

Supporting Information

New 3d-4f heterometallic clusters built from mixed glycine and iminodiacetate acid: dioctahedron {La₂Ni₉} and onion-like {Gd₅} ⊂ {Ni₁₂} with interesting magnetocaloric effect

Zhong-Yi Li,^{a, b} Jiang Zhu,^c Xiao-Qun Wang,^a Jun Ni,^a Jian-Jun Zhang,^{a*} Shu-Qin Liu,^a Chun-Ying Duan^{a, b*}

^a Chemistry College, Dalian University of Technology, Dalian 116024, China

^b State Key Laboratory of Fine Chemicals, Dalian University of Technology, Dalian, 116024, China

^c School of Chemistry and Chemical Engineering, Liaoning Normal University, Dalian 116029, China

contents

Table S1. Selected bond lengths (Å) and angles (°) for 1	1
Table S2. Selected bond lengths (Å) and angles (°) for 2	2
Table S3. Crystal data for 3-7	4
Table S4. Bond-Valence Sums for selected O atoms of 1 and 2	4
Figure S1. Coordination polyhedron of the La ³⁺ ions in 1	5
Figure S2. The possible assembly mechanism of the [La ₂ Ni ₉ (μ ₃ -OH) ₃ (IDA) ₃ (Gly) ₁₂] ³⁺ cationic cluster of 1 from {La ₂ Ni ₆ } and {NiIDA} units.....	5
Figure S3. The coordinated environments of the Gd ³⁺ ions in 1	6
Figure S4. The IR spectrum of 1	7
Figure S5. The IR spectra of 2-7	7
Figure S6. Powder X-ray diffraction patterns of 1	8
Figure S7. Powder X-ray diffraction patterns of 2-7	8
Figure S8. The plot of Δχ _M T(3-7) versus T.....	9
Figure S9. The plot of Δχ _M T(4-7) versus T.....	9
Figure S10. The plot of Δχ _M T(5-7) versus T.....	10
Figure S11. The plot of Δχ _M T(6-7) versus T.....	10
Figure S12. The field-dependent experimental magnetization plot at 2 K for 1	11
Figure S13. The field-dependent experimental magnetization plot at 2 K for 3	11
Figure S14. The field-dependent experimental magnetization plot at 2 K for 4	12
Figure S15. The field-dependent experimental magnetization plot at 2 K for 6	12
Figure S16. The field-dependent experimental magnetization plot at 2 K for 7	13

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

La(1)-O(7)	2.505(3)	Ni(1)-O(3)	2.039(3)
La(1)-O(5)	2.758(3)	Ni(1)-O(2)#2	2.049(4)
La(1)-O(3)	2.772(3)	Ni(1)-N(1)	2.057(4)
La(1)-O(1)	2.808(3)	Ni(1)-O(6)	2.069(3)
La(2)-O(9)	2.501(7)	Ni(2)-O(7)	1.979(4)
La(2)-O(8)	2.522(8)	Ni(2)-O(5)	2.042(3)
Ni(1)-N(2)	2.035(5)	Ni(2)-N(3)	2.078(5)
Ni(1)-O(1)	2.038(3)	Ni(2)-O(4)#1	2.054(3)
Ni(2)-O(5)-La(1)	99.22(12)	O(1)-La(1)-O(1)#2	62.28(11)
O(7)-Ni(2)-O(4)#1	98.98(13)	O(5)-La(1)-O(3)	61.69(10)
O(5)-Ni(2)-O(5)#3	94.01(18)	O(3)-La(1)-O(1)#2	59.63(9)
O(1)-Ni(1)-O(3)	93.04(13)	O(2)#2-Ni(1)-O(6)	179.80(16)
O(4)#1-Ni(2)-N(3)	92.69(17)	O(5)#2-La(1)-O(3)#1	176.06(9)
O(1)-Ni(1)-O(6)	91.21(14)	N(2)-Ni(1)-O(1)	175.23(17)
N(2)-Ni(1)-O(2)#2	90.19(19)	O(7)-La(1)-O(1)#2	175.03(12)
N(1)-Ni(1)-O(6)	90.14(17)	O(7)#1-La(1)-O(1)	175.03(11)
O(3)-Ni(1)-O(2)#2	90.02(15)	O(3)-Ni(1)-N(1)	174.92(16)
N(2)-Ni(1)-O(6)	90.01(18)	O(5)#3-Ni(2)-O(4)#1	173.56(14)
O(3)-Ni(1)-O(6)	89.97(13)	O(7)-Ni(2)-N(3)	163.9(2)
O(2)#2-Ni(1)-N(1)	89.86(18)	O(9)#4-La(2)-O(8)	143.8(2)
O(5)-Ni(2)-O(4)#1	89.44(13)	O(9)#3-La(2)-O(9)#4	132.25(13)
O(9)-La(2)-O(9)#4	89.0(3)	O(7)#1-La(1)-O(3)	120.92(11)
O(1)-Ni(1)-O(2)#2	88.59(15)	O(8)#4-La(2)-O(8)	120.000(2)
O(7)-Ni(2)-O(5)	86.67(12)	O(7)-La(1)-O(1)#1	119.23(10)
O(5)-Ni(2)-N(3)	82.39(15)	O(5)-La(1)-O(1)#1	118.97(10)
N(2)-Ni(1)-O(3)	82.34(16)	O(7)#1-La(1)-O(5)	118.49(10)
O(1)-Ni(1)-N(1)	81.88(16)	O(5)-La(1)-O(5)#2	117.14(4)
O(9)#3-La(2)-O(9)	71.9(4)	O(7)-La(1)-O(3)	116.36(11)
O(9)-La(2)-O(8)#4	69.9(2)	O(3)#2-La(1)-O(3)	115.04(5)
O(5)-La(1)-O(3)#1	65.96(10)	O(7)-La(1)-O(1)	113.74(11)
O(7)-La(1)-O(7)#1	65.01(12)	O(5)-La(1)-O(1)#2	112.02(9)
O(7)-La(1)-O(5)#1	64.81(11)	Ni(2)-O(7)-La(1)	109.97(12)
O(3)-La(1)-O(1)	64.04(9)	La(1)#3-O(7)-La(1)	103.29(15)
O(5)-La(1)-O(1)	63.40(10)	N(2)-Ni(1)-N(1)	102.73(19)
O(7)-La(1)-O(5)	63.02(11)	Ni(1)-O(3)-La(1)	102.01(12)
O(9)-La(2)-O(8)	62.5(2)	Ni(1)-O(1)-La(1)	100.86(12)

