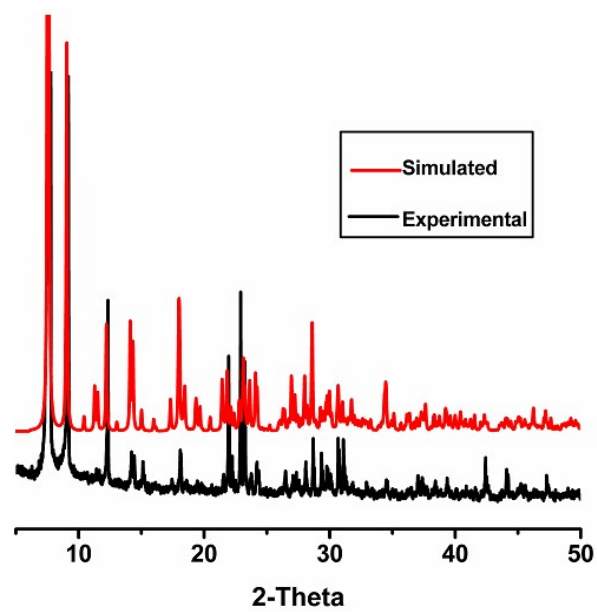


(a)

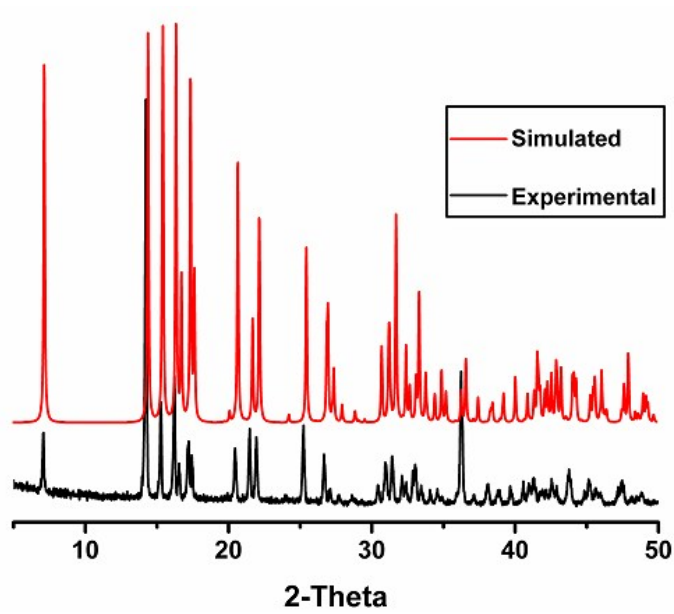


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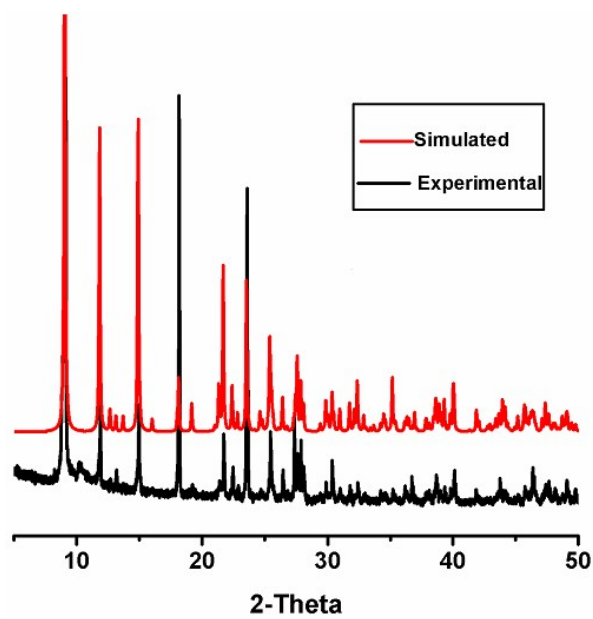
Fig. S2. The TGA curves for **1** (a) and **3** (b).



(a)

