

Supplementary Information

Construction of magnet-type coordination polymers using high-spin $\{\text{Ni}_4\}$ -citrate cubane as secondary building units

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Table S1 The selected bond lengths (Å) and angles (°) for compound **1**.

Ni(1)-O(7)#1	2.0206(18)	Ni(2)-O(18B)#1	2.143(4)
Ni(1)-O(9)	2.0239(17)	Ni(3)-O(14)#4	2.0106(18)
Ni(1)-O(3)	2.0392(17)	Ni(3)-O(14)#5	2.0106(18)
Ni(1)-O(10)	2.0835(15)	Ni(3)-O(15)	2.089(2)
Ni(1)-O(1)	2.1142(17)	Ni(3)-O(15)#6	2.089(2)
Ni(1)-O(3)#1	2.1413(17)	Ni(3)-O(4)#7	2.1068(18)
Ni(2)-O(2)#1	2.041(2)	Ni(3)-O(4)#8	2.1068(18)
Ni(2)-O(2)	2.041(2)	Ni(4)-O(5)#7	2.0267(17)
Ni(2)-O(17)#1	2.048(2)	Ni(4)-O(10)#9	2.0370(16)
Ni(2)-O(17)	2.048(2)	Ni(4)-O(3)#7	2.0659(15)
Ni(2)-O(18A)	2.050(3)	Ni(4)-O(13)#9	2.0779(16)
Ni(2)-O(18A)#1	2.050(3)	Ni(4)-O(11)#7	2.0818(17)
Ni(2)-O(18B)	2.143(4)	Ni(4)-O(10)#7	2.0930(17)
O(7)#1-Ni(1)-O(9)	95.58(8)	O(2)-Ni(2)-O(18B)#1	94.61(14)
O(7)#1-Ni(1)-O(3)	161.26(7)	O(17)#1-Ni(2)-O(18B)#1	82.36(14)
O(9)-Ni(1)-O(3)	102.00(7)	O(17)-Ni(2)-O(18B)#1	80.62(14)
O(7)#1-Ni(1)-O(10)	104.88(7)	O(18A)-Ni(2)-O(18B)#1	177.27(18)
O(9)-Ni(1)-O(10)	92.04(7)	O(18A)#1-Ni(2)-O(18B)#1	23.39(14)
O(3)-Ni(1)-O(10)	81.14(6)	O(18B)-Ni(2)-O(18B)#1	154.7(2)
O(7)#1-Ni(1)-O(1)	85.44(7)	O(14)#4-Ni(3)-O(14)#5	97.06(10)
O(9)-Ni(1)-O(1)	87.57(7)	O(14)#4-Ni(3)-O(15)	179.09(8)
O(3)-Ni(1)-O(1)	88.84(6)	O(14)#5-Ni(3)-O(15)	83.20(10)
O(10)-Ni(1)-O(1)	169.66(7)	O(14)#4-Ni(3)-O(15)#6	83.20(10)
O(7)#1-Ni(1)-O(3)#1	78.62(7)	O(14)#5-Ni(3)-O(15)#6	179.09(8)
O(9)-Ni(1)-O(3)#1	167.41(7)	O(15)-Ni(3)-O(15)#6	96.55(17)
O(3)-Ni(1)-O(3)#1	85.33(7)	O(14)#4-Ni(3)-O(4)#7	95.19(7)
O(10)-Ni(1)-O(3)#1	78.86(6)	O(14)#5-Ni(3)-O(4)#7	96.08(7)
O(1)-Ni(1)-O(3)#1	102.95(7)	O(15)-Ni(3)-O(4)#7	85.65(8)
O(2)#1-Ni(2)-O(2)	95.51(11)	O(15)#6-Ni(3)-O(4)#7	83.03(8)
O(2)#1-Ni(2)-O(17)#1	84.87(8)	O(14)#4-Ni(3)-O(4)#8	96.08(7)
O(2)-Ni(2)-O(17)#1	176.95(9)	O(14)#5-Ni(3)-O(4)#8	95.19(7)
O(2)#1-Ni(2)-O(17)	176.95(9)	O(15)-Ni(3)-O(4)#8	83.03(8)
O(2)-Ni(2)-O(17)	84.87(8)	O(15)#6-Ni(3)-O(4)#8	85.65(8)
O(17)#1-Ni(2)-O(17)	94.91(13)	O(4)#7-Ni(3)-O(4)#8	162.95(11)
O(2)#1-Ni(2)-O(18A)	80.37(12)	O(5)#7-Ni(4)-O(10)#9	104.74(7)
O(2)-Ni(2)-O(18A)	85.32(12)	O(5)#7-Ni(4)-O(3)#7	92.25(7)
O(17)#1-Ni(2)-O(18A)	97.73(12)	O(10)#9-Ni(4)-O(3)#7	81.70(6)
O(17)-Ni(2)-O(18A)	96.66(12)	O(5)#7-Ni(4)-O(13)#9	88.12(7)
O(2)#1-Ni(2)-O(18A)#1	85.32(12)	O(10)#9-Ni(4)-O(13)#9	89.35(6)
O(2)-Ni(2)-O(18A)#1	80.37(12)	O(3)#7-Ni(4)-O(13)#9	170.84(6)
O(17)#1-Ni(2)-O(18A)#1	96.66(12)	O(5)#7-Ni(4)-O(11)#7	93.06(7)
O(17)-Ni(2)-O(18A)#1	97.73(12)	O(10)#9-Ni(4)-O(11)#7	160.77(7)
O(18A)-Ni(2)-O(18A)#1	158.7(2)	O(3)#7-Ni(4)-O(11)#7	105.19(7)
O(2)#1-Ni(2)-O(18B)	94.61(14)	O(13)#9-Ni(4)-O(11)#7	83.92(7)
O(2)-Ni(2)-O(18B)	102.35(14)	O(5)#7-Ni(4)-O(10)#7	166.53(6)
O(17)#1-Ni(2)-O(18B)	80.62(13)	O(10)#9-Ni(4)-O(10)#7	85.39(7)
O(17)-Ni(2)-O(18B)	82.36(14)	O(3)#7-Ni(4)-O(10)#7	80.29(6)
O(18A)-Ni(2)-O(18B)	23.39(13)	O(13)#9-Ni(4)-O(10)#7	101.04(7)
O(18A)#1-Ni(2)-O(18B)	177.27(18)	O(11)#7-Ni(4)-O(10)#7	78.28(7)
O(2)#1-Ni(2)-O(18B)#1	102.35(14)		

Symmetry transformations used to generate equivalent atoms:

#1 $-x+2, y, -z+1/2$; #4 $-x+3/2, y+1/2, -z+1/2$; #5 $x-1/2, y+1/2, z$; #6 $-x+1, y, -z+1/2$; #7 $-x+3/2, -y+3/2, z-1/2$; #8 $x-1/2, -y+3/2, -z+1$; #9 $x-1/2, -y+3/2, -z$

Table S2 The selected bond lengths (Å) and angles (°) for compound **2**.