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

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

Gd(1)-O(1T)	2.329(6)	Gd(5)-O(1T)	2.416(6)	Ni(6)-O(23)	2.048(10)
Gd(1)-O(2T)	2.380(6)	Gd(5)-O(37)	2.418(6)	Ni(6)-O(26)	2.142(8)
Gd(1)-O(3T)	2.393(5)	Gd(5)-O(41)	2.439(6)	Ni(6)-O(48)	2.188(10)
Gd(1)-O(47)	2.421(6)	Gd(5)-O(6T)	2.460(6)	Ni(7)-O(3T)	2.032(6)
Gd(1)-O(23)	2.451(7)	Gd(5)-O(9T)	2.462(5)	Ni(7)-O(20)	2.036(7)
Gd(1)-O(25)	2.472(7)	Gd(5)-O(2T)	2.492(6)	Ni(7)-O(27)	2.037(6)
Gd(1)-O(21)	2.562(8)	Ni(1)-O(3)	2.019(8)	Ni(7)-O(25)	2.046(7)
Gd(1)-O(17)	2.588(8)	Ni(1)-O(1)	2.024(7)	Ni(7)-O(32)	2.053(6)
Gd(1)-O(19)	2.593(8)	Ni(1)-O(6)	2.058(9)	Ni(7)-N(13)	2.109(7)
Gd(2)-O(4T)	2.359(5)	Ni(1)-N(2)	2.069(13)	Ni(8)-O(29)	2.042(6)
Gd(2)-O(6T)	2.388(6)	Ni(1)-N(1)	2.086(11)	Ni(8)-O(8T)	2.044(5)
Gd(2)-O(5T)	2.416(6)	Ni(1)-O(50)	2.209(11)	Ni(8)-O(12)	2.044(7)
Gd(2)-O(33)	2.436(7)	Ni(2)-N(4)	2.012(9)	Ni(8)-O(31)	2.055(6)
Gd(2)-O(39)	2.460(6)	Ni(2)-O(7)	2.016(6)	Ni(8)-O(36)	2.060(7)
Gd(2)-O(5)	2.502(6)	Ni(2)-O(5)	2.025(7)	Ni(8)-N(14)	2.112(8)
Gd(2)-O(7)	2.538(6)	Ni(2)-N(3)	2.085(8)	Ni(9)-O(5T)	2.031(6)
Gd(2)-O(3)	2.548(7)	Ni(2)-O(40)	2.173(8)	Ni(9)-O(4)	2.033(8)
Gd(2)-O(1)	2.593(7)	Ni(2)-O(34)	2.216(8)	Ni(9)-O(35)	2.051(6)
Gd(3)-O(7T)	2.335(5)	Ni(3)-O(11)	2.020(6)	Ni(9)-O(33)	2.061(7)
Gd(3)-O(9T)	2.398(6)	Ni(3)-O(9)	2.029(6)	Ni(9)-O(28)	2.074(7)
Gd(3)-O(8T)	2.406(6)	Ni(3)-N(6)	2.054(9)	Ni(9)-N(15)	2.100(9)
Gd(3)-O(43)	2.442(6)	Ni(3)-O(14)	2.056(7)	Ni(10)-O(6T)	2.029(6)
Gd(3)-O(29)	2.461(6)	Ni(3)-N(5)	2.076(8)	Ni(10)-O(37)	2.038(6)
Gd(3)-O(13)	2.488(6)	Ni(3)-O(49)	2.100(7)	Ni(10)-O(2)	2.046(8)
Gd(3)-O(11)	2.548(6)	Ni(4)-O(15)	2.019(6)	Ni(10)-O(46)	2.047(8)
Gd(3)-O(15)	2.565(6)	Ni(4)-O(13)	2.020(6)	Ni(10)-O(39)	2.065(7)
Gd(3)-O(9)	2.589(6)	Ni(4)-N(8)	2.022(9)	Ni(10)-N(16)	2.087(9)
Gd(4)-O(4T)	2.402(5)	Ni(4)-N(7)	2.067(8)	Ni(11)-O(41)	2.036(6)
Gd(4)-O(7T)	2.406(5)	Ni(4)-O(30)	2.121(7)	Ni(11)-O(9T)	2.042(6)
Gd(4)-O(1T)	2.420(5)	Ni(4)-O(44)	2.143(7)	Ni(11)-O(10)	2.055(6)
Gd(4)-O(31)	2.427(5)	Ni(5)-O(17)	2.018(9)	Ni(11)-O(43)	2.075(6)
Gd(4)-O(35)	2.439(6)	Ni(5)-O(24)	2.022(14)	Ni(11)-N(17)	2.103(8)
Gd(4)-O(27)	2.453(6)	Ni(5)-O(19)	2.054(8)	Ni(11)-O(38)	2.107(6)
Gd(4)-O(8T)	2.465(6)	Ni(5)-N(10)	2.055(14)	Ni(12)-O(18)	2.020(9)
Gd(4)-O(5T)	2.474(5)	Ni(5)-N(9)	2.063(11)	Ni(12)-O(2T)	2.030(6)
Gd(4)-O(3T)	2.483(6)	Ni(5)-O(51)	2.127(11)	Ni(12)-O(45)	2.059(7)
Gd(5)-O(4T)	2.382(5)	Ni(6)-O(21)	2.007(9)	Ni(12)-O(47)	2.060(8)
Gd(5)-O(7T)	2.392(5)	Ni(6)-N(11)	2.011(14)	Ni(12)-O(42)	2.072(7)
Gd(5)-O(45)	2.415(6)	Ni(6)-N(12)	2.027(12)	Ni(12)-N(18)	2.085(9)
O(3T)-Gd(1)-O(47)	155.8(2)	O(8T)-Gd(3)-O(43)	156.72(19)	O(4T)-Gd(5)-O(45)	138.1(2)
O(1T)-Gd(1)-O(23)	141.9(3)	O(9T)-Gd(3)-O(29)	154.38(19)	O(7T)-Gd(5)-O(45)	140.1(2)
O(2T)-Gd(1)-O(23)	132.1(2)	O(43)-Gd(3)-O(29)	127.52(19)	O(7T)-Gd(5)-O(37)	134.0(2)

