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Cryogenic Magnetocaloric Effect in Distorted Double-perovskite Gd₂ZnTiO₆

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1 Experimental Section

Structural Analysis. The products were investigated by powder X-ray diffraction patterns collected on a Rigaku Ultimate IV diffractometer equipped with Cu-*Ka* radiation at room temperature. A Rietveld analysis was performed using the GSAS package with the *EXPGUI* interface.^[1-3] The backgrounds and peak shape were modeled by the first kind of Chebyshev polynomial and pseudo-Voigt function.

Physical Measurements. The magnetic susceptibility and magnetization data were collected in the Physical Property Measurement System (PPMS®DynaCoolTM, Quantum Design) with an applied field of 20 mT in the 2-300 K temperature range. Isothermal magnetization curves were collected in the field range \leq 7 T and temperature range of 2-11 K with a step of 1 K after cooling in zero fields.

Heat capacity measurements were conducted using the thermal-relaxation method on powder samples in a commercial setup Physical Property Measurement System (PPMS-9, Quantum Design) with Apiezon N-grease, under a temperature range of 1.9-30 K and constant external fields of 0, 2, 7, and 9 T, respectively.

2 Supplementary tables

Vector	Leng	th Optr (Cell Ne	eighbor atom coordinates
Gd1_	Gd1	3.7863(20)	2 1-1 0	0.98415 0.06532 0.25302
Gd1_	Gd1	3.7863(20)	2100	0.98415 1.06532 0.25302
Gd1_	Gd1	3.870(6)	-1110	0.48415 0.43468 -0.24698
Gd1_	Gd1	3.963(6)	-1111	0.48415 0.43468 0.75302
Gd1_	01	2.728(12)	2000	0.30294 0.69262 0.55467
Gd1_	01	2.542(13)	-1110	0.80294 0.80738 0.05467
Gd1_	01	2.321(11)	-2111	0.69706 0.30738 0.44533
Gd1_	02	2.661(12)	1000	0.31569 0.70776 -0.05265
Gd1_	02	2.335(11)	-1110	0.68431 0.29224 0.05265
Gd1_	02	2.566(13)	-2121	0.81569 0.79224 0.44735
Gd1_	O3	2.366(6)	1010	0.39080 0.96569 0.23940
Gd1_	O3	2.257(8)	2000	0.10920 0.46569 0.26060
Gd1_	Ti1	3.1096(19)	1010	0.50000 1.00000 0.00000
Gd1_	Ti1	3.4110(17)	2000	0.00000 0.50000 0.50000
Gd1_	Ti1	3.2582(25)	2100	1.00000 0.50000 0.50000
Gd1_	Zn1	3.3687(24)	1000	0.00000 0.50000 0.00000
Gd1_	Zn1	3.2464(17)	1100	1.00000 0.50000 0.00000
Gd1_	Zn1	3.1387(19)	2000	0.50000 1.00000 0.50000
Ti1_G	id1	3.1096(19)	10-10	0.51585 -0.43468 0.24698
	id1	3.4110(17)	20-10	-0.01585 0.06532 0.25302
	id1	3.2582(25)	21-10	0.98415 0.06532 0.25302
	id1	3.1096(19)	-1110	0.48415 0.43468 -0.24698
	id1	3.2582(25)	-2010	0.01585 -0.06532 -0.25302
	id1	3.4110(17)	-2110	1.01585 -0.06532 -0.25302
)1	2.001(12)	1000	0.19706 0.19262 -0.05467

Table S1 Selected interatomic length values of Gd_2ZnTiO_6 .

Ti1_01	2.001(12)	-1100 0.80294 -0.19262 0.05467
Ti1_02	1.969(12)	10-10 0.31569 -0.29224 -0.05265
Ti1_02	1.969(12)	-1110 0.68431 0.29224 0.05265
Ti1_O3	1.943(13)	1000 0.39080 -0.03431 0.23940
Ti1_O3	1.943(13)	-1100 0.60920 0.03431 -0.23940
Zn1_Gd1	3.2464(17)	1-100 -0.48415 0.56532 0.24698
Zn1_Gd1	3.3687(24)	1000 0.51585 0.56532 0.24698
Zn1_Gd1	3.1387(19)	2 0-1 0 -0.01585 0.06532 0.25302
Zn1_Gd1	3.3687(24)	-1010 -0.51585 0.43468 -0.24698
Zn1_Gd1	3.2464(17)	-1110 0.48415 0.43468 -0.24698
Zn1_Gd1	3.1387(19)	-2020 0.01585 0.93468 -0.25302
Zn1_01	2.081(13)	1000 0.19706 0.19262 -0.05467
Zn1_01	2.081(13)	-1010 -0.19706 0.80738 0.05467
Zn1_02	2.104(12)	1000 0.31569 0.70776 -0.05265
Zn1_02	2.104(12)	-1010 -0.31569 0.29224 0.05265
Zn1_O3	2.093(13)	2000 0.10920 0.46569 0.26060
Zn1_03	2.093(13)	-2010 -0.10920 0.53431 -0.26060

Table S2 Selected bond angles of Gd_2ZnTiO_6 .

