Electronic Supplementary Information (ESI)

Two Gd^{III} complexes with different structures and magnetocaloric properties induced by metal ion sources

Teng-Fei Zheng,[a] Xue-Mei Tian,[a] Lin-Hui Wu,[a] Sui-Jun Liu,*[a] Shu-Li Yao,[a] Kun-Huan He,*[b] Haiping Huang,[a] Jinsheng Liao,[a] Jing-Lin Chen[a] and He-Rui Wen*[a]

[a]School of Chemistry and Chemical Engineering, Jiangxi University of Science and Technology, Ganzhou 341000, Jiangxi Province, P.R. China

[b]College of Petroleum and Chemical Engineering, Beibu Gulf University, Qinzhou 535011, Guangxi Province, P.R. China.

E-mail: sjliu@jxust.edu.cn (S.-J. Liu), wenherui63@163.com (H.-R. Wen), hkh821227@163.com (K.-H. He).

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

O1—C1	1.259(5)	Gd1—O4$^{\#1}$	2.383(3)
O1—Gd1	2.371(3)	Gd1—O4	2.383(3)
O3—Gd1	2.371(3)	Gd1—O1W	2.365(3)
Gd1—O1W$^{\#1}$	2.365(4)		
O1—Gd1—O1$^{\#1}$	78.68(17)	O3$^{\#1}$—Gd1—O4	113.60(12)
O1$^{\#1}$—Gd1—O4$^{\#1}$	76.10(12)	O3—Gd1—O4	74.44(11)
O1—Gd1—O4$^{\#1}$	74.85(11)	O4$^{\#1}$—Gd1—O4	142.16(16)
O1—Gd1—O4	76.10(12)	O1W—Gd1—O1	141.57(12)
O1$^{\#1}$—Gd1—O4	74.85(11)	O1W$^{\#1}$—Gd1—O1	114.72(13)
O3$^{\#1}$—Gd1—O1$^{\#1}$	65.34(12)	O1W$^{\#1}$—Gd1—O1$^{\#1}$	141.57(12)
O3—Gd1—O1$^{\#1}$	137.08(11)	O1W—Gd1—O1$^{\#1}$	114.72(13)
O3$^{\#1}$—Gd1—O1	137.08(11)	O1W$^{\#1}$—Gd1—O3	77.73(12)
O3—Gd1—O1	65.34(11)	O1W—Gd1—O3$^{\#1}$	77.73(12)
O3—Gd1—O3$^{\#1}$	156.49(16)	O1W$^{\#1}$—Gd1—O3$^{\#1}$	84.03(13)
O3—Gd1—O4$^{\#1}$	113.60(12)	O1W—Gd1—O3	84.03(13)
O3$^{\#1}$—Gd1—O4$^{\#1}$	74.44(11)	O1W$^{\#1}$—Gd1—O4	141.85(12)
O1W$^{\#1}$—Gd1—O4$^{\#1}$	73.59(12)	O1W—Gd1—O4$^{\#1}$	141.85(12)
O1W—Gd1—O1W$^{\#1}$	78.06(18)	O1W—Gd1—O4	73.59(12)

[a]Symmetry code: #1: −*x*+1/2, *y*, −*z*+3/2.

Table S2. Selected bond lengths (Å) and angles (°) for **2**[a].

O4—Gd1$^{\#1}$	2.645(2)	Gd1—O1	2.366(2)
O4—Gd1$^{\#2}$	2.416(2)	Gd1—O3	2.480(2)
O5—Gd1$^{\#1}$	2.464(2)	Gd1—O6	2.433(2)
O7—Gd1$^{\#3}$	2.428(2)	Gd1—O1W	2.445(2)
O2—Gd1$^{\#4}$	2.384(2)		
O4$^{\#2}$—Gd1—O4$^{\#5}$	63.20(8)	O2$^{\#6}$—Gd1—O6	99.11(9)
O4$^{\#2}$—Gd1—O5$^{\#5}$	113.40(7)	O2$^{\#6}$—Gd1—O1W	78.55(8)
O4$^{\#2}$—Gd1—O7$^{\#3}$	143.84(8)	O1—Gd1—O4$^{\#5}$	70.23(7)
O4$^{\#2}$—Gd1—O3	80.07(7)	O1—Gd1—O4$^{\#2}$	82.38(7)
O4$^{\#2}$—Gd1—O6	146.60(8)	O1—Gd1—O5$^{\#5}$	77.50(7)
O4$^{\#2}$—Gd1—O1W	79.34(8)	O1—Gd1—O7$^{\#3}$	133.10(8)
O5$^{\#5}$—Gd1—O4$^{\#5}$	50.22(7)	O1—Gd1—O2$^{\#6}$	132.95(7)
O5$^{\#5}$—Gd1—O3	137.85(7)	O1—Gd1—O3	64.50(7)
O7$^{\#3}$—Gd1—O4$^{\#5}$	116.24(8)	O1—Gd1—O6	73.39(8)
O7$^{\#3}$—Gd1—O5$^{\#5}$	75.46(8)	O1—Gd1—O1W	139.87(7)
O7$^{\#3}$—Gd1—O3	117.92(8)	O3—Gd1—O4$^{\#5}$	124.41(7)
O7$^{\#3}$—Gd1—O6	66.21(8)	O6—Gd1—O4$^{\#5}$	125.75(8)
O7$^{\#3}$—Gd1—O1W	68.20(9)	O6—Gd1—O5$^{\#5}$	83.74(8)
O2$^{\#6}$—Gd1—O4$^{\#5}$	135.11(7)	O6—Gd1—O3	68.97(8)
O2$^{\#6}$—Gd1—O4$^{\#2}$	80.75(8)	O6—Gd1—O1W	133.69(9)
O2$^{\#6}$—Gd1—O5$^{\#5}$	149.13(7)	O1W—Gd1—O4$^{\#5}$	69.64(7)
O2$^{\#6}$—Gd1—C4$^{\#5}$	149.59(7)	O1W—Gd1—O5$^{\#5}$	77.56(8)
O2$^{\#6}$—Gd1—O7$^{\#3}$	77.68(9)	O1W—Gd1—O3	144.21(8)
O2$^{\#6}$—Gd1—O3	69.47(7)		