O(3T)-Gd(1)-O(23)	130.1(2)	O(7T)-Gd(3)-O(13)	141.4(2)	O(1T)-Gd(5)-O(37)	139.9(2)
O(2T)-Gd(1)-O(25)	155.2(2)	O(9T)-Gd(3)-O(13)	132.0(2)	O(4T)-Gd(5)-O(41)	140.4(2)
O(47)-Gd(1)-O(25)	128.5(2)	O(8T)-Gd(3)-O(13)	130.6(2)	O(1T)-Gd(5)-O(41)	137.8(2)
O(2T)-Gd(1)-O(21)	117.9(2)	O(7T)-Gd(3)-O(11)	139.8(2)	O(7T)-Gd(5)-O(6T)	133.5(2)
O(3T)-Gd(1)-O(21)	117.2(2)	O(9T)-Gd(3)-O(11)	115.7(2)	O(41)-Gd(5)-O(6T)	134.8(2)
O(1T)-Gd(1)-O(17)	138.5(2)	O(43)-Gd(3)-O(11)	127.2(2)	O(45)-Gd(5)-O(9T)	135.1(2)
O(3T)-Gd(1)-O(17)	114.5(3)	O(9T)-Gd(3)-O(15)	114.7(2)	O(1T)-Gd(5)-O(9T)	133.9(2)
O(25)-Gd(1)-O(17)	129.2(3)	O(8T)-Gd(3)-O(15)	117.8(2)	O(6T)-Gd(5)-O(9T)	120.1(2)
O(21)-Gd(1)-O(17)	127.4(3)	O(11)-Gd(3)-O(15)	128.6(2)	O(4T)-Gd(5)-O(2T)	131.8(2)
O(1T)-Gd(1)-O(19)	138.5(3)	O(7T)-Gd(3)-O(9)	138.45(18)	O(37)-Gd(5)-O(2T)	136.7(2)
O(2T)-Gd(1)-O(19)	112.5(3)	O(8T)-Gd(3)-O(9)	114.3(2)	O(6T)-Gd(5)-O(2T)	119.7(2)
O(47)-Gd(1)-O(19)	129.2(3)	O(29)-Gd(3)-O(9)	131.0(2)	O(9T)-Gd(5)-O(2T)	120.1(2)
O(21)-Gd(1)-O(19)	129.0(3)	O(15)-Gd(3)-O(9)	127.6(2)	O(1)-Ni(1)-N(2)	166.2(4)
O(6T)-Gd(2)-O(33)	155.2(2)	O(4T)-Gd(4)-O(31)	141.31(18)	O(3)-Ni(1)-N(1)	166.6(4)
O(5T)-Gd(2)-O(39)	156.1(2)	O(1T)-Gd(4)-O(31)	137.7(2)	N(2)-Ni(1)-N(1)	110.8(5)
O(33)-Gd(2)-O(39)	128.0(2)	O(7T)-Gd(4)-O(35)	136.83(19)	O(6)-Ni(1)-O(50)	175.7(5)
O(4T)-Gd(2)-O(5)	143.5(2)	O(1T)-Gd(4)-O(35)	141.02(19)	N(4)-Ni(2)-O(5)	174.0(3)
O(6T)-Gd(2)-O(5)	131.4(2)	O(4T)-Gd(4)-O(27)	137.51(19)	N(4)-Ni(2)-N(3)	102.0(4)
O(5T)-Gd(2)-O(5)	130.7(2)	O(7T)-Gd(4)-O(27)	141.07(19)	O(7)-Ni(2)-N(3)	175.0(4)
O(6T)-Gd(2)-O(7)	116.7(2)	O(1T)-Gd(4)-O(8T)	133.7(2)	O(40)-Ni(2)-O(34)	171.1(3)
O(5T)-Gd(2)-O(7)	118.2(2)	O(27)-Gd(4)-O(8T)	135.19(19)	O(9)-Ni(3)-N(6)	167.7(3)
O(4T)-Gd(2)-O(3)	138.0(2)	O(7T)-Gd(4)-O(5T)	132.49(18)	O(11)-Ni(3)-N(5)	167.5(3)
O(6T)-Gd(2)-O(3)	112.1(3)	O(31)-Gd(4)-O(5T)	134.7(2)	N(6)-Ni(3)-N(5)	108.9(4)
O(39)-Gd(2)-O(3)	127.6(2)	O(8T)-Gd(4)-O(5T)	120.17(19)	O(14)-Ni(3)-O(49)	177.8(3)
O(7)-Gd(2)-O(3)	130.2(3)	O(4T)-Gd(4)-O(3T)	133.43(18)	O(13)-Ni(4)-N(8)	176.6(3)
O(4T)-Gd(2)-O(1)	139.4(2)	O(35)-Gd(4)-O(3T)	134.9(2)	O(15)-Ni(4)-N(7)	175.0(3)
O(5T)-Gd(2)-O(1)	116.0(2)	O(8T)-Gd(4)-O(3T)	120.2(2)	N(8)-Ni(4)-O(44)	91.0(3)
O(33)-Gd(2)-O(1)	129.3(2)	O(5T)-Gd(4)-O(3T)	119.6(2)	O(30)-Ni(4)-O(44)	172.5(2)
O(17)-Ni(5)-N(10)	167.7(5)	O(8T)-Ni(8)-O(12)	100.3(3)	O(37)-Ni(10)-O(2)	176.8(3)
O(19)-Ni(5)-N(9)	167.4(4)	O(12)-Ni(8)-O(31)	174.5(3)	O(6T)-Ni(10)-O(46)	94.9(3)
N(10)-Ni(5)-N(9)	109.4(5)	O(29)-Ni(8)-O(36)	177.0(3)	O(46)-Ni(10)-O(39)	178.5(3)
O(24)-Ni(5)-O(51)	179.5(5)	O(8T)-Ni(8)-N(14)	159.5(3)	O(6T)-Ni(10)-N(16)	160.6(3)
O(21)-Ni(6)-N(12)	173.7(5)	O(36)-Ni(8)-N(14)	101.7(3)	O(41)-Ni(11)-O(10)	176.0(3)
N(11)-Ni(6)-N(12)	101.0(5)	O(4)-Ni(9)-O(35)	175.7(3)	O(9T)-Ni(11)-N(17)	158.7(3)
N(11)-Ni(6)-O(23)	176.2(4)	O(33)-Ni(9)-O(28)	177.5(3)	O(43)-Ni(11)-O(38)	179.1(3)
O(26)-Ni(6)-O(48)	169.0(3)	O(5T)-Ni(9)-N(15)	159.3(3)	N(17)-Ni(11)-O(38)	100.1(3)
O(20)-Ni(7)-O(27)	174.0(3)	O(28)-Ni(9)-N(15)	101.7(3)	O(18)-Ni(12)-O(45)	174.1(3)
O(25)-Ni(7)-O(32)	178.7(3)	O(42)-Ni(12)-N(18)	102.5(3)	O(47)-Ni(12)-O(42)	176.0(3)
O(3T)-Ni(7)-N(13)	159.9(3)	O(2T)-Ni(12)-N(18)	159.3(4)	Ni(11)-O(9T)-Gd(5)	101.6(2)
Gd(1)-O(1T)-Gd(5)	115.3(2)	Ni(1)-O(1)-Gd(2)	104.2(3)	Ni(3)-O(9)-Gd(3)	103.8(2)
Gd(1)-O(1T)-Gd(4)	114.0(2)	Ni(12)-O(2T)-Gd(1)	104.2(3)	Ni(3)-O(11)-Gd(3)	105.5(2)
Gd(5)-O(1T)-Gd(4)	91.3(2)	Ni(12)-O(2T)-Gd(5)	100.3(2)	Ni(4)-O(13)-Gd(3)	98.7(3)
Gd(1)-O(2T)-Gd(5)	110.7(2)	Ni(7)-O(3T)-Gd(1)	104.2(2)	Ni(4)-O(15)-Gd(3)	96.3(3)
Gd(1)-O(3T)-Gd(4)	109.5(2)	Ni(7)-O(3T)-Gd(4)	101.5(2)	Ni(5)-O(17)-Gd(1)	104.7(3)