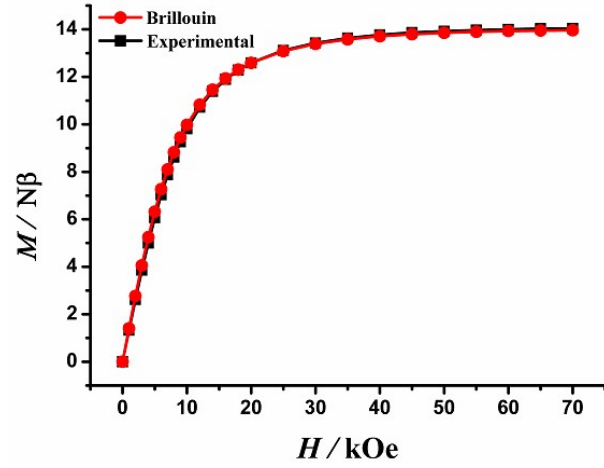


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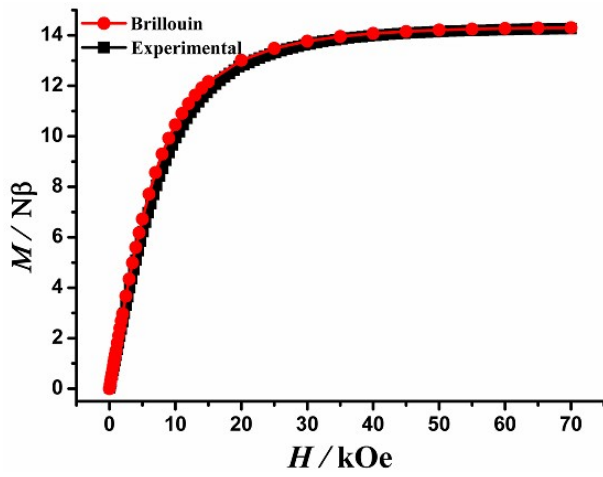


(c)

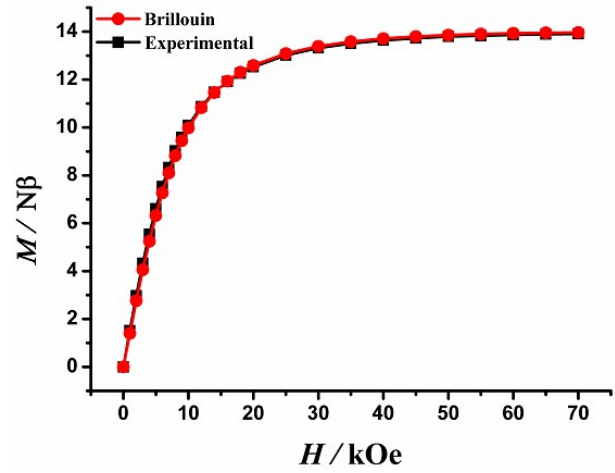
Fig. S3. Powder X-ray diffraction (PXRD) patterns of (a) **1**, (b) **2** and (c) **3**.



(a)

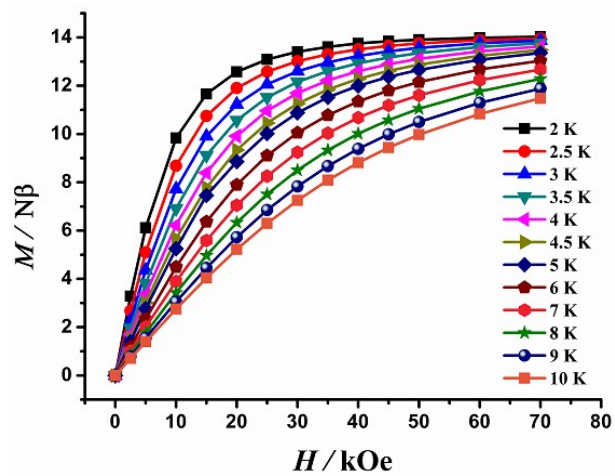


(b)

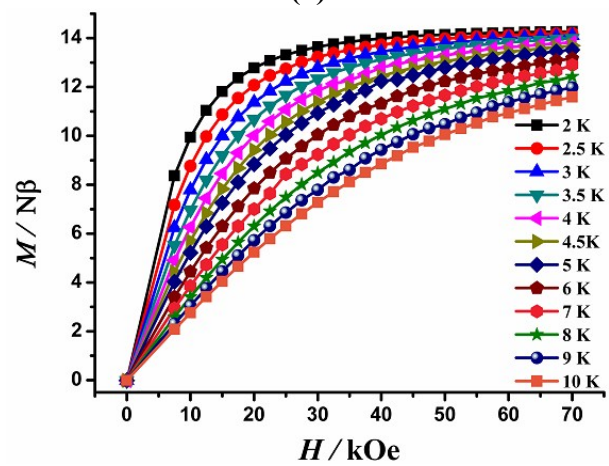


(c)

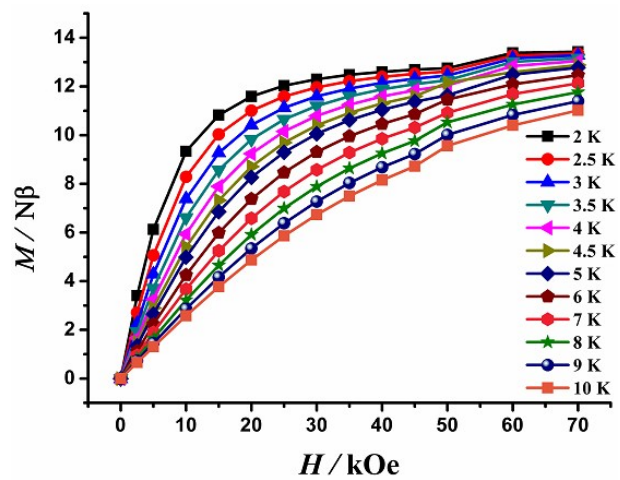
Fig. S4. The M vs. H plots of 1 (a), 2 (b) and 3 (c) in the field range 0-70 kOe.



(a)



(b)



(c)

Fig. S5. The M vs. H curves of 1 (a), 2 (b) and 3 (c) in the temperature range 2-10 K.