

Supporting Information for

Alkylamine-Templated Niccolite Frameworks of $[\text{Ga}^{\text{III}}\text{M}^{\text{II}}(\text{HCOO})_6]^-$ ($\text{M} = \text{Fe}, \text{Ni}$): Structure, Magnetism, and Dielectricity

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Table S1. Crystallographic data and structural refinement for complexes **1-5**

Complex	1	
Empirical formula	C ₈ H ₁₄ NO ₁₂ GaFe	
Formula weight	442	
Temperature	110 K	300 K
Crystal system	Trigonal	Trigonal
Space group	<i>P</i> -3 ₁ <i>c</i>	<i>P</i> -3 ₁ <i>c</i>
<i>a</i> /Å	8.1712(7)	8.1821(6)
<i>b</i> /Å	8.1712(7)	8.1821(6)
<i>c</i> /Å	13.9019(15)	13.950(2)
α /°	90	90
β /°	90	90
γ /°	120	120
<i>V</i> /Å ³	803.85(13)	808.79(14)
<i>Z</i>	2	2
<i>D</i> _{calc} /g cm ⁻³	1.804	1.793
μ /mm ⁻¹	2.637	2.621
<i>F</i> (000)	434	434
θ range for data collection/°	3.23 to 27.46	3.22 to 27.47
Reflections collected/unique	7706 / 625	7718 / 626
<i>R</i> _{int}	0.0366	0.0278
Completeness	99.7%	99.7%
Data / restraints / parameters	625 / 6 / 44	626 / 0 / 44
Goodness-of-fit on <i>F</i> ²	1.246	1.325
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0395, <i>wR</i> ₂ = 0.1262	<i>R</i> ₁ = 0.0336, <i>wR</i> ₂ = 0.1210
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0402, <i>wR</i> ₂ = 0.1266	<i>R</i> ₁ = 0.0345, <i>wR</i> ₂ = 0.1214
Complex	2	
Empirical formula	C ₈ H ₁₄ NO ₁₂ GaFe	
Formula weight	442	
Temperature	110 K	300 K
Crystal system	Trigonal	Trigonal
Space group	<i>P</i> -3 ₁ <i>c</i>	<i>P</i> -3 ₁ <i>c</i>
<i>a</i> /Å	8.215(2)	8.242(5)
<i>b</i> /Å	8.215(2)	8.242(5)
<i>c</i> /Å	13.616(5)	13.674(6)
α /°	90	90
β /°	90	90
γ /°	120	120
<i>V</i> /Å ³	795.9(4)	804.4(8)

<i>Z</i>	2	2
<i>D</i> _{calc} /g cm ⁻³	1.810	1.791
μ/mm ⁻¹	2.662	2.634
<i>F</i> (000)	428	428
<i>θ</i> range for data collection/°	3.23 to 27.48	3.22 to 27.46
Reflections collected/ unique	7651 / 622	7660 / 629
<i>R</i> _{int}	0.0497	0.0561
Completeness	99.7%	99.7%
Data / restraints / parameters	622 / 0 / 40	629 / 0 / 40
Goodness-of-fit on <i>F</i> ²	1.140	1.113
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0232, <i>wR</i> ₂ = 0.0615	<i>R</i> ₁ = 0.0284, <i>wR</i> ₂ = 0.0669
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0274, <i>wR</i> ₂ = 0.0644	<i>R</i> ₁ = 0.0359, <i>wR</i> ₂ = 0.0708

Complex

3

Empirical formula	C ₁₀ H ₁₈ NO ₁₂ GaFe	
Formula weight	470	
Temperature	110 K	300 K
Crystal system	Trigonal	Trigonal
Space group	<i>P</i> -3 ₁ <i>c</i>	<i>P</i> -3 ₁ <i>c</i>
<i>a</i> /Å	8.294(4)	8.3950(6)
<i>b</i> /Å	8.294(4)	8.3950(6)
<i>c</i> /Å	13.580(11)	13.5962(14)
α/°	90	90
β/°	90	90
γ/°	120	120
<i>V</i> /Å ³	809.0(10)	829.83(15)
<i>Z</i>	2	2
<i>D</i> _{calc} /g cm ⁻³	1.904	1.856
μ/mm ⁻¹	2.626	2.560
<i>F</i> (000)	464	464
<i>θ</i> range for data collection/°	3.208 to 27.652	2.996 to 27.389
Reflections collected/ unique	7436 / 634	7937 / 633
<i>R</i> _{int}	0.1209	0.0457
Completeness	99.4%	99.4%
Data / restraints / parameters	634 / 6 / 47	633 / 0 / 47
Goodness-of-fit on <i>F</i> ²	1.086	1.330
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0761, <i>wR</i> ₂ = 0.1957	<i>R</i> ₁ = 0.0262, <i>wR</i> ₂ = 0.0841
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0885, <i>wR</i> ₂ = 0.2049	<i>R</i> ₁ = 0.0341, <i>wR</i> ₂ = 0.1139

Complex

4

Empirical formula	C ₇ H ₁₂ NO ₁₂ GaNi
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Formula weight	431	
Temperature	110 K	300 K
Crystal system	Trigonal	Trigonal
Space group	$P\bar{3}_1c$	$P\bar{3}_1c$
$a/\text{\AA}$	8.0822(9)	8.0926(2)
$b/\text{\AA}$	8.0822(9)	8.0926(2)
$c/\text{\AA}$	13.701(2)	13.7165(4)
$\alpha/^\circ$	90	90
$\beta/^\circ$	90	90
$\gamma/^\circ$	120	120
$V/\text{\AA}^3$	775.05(17)	777.95(4)
Z	2	2
$D_{\text{calc}}/\text{g cm}^{-3}$	1.819	1.812
μ/mm^{-1}	3.010	2.999
$F(000)$	420	420
θ range for data collection/ $^\circ$	3.27 to 27.52	2.91 to 29.27
Reflections collected/ unique	9441 / 604	7660 / 622
R_{int}	0.0311	0.1200
Completeness	99.5%	97.2%
Data / restraints / parameters	604 / 0 / 49	622 / 0 / 43
Goodness-of-fit on F^2	1.171	1.009
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0173$, $wR_2 = 0.0501$	$R_1 = 0.0679$, $wR_2 = 0.1698$
R indices (all data)	$R_1 = 0.0176$, $wR_2 = 0.0502$	$R_1 = 0.0783$, $wR_2 = 0.1827$

Complex

5

Empirical formula	$\text{C}_8\text{H}_{14}\text{NO}_{12}\text{GaNi}$	
Formula weight	445	
Temperature	110 K	300 K
Crystal system	Trigonal	Trigonal
Space group	$P\bar{3}_1c$	$P\bar{3}_1c$
$a/\text{\AA}$	8.1561(15)	8.1520(2)
$b/\text{\AA}$	8.1561(15)	8.1520(2)
$c/\text{\AA}$	13.418(3)	13.4489(4)
$\alpha/^\circ$	90	90
$\beta/^\circ$	90	90
$\gamma/^\circ$	120	120
$V/\text{\AA}^3$	773.0(3)	774.01(4)
Z	2	2
$D_{\text{calc}}/\text{g cm}^{-3}$	1.876	1.873
μ/mm^{-1}	3.021	3.017
$F(000)$	432	432
θ range for data collection/ $^\circ$	3.04 to 27.51	2.89 to 28.98
Reflections collected/ unique	7300 / 606	7917 / 617

unique		
R_{int}	0.0216	0.0427
Completeness	99.7%	99.3%
Data / restraints / parameters	606 / 0 / 40	617 / 0 / 40
Goodness-of-fit on F^2	1.247	1.170
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0199$, $wR_2 = 0.0557$	$R_1 = 0.0352$, $wR_2 = 0.0860$
R indices (all data)	$R_1 = 0.0205$, $wR_2 = 0.0560$	$R_1 = 0.0466$, $wR_2 = 0.0936$