Ni(1)-O(4)	2.024(6)	Ni(5)-O(4)	2.072(6)
Ni(1)-O(29)	2.039(6)	Ni(5)-O(3)	2.079(6)
Ni(1)-O(33)	2.066(6)	Ni(5)-O(1)#1	2.097(6)
Ni(1)-O(2)	2.067(6)	Ni(6)-O(6)	2.023(6)
Ni(1)-O(32)	2.101(6)	Ni(6)-O(2)	2.035(6)
Ni(1)-O(3)	2.109(6)	Ni(6)-O(7)#1	2.055(7)
Ni(2)-O(31)	2.011(6)	Ni(6)-O(5)	2.078(6)
Ni(2)-O(41)	2.022(6)	Ni(6)-O(3)	2.082(6)
Ni(2)-O(1)#1	2.032(6)	Ni(6)-O(1)#1	2.089(6)
Ni(2)-O(4)	2.082(6)	Ni(7)-O(28)#3	2.021(8)
Ni(2)-O(30)#1	2.082(6)	Ni(7)-O(22)#3	2.033(6)
Ni(2)-O(2)	2.105(6)	Ni(7)-O(27)	2.048(7)
Ni(3)-O(16)#2	2.047(6)	Ni(7)-O(26)#3	2.070(6)
Ni(3)-O(14)	2.052(6)	Ni(7)-O(39)#3	2.089(6)
Ni(3)-O(17)	2.067(6)	Ni(7)-O(22)	2.109(6)
Ni(3)-O(18)	2.067(6)	Ni(8)-O(19)#2	2.023(7)
Ni(3)-O(37)	2.072(6)	Ni(8)-O(19)#5	2.023(7)
Ni(3)-O(15)	2.081(6)	Ni(8)-O(20)#3	2.058(7)
Ni(4)-O(24)	2.036(7)	Ni(8)-O(20)	2.058(7)
Ni(4)-O(25)	2.049(7)	Ni(8)-O(21)	2.142(7)
Ni(4)-O(26)#3	2.059(6)	Ni(8)-O(21)#3	2.142(7)
Ni(4)-O(23)#3	2.061(6)	Ni(9)-O(10)	2.052(6)
Ni(4)-O(22)	2.071(6)	Ni(9)-O(9)	2.053(6)
Ni(4)-O(26)	2.107(6)	Ni(9)-O(12)#6	2.058(6)
Ni(5)-O(34)#1	2.018(6)	Ni(9)-O(13)	2.069(7)
Ni(5)-O(35)	2.044(6)	Ni(9)-O(11)	2.075(7)
Ni(5)-O(36)	2.050(6)	Ni(9)-O(8)	2.076(7)
O(4)-Ni(1)-O(29)	102.8(3)	O(35)-Ni(5)-O(1)#1	108.3(2)
O(4)-Ni(1)-O(33)	161.2(2)	O(36)-Ni(5)-O(1)#1	168.1(2)
O(29)-Ni(1)-O(33)	94.8(2)	O(4)-Ni(5)-O(1)#1	80.2(2)
O(4)-Ni(1)-O(2)	81.5(2)	O(3)-Ni(5)-O(1)#1	80.9(2)
O(29)-Ni(1)-O(2)	92.4(2)	O(6)-Ni(6)-O(2)	101.1(3)
O(33)-Ni(1)-O(2)	104.7(2)	O(6)-Ni(6)-O(7)#1	96.4(3)
O(4)-Ni(1)-O(32)	89.0(2)	O(2)-Ni(6)-O(7)#1	160.6(2)
O(29)-Ni(1)-O(32)	89.3(2)	O(6)-Ni(6)-O(5)	87.1(3)
O(33)-Ni(1)-O(32)	84.5(2)	O(2)-Ni(6)-O(5)	88.8(2)
O(2)-Ni(1)-O(32)	170.5(2)	O(7)#1-Ni(6)-O(5)	83.8(2)
O(4)-Ni(1)-O(3)	85.0(2)	O(6)-Ni(6)-O(3)	92.2(2)
O(29)-Ni(1)-O(3)	168.1(2)	O(2)-Ni(6)-O(3)	81.1(2)
O(33)-Ni(1)-O(3)	78.8(2)	O(7)#1-Ni(6)-O(3)	106.6(2)
O(2)-Ni(1)-O(3)	79.7(2)	O(5)-Ni(6)-O(3)	169.6(3)
O(32)-Ni(1)-O(3)	99.9(2)	O(6)-Ni(6)-O(1)#1	170.1(3)
O(31)-Ni(2)-O(41)	95.3(3)	O(2)-Ni(6)-O(1)#1	85.1(2)
O(31)-Ni(2)-O(1)#1	101.3(3)	O(7)#1-Ni(6)-O(1)#1	78.7(2)
O(41)-Ni(2)-O(1)#1	162.2(2)	O(5)-Ni(6)-O(1)#1	100.9(2)
O(31)-Ni(2)-O(4)	92.7(2)	O(3)-Ni(6)-O(1)#1	81.0(2)
O(41)-Ni(2)-O(4)	104.2(2)	O(28)#3-Ni(7)-O(22)#3	100.4(3)
O(1)#1-Ni(2)-O(4)	81.5(2)	O(28)#3-Ni(7)-O(27)	96.0(3)
O(31)-Ni(2)-O(30)#1	89.4(2)	O(22)#3-Ni(7)-O(27)	162.9(3)
O(41)-Ni(2)-O(30)#1	85.4(2)	O(28)#3-Ni(7)-O(26)#3	90.3(3)
O(1)#1-Ni(2)-O(30)#1	88.4(2)	O(22)#3-Ni(7)-O(26)#3	81.5(2)