Gd(2)-O(4T)-Gd(5)	114.1(2)	Ni(1)-O(3)-Gd(2)	106.0(3)	Ni(5)-O(19)-Gd(1)	103.5(4)
Gd(2)-O(4T)-Gd(4)	115.0(2)	Ni(9)-O(5T)-Gd(2)	103.4(2)	Ni(6)-O(21)-Gd(1)	97.7(4)
Gd(5)-O(4T)-Gd(4)	92.5(2)	Ni(9)-O(5T)-Gd(4)	100.5(2)	Ni(6)-O(23)-Gd(1)	100.1(3)
Gd(2)-O(5T)-Gd(4)	110.4(2)	Ni(2)-O(5)-Gd(2)	98.1(2)	Ni(7)-O(25)-Gd(1)	101.1(3)
Gd(2)-O(6T)-Gd(5)	110.2(2)	Ni(10)-O(6T)-Gd(2)	104.1(3)	Ni(7)-O(27)-Gd(4)	102.4(2)
Gd(3)-O(7T)-Gd(5)	114.6(2)	Ni(10)-O(6T)-Gd(5)	101.6(3)	Ni(8)-O(29)-Gd(3)	102.1(2)
Gd(3)-O(7T)-Gd(4)	114.7(2)	Ni(2)-O(7)-Gd(2)	97.2(2)	Ni(8)-O(31)-Gd(4)	102.5(2)
Gd(5)-O(7T)-Gd(4)	92.2(2)	Ni(8)-O(8T)-Gd(3)	103.9(2)	Ni(9)-O(33)-Gd(2)	101.8(3)
Gd(3)-O(8T)-Gd(4)	110.0(2)	Ni(8)-O(8T)-Gd(4)	101.5(2)	Ni(9)-O(35)-Gd(4)	101.1(3)
Gd(3)-O(9T)-Gd(5)	109.9(2)	Ni(11)-O(9T)-Gd(3)	104.0(2)	Ni(10)-O(37)-Gd(5)	102.8(2)
Ni(12)-O(47)-Gd(1)	101.8(3)	Ni(12)-O(45)-Gd(5)	102.0(3)	Ni(10)-O(39)-Gd(2)	100.6(3)
Ni(11)-O(43)-Gd(3)	101.5(2)	Ni(11)-O(41)-Gd(5)	102.5(2)		

Table S3. Crystal data for **3-7**.

	3	4	5	6	7
Formula	C ₄₈ H ₁₁₅ Cl ₆ Nd ₅ N ₁₈ Ni ₁₂ O ₉₅	C ₄₈ H ₁₁₅ Cl ₆ Sm ₅ N ₁₈ Ni ₁₂ O ₉₅	C ₄₈ H ₁₁₅ Cl ₆ Tb ₅ N ₁₈ Ni ₁₂ O ₉₅	C ₄₈ H ₁₁₅ Cl ₆ Dy ₅ N ₁₈ Ni ₁₂ O ₉₅	C ₄₈ H ₁₁₅ Cl ₆ Y ₅ N ₁₈ Ni ₁₂ O ₉₅
Mr.	4102.74	4133.33	4176.15	4281.10	3828.06
Cryst. system	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic
Space group	P2 ₁ 2 ₁ 2 ₁	P2 ₁ 2 ₁ 2 ₁	P2 ₁ 2 ₁ 2 ₁	P2 ₁ 2 ₁ 2 ₁	P2 ₁ 2 ₁ 2 ₁
<i>a</i> / Å	17.1835(7)	17.104(4)	17.61(3)	17.070(6)	17.213(4)
<i>b</i> / Å	26.6609(10)	26.684(6)	27.66(4)	26.704(9)	26.471(6)
<i>c</i> / Å	26.8884(10)	26.684(6)	27.66(4)	26.704(9)	26.471(6)
<i>α</i> / °	90	90	90	90	90
<i>β</i> / °	90	90	90	90	90
<i>γ</i> / °	90	90	90	90	90
<i>V</i> (Å ³)/ <i>Z</i>	12318.3(8)/4	12178(4)/4	13470(4)/4	12172(7)/4	12061(4)/4

Table S4. Bond-Valence Sums for selected O atoms of **1** and **2**.^a

compound	atom	OH ⁻	atom	OH ⁻
1	O7	1.18		
2	O1T	1.15	O6T	1.05
	O2T	1.04	O7T	1.18
	O3T	1.03	O8T	1.02
	O4T	1.16	O9T	1.03
	O5T	1.02		

^a Bond-Valence Sum (BVS) calculations confirm that the μ₃-O atoms are μ₃-OH⁻ groups.^{1,2}

References:

- 1 C. Papatriantafyllopoulou, W. Wernsdorfer, K. A. Abboud and G. Christou, *Inorg. Chem.*, 2011, **50**, 421 and references therein.
- 2 A. Saha, M. Thompson, K. A. Abboud, W. Wernsdorfer and G. Christou, *Inorg. Chem.*, 2011, **50**, 10476.