Table S2. Selected bond lengths (Å) and angles (°) for complexes **1-5**

Bond lengths of complex 1			
	110 K		300 K
Fe(1)-O(1)#1	2.112(3)	Fe(1)-O(1)#1	2.114(3)
Fe(1)-O(1)#2	2.112(3)	Fe(1)-O(1)#2	2.114(3)
Fe(1)-O(1)#3	2.112(3)	Fe(1)-O(1)#3	2.114(3)
Fe(1)-O(1)#4	2.112(3)	Fe(1)-O(1)#4	2.114(3)
Fe(1)-O(1)#5	2.112(3)	Fe(1)-O(1)#5	2.114(3)
Fe(1)-O(1)	2.112(3)	Fe(1)-O(1)	2.114(3)
Ga(1)-O(2)#6	1.977(3)	Ga(1)-O(2)#6	1.977(3)
Ga(1)-O(2)	1.977(3)	Ga(1)-O(2)	1.977(3)
Ga(1)-O(2)#7	1.977(3)	Ga(1)-O(2)#7	1.977(3)
Ga(1)-O(2)#8	1.977(3)	Ga(1)-O(2)#8	1.977(3)
Ga(1)-O(2)#9	1.977(3)	Ga(1)-O(2)#9	1.977(3)
Ga(1)-O(2)#10	1.977(3)	Ga(1)-O(2)#10	1.977(3)
Bond angles of complex 1			
	110 K		300 K
O(2)#1-Fe(1)-O(2)	89.06(16)	O(1)#1-Fe(1)-O(1)	92.67(11)
O(2)#1-Fe(1)-O(2)#2	92.89(11)	O(1)#1-Fe(1)-O(1)#2	86.15(15)
O(2)-Fe(1)-O(2)#2	85.21(16)	O(1)-Fe(1)-O(1)#2	88.53(16)
O(2)#1-Fe(1)-O(2)#3	85.21(16)	O(1)#1-Fe(1)-O(1)#3	178.35(16)
O(2)-Fe(1)-O(2)#3	92.89(11)	O(1)-Fe(1)-O(1)#3	86.15(15)
O(2)#2-Fe(1)-O(2)#3	177.35(16)	O(1)#2-Fe(1)-O(1)#3	92.67(11)
O(2)#1-Fe(1)-O(2)#4	177.35(16)	O(1)#1-Fe(1)-O(1)#4	88.53(16)
O(2)-Fe(1)-O(2)#4	92.89(11)	O(1)-Fe(1)-O(1)#4	178.35(16)
O(2)#2-Fe(1)-O(2)#4	89.06(17)	O(1)#2-Fe(1)-O(1)#4	92.67(11)
O(2)#3-Fe(1)-O(2)#4	92.89(11)	O(1)#3-Fe(1)-O(1)#4	92.67(11)
O(2)#1-Fe(1)-O(2)#5	92.89(11)	O(1)#1-Fe(1)-O(1)#5	92.67(11)
O(2)-Fe(1)-O(2)#5	177.35(16)	O(1)-Fe(1)-O(1)#5	92.67(11)
O(2)#2-Fe(1)-O(2)#5	92.89(11)	O(1)#2-Fe(1)-O(1)#5	178.35(16)
O(2)#3-Fe(1)-O(2)#5	89.06(17)	O(1)#3-Fe(1)-O(1)#5	88.53(16)
O(2)#4-Fe(1)-O(2)#5	85.21(15)	O(1)#4-Fe(1)-O(1)#5	86.15(15)
O(1)#6-Ga(1)-O(1)#7	180.00(13)	O(2)#6-Ga(1)-O(2)#7	91.06(11)
O(1)#6-Ga(1)-O(1)#8	88.93(11)	O(2)#6-Ga(1)-O(2)	88.94(11)
O(1)#7-Ga(1)-O(1)#8	91.07(11)	O(2)#7-Ga(1)-O(2)	180.00(15)

O(1)#6-Ga(1)-O(1)	88.93(11)	O(2)#6-Ga(1)-O(2)#8	88.94(11)
O(1)#7-Ga(1)-O(1)	91.07(11)	O(2)#7-Ga(1)-O(2)#8	88.94(11)
O(1)#8-Ga(1)-O(1)	91.07(11)	O(2)-Ga(1)-O(2)#8	91.06(11)
O(1)#6-Ga(1)-O(1)#9	91.07(11)	O(2)#6-Ga(1)-O(2)#9	180.00(12)
O(1)#7-Ga(1)-O(1)#9	88.93(11)	O(2)#7-Ga(1)-O(2)#9	88.94(11)
O(1)#8-Ga(1)-O(1)#9	88.93(11)	O(2)-Ga(1)-O(2)#9	91.06(11)
O(1)-Ga(1)-O(1)#9	180.00(16)	O(2)#8-Ga(1)-O(2)#9	91.06(11)
O(1)#6-Ga(1)-O(1)#10	91.07(11)	O(2)#6-Ga(1)-O(2)#10	91.06(11)
O(1)#7-Ga(1)-O(1)#10	88.93(11)	O(2)#7-Ga(1)-O(2)#10	91.06(11)
O(1)#8-Ga(1)-O(1)#10	180.00(13)	O(2)-Ga(1)-O(2)#10	88.94(11)
O(1)-Ga(1)-O(1)#10	88.93(11)	O(2)#8-Ga(1)-O(2)#10	180.00(16)
O(1)#9-Ga(1)-O(1)#10	91.07(11)	O(2)#9-Ga(1)-O(2)#10	88.94(11)
C(1)-O(2)-Fe(1)	125.6(3)	C(1)-O(1)-Fe(1)	126.5(3)
C(1)-O(1)-Ga(1)	125.0(2)	C(1)-O(2)-Ga(1)	126.0(2)
Symmetry transformations used to generate equivalent atoms: #1 -y+1,-x+1,-z+1/2; #2 -x+y+1,y,-z+1/2; #3 -y+1,x-y,z; #4 -x+y+1,-x+1,z; #5 x,x-y,-z+1/2; #6 x-y,x-1,-z; #7 -x+y+2,-x+1,z; #8 -y+1,x-y-1,z; #9 -x+2,-y,-z; #10 y+1,-x+y+1,-z		Symmetry transformations used to generate equivalent atoms: #1 -y+1,x-y+1,z; #2 -y+1,-x+1,-z+1/2; #3 -x+y,y,-z+1/2; #4 x,x-y+1,-z+1/2; #5 -x+y,-x+1,z; #6 y-1,-x+y,-z; #7 -x,-y+2,-z; #8 -x+y-1,-x+1,z; #9 -y+1,x-y+2,z; #10 x-y+1,x+1,-z	