O(4)-Ni(2)-O(30)#1	169.9(2)	O(27)-Ni(7)-O(26)#3	103.5(2)
O(31)-Ni(2)-O(2)	169.2(2)	O(28)#3-Ni(7)-O(39)#3	89.1(3)
O(41)-Ni(2)-O(2)	79.8(2)	O(22)#3-Ni(7)-O(39)#3	88.3(2)
O(1)#1-Ni(2)-O(2)	84.8(2)	O(27)-Ni(7)-O(39)#3	87.0(3)
O(4)-Ni(2)-O(2)	79.3(2)	O(26)#3-Ni(7)-O(39)#3	169.5(3)
O(30)#1-Ni(2)-O(2)	99.8(2)	O(28)#3-Ni(7)-O(22)	166.5(3)
O(16)#2-Ni(3)-O(14)	94.8(3)	O(22)#3-Ni(7)-O(22)	86.5(2)
O(16)#2-Ni(3)-O(17)	86.3(2)	O(27)-Ni(7)-O(22)	78.6(3)
O(14)-Ni(3)-O(17)	87.5(3)	O(26)#3-Ni(7)-O(22)	79.1(2)
O(16)#2-Ni(3)-O(18)	175.5(3)	O(39)#3-Ni(7)-O(22)	102.8(3)
O(14)-Ni(3)-O(18)	87.6(3)	O(28)#3-Ni(7)-Ni(7)#3	145.6(2)
O(17)-Ni(3)-O(18)	97.7(3)	O(22)#3-Ni(7)-Ni(7)#3	45.50(17)
O(16)#2-Ni(3)-O(37)	88.8(3)	O(27)-Ni(7)-Ni(7)#3	117.7(2)
O(14)-Ni(3)-O(37)	173.1(3)	O(26)#3-Ni(7)-Ni(7)#3	88.15(17)
O(17)-Ni(3)-O(37)	86.8(3)	O(39)#3-Ni(7)-Ni(7)#3	86.4(2)
O(18)-Ni(3)-O(37)	89.3(3)	O(22)-Ni(7)-Ni(7)#3	43.43(16)
O(16)#2-Ni(3)-O(15)	88.9(2)	O(19)#2-Ni(8)-O(19)#5	94.7(4)
O(14)-Ni(3)-O(15)	93.2(3)	O(19)#2-Ni(8)-O(20)#3	81.4(3)
O(17)-Ni(3)-O(15)	175.1(3)	O(19)#5-Ni(8)-O(20)#3	175.8(3)
O(18)-Ni(3)-O(15)	87.1(3)	O(19)#2-Ni(8)-O(20)	175.8(3)
O(37)-Ni(3)-O(15)	92.8(3)	O(19)#5-Ni(8)-O(20)	81.4(3)
O(24)-Ni(4)-O(25)	94.2(3)	O(20)#3-Ni(8)-O(20)	102.5(4)
O(24)-Ni(4)-O(26)#3	162.3(2)	O(19)#2-Ni(8)-O(21)	99.3(3)
O(25)-Ni(4)-O(26)#3	102.7(3)	O(19)#5-Ni(8)-O(21)	92.7(3)
O(24)-Ni(4)-O(23)#3	86.9(3)	O(20)#3-Ni(8)-O(21)	86.5(3)
O(25)-Ni(4)-O(23)#3	86.7(2)	O(20)-Ni(8)-O(21)	82.5(3)
O(26)#3-Ni(4)-O(23)#3	88.7(2)	O(19)#2-Ni(8)-O(21)#3	92.7(3)
O(24)-Ni(4)-O(22)	104.8(3)	O(19)#5-Ni(8)-O(21)#3	99.3(3)
O(25)-Ni(4)-O(22)	92.1(2)	O(20)#3-Ni(8)-O(21)#3	82.5(3)
O(26)#3-Ni(4)-O(22)	80.3(2)	O(20)-Ni(8)-O(21)#3	86.5(3)
O(23)#3-Ni(4)-O(22)	168.3(3)	O(21)-Ni(8)-O(21)#3	162.3(4)
O(24)-Ni(4)-O(26)	78.9(2)	O(10)-Ni(9)-O(9)	96.6(2)
O(25)-Ni(4)-O(26)	167.5(2)	O(10)-Ni(9)-O(12)#6	84.8(3)
O(26)#3-Ni(4)-O(26)	85.5(3)	O(9)-Ni(9)-O(12)#6	177.6(3)
O(23)#3-Ni(4)-O(26)	103.2(2)	O(10)-Ni(9)-O(13)	175.8(3)
O(22)-Ni(4)-O(26)	79.8(2)	O(9)-Ni(9)-O(13)	83.0(3)
O(34)#1-Ni(5)-O(35)	96.2(3)	O(12)#6-Ni(9)-O(13)	95.7(3)
O(34)#1-Ni(5)-O(36)	86.9(2)	O(10)-Ni(9)-O(11)	90.8(3)
O(35)-Ni(5)-O(36)	83.5(2)	O(9)-Ni(9)-O(11)	87.7(3)
O(34)#1-Ni(5)-O(4)	168.1(2)	O(12)#6-Ni(9)-O(11)	90.3(3)
O(35)-Ni(5)-O(4)	79.7(2)	O(13)-Ni(9)-O(11)	93.3(3)
O(36)-Ni(5)-O(4)	103.6(2)	O(10)-Ni(9)-O(8)	90.0(3)
O(34)#1-Ni(5)-O(3)	101.6(2)	O(9)-Ni(9)-O(8)	92.6(3)
O(35)-Ni(5)-O(3)	159.9(2)	O(12)#6-Ni(9)-O(8)	89.4(3)
O(36)-Ni(5)-O(3)	88.2(2)	O(13)-Ni(9)-O(8)	85.8(3)
O(4)-Ni(5)-O(3)	84.6(2)	O(11)-Ni(9)-O(8)	179.1(3)
O(34)#1-Ni(5)-O(1)#1	90.6(2)		

Symmetry transformations used to generate equivalent atoms:

#1 $x, -y+3/2, z-1/2$; #2 $x, -y+1/2, z-1/2$; #3 $-x+1/2, -y+1/2, z$; #5 $-x+1/2, y, z-1/2$; #6 $x, -y+3/2, z+1/2$

Table S3 The selected bond lengths (Å) and angles (°) for compound **3**.