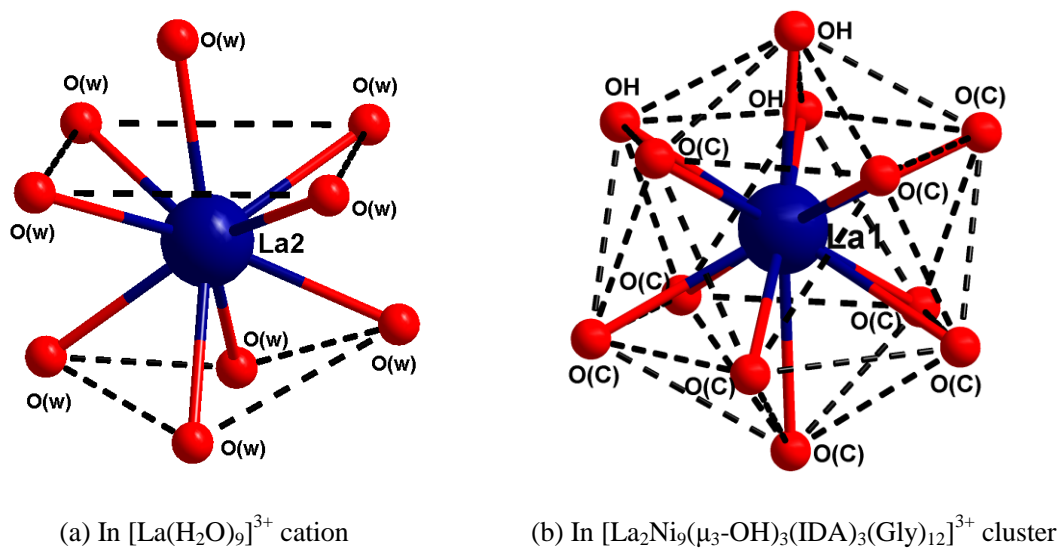


Figure S1. The coordination environments of the La^{3+} ions in **1**. O(C) means carboxylate oxygen.

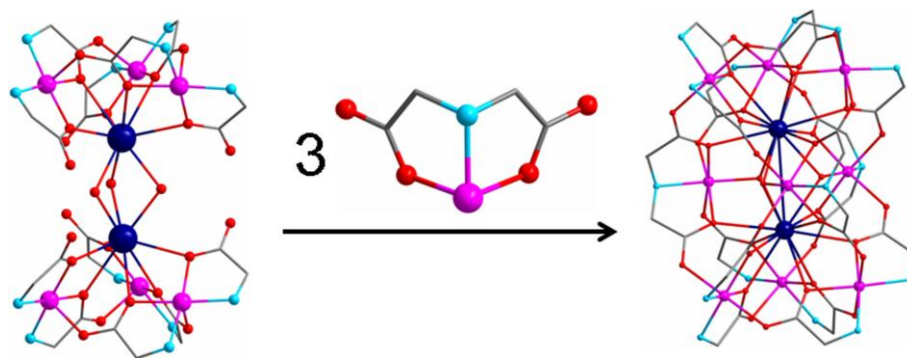


Figure S2. The possible assembly mechanism of the $[\text{La}_2\text{Ni}_9(\mu_3\text{-OH})_3(\text{IDA})_3(\text{Gly})_{12}]^{3+}$ cationic cluster of **1** from $\{\text{La}_2\text{Ni}_6\}$ and $\{\text{NiIDA}\}$ units.

Reference:

[1] Hosoi, A.; Yukawa, Y.; Igarashi, S.; Teat, S. J.; Roubeau, O.; Evangelisti, M.; Cremades, W.; Ruiz, E.; Barrios, L. A.; Arom G. *Chem. Eur. J.* **2011**, *17*, 8264.

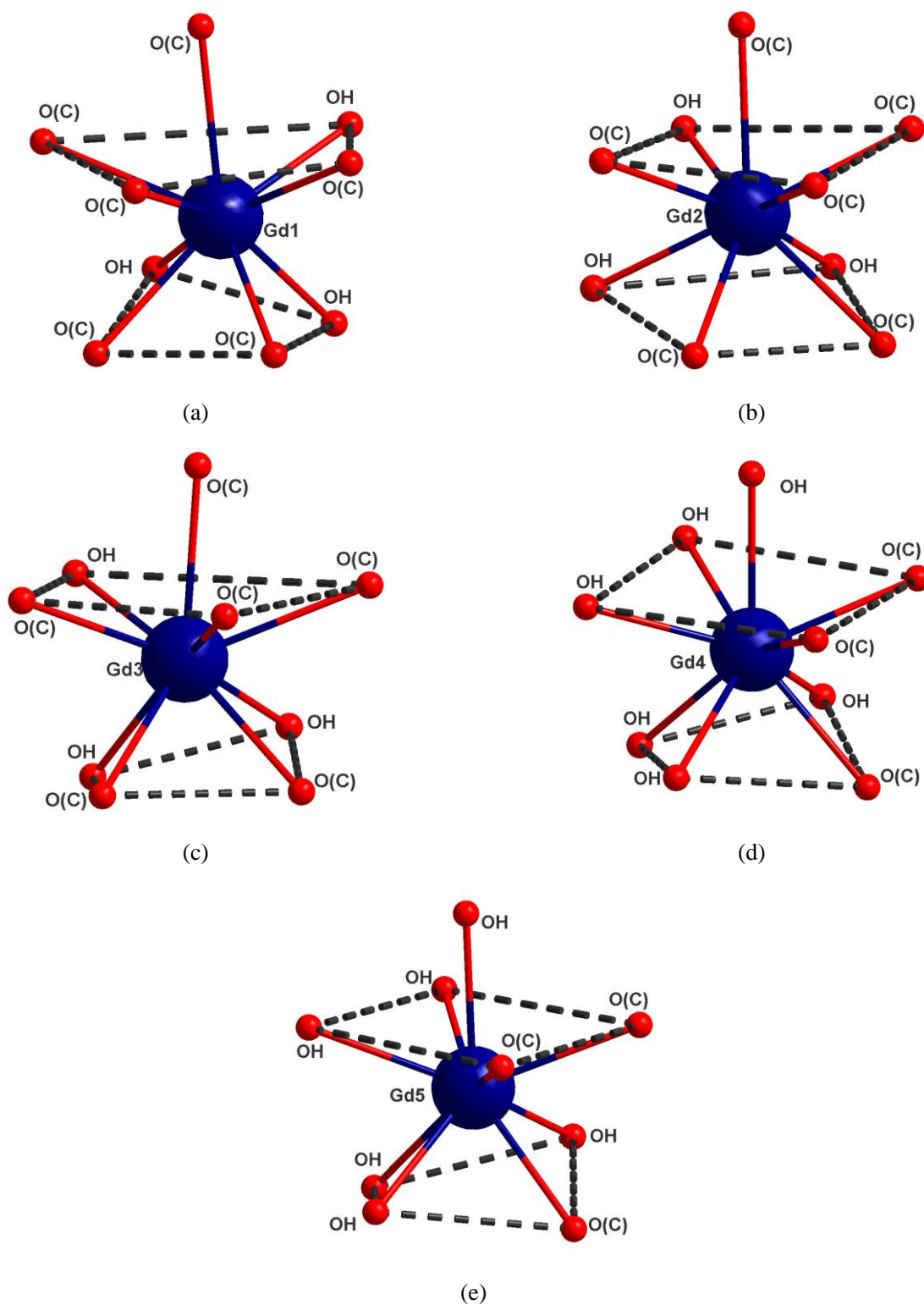


Figure S3. The coordination environments of the Gd^{3+} ions in **2**. O(C) means carboxylate oxygen.