Bond lengths of complex 2

110 K		300 K	
Fe(1)-O(1)#6	2.1186(19)	Fe(1)-O(1)#1	2.1157(15)
Fe(1)-O(1)#7	2.1186(19)	Fe(1)-O(1)#2	2.1157(15)
Fe(1)-O(1)#8	2.1186(19)	Fe(1)-O(1)#3	2.1157(15)
Fe(1)-O(1)#9	2.1186(19)	Fe(1)-O(1)#4	2.1157(15)
Fe(1)-O(1)#10	2.1186(19)	Fe(1)-O(1)#5	2.1157(15)
Fe(1)-O(1)	2.1186(19)	Fe(1)-O(1)	2.1157(15)
Ga(1)-O(2)#1	1.9721(18)	Ga(1)-O(2)#6	1.9712(13)
Ga(1)-O(2)	1.9721(18)	Ga(1)-O(2)	1.9712(13)
Ga(1)-O(2)#2	1.9721(18)	Ga(1)-O(2)#7	1.9712(13)
Ga(1)-O(2)#3	1.9721(18)	Ga(1)-O(2)#8	1.9712(13)
Ga(1)-O(2)#4	1.9721(18)	Ga(1)-O(2)#9	1.9712(13)
Ga(1)-O(2)#5	1.9721(18)	Ga(1)-O(2)#10	1.9712(13)

Bond angles of complex 2

110 K		300 K	
O(2)#1-Ga(1)-O(2)#2	88.76(8)	O(1)-Fe(1)-O(1)#1	89.04(8)
O(2)#1-Ga(1)-O(2)#3	180.00(12)	O(1)-Fe(1)-O(1)#2	93.30(6)
O(2)#2-Ga(1)-O(2)#3	91.24(8)	O(1)#1-Fe(1)-O(1)#2	84.43(8)
O(2)#1-Ga(1)-O(2)	91.24(8)	O(1)-Fe(1)-O(1)#3	84.43(8)
O(2)#2-Ga(1)-O(2)	180.00(12)	O(1)#1-Fe(1)-O(1)#3	93.30(6)
O(2)#3-Ga(1)-O(2)	88.76(8)	O(1)#2-Fe(1)-O(1)#3	176.84(8)

O(2)#1-Ga(1)-O(2)#4	88.76(8)	O(1)-Fe(1)-O(1)#4	93.30(6)
O(2)#2-Ga(1)-O(2)#4	91.24(8)	O(1)#1-Fe(1)-O(1)#4	176.84(8)
O(2)#3-Ga(1)-O(2)#4	91.24(8)	O(1)#2-Fe(1)-O(1)#4	93.30(6)
O(2)-Ga(1)-O(2)#4	88.76(8)	O(1)#3-Fe(1)-O(1)#4	89.04(8)
O(2)#1-Ga(1)-O(2)#5	91.24(8)	O(1)-Fe(1)-O(1)#5	176.84(8)
O(2)#2-Ga(1)-O(2)#5	88.76(8)	O(1)#1-Fe(1)-O(1)#5	93.30(6)
O(2)#3-Ga(1)-O(2)#5	88.76(8)	O(1)#2-Fe(1)-O(1)#5	89.04(8)
O(2)-Ga(1)-O(2)#5	91.24(8)	O(1)#3-Fe(1)-O(1)#5	93.30(6)
O(2)#4-Ga(1)-O(2)#5	180.00(12)	O(1)#4-Fe(1)-O(1)#5	84.44(8)
O(1)#6-Fe(1)-O(1)	85.21(10)	O(2)#6-Ga(1)-O(2)#7	180.00(6)
O(1)#6-Fe(1)-O(1)#7	93.18(8)	O(2)#6-Ga(1)-O(2)#8	88.83(5)
O(1)-Fe(1)-O(1)#7	177.76(10)	O(2)#7-Ga(1)-O(2)#8	91.17(6)
O(1)#6-Fe(1)-O(1)#8	88.47(11)	O(2)#6-Ga(1)-O(2)#9	88.83(6)
O(1)-Fe(1)-O(1)#8	93.18(8)	O(2)#7-Ga(1)-O(2)#9	91.17(5)
O(1)#7-Fe(1)-O(1)#8	85.21(10)	O(2)#8-Ga(1)-O(2)#9	91.17(6)
O(1)#6-Fe(1)-O(1)#9	93.18(8)	O(2)#6-Ga(1)-O(2)	91.17(5)
O(1)-Fe(1)-O(1)#9	88.47(11)	O(2)#7-Ga(1)-O(2)	88.83(6)
O(1)#7-Fe(1)-O(1)#9	93.18(8)	O(2)#8-Ga(1)-O(2)	180.00(8)
O(1)#8-Fe(1)-O(1)#9	177.76(10)	O(2)#9-Ga(1)-O(2)	88.83(5)
O(1)#6-Fe(1)-O(1)#10	177.76(10)	O(2)#6-Ga(1)-O(2)#10	91.17(6)
O(1)-Fe(1)-O(1)#10	93.18(8)	O(2)#7-Ga(1)-O(2)#10	88.83(6)
O(1)#7-Fe(1)-O(1)#10	88.47(11)	O(2)#8-Ga(1)-O(2)#10	88.83(5)
O(1)#8-Fe(1)-O(1)#10	93.18(8)	O(2)#9-Ga(1)-O(2)#10	180.00(9)
O(1)#9-Fe(1)-O(1)#10	85.21(10)	O(2)-Ga(1)-O(2)#10	91.17(5)
C(1)-O(1)-Fe(1)	126.08(17)	C(1)-O(1)-Fe(1)	125.28(13)
C(1)-O(2)-Ga(1)	125.26(15)	C(1)-O(2)-Ga(1)	124.21(12)
Symmetry transformations used to generate equivalent atoms: #1 -y,x-y,z; #2 -x,-y,-z; #3 y,-x+y,-z; #4 x-y,x,-z; #5 -x+y,-x,z; #6 -x+y+1,y,-z+1/2; #7 -y+1,-x+1,-z+1/2; #8 -y+1,x-y,z; #9 x,x-y,-z+1/2; #10 -x+y+1,-x+1,z		Symmetry transformations used to generate equivalent atoms: #1 -y+1,-x+1,-z+1/2; #2 -y+1,x-y,z; #3 -x+y+1,y,-z+1/2; #4 -x+y+1,-x+1,z; #5 x,x-y,-z+1/2; #6 -x+y+2,-x+1,z; #7 x-y,x-1,-z; #8 -x+2,-y,-z; #9 y+1,-x+y+1,-z; #10 -y+1,x-y-1,z	

