Strong Antiferromagnetic Interaction in a 3D Copper-Organic Framework and Spin-glass-like Behaviour in a 1D Nickel Compound

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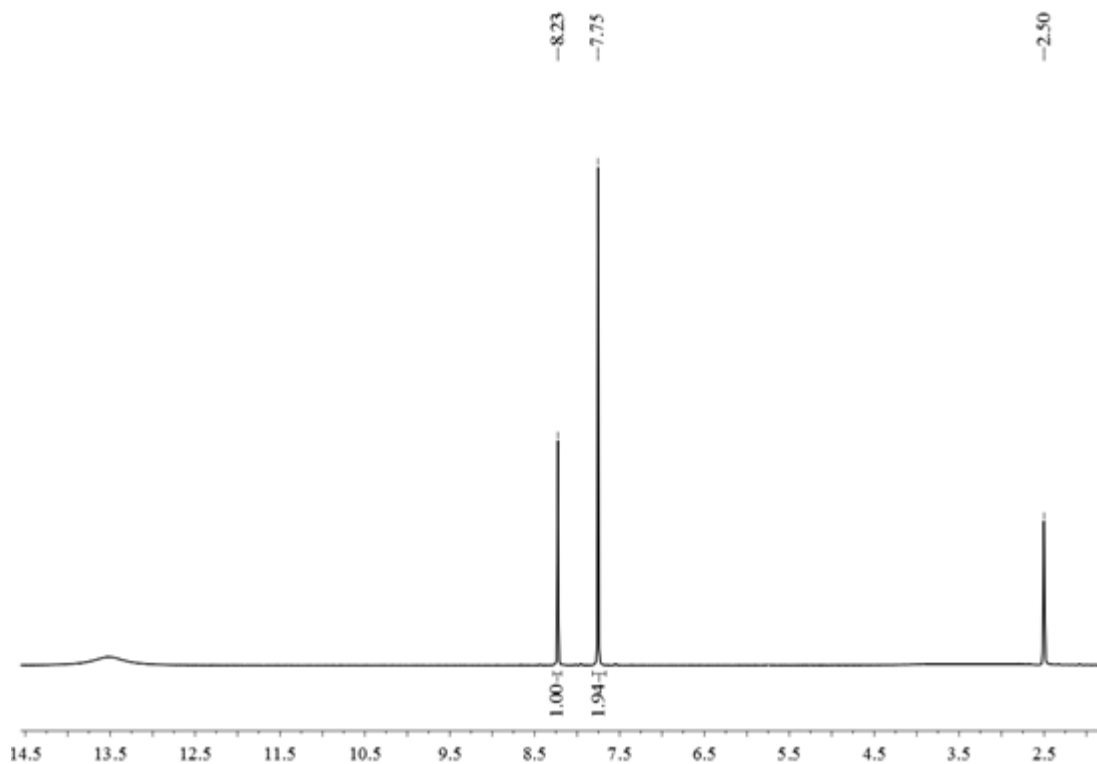
1