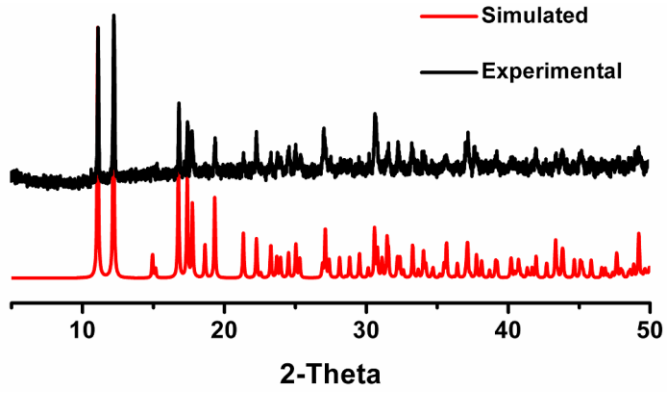
[a]Symmetry codes: #1: *x*, *y*+1, *z*; #2: −*x*+1, −*y*+2, −*z*+2; #3: −*x*+1, −*y*+1, −*z*+1; #4: *x*−1, *y*, *z*; #5: *x*, *y*−1, *z*; #6: *x*+1, *y*, *z*.

Table S3. SHAPE analysis of Gd^{III} ions in **1** and **2**.

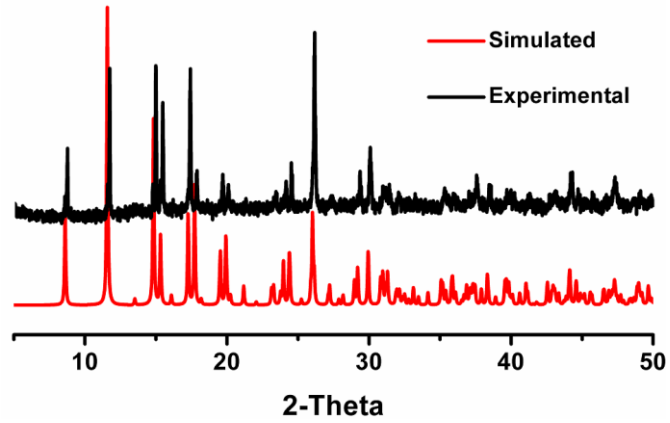
Complex	Label	Shape	Symmetry	Distortion (τ)
1	OP-8	Octagon	D_{8h}	29.709
1	HPY-8	Heptagonal pyramid	C_{7v}	22.376
1	HBPY-8	Hexagonal bipyramid	D_{6h}	16.246
1	CU-8	Cube	O_h	9.047
1	SAPR-8	Square antiprism	D_{4d}	**0.461**
1	TDD-8	Triangular dodecahedron	D_{2d}	2.547
1	JGBF-8	Johnson gyrobifastigium J26	D_{2d}	15.898
1	JETBPY-8	Johnson elongated triangular bipyramid J14	D_{3h}	27.624
1	JBTPR-8	Biaugmented trigonal prism J50	C_{2v}	3.230
1	BTPR-8	Biaugmented trigonal prism	C_{2v}	2.643
1	JSD-8	Snub diphenoid J84	D_{2d}	5.653
1	TT-8	Triakis tetrahedron	T_d	9.911
1	ETBPY-8	Elongated trigonal bipyramid	D_{3h}	23.678
2	EP-9	Enneagon	D_{9h}	32.880
2	OPY-9	Octagonal pyramid	C_{8v}	22.756
2	HBPY-9	Heptagonal bipyramid	D_{7h}	18.137
2	JTC-9	Johnson triangular cupola J3	C_{3v}	13.481
2	JCCU-9	Capped cube J8	C_{4v}	9.741
2	CCU-9	Spherical-relaxed capped cube	C_{4v}	9.023
2	JCSAPR-9	Capped square antiprism J10	C_{4v}	1.704
2	CSAPR-9	Spherical capped square antiprism	C_{4v}	**1.382**
2	JTCTPR-9	Tricapped trigonal prism J51	D_{3h}	2.433
2	TCTPR-9	Spherical tricapped trigonal prism	D_{3h}	1.835
2	JTDIC-9	Tridiminished icosahedron J63	C_{3v}	11.460
2	HH-9	Hula-hoop	C_{2v}	12.001
2	MFF-9	Muffin	C_s	1.895

Table S4. Hydrogen-bonding geometry (Å, °) for **1**.

