Supplementary Information

Solvents and auxiliary ligands co-regulate three antiferromagnetic Co(II) MOFs based on a semi-rigid carboxylate ligand

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Table S1 Crystal data and structural parameters of CPs 1-3.

Complex	**1**	**2**	**3**
Empirical formula	$C_{66}H_{52}Co_3N_6O_{18}$	$C_{36}H_{50}O_{16}N_5Co_2$	$C_{78}H_{62}Co_3N_8O_{14}$
Formula weight	1393.95	926.67	1512.15
Crystal System	triclinic	Triclinic	Monoclinic
Space Group	*P*$\bar{1}$	*P*$\bar{1}$	*P2/c*
a/Å	11.3568(12)	10.3914(7)	12.856(3)
b/Å	12.0897(13)	12.7364(9)	11.081(3)
c/Å	12.9531(13)	13.0153(9)	27.351(6)
α/°	95.237(2)	107.453(7)	90.00
β/°	97.074(2)	105.230(8)	114.913(9)
γ/°	107.616(2)	97.342(8)	90.00
V/Å^3	1666.6(3)	1545.10(18)	3533.8(15)
Z	1	2	2
ρ_c/g cm^{-3}	1.389	1.404	1.421
μ/mm^{-1}	0.811	1.127	0.768
F(000)	715	666	1558
Crystal size/mm	0.32 0.25 0.20	0.30 0.24 0.21	0.30 0.27 0.22
Reflections	8559 / 5900	7913 / 5406	21559 / 8638
R_{int}	0.0258	0.0314	0.0947
T_{man}/T_{min}	0.8545 / 0.7813	0.7977 / 0.7285	0.8491 / 0.8022
Data/parameters	4044 / 334	5406 / 370	8638 / 465
S	1.007	1.045	1.022
$R_1{}^a$, $wR_2{}^b[I>2\sigma(I)]$	0.0484, 0.1017	0.0681, 0.1921	0.0732, 0.1760
R_1, wR_2 *(all data)*	0.0627, 0.1084	0.0877, 0.2082	0.1692, 0.2451
$\Delta\rho_{max}/\Delta\rho_{min}$/eA^{-3}	0.772 / -0.410	2.853 / -0.538	1.237 / -0.587

$R_1 = \sum||F_o|-|F_c||/\sum|F_o|$, $wR_2 = \{\sum[w(F_o^2-F_c^2)^2]/\sum(F_o^2)^2\}^{1/2}$

Table S2 Selected bond lengths (Å) and bond angles (°) for CPs 1-3.

Complex 1			
Co(1)-O(6)#1	2.061(2)	Co(2)-N(1)	2.150(3)
Co(1)-O(6)	2.061(2)	Co(2)-O(3)#2	2.158(2)
Co(1)-O(10)	2.127(2)	Co(2)-O(9)	2.180(2)

Co(1)-O(10)#1	2.127(2)	Co(2)-O(4)#2	2.185(2)
Co(1)-N(3)	2.221(3)	Co(2)-C(33)#2	2.494(3)
Co(1)-N(3)#1	2.221(3)	O(3)-Co(2)#2	2.158(2)
Co(2)-O(1)	2.044(2)	O(4)-Co(2)#2	2.185(2)
Co(2)-N(2)	2.087(3)		
O(6)#1-Co(1)-O(6)	180.000(1)	O(1)-Co(2)-N(2)	103.83(10)
O(6)#1-Co(1)-O(10)	89.38(9)	O(1)-Co(2)-N(1)	88.25(9)
O(6)-Co(1)-O(10)	90.62(9)	N(2)-Co(2)-N(1)	87.46(11)
O(6)#1-Co(1)-O(10)#1	90.62(9)	O(1)-Co(2)-O(3)#2	97.80(9)
O(6)-Co(1)-O(10)#1	89.38(9)	N(2)-Co(2)-O(3)#2	158.38(10)
O(10)-Co(1)-O(10)#1	180	N(1)-Co(2)-O(3)#2	93.32(10)
O(6)#1-Co(1)-N(3)	87.30(10)	O(1)-Co(2)-O(9)	92.46(9)
O(6)-Co(1)-N(3)	92.70(10)	N(2)-Co(2)-O(9)	87.38(10)
O(10)-Co(1)-N(3)	86.77(9)	N(1)-Co(2)-O(9)	174.81(10)
O(10)#1-Co(1)-N(3)	93.23(9)	O(3)#2-Co(2)-O(9)	91.67(9)
O(6)#1-Co(1)-N(3)#1	92.70(10)	O(1)-Co(2)-O(4)#2	158.20(9)
O(6)-Co(1)-N(3)#1	87.30(10)	N(2)-Co(2)-O(4)#2	97.87(10)
O(10)-Co(1)-N(3)#1	93.23(9)	N(1)-Co(2)-O(4)#2	94.79(10)
O(10)#1-Co(1)-N(3)#1	86.77(9)	O(3)#2-Co(2)-O(4)#2	60.51(8)
N(3)-Co(1)-N(3)#1	180.00(10)	O(9)-Co(2)-O(4)#2	86.44(9)
O(3)#2-Co(2)-C(33)#2	30.31(9)	O(1)-Co(2)-C(33)#2	127.86(10)
O(9)-Co(2)-C(33)#2	86.72(10)	N(2)-Co(2)-C(33)#2	128.15(11)
O(4)#2-Co(2)-C(33)#2	30.35(9)	N(1)-Co(2)-C(33)#2	96.90(10)
Complex 2			
Co(1)-O(15)#1	2.067(4)	Co(2)-N(1)#4	2.136(4)
Co(1)-O(6)#2	2.087(4)	Co(2)-O(28)	2.153(6)
Co(1)-O(15)	2.092(4)	Co(2)-O(17)#1	2.255(4
Co(1)-O(1)	2.102(4)	O(7)-Co(2)#5	2.067(4)
Co(1)-N(2)	2.102(5)	O(15)-Co(2)#1	2.062(4)
Co(1)-O(17)	2.252(4)	O(15)-Co(1)#1	2.067(4)
Co(2)-O(2)	2.046(4)	O(17)-Co(2)#1	2.255(4)
Co(2)-O(15)#1	2.062(4)	N(1)-Co(2)#4	2.136(4)
Co(2)-O(7)#3	2.067(4)		
O(15)#1-Co(1)-O(6)#2	173.68(14)	N(2)-Co(1)-O(17)	86.43(16)
O(15)#1-Co(1)-O(15)	80.92(15)	O(2)-Co(2)-O(15)#1	103.04(15)
O(6)#2-Co(1)-O(15)	93.29(14)	O(2)-Co(2)-O(7)#3	162.59(17)
O(15)#1-Co(1)-O(1)	97.45(15)	O(15)#1-Co(2)-O(7)#3	92.65(16)
O(6)#2-Co(1)-O(1)	80.84(15)	O(2)-Co(2)-N(1)#4	93.82(17)