NMR spectra of ligand

Fig. S1 ^{1}HNMR spectrum (400 Hz) of 5-azidoisophthalic acid in DMSO-d$_6$.
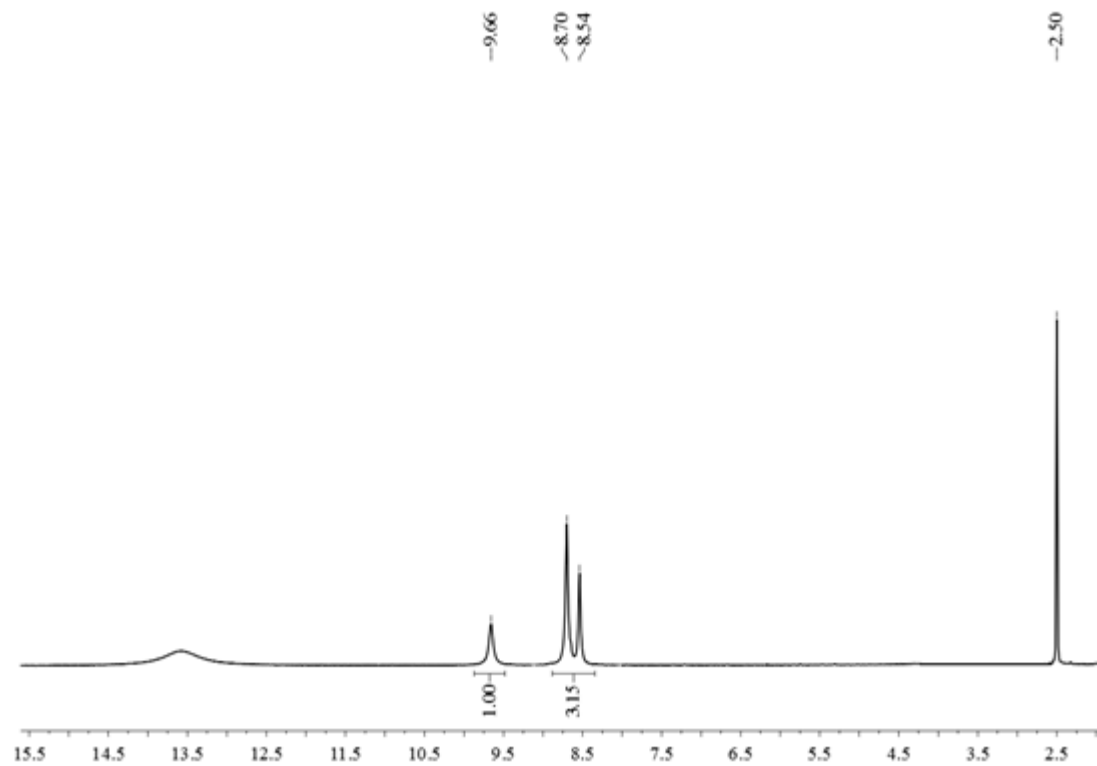

Fig. S2 ^{1}HNMR spectrum (400 Hz) of H$_3$ctia in DMSO-d$_6$

Selected bond distances and angles

Table S1. Selected Bond Distances (Å) and Angles (deg) for **1**

bonds (Å) and angles (deg)			
Cu(1)-O(14)	1.941(4)	O(2)-Cu(1)-N(3)#2	100.85(16)
Cu(1)-O(6)	1.954(4)	O(1)-Cu(2)-O(9)#1	168.88(16)
Cu(1)-O(10)#1	1.955(4)	O(1)-Cu(2)-O(5)	86.32(18)
Cu(1)-O(2)	2.019(4)	O(9)#1-Cu(2)-O(5)	90.41(17)
Cu(1)-N(3)#2	2.147(4)	O(1)-Cu(2)-O(13)	86.09(18)
Cu(2)-O(1)	1.929(4)	O(9)#1-Cu(2)-O(13)	94.95(17)
Cu(2)-O(9)#1	1.933(4)	O(5)-Cu(2)-O(13)	166.58(16)
Cu(2)-O(5)	1.981(4)	O(1)-Cu(2)-N(12)#3	92.66(16)
Cu(2)-O(13)	1.980(4)	O(9)#1-Cu(2)-N(12)#3	98.36(16)
Cu(2)-N(12)#3	2.168(4)	O(5)-Cu(2)-N(12)#3	99.24(17)
Cu(3)-O(12)	1.906(4)	O(13)-Cu(2)-N(12)#3	92.15(17)
Cu(3)-O(16)	1.924(4)	O(12)-Cu(3)-O(16)	177.01(17)
Cu(3)-O(18)	1.980(5)	O(12)-Cu(3)-O(18)	88.00(19)
Cu(3)-N(9)	2.083(5)	O(16)-Cu(3)-O(18)	94.8(2)
Cu(3)-O(17)	2.158(6)	O(12)-Cu(3)-N(9)	90.52(18)
Cu(4)-O(19)	1.910(5)	O(16)-Cu(3)-N(9)	86.99(18)
Cu(4)-O(8)	1.926(4)	O(18)-Cu(3)-N(9)	127.3(3)
Cu(4)-O(4)	1.932(4)	O(12)-Cu(3)-O(17)	90.7(2)
Cu(4)-N(6)#4	2.010(5)	O(16)-Cu(3)-O(17)	89.3(2)
O(14)-Cu(1)-O(6)	168.67(16)	O(18)-Cu(3)-O(17)	108.5(4)
O(14)-Cu(1)-O(10)#1	90.53(18)	N(9)-Cu(3)-O(17)	124.2(3)
O(6)-Cu(1)-O(10)#1	89.51(17)	O(19)-Cu(4)-O(8)	94.5(2)
O(14)-Cu(1)-O(2)	89.64(18)	O(19)-Cu(4)-O(4)	86.4(2)
O(6)-Cu(1)-O(2)	87.80(17)	O(8)-Cu(4)-O(4)	177.1(2)
O(10)#1-Cu(1)-O(2)	167.02(16)	O(19)-Cu(4)-N(6)#4	177.4(2)
O(14)-Cu(1)-N(3)#2	89.63(17)	O(8)-Cu(4)-N(6)#4	88.11(18)
O(6)-Cu(1)-N(3)#2	101.69(17)	O(4)-Cu(4)-N(6)#4	91.02(18)
O(10)#1-Cu(1)-N(3)#2	92.13(16)		