Ni(1)-O(16)	2.006(4)	Ni(7)-O(39)	2.123(4)
Ni(1)-O(25)	2.024(4)	Ni(7)-O(31)	2.185(4)
Ni(1)-O(7)	2.030(4)	Ni(7)-O(54)	2.001(4)
Ni(1)-O(24)	2.090(3)	Ni(7)-O(38)	2.009(4)
Ni(1)-O(17)	2.097(3)	Ni(7)-O(32)	2.030(3)
Ni(1)-O(1)	2.099(4)	Ni(7)-O(53)	2.120(4)
Ni(2)-O(6)	1.997(4)	Ni(8)-O(36)	1.986(4)
Ni(2)-O(12)	2.042(3)	Ni(8)-O(46)	2.024(3)
Ni(2)-O(19)	2.067(4)	Ni(8)-O(43)	2.045(4)
Ni(2)-O(17)	2.085(3)	Ni(8)-O(32)	2.087(3)
Ni(2)-O(7)	2.093(4)	Ni(8)-O(39)	2.104(4)
Ni(2)-O(9)	2.121(3)	Ni(8)-O(44)	2.177(4)
Ni(3)-O(11)	2.032(4)	Ni(9)-O(45)	1.977(4)
Ni(3)-O(22)	2.034(4)	Ni(9)-O(41)	1.979(5)
Ni(3)-O(17)	2.053(4)	Ni(9)-O(2)#5	2.010(5)
Ni(3)-O(24)	2.074(3)	Ni(9)-O(28)#5	2.016(4)
Ni(3)-O(21)	2.080(4)	Ni(9)-O(40)	2.315(4)
Ni(3)-O(12)	2.134(4)	Ni(10)-O(47)	2.019(4)
Ni(4)-O(14)	2.000(4)	Ni(10)-O(34)	2.032(4)
Ni(4)-O(24)	2.048(4)	Ni(10)-O(53)	2.047(4)
Ni(4)-O(3)	2.052(4)	Ni(10)-O(46)	2.059(3)
Ni(4)-O(12)	2.056(3)	Ni(10)-O(32)	2.119(3)
Ni(4)-O(7)	2.098(4)	Ni(10)-O(56)	2.182(4)
Ni(4)-O(27)	2.104(4)	Ni(11)-O(49)	2.002(4)
Ni(5)-O(15)#2	2.019(4)	Ni(11)-O(51)	2.017(4)
Ni(5)-O(58)	2.030(4)	Ni(11)-O(39)	2.042(4)
Ni(5)-O(13)#3	2.076(4)	Ni(11)-O(53)	2.110(4)
Ni(5)-O(23)	2.078(4)	Ni(11)-O(46)	2.163(4)
Ni(5)-O(59)	2.087(4)	Ni(11)-O(40)	2.195(4)
Ni(5)-O(18)#2	2.114(4)	Ni(12)-O(42)#7	2.019(4)
Ni(6)-O(20)	1.981(4)	Ni(12)-O(37)#7	2.024(4)
Ni(6)-O(8)	1.985(4)	Ni(12)-O(48)#8	2.064(4)
Ni(6)-O(30)	1.987(4)	Ni(12)-O(52)	2.066(4)
Ni(6)-O(57)	2.032(4)	Ni(12)-O(70)	2.094(4)
Ni(6)-O(56)	2.324(4)	Ni(12)-O(69)	2.109(4)
Ni(6)-O(31)	2.343(4)	O(6)-Ni(2)-O(12)	102.43(15)
O(16)-Ni(1)-O(25)	91.33(15)	O(6)-Ni(2)-O(19)	93.36(15)
O(16)-Ni(1)-O(7)	102.68(14)	O(12)-Ni(2)-O(19)	163.21(14)
O(25)-Ni(1)-O(7)	164.51(14)	O(6)-Ni(2)-O(17)	166.09(14)
O(16)-Ni(1)-O(24)	166.55(14)	O(12)-Ni(2)-O(17)	86.46(14)
O(25)-Ni(1)-O(24)	79.75(14)	O(19)-Ni(2)-O(17)	79.16(14)
O(7)-Ni(1)-O(24)	87.51(14)	O(6)-Ni(2)-O(7)	93.40(14)
O(16)-Ni(1)-O(17)	93.79(14)	O(12)-Ni(2)-O(7)	79.01(14)
O(25)-Ni(1)-O(17)	107.17(14)	O(19)-Ni(2)-O(7)	105.96(14)
O(7)-Ni(1)-O(17)	78.77(14)	O(17)-Ni(2)-O(7)	77.65(13)
O(24)-Ni(1)-O(17)	79.46(13)	O(6)-Ni(2)-O(9)	86.63(14)
O(16)-Ni(1)-O(1)	87.16(14)	O(12)-Ni(2)-O(9)	88.85(14)
O(25)-Ni(1)-O(1)	86.39(15)	O(19)-Ni(2)-O(9)	86.42(14)
O(7)-Ni(1)-O(1)	87.74(14)	O(17)-Ni(2)-O(9)	104.41(14)
O(24)-Ni(1)-O(1)	102.16(14)	O(7)-Ni(2)-O(9)	167.59(14)
O(17)-Ni(1)-O(1)	166.36(14)	O(14)-Ni(4)-O(24)	102.18(14)