D–H···A	**D–H**	**H···A**	**D···A**	**D–H···A**
O1W–H1WA···O1	0.85	1.90	2.742(5)	174
O1W–H1WB···O5	0.85	1.86	2.683(5)	161
O3–H3···O2	0.86(2)	1.833(18)	2.660(4)	161(4)
O2W–H2WA···O2	0.87	1.84	2.614(6)	147
O2W–H2WB···O2	0.87	1.76	2.625(6)	172



(a)



(b)

Fig. S1. PXRD patterns of **1** (a) and **2** (b).

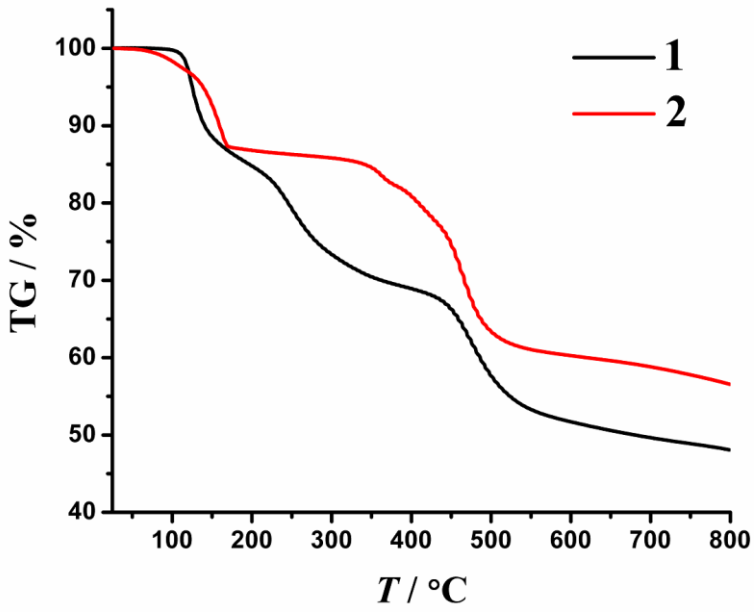


Fig. S2. Thermogravimetric analysis (TGA) curves of **1** and **2**.

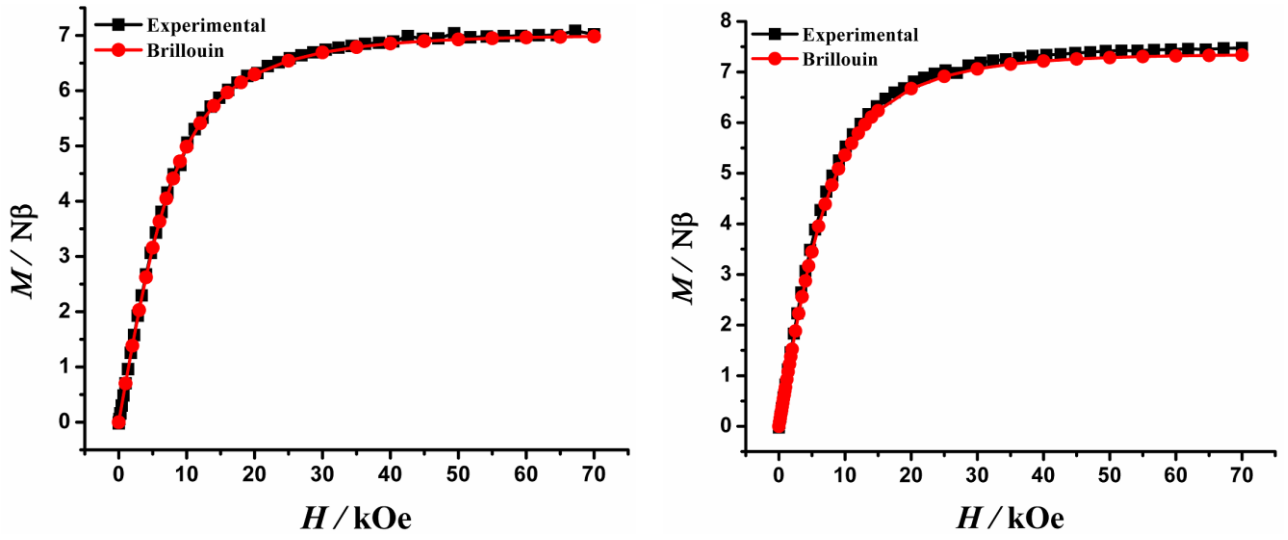


Fig. S3. The *M vs. H* curves at 2 K of **1** (a) and **2** (b).