Electronic Supplementary Information

A Cobalt (II) Chain Based on Pymca Generated in Situ from the Hydrolysis of 2-Cyanopyrimidine: Spin Canting and Magnetic relaxation

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Table S1. Crystallographic data of complex **1**

complex	**1**
Empirical formula	$C_{10}H_{18}Co_2N_4O_{14}S$
Formula weight	568.20
Crystal system	Tetragonal
space group	$P\bar{4}2_1c$
a (Å)	9.5941(13)
b (Å)	9.5941(13)
c (Å)	20.329(3)
α (°)	90
β (°)	90
γ (°)	90
V (Å^3)	1871.2(6)
T (K)	296(2)
Z	4
ρ_{calcd} (g cm^{-3})	2.017
F(000)	1152
□ (Å)	0.71073
R(int)	0.0568
final R_1, □R_2 [$I > 2$□(I)]	0.0568, 0.1387
R_1, □R_2 all data	0.0630, 0.1387
Data / restraints / parameters	2103 / 1 / 143
Largest diff. Peak and hole[e·Å^{-3}]	0.924 and -0.573
goodness of fit, GOF	1.071
CCDC number	1949664

Table S2. Bond lengths [Å] and angles [°] for complex **1**.

Complex **1**			
Co1 -O1W^{i}	2.077(6)	Co1-N1	2.158(6)
Co1-O1W	2.077(6)	Co1-O1^{i}	2.108(5)
Co1-N1^{i}	2.158(6)	Co1-O1	2.108(5)
Co2-O2^{ii}	2.119(6)	Co2-N2^{ii}	2.141(6)
Co2-O2W^{ii}	2.069(8)	Co2-O2	2.119(6)
Co2-O2W	2.069(8)	Co2-N2	2.141(6)
O1-Co1-N1^{i}	86.8(2)	O1-Co1-N1	78.4(2)
O1^{i}-Co1-N1	86.8(2)	O1^{i}-Co1-O1	157.0(3)
O1W^{i}-Co1-O1W	88.1(3)	O1W-Co1-O1^{i}	93.4(2)
O2W^{ii}-Co2-O2W	88.7(5)	O2W-Co2-N2	99.8(2)
O2W-Co2-N2^{ii}	91.0(2)	O2-Co2-N2	78.3(2)
O2W-Co2-O2^{ii}	87.8(3)	O2-Co2-N2^{ii}	91.6(2)
O1W-Co1-N1	174.3(2)	O1W-Co1-O1	103.1(2)
O1W^{i}-Co1-N1	86.3(2)	O1W^{i}-Co1-O1	93.4(2)
O1W-Co1-N1^{i}	86.3(2)	N1-Co1-N1^{i}	99.3(3)
O1W^{i}-Co1-N1^{i}	174.3(2)	O1^{i}-Co1-N1^{i}	78.4(2)
O1W^{i}-Co1-O1^{i}	103.1(2)	O2W^{ii}-Co2-N2	91.0(2)
O2W^{ii}-Co2-O2	87.8(3)	O2W^{ii}-Co2-N2^{ii}	99.8(2)
O2W^{ii}-Co2-O2^{ii}	175.9(3)	O2-Co2-O2^{ii}	95.8(3)
O2W-Co2-O2	175.9(3)		

Symmetry transformations used to generate equivalent atoms: i: -x+1, -y, z, ii: -x+1, -y+1, z.

Table S3.

Hydrogen bonds for complex **1**. Bond lengths [Å] and angles [°].