Angle	Degr	ees	atom	1 loc atom	3		loc	
01_G	d1_01	117.92	2(22)	-111	C)	-2111	
01_G	d1_02	64.9(4	1)	-111	C)	1000	
01_G	d1_02	75.4(5	5)	-111	C)	-1110	
01_G	d1_02	72.47	(21)	-111	C)	-2121	
01_G	d1_03	69.0(4	1)	-111	C)	1010	
01_G	d1_03	138.7(4)	-111	C)	2000	
01_G	d1_Ti1	39.90(28)	-111	C)	1010	
01_G	d1_Ti1	85.67(25)	-111	C)	2100	
01_G	d1_Zn1	87.45	(26)	-111	C)	2000	
01_G	d1_02	157.7(5)	-211	1	_	1000	
01_G	d1_02	80.84	(29)	-211	1	_	-1110	
01_G	d1_02	70.2(5	5)	-211	1	_	-2121	
01_G	d1_03	137.5(5)	-211	1	_	1010	
01_G	d1_O3	102.4(4)	-211	1	_	2000	
01_G	d1_Ti1	155.39	(31)	-211	1	_	1010	
01_G	d1_Ti1	37.49(31)	-211	1	_	2100	
01_G	d1_Zn1	95.7(4	4)	-211	1	_	2000	
O2_G	d1_02	78.7(5	5)	100	C)	-1110	
O2_G	d1_02	128.05	5(17)	100	C)	-2121	
O2_G	d1_O3	64.8(4	1)	100	C)	1010	
O2_G	d1_O3	74.3(4	1)	100	C)	2000	
O2_G	d1_Ti1	38.93(27)	100	C)	1010	
O2_G	d1_Ti1	150.22	(25)	100	C)	2100	
O2_G	d1_Zn1	106.63	3(25)	100	C)	2000	
O2_G	d1_02	118.16	6(24)	-111	C)	-2121	
O2_G	d1_03	136.9(5)	-111	C)	1010	
O2_G	d1_03	104.0(4)	-111	C)	2000	

O2_Gd1_Ti1	98.25(33)	-111	0 1010
O2_Gd1_Ti1	89.79(31)	-111	0 2100
O2_Gd1_Zn1	158.05(29)	-111	0 2000
O2_Gd1_O3	73.2(4)	-212	1 1010
O2_Gd1_O3	134.5(4)	-212	1 2000
O2_Gd1_Ti1	89.13(25)	-212	1 1010
O2_Gd1_Ti1	37.18(28)	-212	1 2100
O2_Gd1_Zn1	41.78(26)	-212	1 2000
O3_Gd1_O3	88.09(17)	101	0 2000
O3_Gd1_Ti1	38.66(31)	101	0 1010
O3_Gd1_Ti1	110.41(26)	101	0 2100
O3_Gd1_Zn1	41.82(31)	101	0 2000
O3_Gd1_Ti1	101.70(25)	200	0 1010
O3_Gd1_Ti1	135.41(33)	200	0 2100
O3_Gd1_Zn1	97.94(26)	200	0 2000
Ti1_Gd1_Ti1	118.26(4)	101	0 2100
Ti1_Gd1_Zn1	75.897(18)	101	0 2000
Ti1_Gd1_Zn1	75.13(6)	210	0 2000
Gd1_O1_Gd1	102.2(4)	-111	0 -2010
Gd1_O1_Ti1	85.5(4)	-111	0 1000
Gd1_O1_Zn1	88.6(5)	-111	0 1000
Gd1_O1_Ti1	97.6(5)	-201	0 1000
Gd1_O1_Zn1	116.6(5)	-201	0 1000
Ti1_O1_Zn1	145.8(6)	100	0 1000
Gd1_O2_Gd1	101.3(5)	100	0 -1110
Gd1_O2_Gd1	156.9(4)	100	0 -2020
Gd1_O2_Ti1	82.9(4)	100	0 1010
Gd1_O2_Zn1	89.2(4)	100	0 1000
Gd1_O2_Gd1	101.0(4)	-111	0 -2020