Symmetry transformations used to generate equivalent atoms: #1 x, y-1, z; #2 -x, -y+1, -z; #3 -x+1, -y+2, -z+1; #4 x-1, y, z; #5 x, y+1, z; #6 x+1, y, z; #7 x+1, y+1, z; #8 x-1, y-1, .z.

Table S2. Selected Bond Distances (Å) and Angles (deg) for **2**

bonds (Å) and angles (deg)			
Ni(1)-O(1)#1	2.026(3)	O(7)#1-Ni(1)-O(7)	180.000(1)
Ni(1)-O(1)	2.026(3)	N(3)#2-Ni(2)-N(3)	180.0(2)
Ni(1)-O(8)	2.045(3)	N(3)#2-Ni(2)-O(6)	100.07(13)
Ni(1)-O(8)#1	2.045(3)	N(3)-Ni(2)-O(6)	79.93(13)
Ni(1)-O(7)#1	2.099(4)	N(3)#2-Ni(2)-O(6)#2	79.93(13)
Ni(1)-O(7)	2.099(4)	N(3)-Ni(2)-O(6)#2	100.07(13)
Ni(2)-N(3)#2	2.011(4)	O(6)-Ni(2)-O(6)#2	180.0
Ni(2)-N(3)	2.011(4)	N(3)#2-Ni(2)-O(9)	91.03(14)
Ni(2)-O(6)	2.076(3)	N(3)-Ni(2)-O(9)	88.97(14)
Ni(2)-O(6)#2	2.076(3)	O(6)-Ni(2)-O(9)	89.27(12)
Ni(2)-O(9)	2.117(3)	O(6)#2-Ni(2)-O(9)	90.73(12)
Ni(2)-O(9)#2	2.117(3)	N(3)#2-Ni(2)-O(9)#2	88.97(14)
Ni(3)-O(11)#3	2.016(3)	N(3)-Ni(2)-O(9)#2	91.03(14)
Ni(3)-O(11)	2.016(3)	O(6)-Ni(2)-O(9)#2	90.73(12)
Ni(3)-O(10)	2.028(4)	O(6)#2-Ni(2)-O(9)#2	89.27(12)
Ni(3)-O(10)#3	2.028(4)	O(9)-Ni(2)-O(9)#2	180.00(18)
Ni(3)-O(12)	2.056(4)	O(11)#3-Ni(3)-O(11)	180.0(3)
Ni(3)-O(12)#3	2.056(4)	O(11)#3-Ni(3)-O(10)	87.21(16)
O(1)#1-Ni(1)-O(1)	180.000(1)	O(11)-Ni(3)-O(10)	92.79(16)
O(1)#1-Ni(1)-O(8)	91.35(13)	O(11)#3-Ni(3)-O(10)#3	92.79(16)
O(1)-Ni(1)-O(8)	88.65(13)	O(11)-Ni(3)-O(10)#3	87.21(16)
O(1)#1-Ni(1)-O(8)#1	88.65(13)	O(10)-Ni(3)-O(10)#3	180.000(1)
O(1)-Ni(1)-O(8)#1	91.35(13)	O(11)#3-Ni(3)-O(12)	89.82(15)
O(8)-Ni(1)-O(8)#1	180.000(1)	O(11)-Ni(3)-O(12)	90.18(15)
O(1)#1-Ni(1)-O(7)#1	93.44(14)	O(10)-Ni(3)-O(12)	88.40(17)
O(1)-Ni(1)-O(7)#1	86.56(14)	O(10)#3-Ni(3)-O(12)	91.60(17)
O(8)-Ni(1)-O(7)#1	86.63(17)	O(11)#3-Ni(3)-O(12)#3	90.18(15)
O(8)#1-Ni(1)-O(7)#1	93.37(17)	O(11)-Ni(3)-O(12)#3	89.82(15)
O(1)#1-Ni(1)-O(7)	86.56(14)	O(10)-Ni(3)-O(12)#3	91.60(17)
O(1)-Ni(1)-O(7)	93.44(14)	O(10)#3-Ni(3)-O(12)#3	88.40(17)
O(8)-Ni(1)-O(7)	93.37(17)	O(12)-Ni(3)-O(12)#3	180.00(16)
O(8)#1-Ni(1)-O(7)	86.63(17)		