D—H···A	d(D—H)	d(H···A)	d(D···A)	<(D—H···A)
O(1W)—H(1A) ···O(4)	0.85	1.91	2.735(9)	164
O(1W)—H(1B) ···O(2)	0.85	1.96	2.793(8)	168
O(2W)—H(2A) ···O(3)	0.87	2.06	2.913(12)	168
O(2W)—H(2B) ···O(3W)	0.74	2.34	2.961(14)	143
O(3W)—H(10A)···O(4)	0.85	2.16	2.847(16)	137
O(3W)—H(10B) ···O(3)	0.85	2.40	2.683(12)	100

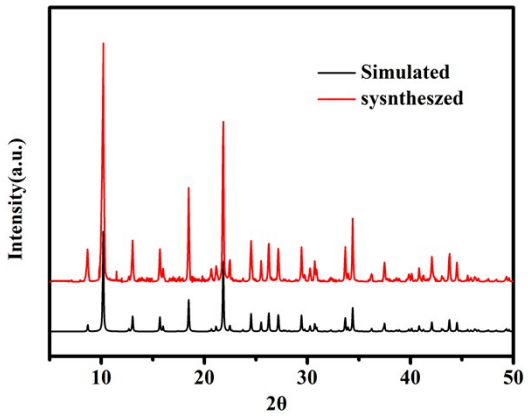

Fig. S1 The PXRD pattern of **1.**

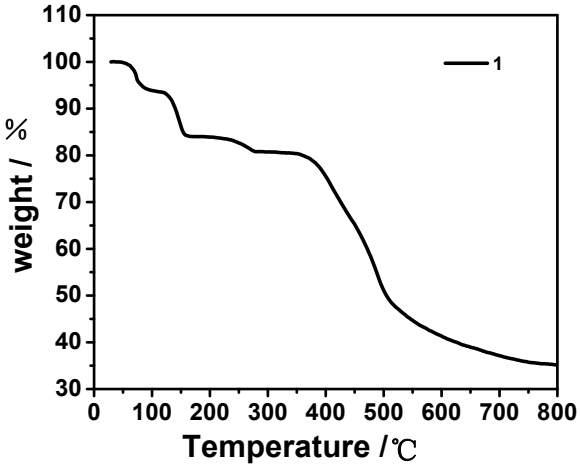

Fig. S2 The TG curves of complex **1.**

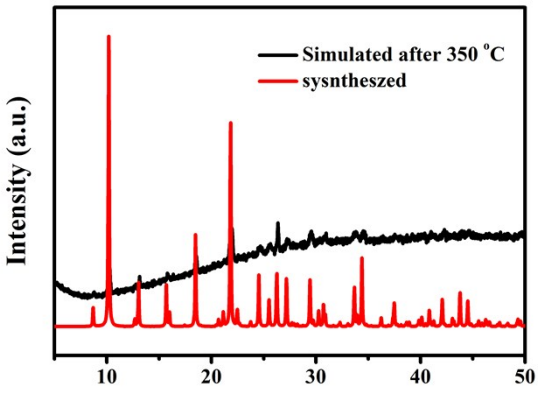

Fig. S3 The PXRD pattern of the **1** heated to 350 °C.

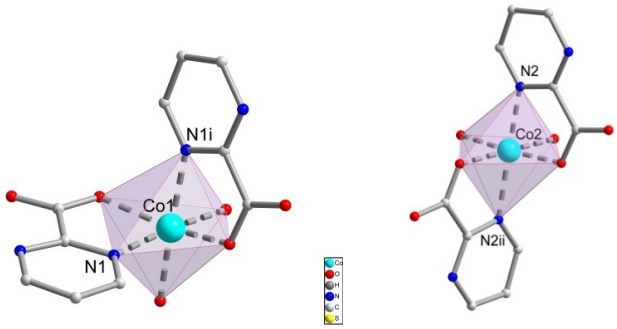

Fig. S4 The distorted octahedral coordination geometry of Co1 and Co2 (N1-Co1-N1i = 99.3(3)° (left), N2-Co2-N2i = 164.9(3)°) (right).