O(11)-Ni(3)-O(22)	97.82(14)	O(14)-Ni(4)-O(3)	94.03(15)
O(11)-Ni(3)-O(17)	160.65(14)	O(24)-Ni(4)-O(3)	162.68(14)
O(22)-Ni(3)-O(17)	100.32(14)	O(14)-Ni(4)-O(12)	90.73(14)
O(11)-Ni(3)-O(24)	105.27(14)	O(24)-Ni(4)-O(12)	81.88(14)
O(22)-Ni(3)-O(24)	92.03(14)	O(3)-Ni(4)-O(12)	104.21(14)
O(17)-Ni(3)-O(24)	80.84(14)	O(14)-Ni(4)-O(7)	165.00(15)
O(11)-Ni(3)-O(21)	87.01(14)	O(24)-Ni(4)-O(7)	86.84(14)
O(22)-Ni(3)-O(21)	85.91(14)	O(3)-Ni(4)-O(7)	78.68(14)
O(17)-Ni(3)-O(21)	87.60(14)	O(12)-Ni(4)-O(7)	78.58(14)
O(24)-Ni(3)-O(21)	167.71(14)	O(14)-Ni(4)-O(27)	86.12(14)
O(11)-Ni(3)-O(12)	78.40(14)	O(24)-Ni(4)-O(27)	87.57(14)
O(22)-Ni(3)-O(12)	169.22(14)	O(3)-Ni(4)-O(27)	87.47(14)
O(17)-Ni(3)-O(12)	84.89(13)	O(12)-Ni(4)-O(27)	168.11(14)
O(24)-Ni(3)-O(12)	79.40(13)	O(7)-Ni(4)-O(27)	106.43(14)
O(21)-Ni(3)-O(12)	103.84(14)	O(20)-Ni(6)-O(8)	103.36(15)
O(15)#2-Ni(5)-O(58)	83.58(15)	O(20)-Ni(6)-O(30)	99.45(16)
O(15)#2-Ni(5)-O(13)#3	167.42(15)	O(8)-Ni(6)-O(30)	97.30(15)
O(58)-Ni(5)-O(13)#3	96.37(14)	O(20)-Ni(6)-O(57)	99.15(15)
O(15)#2-Ni(5)-O(23)	107.34(15)	O(8)-Ni(6)-O(57)	99.18(15)
O(58)-Ni(5)-O(23)	90.11(15)	O(30)-Ni(6)-O(57)	151.49(15)
O(13)#3-Ni(5)-O(23)	85.24(14)	O(20)-Ni(6)-O(56)	150.68(14)
O(15)#2-Ni(5)-O(59)	85.19(15)	O(8)-Ni(6)-O(56)	100.74(14)
O(58)-Ni(5)-O(59)	92.91(15)	O(30)-Ni(6)-O(56)	93.77(14)
O(13)#3-Ni(5)-O(59)	82.25(14)	O(57)-Ni(6)-O(56)	60.38(14)
O(23)-Ni(5)-O(59)	167.37(15)	O(20)-Ni(6)-O(31)	93.54(14)
O(15)#2-Ni(5)-O(18)#2	92.99(14)	O(8)-Ni(6)-O(31)	154.38(14)
O(58)-Ni(5)-O(18)#2	176.04(15)	O(30)-Ni(6)-O(31)	60.54(14)
O(13)#3-Ni(5)-O(18)#2	87.41(14)	O(57)-Ni(6)-O(31)	96.92(14)
O(23)-Ni(5)-O(18)#2	89.01(15)	O(56)-Ni(6)-O(31)	70.44(12)
O(59)-Ni(5)-O(18)#2	88.77(15)	O(36)-Ni(8)-O(46)	100.00(14)
O(54)-Ni(7)-O(38)	94.33(15)	O(36)-Ni(8)-O(43)	95.54(15)
O(54)-Ni(7)-O(32)	164.66(14)	O(46)-Ni(8)-O(43)	162.46(15)
O(38)-Ni(7)-O(32)	99.32(14)	O(36)-Ni(8)-O(32)	93.64(14)
O(54)-Ni(7)-O(53)	79.31(14)	O(46)-Ni(8)-O(32)	79.51(14)
O(38)-Ni(7)-O(53)	166.47(14)	O(43)-Ni(8)-O(32)	107.70(14)
O(32)-Ni(7)-O(53)	88.71(14)	O(36)-Ni(8)-O(39)	166.78(14)
O(54)-Ni(7)-O(39)	108.05(15)	O(46)-Ni(8)-O(39)	87.99(14)
O(38)-Ni(7)-O(39)	93.72(14)	O(43)-Ni(8)-O(39)	78.35(14)
O(32)-Ni(7)-O(39)	78.15(13)	O(32)-Ni(8)-O(39)	77.37(13)
O(53)-Ni(7)-O(39)	77.19(13)	O(36)-Ni(8)-O(44)	83.44(14)
O(54)-Ni(7)-O(31)	87.51(14)	O(46)-Ni(8)-O(44)	87.63(14)
O(38)-Ni(7)-O(31)	85.23(14)	O(43)-Ni(8)-O(44)	86.09(14)
O(32)-Ni(7)-O(31)	86.68(13)	O(32)-Ni(8)-O(44)	166.14(13)
O(53)-Ni(7)-O(31)	106.23(13)	O(39)-Ni(8)-O(44)	107.57(14)
O(39)-Ni(7)-O(31)	164.44(14)	O(47)-Ni(10)-O(34)	94.45(15)
O(45)-Ni(9)-O(41)	148.0(2)	O(47)-Ni(10)-O(53)	100.40(14)
O(45)-Ni(9)-O(2)#5	102.35(17)	O(34)-Ni(10)-O(53)	163.91(15)
O(41)-Ni(9)-O(2)#5	94.64(17)	O(47)-Ni(10)-O(46)	91.16(14)
O(45)-Ni(9)-O(28)#5	94.94(16)	O(34)-Ni(10)-O(46)	105.12(14)
O(41)-Ni(9)-O(28)#5	104.98(17)	O(53)-Ni(10)-O(46)	80.88(14)
O(2)#5-Ni(9)-O(28)#5	109.0(2)	O(47)-Ni(10)-O(32)	164.91(14)
O(45)-Ni(9)-O(40)	92.82(17)	O(34)-Ni(10)-O(32)	78.60(14)

O(41)-Ni(9)-O(40)	61.08(16)	O(53)-Ni(10)-O(32)	88.30(14)
O(2)#5-Ni(9)-O(40)	149.96(17)	O(46)-Ni(10)-O(32)	77.97(13)
O(28)#5-Ni(9)-O(40)	95.09(15)	O(47)-Ni(10)-O(56)	84.31(14)
O(49)-Ni(11)-O(51)	97.45(15)	O(34)-Ni(10)-O(56)	88.96(14)
O(49)-Ni(11)-O(39)	161.10(15)	O(53)-Ni(10)-O(56)	86.42(14)
O(51)-Ni(11)-O(39)	100.12(15)	O(46)-Ni(10)-O(56)	165.53(14)
O(49)-Ni(11)-O(53)	106.80(14)	O(32)-Ni(10)-O(56)	108.71(13)
O(51)-Ni(11)-O(53)	93.15(14)	O(69)-Ni(12)-O(37)#7	85.85(15)
O(39)-Ni(11)-O(53)	79.20(14)	O(69)-Ni(12)-O(48)#8	95.31(15)
O(49)-Ni(11)-O(46)	78.23(14)	O(37)#7-Ni(12)-O(48)#8	164.50(15)
O(51)-Ni(11)-O(46)	167.48(14)	O(69)-Ni(12)-O(52)	89.27(15)
O(39)-Ni(11)-O(46)	85.93(14)	O(37)#7-Ni(12)-O(52)	110.23(15)
O(53)-Ni(11)-O(46)	77.11(13)	O(48)#8-Ni(12)-O(52)	85.26(14)
O(49)-Ni(11)-O(40)	88.73(14)	O(69)-Ni(12)-O(70)	95.89(15)
O(51)-Ni(11)-O(40)	84.98(14)	O(37)#7-Ni(12)-O(70)	83.19(15)
O(39)-Ni(11)-O(40)	85.94(14)	O(48)#8-Ni(12)-O(70)	81.31(14)
O(53)-Ni(11)-O(40)	164.46(14)	O(52)-Ni(12)-O(70)	165.99(15)
O(46)-Ni(11)-O(40)	106.50(13)	O(69)-Ni(12)-O(42)#7	174.26(15)
O(52)-Ni(12)-O(42)#7	85.72(14)	O(37)#7-Ni(12)-O(42)#7	93.24(15)
O(70)-Ni(12)-O(42)#7	89.63(15)	O(48)#8-Ni(12)-O(42)#7	87.09(14)