Symmetry transformations used to generate equivalent atoms: #1 -x+1, -y+2, -z+1; #2 -x+1, -y+1, -z; #3 -x, -y+2, -z+2.
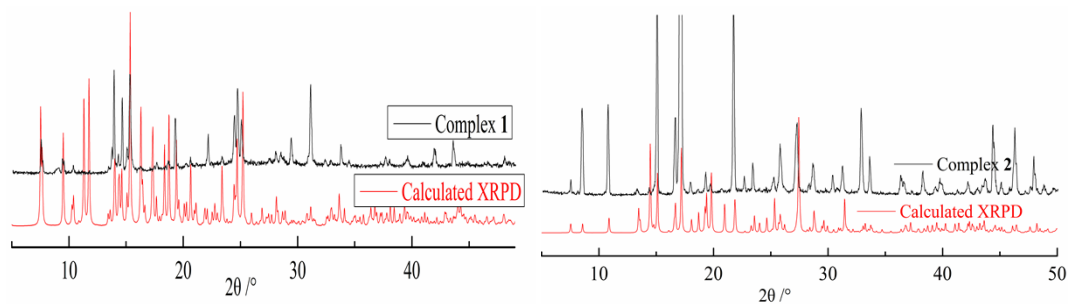
XRD patterns of 1 and 2

Fig. S3 XRD patterns of **1** and **2** compared with a simulated pattern.

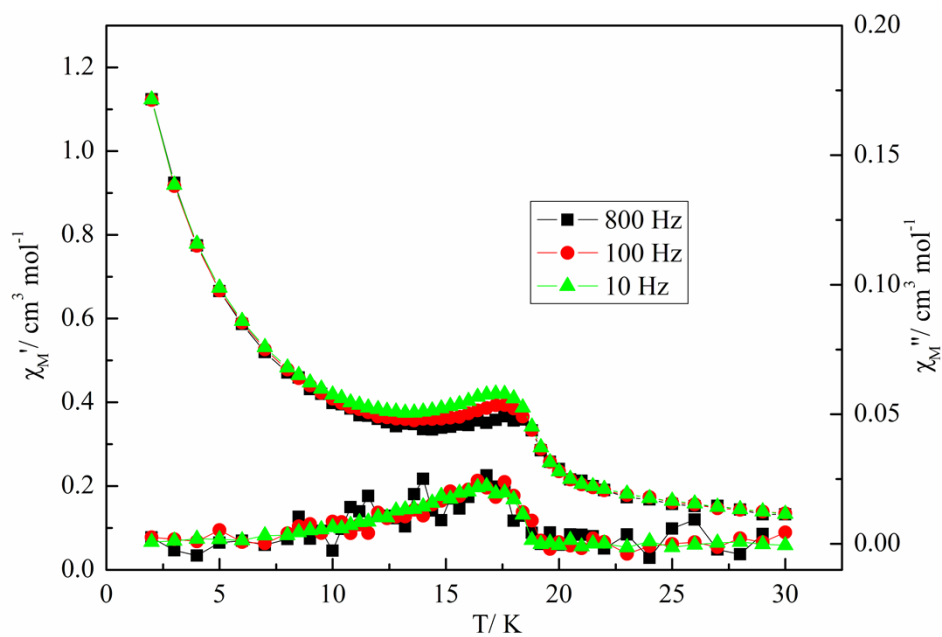# Temperature dependence of ac susceptibility of 2