Gd1_O2_Ti1	119.5(5)	-111	0 1010
Gd1_O2_Zn1	93.9(5)	-111	0 1000
Gd1_O2_Ti1	90.9(5)	-202	0 1010
Gd1_O2_Zn1	83.8(4)	-202	0 1000
	146.6(5)	101	0 1000
Gd1_O3_Gd1	120.85(33)	10-1	0 20-10
Gd1_O3_Ti1	91.9(4)	10-1	0 1000
Gd1_O3_Zn1	89.3(4)	10-1	0 20-10
Gd1_O3_Ti1	108.4(5)	20-1	0 1000
Gd1_O3_Zn1	101.4(5)	2 0-1	0 20-10
Ti1_O3_Zn1	144.3(4)	100	0 20-10
Gd1_Ti1_Gd1	72.926(28)	10-1	0 21-10
Gd1_Ti1_Gd1	180.000(0)	10-1	0 -1110
Gd1_Ti1_Gd1	107.074(28)	10-1	0 -2010
Gd1_Ti1_O1	125.4(4)	10-1	0 1000
Gd1_Ti1_O1	54.6(4)	10-1	0 -1100
Gd1_Ti1_O2	58.1(4)	10-1	0 10-10
Gd1_Ti1_O2	121.9(4)	10-1	0 -1110
Gd1_Ti1_O3	49.49(18)	10-1	0 1000
Gd1_Ti1_O3	130.51(18)	10-1	0 -1100
Gd1_Ti1_Gd1	107.074(28)	21-1	0 -1110
Gd1_Ti1_Gd1	180.000(0)	21-1	0 -2010
Gd1_Ti1_O1	135.07(32)	2 1-1	0 1000
Gd1_Ti1_O1	44.93(32)	2 1-1	0 -1100
Gd1_Ti1_O2	128.0(4)	2 1-1	0 10-10
Gd1_Ti1_O2	52.0(4)	2 1-1	0 -1110
Gd1_Ti1_O3	71.93(26)	2 1-1	0 1000
Gd1_Ti1_O3	108.07(26)	2 1-1	0 -1100
Gd1_Ti1_Gd1	72.926(28)	-111	0 -2010

Gd1_Ti1_O1	54.6(4)	-111	0	1000
Gd1_Ti1_O1	125.4(4)	-111	0	-1100
Gd1_Ti1_O2	121.9(4)	-111	0	10-10
Gd1_Ti1_O2	58.1(4)	-111	0	-1110
Gd1_Ti1_O3	130.51(18)	-111	0	1000
Gd1_Ti1_O3	49.49(18)	-111	0	-1100
Gd1_Ti1_O1	44.93(32)	-201	0	1000
Gd1_Ti1_O1	135.07(32)	-201	0	-1100
Gd1_Ti1_O2	52.0(4)	-201	0	10-10
Gd1_Ti1_O2	128.0(4)	-201	0	-1110
Gd1_Ti1_O3	108.07(26)	-201	0	1000
Gd1_Ti1_O3	71.93(26)	-201	0	-1100
01_Ti1_01	180.000(0)	100	0	-1100
O1_Ti1_O2	90.5(6)	100	0	10-10
O1_Ti1_O2	89.5(6)	100	0	-1110
O1_Ti1_O3	90.3(4)	100	0	1000
O1_Ti1_O3	89.7(4)	100	0	-1100
O1_Ti1_O2	89.5(6)	-110	0	10-10
O1_Ti1_O2	90.5(6)	-110	0	-1110
O1_Ti1_O3	89.7(4)	-110	0	1000
O1_Ti1_O3	90.3(4)	-110	0	-1100
O2_Ti1_O2	180.000(0)	10-1	0	-1110
O2_Ti1_O3	87.5(4)	10-1	0	1000
O2_Ti1_O3	92.5(4)	10-1	0	-1100
O2_Ti1_O3	92.5(4)	-111	0	1000
O2_Ti1_O3	87.5(4)	-111	0	-1100
O3_Ti1_O3	180.000(0)	100	0	-1100
Gd1_Zn1_Gd1	180.000(0)	20-1	0	-2020
Gd1_Zn1_O1	58.9(4)	20-1	0	1000