Symmetry transformations used to generate equivalent atoms:

#2 -x+1,-y+2,-z; #3 -x,-y+2,-z; #5 x+1,y,z+1; #7 -x+2,-y+2,-z+1; #8 -x+1,-y+2,-z+1

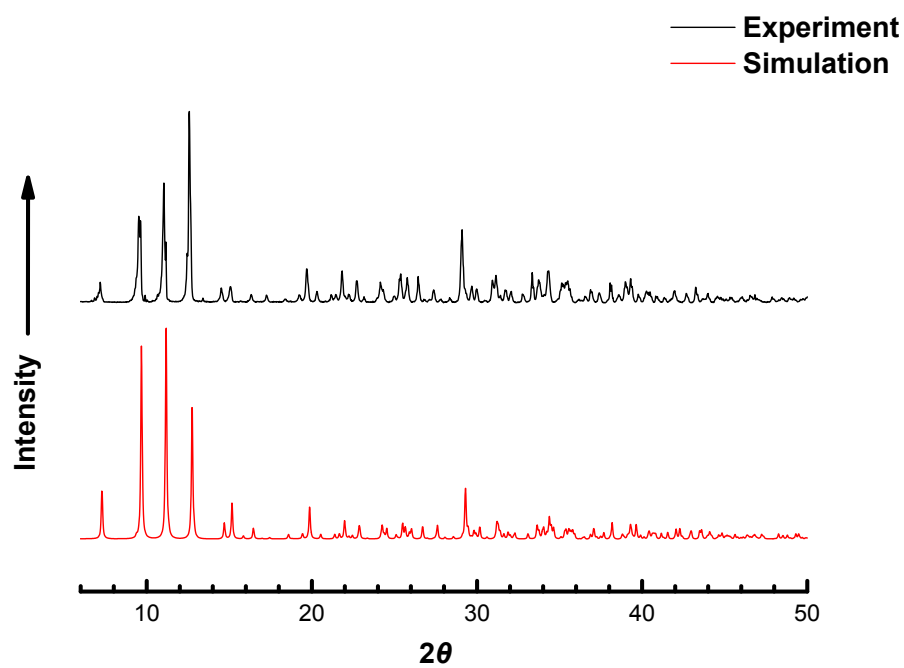


Fig. S1. The powder X-ray diffractions of **1**.

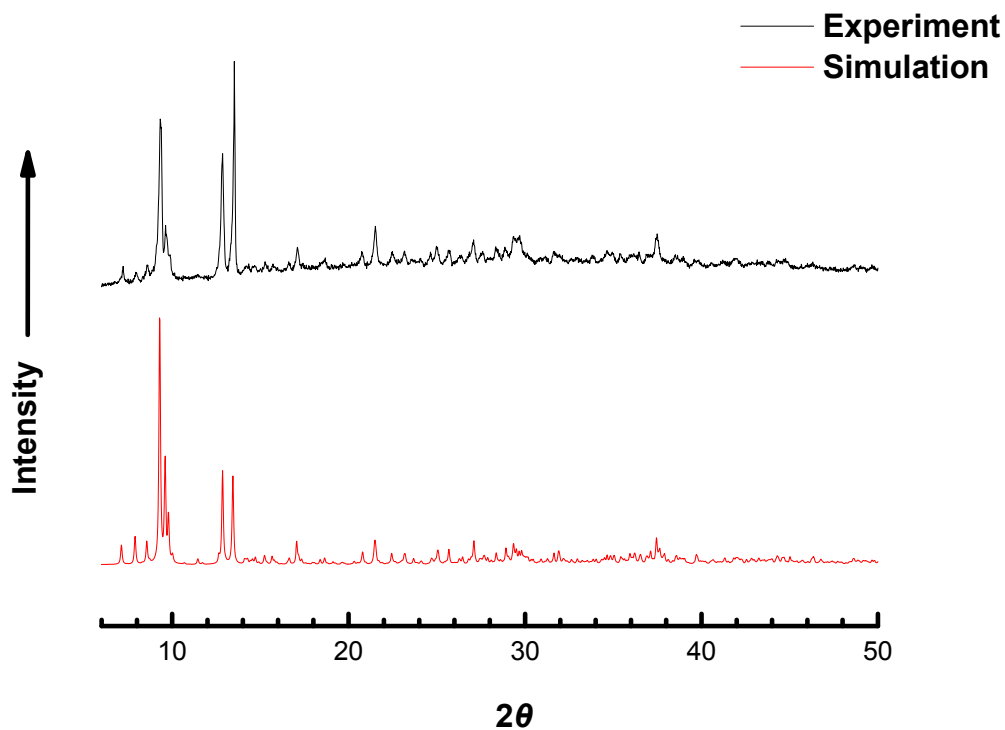


Fig. S2. The powder X-ray diffractions of **2**.