Fig. S4 Temperature dependence of ac susceptibility at various frequencies of **2.**
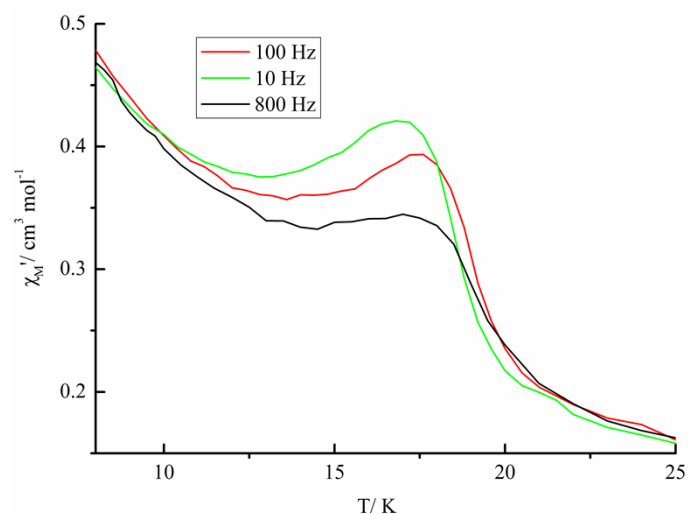
Fig. S4' The χ_M' of ac susceptibility at various frequencies of **2**。

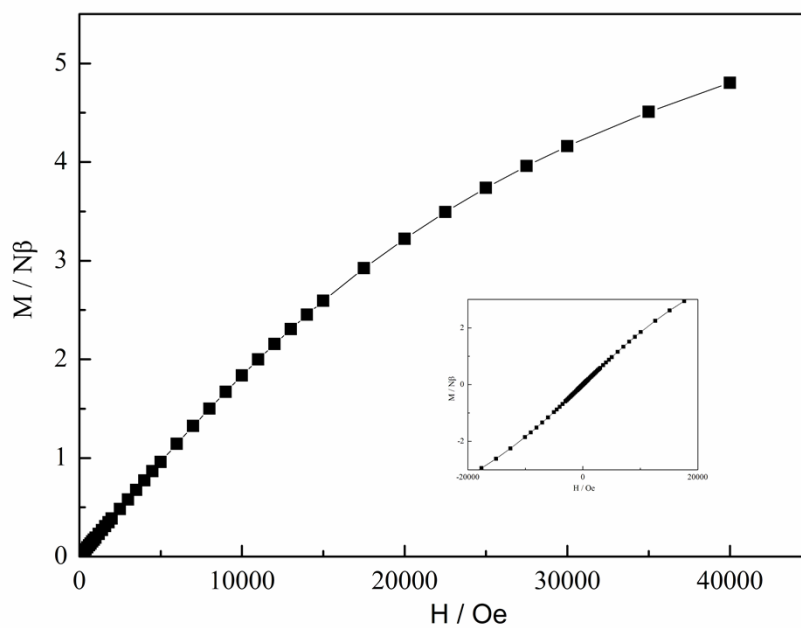# Field dependence of magnetization and the hysteresis loop

Fig. S5. Field dependence of magnetization and the hysteresis loop at 2 K (inset) for **2.**