Bond lengths of complex 3

	110 K		300 K
Fe(1)-O(1)#6	2.115(4)	Fe(1)-O(1)#1	2.119(2)
Fe(1)-O(1)#7	2.115(4)	Fe(1)-O(1)#2	2.119(2)
Fe(1)-O(1)#8	2.115(4)	Fe(1)-O(1)#3	2.119(2)
Fe(1)-O(1)#9	2.115(4)	Fe(1)-O(1)#4	2.119(2)
Fe(1)-O(1)#10	2.115(4)	Fe(1)-O(1)#5	2.119(2)
Fe(1)-O(1)	2.115(4)	Fe(1)-O(1)	2.119(2)
Ga(1)-O(2)#1	1.977(4)	Ga(1)-O(2)#6	1.977(2)
Ga(1)-O(2)	1.977(4)	Ga(1)-O(2)	1.977(2)
Ga(1)-O(2)#2	1.977(4)	Ga(1)-O(2)#7	1.977(2)

Ga(1)-O(2)#3	1.977(4)	Ga(1)-O(2)#8	1.977(2)
Ga(1)-O(2)#4	1.977(4)	Ga(1)-O(2)#9	1.977(2)
Ga(1)-O(2)#5	1.977(4)	Ga(1)-O(2)#10	1.977(2)

Bond angles of complex 3

110 K		300 K	
O(2)#1-Ga(1)-O(2)#2	180.0(3)	C(1)-O(2)-Ga(1)	128.02(18)
O(2)#1-Ga(1)-O(2)#3	90.97(17)	C(1)-O(1)-Fe(1)	127.78(19)
O(2)#2-Ga(1)-O(2)#3	89.03(17)	O(1)-Fe(1)-O(1)#1	85.52(12)
O(2)#1-Ga(1)-O(2)#4	90.97(17)	O(1)-Fe(1)-O(1)#2	93.38(8)
O(2)#2-Ga(1)-O(2)#4	89.03(17)	O(1)#1-Fe(1)-O(1)#2	87.74(11)
O(2)#3-Ga(1)-O(2)#4	90.97(17)	O(1)-Fe(1)-O(1)#3	178.48(11)
O(2)#1-Ga(1)-O(2)#5	89.03(17)	O(1)#1-Fe(1)-O(1)#3	93.38(9)
O(2)#2-Ga(1)-O(2)#5	90.97(17)	O(1)#2-Fe(1)-O(1)#3	85.52(12)
O(2)#3-Ga(1)-O(2)#5	89.03(17)	O(1)-Fe(1)-O(1)#4	87.74(12)
O(2)#4-Ga(1)-O(2)#5	180.0(5)	O(1)#1-Fe(1)-O(1)#4	93.38(9)
O(2)#1-Ga(1)-O(2)	89.03(17)	O(1)#2-Fe(1)-O(1)#4	178.47(11)
O(2)#2-Ga(1)-O(2)	90.97(17)	O(1)#3-Fe(1)-O(1)#4	93.38(9)
O(2)#3-Ga(1)-O(2)	180.0	O(1)-Fe(1)-O(1)#5	93.38(9)
O(2)#4-Ga(1)-O(2)	89.03(17)	O(1)#1-Fe(1)-O(1)#5	178.47(11)
O(2)#5-Ga(1)-O(2)	90.97(17)	O(1)#2-Fe(1)-O(1)#5	93.38(9)
O(1)-Fe(1)-O(1)#6	86.1(2)	O(1)#3-Fe(1)-O(1)#5	87.74(11)
O(1)-Fe(1)-O(1)#7	93.74(16)	O(1)#4-Fe(1)-O(1)#5	85.52(12)
O(1)#6-Fe(1)-O(1)#7	86.4(2)	O(2)-Ga(1)-O(2)#6	88.87(9)
O(1)-Fe(1)-O(1)#8	179.8(2)	O(2)-Ga(1)-O(2)#7	180.00(9)
O(1)#6-Fe(1)-O(1)#8	93.74(16)	O(2)#6-Ga(1)-O(2)#7	91.13(9)
O(1)#7-Fe(1)-O(1)#8	86.1(2)	O(2)-Ga(1)-O(2)#8	91.13(9)
O(1)-Fe(1)-O(1)#9	93.74(16)	O(2)#6-Ga(1)-O(2)#8	180.00(13)
O(1)#6-Fe(1)-O(1)#9	179.8(2)	O(2)#7-Ga(1)-O(2)#8	88.87(9)
O(1)#7-Fe(1)-O(1)#9	93.74(16)	O(2)-Ga(1)-O(2)#9	91.13(9)
O(1)#8-Fe(1)-O(1)#9	86.4(2)	O(2)#6-Ga(1)-O(2)#9	88.87(9)
O(1)-Fe(1)-O(1)#10	86.4(2)	O(2)#7-Ga(1)-O(2)#9	88.87(9)
O(1)#6-Fe(1)-O(1)#10	93.74(16)	O(2)#8-Ga(1)-O(2)#9	91.13(9)
O(1)#7-Fe(1)-O(1)#10	179.8(2)	O(2)-Ga(1)-O(2)#10	88.87(9)
O(1)#8-Fe(1)-O(1)#10	93.74(16)	O(2)#6-Ga(1)-O(2)#10	91.13(9)
O(1)#9-Fe(1)-O(1)#10	86.1(2)	O(2)#7-Ga(1)-O(2)#10	91.13(9)
C(1)-O(1)-Fe(1)	126.5(4)	O(2)#8-Ga(1)-O(2)#10	88.87(9)
C(1)-O(2)-Ga(1)	125.9(4)	O(2)#9-Ga(1)-O(2)#10	180.0(2)
Symmetry transformations used to generate equivalent atoms: #1 y,-x+y,-z; #2 -y,x-y,z; #3 -x,-y,-z; #4 x-y,x,-z; #5 -x+y,-x,z; #6 -x+y+1,y,-z+1/2; #7 -y+1,x-y,z; #8 -y+1,-x+1,-z+1/2; #9 -x+y+1,-x+1,z; #10 x,x-y,-z+1/2		Symmetry transformations used to generate equivalent atoms: #1 -x+y,y,-z+1/2; #2 -y+1,x-y+1,z; #3 -y+1,-x+1,-z+1/2; #4 x,x-y+1,-z+1/2; #5 -x+y,-x+1,z; #6 x-y,x,-z; #7 -x,-y,-z; #8 -x+y,-x,z; #9 -y,x-y,z; #10 y,-x+y,-z	

Bond lengths of complex 4

110 K		300 K	
Ni(1)-O(1)#1	2.0419(11)	Ni(1)-O(1)#1	2.051(4)
Ni(1)-O(1)#2	2.0419(11)	Ni(1)-O(1)#2	2.051(4)
Ni(1)-O(1)#3	2.0419(11)	Ni(1)-O(1)#3	2.051(4)
Ni(1)-O(1)#4	2.0419(11)	Ni(1)-O(1)#4	2.051(4)
Ni(1)-O(1)#5	2.0419(11)	Ni(1)-O(1)#5	2.051(4)
Ni(1)-O(1)	2.0419(11)	Ni(1)-O(1)	2.051(4)
Ga(1)-O(2)#6	1.9754(11)	Ga(1)-O(2)#6	1.984(3)
Ga(1)-O(2)	1.9754(11)	Ga(1)-O(2)	1.984(3)
Ga(1)-O(2)#7	1.9754(11)	Ga(1)-O(2)#7	1.984(3)
Ga(1)-O(2)#8	1.9754(11)	Ga(1)-O(2)#8	1.984(3)
Ga(1)-O(2)#9	1.9754(11)	Ga(1)-O(2)#9	1.984(3)
Ga(1)-O(2)#10	1.9754(11)	Ga(1)-O(2)#10	1.984(3)