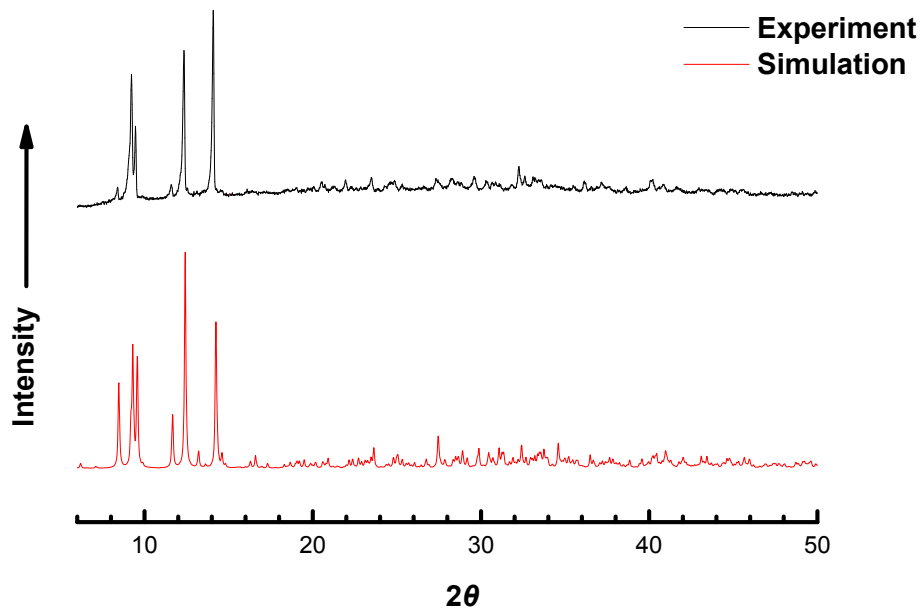
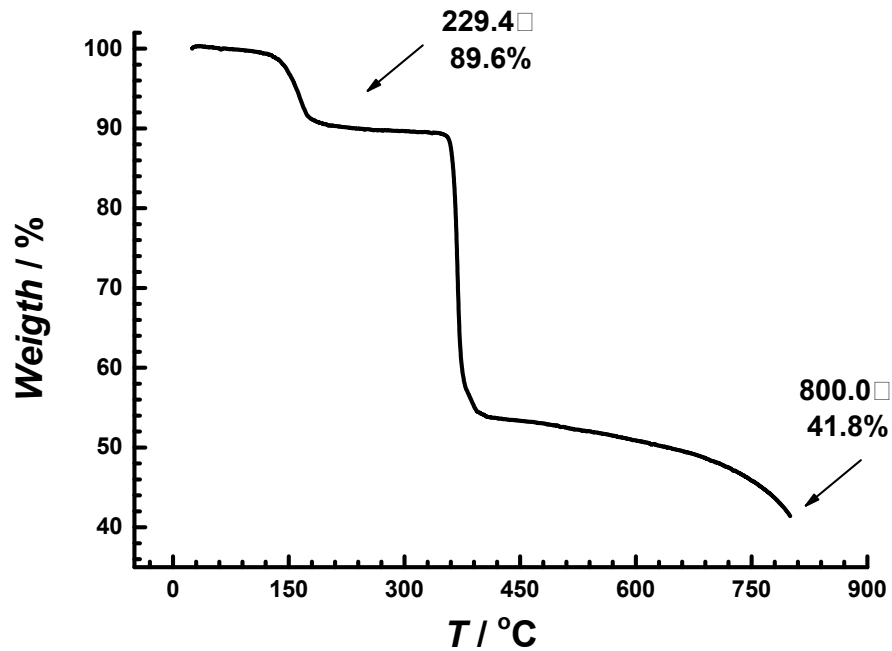


Fig. S3. The powder X-ray diffractions of **3**.



ig. S4. Thermogravimetric curves of **1**.

F

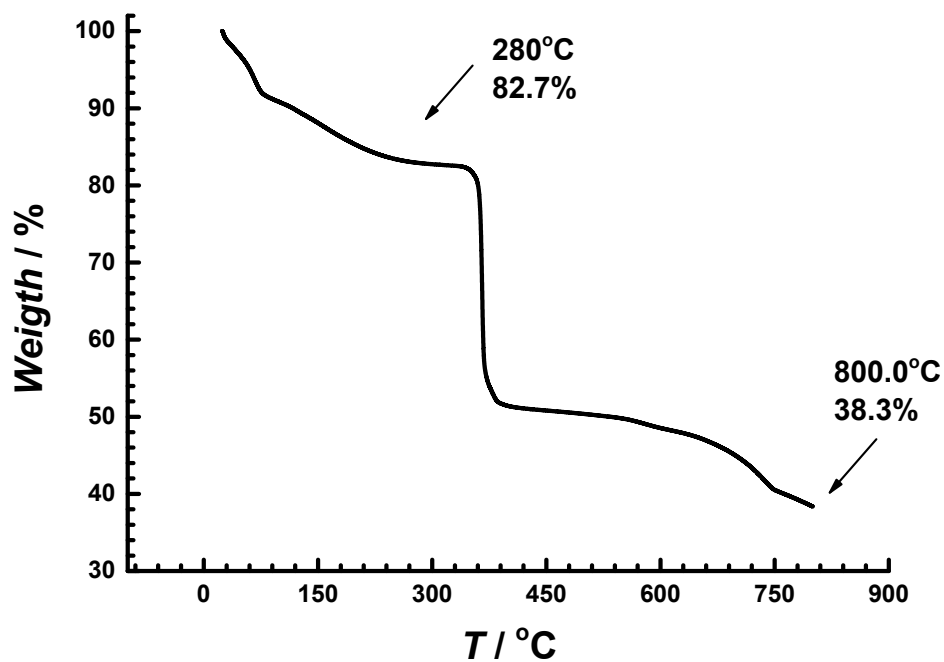


Fig. S5. Thermogravimetric curves of 2.

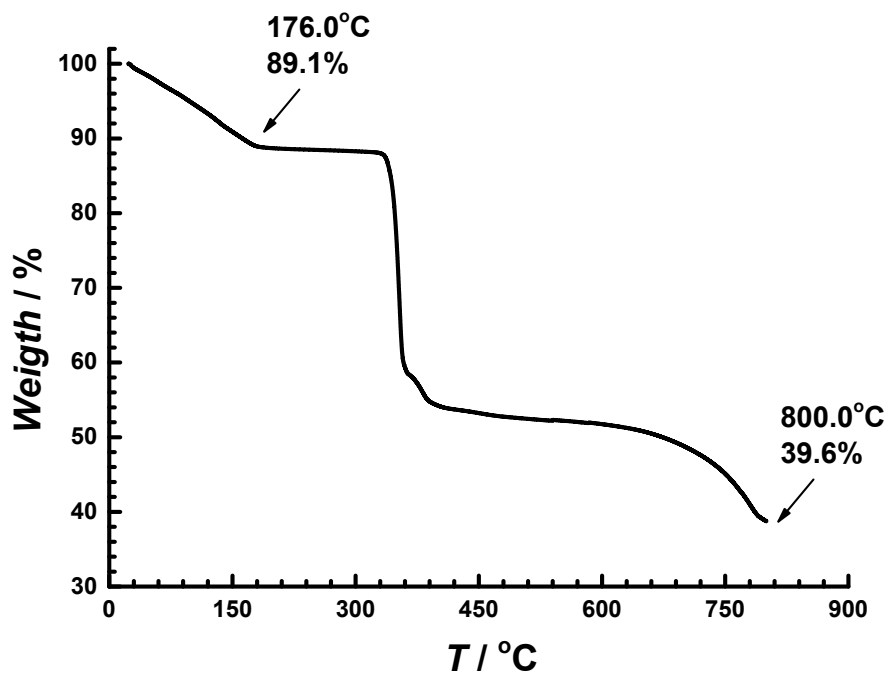


Fig. S6. Thermogravimetric curves of 3.