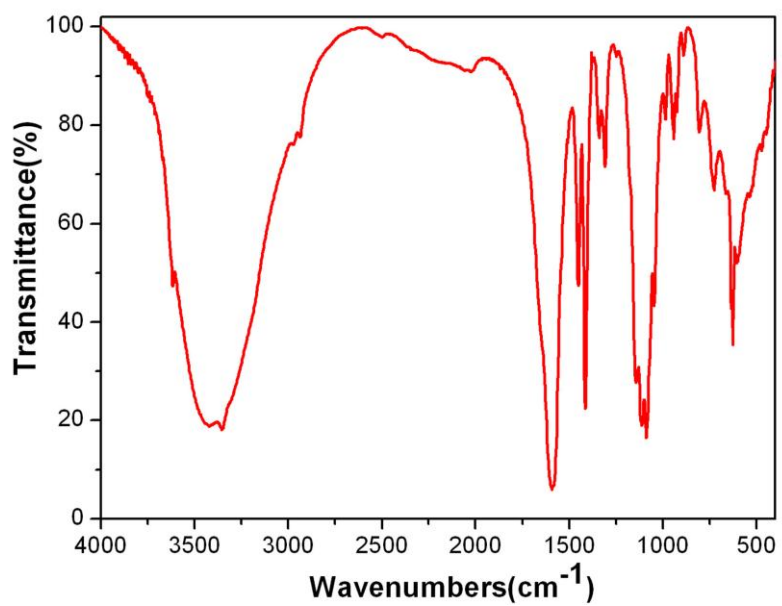


Figure S4. The IR spectrum of **1**.

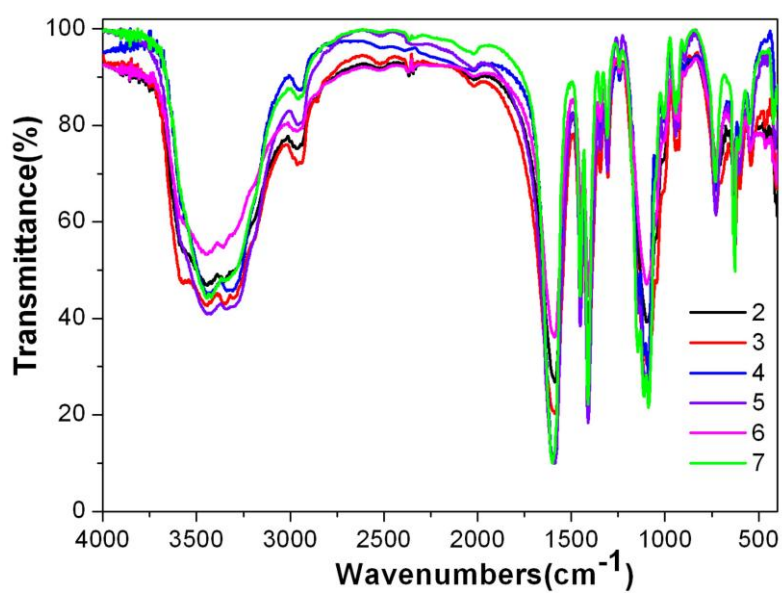


Figure S5. The IR spectra of **2-7**.

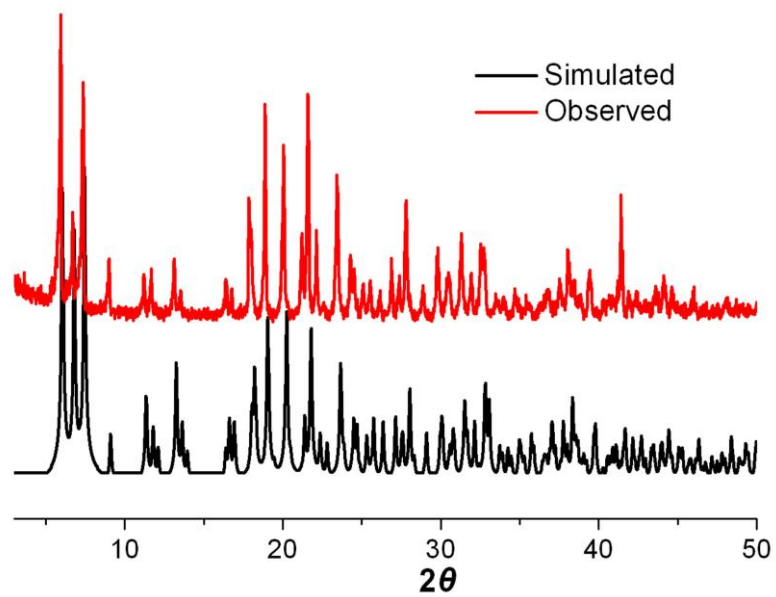


Figure S6. Powder X-ray diffraction patterns of **1**.

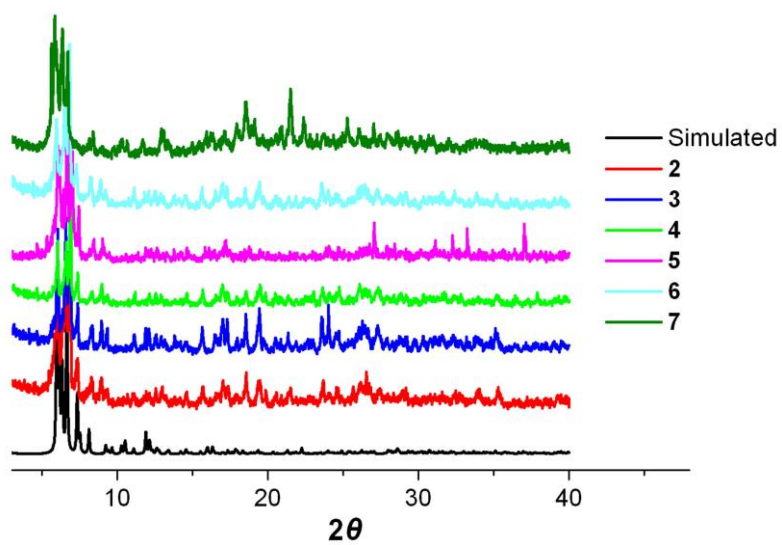


Figure S7. Powder X-ray diffraction patterns of **2-7**.