Bond angles of complex 4

110 K		300 K	
O(1)#1-Ni(1)-O(1)#2	89.42(6)	O(1)#1-Ni(1)-O(1)	89.18(19)
O(1)#1-Ni(1)-O(1)#3	93.22(4)	O(1)#1-Ni(1)-O(1)#2	84.95(18)
O(1)#2-Ni(1)-O(1)#3	84.25(6)	O(1)-Ni(1)-O(1)#2	92.97(14)
O(1)#1-Ni(1)-O(1)#4	84.25(6)	O(1)#1-Ni(1)-O(1)#3	92.97(14)
O(1)#2-Ni(1)-O(1)#4	93.22(4)	O(1)-Ni(1)-O(1)#3	84.95(18)
O(1)#3-Ni(1)-O(1)#4	176.45(6)	O(1)#2-Ni(1)-O(1)#3	177.09(17)
O(1)#1-Ni(1)-O(1)	176.45(6)	O(1)#1-Ni(1)-O(1)#4	92.97(14)
O(1)#2-Ni(1)-O(1)	93.22(4)	O(1)-Ni(1)-O(1)#4	177.09(17)
O(1)#3-Ni(1)-O(1)	89.42(6)	O(1)#2-Ni(1)-O(1)#4	89.18(19)
O(1)#4-Ni(1)-O(1)	93.22(4)	O(1)#3-Ni(1)-O(1)#4	92.97(14)
O(1)#1-Ni(1)-O(1)#5	93.22(4)	O(1)#1-Ni(1)-O(1)#5	177.09(17)
O(1)#2-Ni(1)-O(1)#5	176.45(6)	O(1)-Ni(1)-O(1)#5	92.97(14)
O(1)#3-Ni(1)-O(1)#5	93.22(4)	O(1)#2-Ni(1)-O(1)#5	92.97(14)
O(1)#4-Ni(1)-O(1)#5	89.42(6)	O(1)#3-Ni(1)-O(1)#5	89.18(19)
O(1)-Ni(1)-O(1)#5	84.25(6)	O(1)#4-Ni(1)-O(1)#5	84.95(18)
O(2)#6-Ga(1)-O(2)	180.00(12)	O(2)#6-Ga(1)-O(2)#7	180.0
O(2)#6-Ga(1)-O(2)#7	91.31(4)	O(2)#6-Ga(1)-O(2)#8	88.69(14)
O(2)-Ga(1)-O(2)#7	88.69(4)	O(2)#7-Ga(1)-O(2)#8	91.31(14)
O(2)#6-Ga(1)-O(2)#8	88.69(4)	O(2)#6-Ga(1)-O(2)	91.31(14)
O(2)-Ga(1)-O(2)#8	91.31(4)	O(2)#7-Ga(1)-O(2)	88.69(14)
O(2)#7-Ga(1)-O(2)#8	180.00(6)	O(2)#8-Ga(1)-O(2)	88.69(14)
O(2)#6-Ga(1)-O(2)#9	91.31(4)	O(2)#6-Ga(1)-O(2)#9	88.69(14)
O(2)-Ga(1)-O(2)#9	88.69(4)	O(2)#7-Ga(1)-O(2)#9	91.31(14)
O(2)#7-Ga(1)-O(2)#9	91.31(4)	O(2)#8-Ga(1)-O(2)#9	91.31(14)
O(2)#8-Ga(1)-O(2)#9	88.69(4)	O(2)-Ga(1)-O(2)#9	180.0(2)
O(2)#6-Ga(1)-O(2)#10	88.69(4)	O(2)#6-Ga(1)-O(2)#10	91.31(14)
O(2)-Ga(1)-O(2)#10	91.31(4)	O(2)#7-Ga(1)-O(2)#10	88.69(14)

O(2)#7-Ga(1)-O(2)#10	88.69(4)	O(2)#8-Ga(1)-O(2)#10	180.0
O(2)#8-Ga(1)-O(2)#10	91.31(4)	O(2)-Ga(1)-O(2)#10	91.31(14)
O(2)#9-Ga(1)-O(2)#10	180.00(7)	O(2)#9-Ga(1)-O(2)#10	88.69(14)
C(1)-O(1)-Ni(1)	125.19(10)	C(1)-O(1)-Ni(1)	125.5(3)
C(1)-O(2)-Ga(1)	124.87(10)	C(1)-O(2)-Ga(1)	125.6(3)
Symmetry transformations used to generate equivalent atoms: #1 x,x-y+1,-z+1/2; #2 -x+y,-x+1,z; #3 -x+y,y,-z+1/2; #4 -y+1,x-y+1,z; #5 -y+1,-x+1,-z+1/2; #6 -x,-y,-z; #7 y,-x+y,-z; #8 -y,x-y,z; #9 x-y,x,-z; #10 -x+y,-x,z		Symmetry transformations used to generate equivalent atoms: #1 -y+1,-x+1,-z+1/2; #2 -x+y,-x+1,z; #3 x,x-y+1,-z+1/2; #4 -x+y,y,-z+1/2; #5 -y+1,x-y+1,z; #6 -y+1,x-y+2,z; #7 y-1,-x+y,-z; #8 x-y+1,x+1,-z; #9 -x,-y+2,-z; #10 -x+y-1,-x+1,z	

Bond lengths of complex 5

110 K		300 K	
Ni(1)-O(1)#6	2.0313(14)	Ni(1)-O(1)#1	2.030(2)
Ni(1)-O(1)#7	2.0313(14)	Ni(1)-O(1)#2	2.030(3)
Ni(1)-O(1)#8	2.0313(14)	Ni(1)-O(1)#3	2.030(3)
Ni(1)-O(1)#9	2.0313(14)	Ni(1)-O(1)#4	2.030(3)
Ni(1)-O(1)#10	2.0313(14)	Ni(1)-O(1)#5	2.030(2)
Ni(1)-O(1)	2.0313(14)	Ni(1)-O(1)	2.030(2)
Ga(1)-O(2)#1	1.9866(14)	Ga(1)-O(2)#6	1.985(2)
Ga(1)-O(2)	1.9866(14)	Ga(1)-O(2)	1.985(2)
Ga(1)-O(2)#2	1.9866(14)	Ga(1)-O(2)#7	1.985(2)
Ga(1)-O(2)#3	1.9866(14)	Ga(1)-O(2)#8	1.985(2)
Ga(1)-O(2)#4	1.9866(14)	Ga(1)-O(2)#9	1.985(2)
Ga(1)-O(2)#5	1.9866(14)	Ga(1)-O(2)#10	1.985(2)