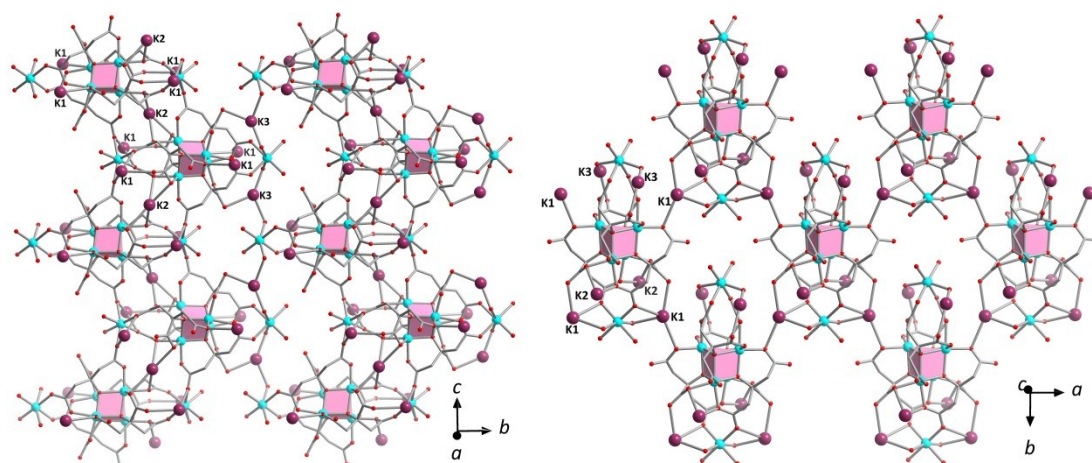


Fig. S7. Polymeric structure of compound **1**. Colour codes: Ni, cyan; K, plum; O, red and C, grey; and the same settings in the following figures.

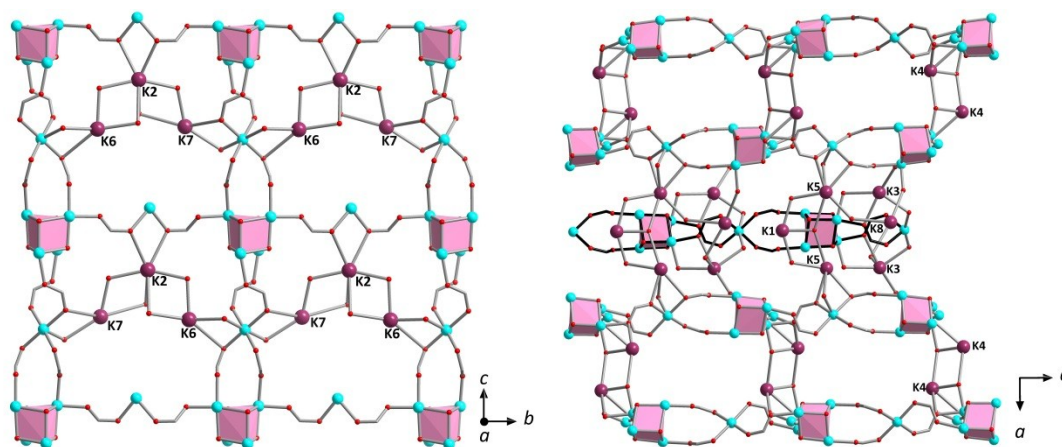


Fig. S8. Polymeric structure of compound **2**.

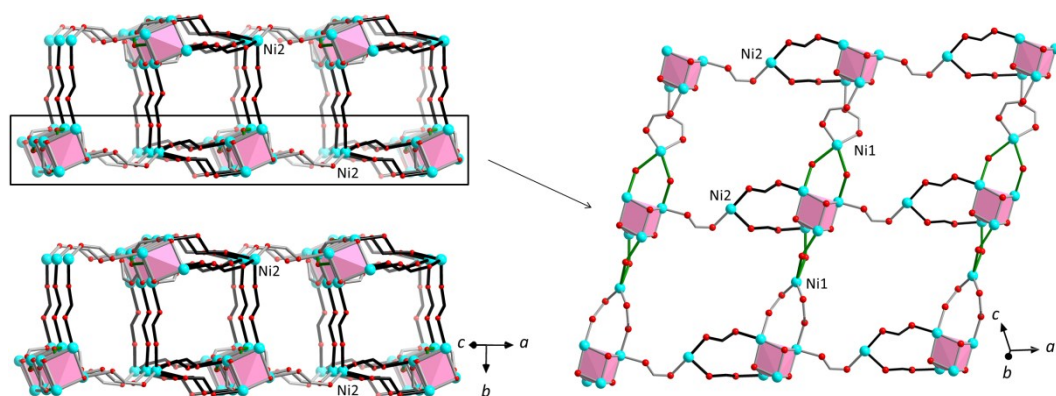


Fig. S9. Connections between Ni(II) ions of compound **3**.

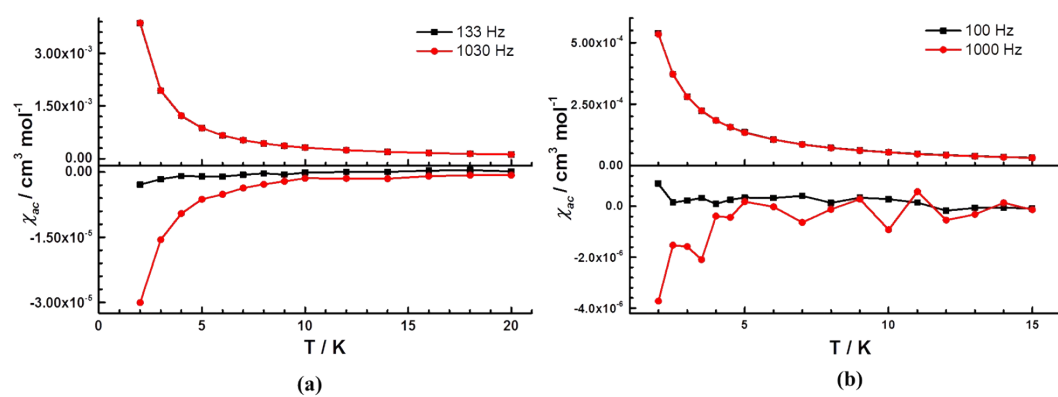


Fig. S10. (a) Temperature dependence of the χ' and χ'' for **1** under 0 field. (b) Temperature dependence of the χ' and χ'' for **2** under 0 field.