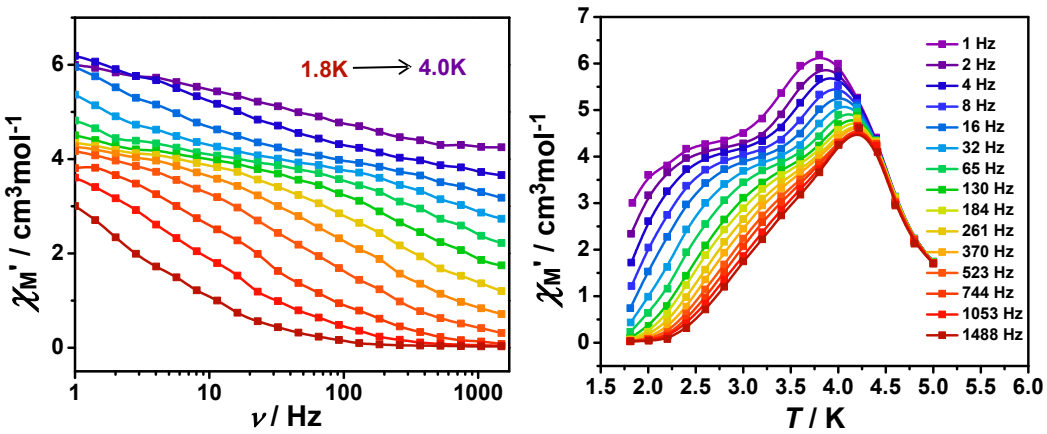

Fig. S5 Frequency dependence of in-phase (left) and temperature dependence of in-phase (right) components of the ac susceptibility for the complex **1** in zero applied static field with a 5 Oe oscillating field at a frequency of 1–1488 Hz.

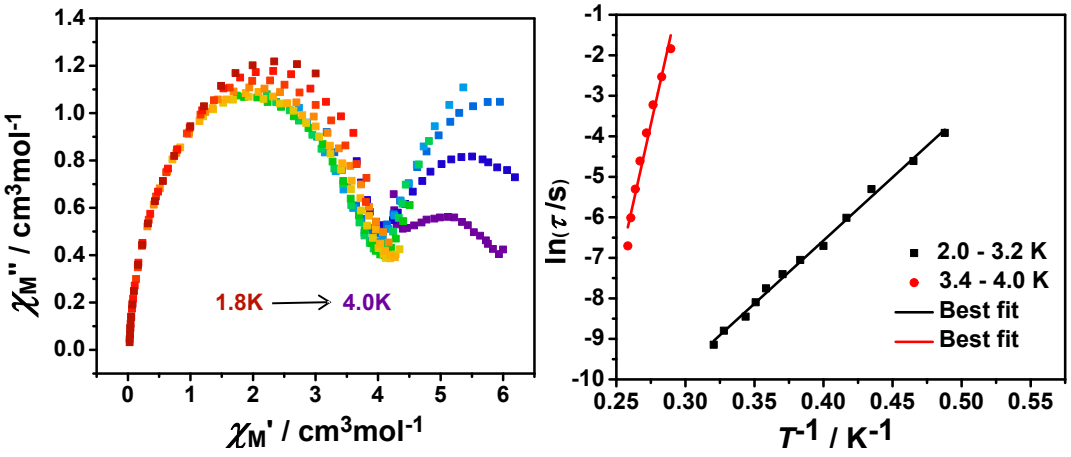

Fig. S6 (a) A plot of cole-cole curve, (b) the plot of lnτ vs. 1/T.

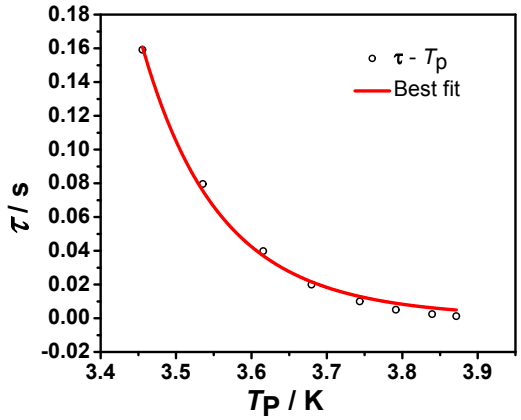

Fig. S7 The plot of τ vs. Tp for **1** was fitted by the conventional critical scaling law of the spin dynamics as described by $\tau = \tau_0 [(T_P - T_f)/T_f]^{-zv}$.