Bond angles of complex 5

110 K		300 K	
O(2)#1-Ga(1)-O(2)	180.00(10)	O(1)#1-Ni(1)-O(1)#2	88.97(15)
O(2)#1-Ga(1)-O(2)#2	88.64(6)	O(1)#1-Ni(1)-O(1)#3	84.32(14)
O(2)-Ga(1)-O(2)#2	91.36(6)	O(1)#2-Ni(1)-O(1)#3	93.40(10)
O(2)#1-Ga(1)-O(2)#3	91.36(6)	O(1)#1-Ni(1)-O(1)#4	93.40(10)
O(2)-Ga(1)-O(2)#3	88.64(6)	O(1)#2-Ni(1)-O(1)#4	84.32(14)
O(2)#2-Ga(1)-O(2)#3	88.64(6)	O(1)#3-Ni(1)-O(1)#4	176.81(14)
O(2)#1-Ga(1)-O(2)#4	88.64(6)	O(1)#1-Ni(1)-O(1)	93.40(10)
O(2)-Ga(1)-O(2)#4	91.36(6)	O(1)#2-Ni(1)-O(1)	176.81(14)
O(2)#2-Ga(1)-O(2)#4	91.36(6)	O(1)#3-Ni(1)-O(1)	88.97(15)
O(2)#3-Ga(1)-O(2)#4	180.00(10)	O(1)#4-Ni(1)-O(1)	93.40(10)
O(2)#1-Ga(1)-O(2)#5	91.36(6)	O(1)#1-Ni(1)-O(1)#5	176.81(14)
O(2)-Ga(1)-O(2)#5	88.64(6)	O(1)#2-Ni(1)-O(1)#5	93.40(10)
O(2)#2-Ga(1)-O(2)#5	180.00(6)	O(1)#3-Ni(1)-O(1)#5	93.40(10)
O(2)#3-Ga(1)-O(2)#5	91.36(6)	O(1)#4-Ni(1)-O(1)#5	88.97(15)
O(2)#4-Ga(1)-O(2)#5	88.64(6)	O(1)-Ni(1)-O(1)#5	84.32(14)

O(1)#6-Ni(1)-O(1)#7	89.48(9)	O(2)-Ga(1)-O(2)#6	180.00(18)
O(1)#6-Ni(1)-O(1)#8	83.79(8)	O(2)-Ga(1)-O(2)#7	88.51(10)
O(1)#7-Ni(1)-O(1)#8	93.43(6)	O(2)#6-Ga(1)-O(2)#7	91.49(10)
O(1)#6-Ni(1)-O(1)#9	93.43(6)	O(2)-Ga(1)-O(2)#8	91.49(10)
O(1)#7-Ni(1)-O(1)#9	83.79(8)	O(2)#6-Ga(1)-O(2)#8	88.51(10)
O(1)#8-Ni(1)-O(1)#9	176.10(8)	O(2)#7-Ga(1)-O(2)#8	180.00(17)
O(1)#6-Ni(1)-O(1)	93.43(6)	O(2)-Ga(1)-O(2)#9	91.49(10)
O(1)#7-Ni(1)-O(1)	176.10(9)	O(2)#6-Ga(1)-O(2)#9	88.51(10)
O(1)#8-Ni(1)-O(1)	89.48(9)	O(2)#7-Ga(1)-O(2)#9	88.51(10)
O(1)#9-Ni(1)-O(1)	93.43(6)	O(2)#8-Ga(1)-O(2)#9	91.49(10)
O(1)#6-Ni(1)-O(1)#10	176.10(8)	O(2)-Ga(1)-O(2)#10	88.51(10)
O(1)#7-Ni(1)-O(1)#10	93.43(6)	O(2)#6-Ga(1)-O(2)#10	91.49(10)
O(1)#8-Ni(1)-O(1)#10	93.43(6)	O(2)#7-Ga(1)-O(2)#10	91.49(10)
O(1)#9-Ni(1)-O(1)#10	89.48(9)	O(2)#8-Ga(1)-O(2)#10	88.51(10)
O(1)-Ni(1)-O(1)#10	83.79(8)	O(2)#9-Ga(1)-O(2)#10	180.00(14)
C(1)-O(2)-Ga(1)	124.26(13)	C(1)-O(1)-Ni(1)	125.6(2)
C(1)-O(1)-Ni(1)	124.95(14)	C(1)-O(2)-Ga(1)	125.5(2)
Symmetry transformations used to generate equivalent atoms: #1 -x,-y,-z; #2 -y,x-y,z; #3 x-y,x,-z; #4 -x+y,-x,z; #5 y,-x+y,-z; #6 -y+1,x-y,z; #7 -x+y+1,y,-z+1/2; #8 x,x-y,-z+1/2; #9 -x+y+1,-x+1,z; #10 -y+1,-x+1,-z+1/2		Symmetry transformations used to generate equivalent atoms: #1 -y+1,x-y,z; #2 -x+y+1,y,-z+1/2; #3 x,x-y,-z+1/2; #4 -x+y+1,-x+1,z; #5 -y+1,-x+1,-z+1/2; #6 -x,-y,-z; #7 x-y,x,-z; #8 -x+y,-x,z; #9 -y,x-y,z; #10 y,-x+y,-z	