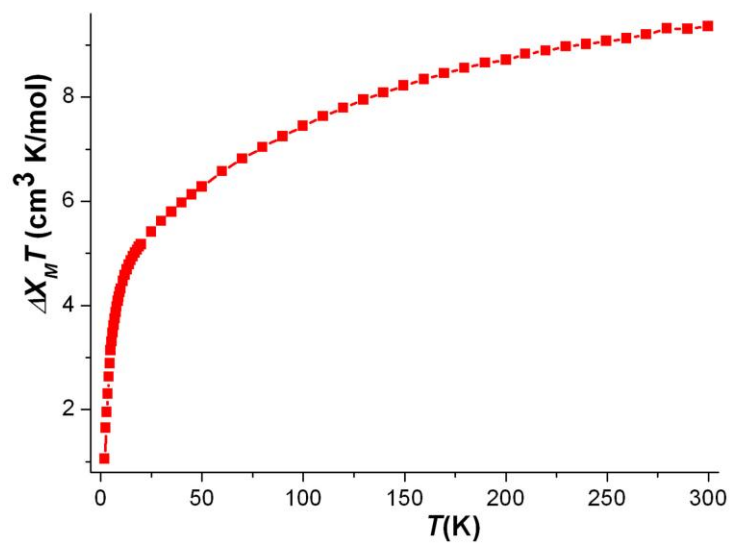


Figure S8. The plot of $\Delta\chi_M T$ (3-7) versus T .

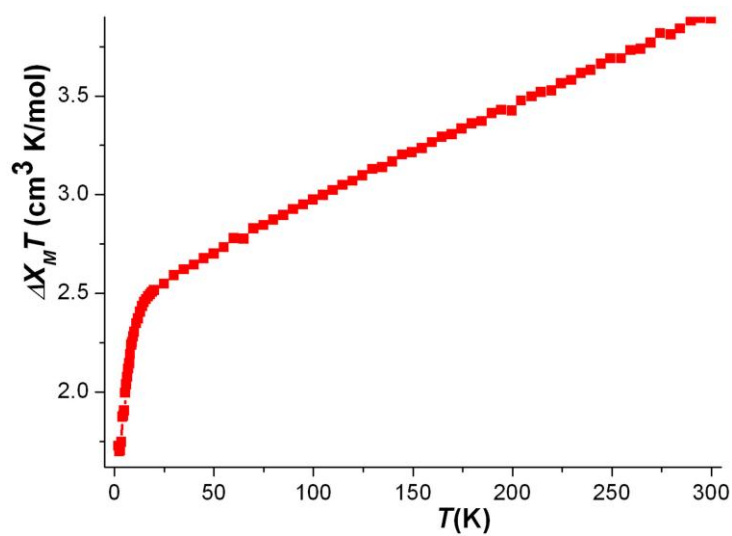


Figure S9. The plot of $\Delta\chi_M T$ (4-7) versus T .

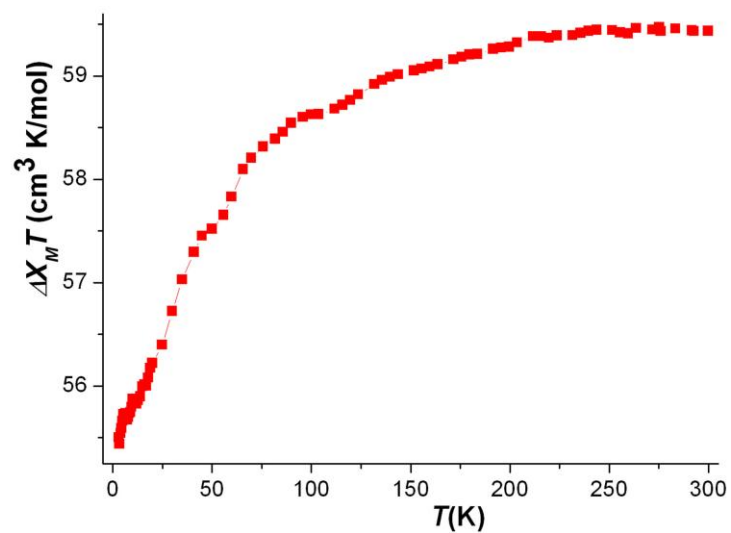


Figure S10. The plot of $\Delta\chi_M T(5-7)$ versus T .

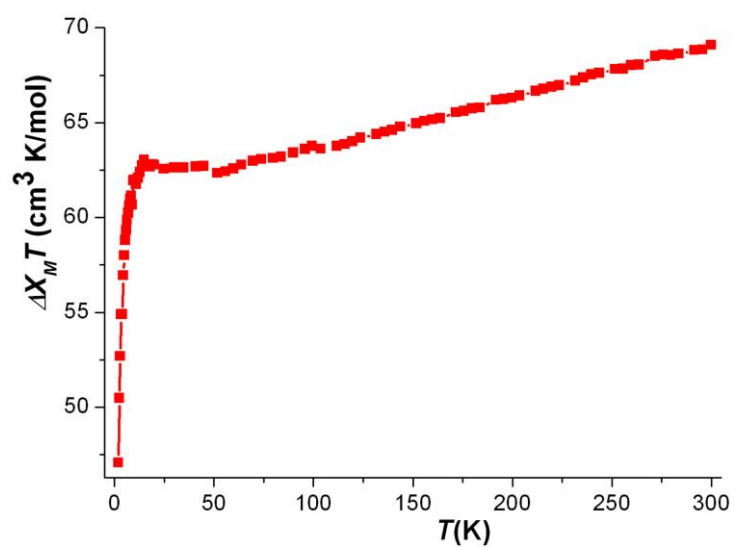


Figure S11. The plot of $\Delta\chi_M T(6-7)$ versus T .

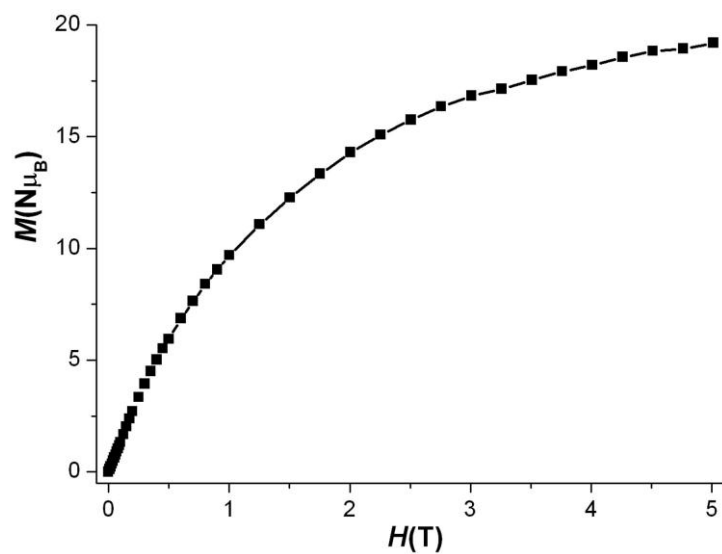


Figure S12. The field-dependent experimental magnetization plot at 2 K for **1**.