Gd1_Zn1_O1	121.1(4)	20-1	0 -1010
Gd1_Zn1_O2	125.62(35)	20-1	0 1000
Gd1_Zn1_O2	54.38(35)	2 0-1	0 -1010
Gd1_Zn1_O3	48.90(18)	2 0-1	0 2000
Gd1_Zn1_O3	131.10(18)	20-1	0 -2010
Gd1_Zn1_O1	121.1(4)	-202	0 1000
Gd1_Zn1_O1	58.9(4)	-202	0 -1010
Gd1_Zn1_O2	54.38(35)	-202	0 1000
Gd1_Zn1_O2	125.62(35)	-202	0 -1010
Gd1_Zn1_O3	131.10(18)	-202	0 2000
Gd1_Zn1_O3	48.90(18)	-202	0 -2010
01_Zn1_01	180.000(0)	100	0 -1010
O1_Zn1_O2	91.1(6)	100	0 1000
O1_Zn1_O2	88.9(6)	100	0 -1010
O1_Zn1_O3	88.6(4)	100	0 2000
O1_Zn1_O3	91.4(4)	100	0 -2010
O1_Zn1_O2	88.9(6)	-101	0 1000
O1_Zn1_O2	91.1(6)	-101	0 -1010
O1_Zn1_O3	91.4(4)	-101	0 2000
O1_Zn1_O3	88.6(4)	-101	0 -2010
O2_Zn1_O2	180.000(0)	100	0 -1010
O2_Zn1_O3	90.8(4)	100	0 2000
O2_Zn1_O3	89.2(4)	100	0 -2010
O2_Zn1_O3	89.2(4)	-101	0 2000
O2_Zn1_O3	90.8(4)	-101	0 -2010
O3_Zn1_O3	180.000(0)	200	0 -2010

Formula	- Δ <i>S</i> M I·K ⁻¹ ·Kα ⁻¹	$-\Delta S_{M}$	7/ K	<i>∆H</i> // T	Ref
Gd ₃ BWO ₉	58.1	452	2	9	[36]
Gd ₂ ZnTiO ₆	53.5	398.7	3.1	9	This work
GdBO ₃	57.8	366.3	2	9	[26]
GdAIO3	40.9	317	2	9	[22]
GdCrO ₃	41.24	303	4	9	[32]
[Gd(HCOO)(bdc)]n	47	125	2	9	[8]
[Gd(C4O4)(OH)(H2O)4]n	47.3	112.7	3	9	[10]
K ₂ Gd(BH ₄) ₅	54.6	59.8	5	9	[24]
EuHo ₂ O ₄	30	267	2	8	[33]
EuDy ₂ O ₄	25	224	2	8	[33]
Gd ₂ Cu(SO ₄₎₂ (OH) ₄	45.52	212.8	4	8	[17]
GdF ₃	71	506	3	7	[20]
Gd ₅ BSi ₂ O ₁₃	67	461	3	7	[27]
GdPO ₄	62	375.8	2	7	[21]
Gd(OH)CO ₃	66.4	355	2	7	[4]
Gd(OH) ₃	62	346.08	2	7	[16]
EuTiO₃	49	331	5	7	[29]
GdFeO ₃	44	321	3	7	[35]
[Gd ₃ (OH) ₈ Cl] _n	61.8	318.9	3	7	[19]
K3Li3Gd7(BO3)9	56.6	277.2	2	7	[25]
Gd(OH)SO4	53.5	276	2	7	[18]
Gd ₂ NiMnO ₆	35.5	268	4	7	[31]
Gd(HCOO) ₃	55.9	215.7	2	7	[5]
$\{[Gd_6O(OH)_8(CIO_4)_4(H_2O)_6](OH)_4\}_n$	46.6	215.6	3	7	[6]
$[Gd_4(SO_4)_4(\mu_3-OH)_4(H_2O)]_n$	51.3	198.9	2	7	[7]
[Gd48O6(OH)84(CAA)36(NO3)6(H2O)24(EtOH)12(NO3)Cl2]Cl3·6DMF·5EtOH·20H2O	43.6	120.7	2	7	[9]
[MnII(glc) ₂ (H ₂ O) ₂]	60.3	112	2	7	[11]
[Gd(HCOO)(OAc) ₂ (H ₂ O) ₂] _n	45.9	110	2	7	[12]
[Gd(OAc)3(H2O)05]n	47.7	106.3	2	7	[13]
$\{[Gd_2(IDA)_3] \cdot 2H_2O\}_n$	40.6	100.7	2	7	[14]
$\{[Gd_{36}O_6(OH)_{49}(NA)_{36}(NO_3)_6(N_3)_3(H_2O)_{20}]Cl_2\cdot 28H_2O\}_n$	39.66	91.3	3	7	[15]
GdCrTiO ₅	36	\	5	7	[28]
GdFeTeO ₆	38.5	١	5	7	[34]

Table S3 State of the art collections of solid-state cryogenic refrigeration (CR) materials.

EuSe	37.5	244.8	5	5	[30]
GdVO ₄	41.1	227	3	5	[23]

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