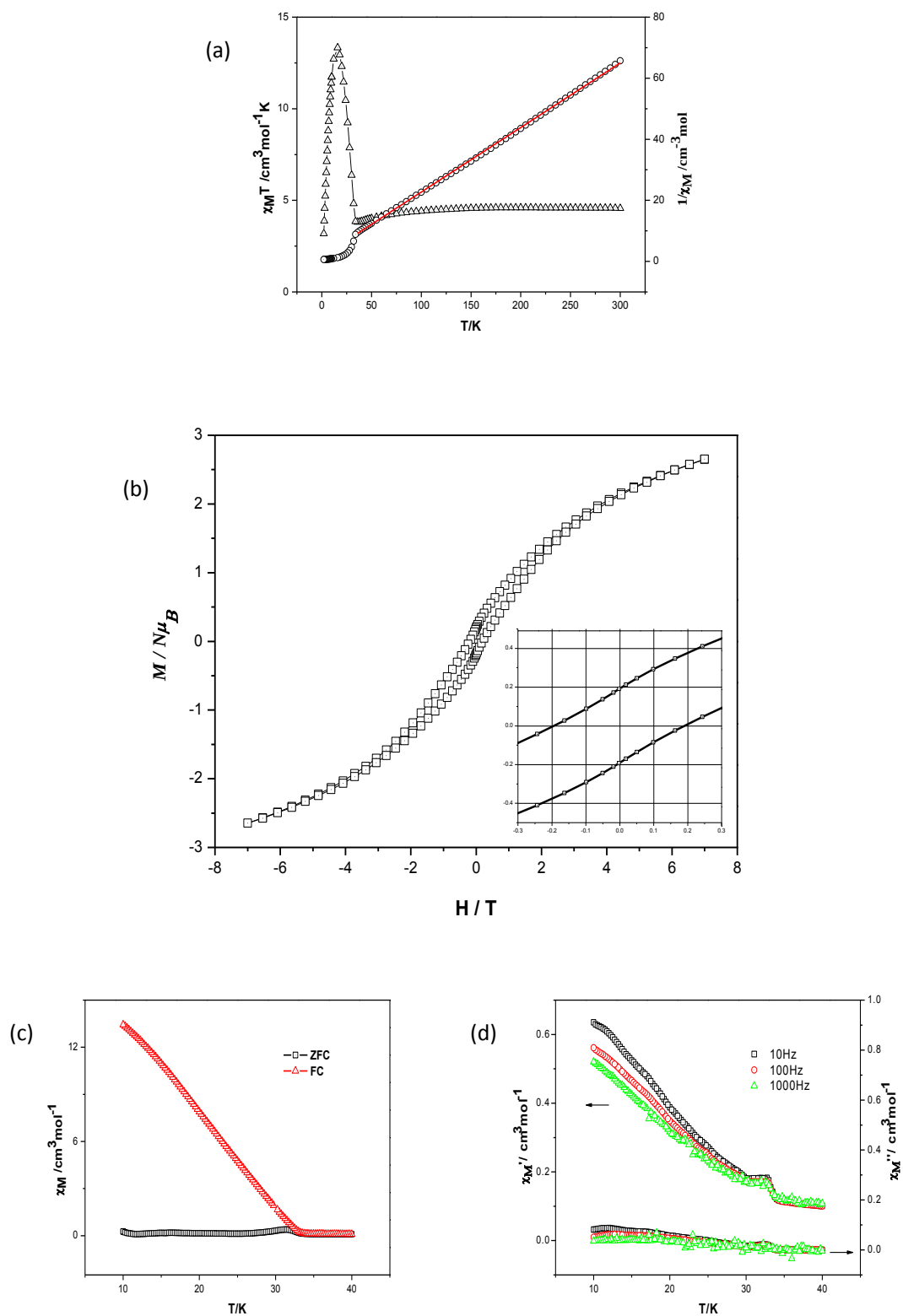


Figure S1. (a) The $\chi_M T$ vs. T and χ_M^{-1} vs. T plots of **2** under applied field 1000Oe; (b) M vs. H plot of **2** at 2K; (c) ZFC/FC measurements under a 50 Oe field for **2**; (d) zero-field ac in-phase (χ_M') and out-of-phase (χ_M'') susceptibility vs. T at various frequencies for **2**.

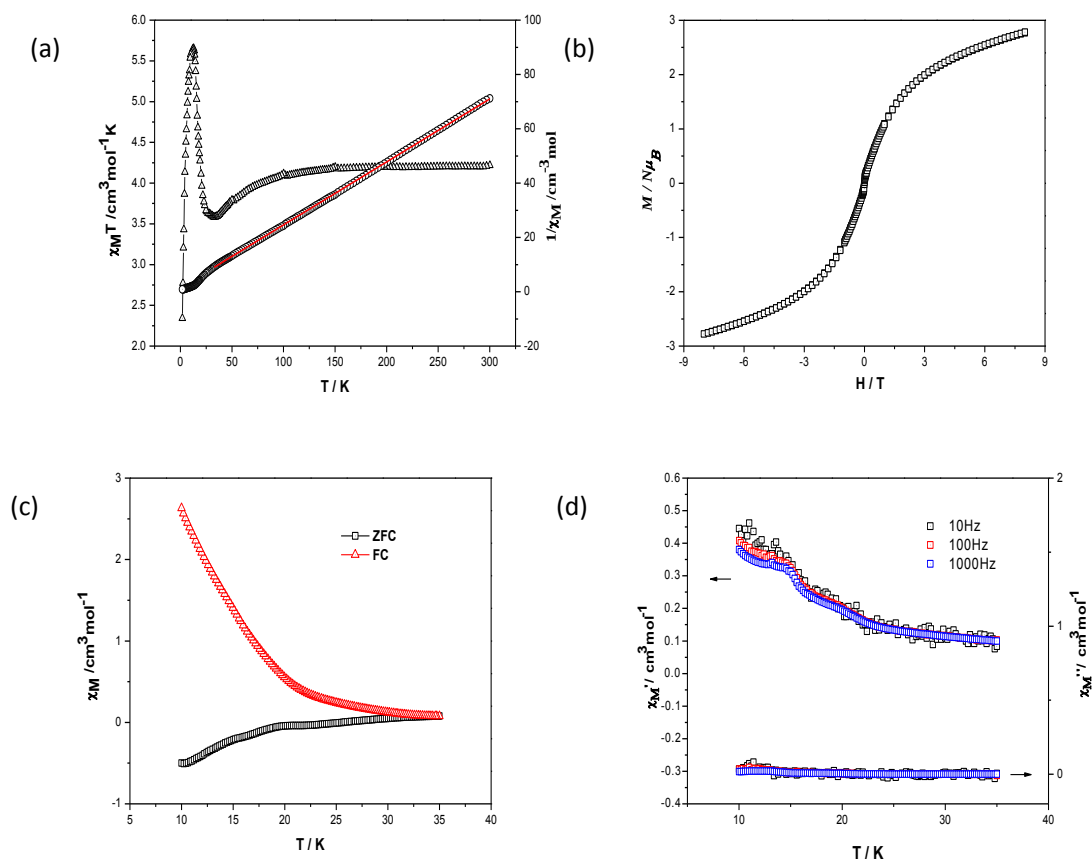


Figure S2. (a) The $\chi_M T$ vs. T and χ_M^{-1} vs. T plots of **3** under applied field 1000Oe; (b) M vs. H plot of **3** at 2K; (c) ZFC/FC measurements under a 50 Oe field for **3**; (d) zero-field ac in-phase (χ_M') and out-of-phase (χ_M'') susceptibility vs. T at various frequencies for **3**.