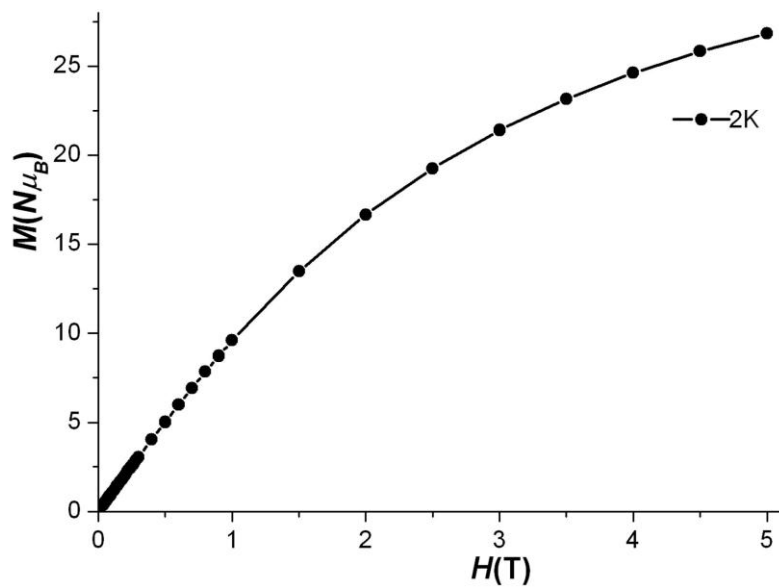


Figure S13. The field-dependent experimental magnetization plot at 2 K for **3**.

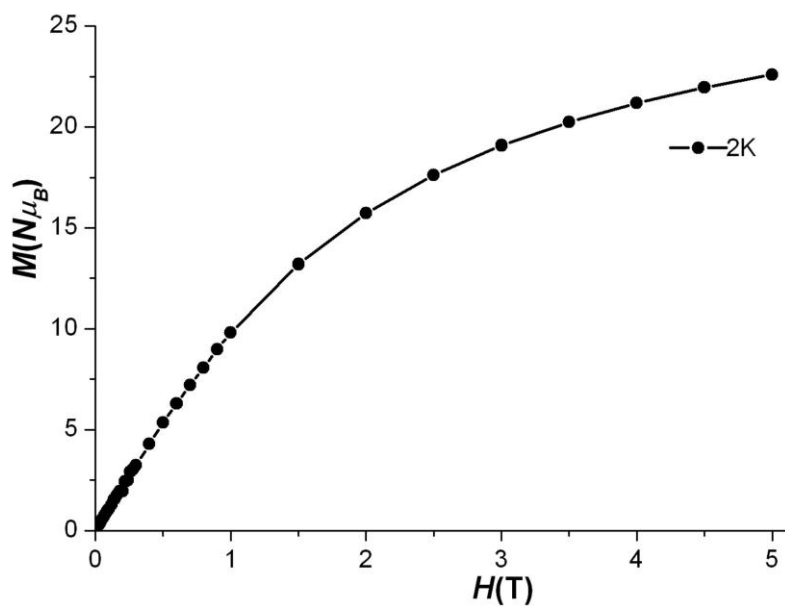


Figure S14. The field-dependent experimental magnetization plot at 2 K for **4**.

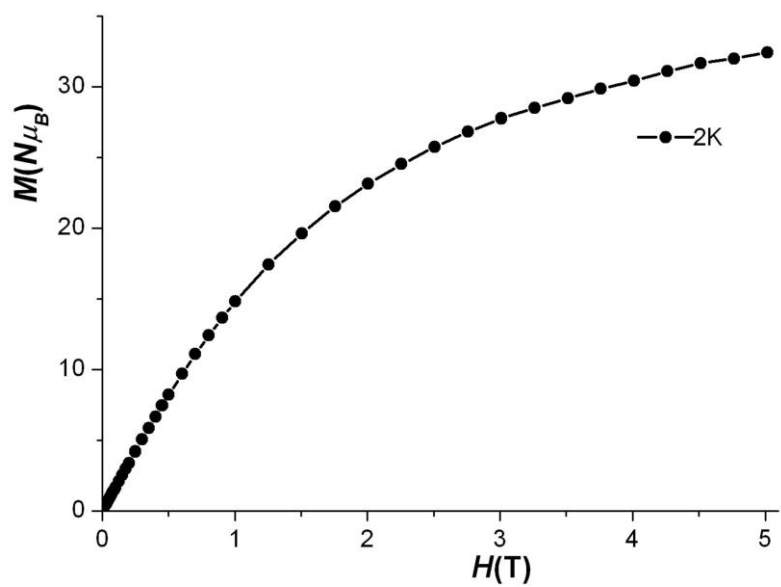


Figure S15. The field-dependent experimental magnetization plot at 2 K for **6**.

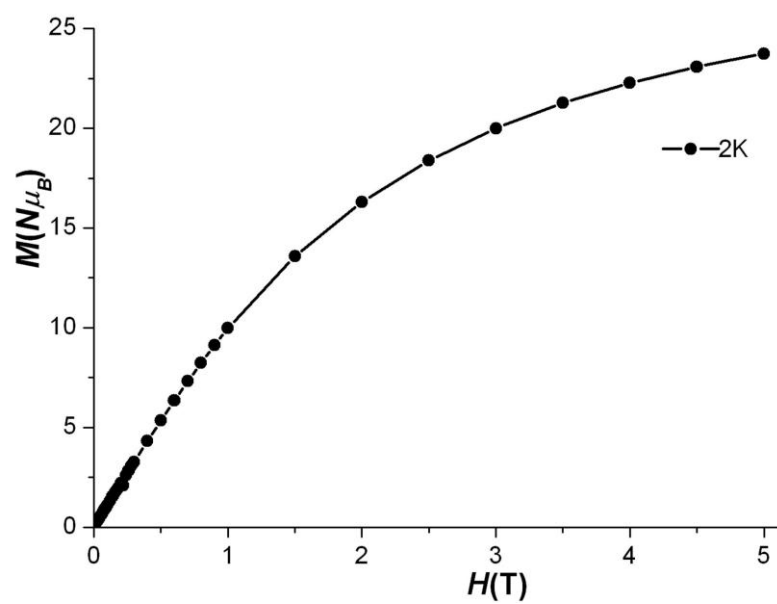


Figure S16. The field-dependent experimental magnetization plot at 2 K for 7.