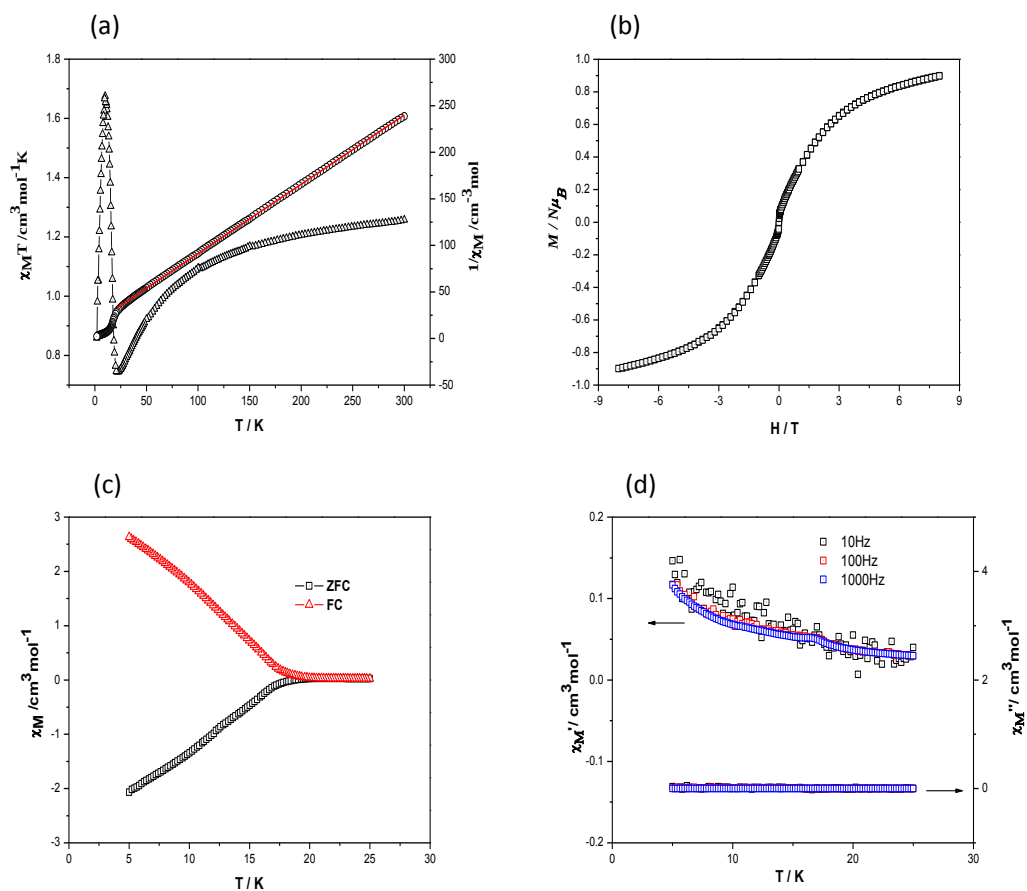


Figure S3. (a) The $\chi_M T$ vs. T and χ_M^{-1} vs. T plots of **4** under applied field 1000Oe; (b) M vs. H plot of **4** at 2K; (c) ZFC/FC measurements under a 50 Oe field for **4**; (d) zero-field ac in-phase (χ_M') and out-of-phase (χ_M'') susceptibility vs. T at various frequencies for **4**.

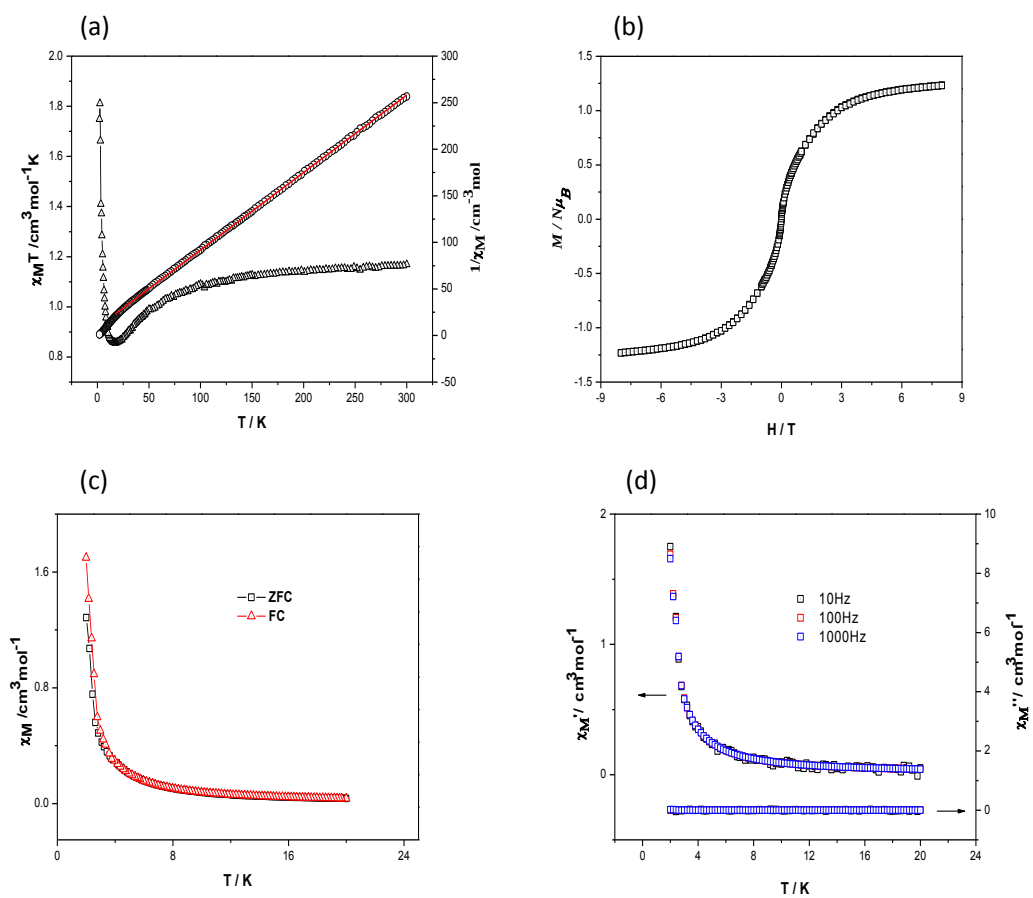


Figure S4. (a) The $\chi_M T$ vs. T and χ_M^{-1} vs. T plots of **5** under applied field 1000 Oe; (b) M vs. H plot of **5** at 2 K; (c) ZFC/FC measurements under a 50 Oe field for **5**; (d) zero-field ac in-phase (χ_M') and out-of-phase (χ_M'') susceptibility vs. T at various frequencies for **5**.

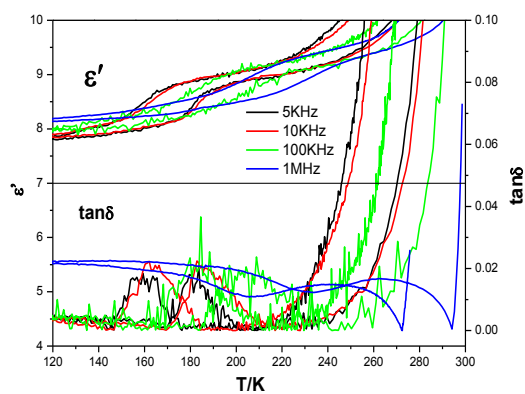


Figure S5. The temperature-dependent traces of the dielectric permittivities for **1**.

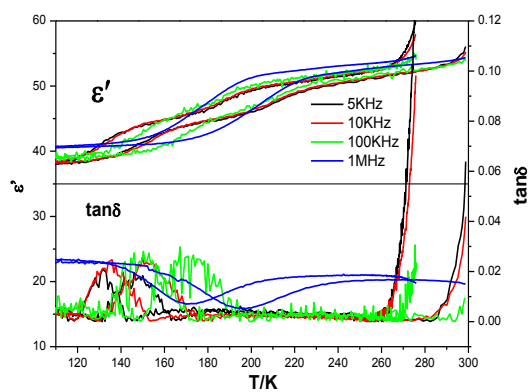


Figure S6. The temperature-dependent traces of the dielectric permittivities for **3**.

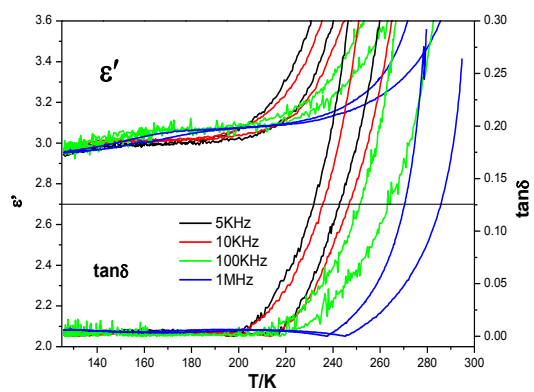


Figure S7. The temperature-dependent traces of the dielectric permittivities for **4**.