O(15)-Co(1)-O(1)	98.53(15)	O(15)#1-Co(2)-N(1)#4	90.21(16)
O(15)#1-Co(1)-N(2)	95.44(17)	O(7)#3-Co(2)-N(1)#4	93.62(17)
O(6)#2-Co(1)-N(2)	90.79(17)	O(2)-Co(2)-O(28)	81.9(2)
O(15)-Co(1)-N(2)	165.68(17)	O(15)#1-Co(2)-O(28)	171.7(2)
O(1)-Co(1)-N(2)	95.67(17)	O(7)#3-Co(2)-O(28)	81.7(2)
O(15)#1-Co(1)-O(17)	99.01(14)	N(1)#4-Co(2)-O(28)	96.1(2)
O(6)#2-Co(1)-O(17)	82.40(15)	O(2)-Co(2)-O(17)#1	82.54(15)
O(15)-Co(1)-O(17)	80.52(13)	O(15)#1-Co(2)-O(17)#1	81.10(14)
O(1)-Co(1)-O(17)	163.13(15)	O(7)#3-Co(2)-O(17)#1	92.64(15)
O(28)-Co(2)-O(17)#1	93.1(2)	N(1)#4-Co(2)-O(17)#1	169.52(16)
Complex 3			
Co(1)-O(2)	2.136(4)	Co(2)-O(6)	2.068(4)
Co(1)-O(2)#1	2.136(4)	Co(2)-O(4)	2.085(4)
Co(1)-O(1)	2.141(4)	Co(2)-N(3)	2.100(4)
Co(1)-O(1)#1	2.141(4)	Co(2)-O(5)#2	2.155(4)
Co(1)-N(4)#1	2.176(5)	Co(2)-N(1)	2.207(4)
Co(1)-N(4)	2.176(5)	Co(2)-N(2)#3	2.214(4)
Co(1)-C(1)	2.460(6)	N(2)-Co(2)#6	2.214(4)
Co(1)-C(1)#1	2.460(6)	O(5)-Co(2)#2	2.155(4)
O(2)-Co(1)-O(2)#1	115.2(2)	O(2)#1-Co(1)-C(1)#1	30.56(17)
O(2)-Co(1)-O(1)	62.15(16)	O(1)-Co(1)-C(1)#1	152.1(2)
O(2)#1-Co(1)-O(1)	177.34(16)	O(1)#1-Co(1)-C(1)#1	31.64(17)
O(2)-Co(1)-O(1)#1	177.34(16)	N(4)#1-Co(1)-C(1)#1	90.86(19)
O(2)#1-Co(1)-O(1)#1	62.15(16)	N(4)-Co(1)-C(1)#1	89.34(19)
O(1)-Co(1)-O(1)#1	120.5(2)	C(1)-Co(1)-C(1)#1	176.3(3)
O(2)-Co(1)-N(4)#1	92.45(17)	O(6)-Co(2)-O(4)	86.32(15)
O(2)#1-Co(1)-N(4)#1	90.97(18)	O(6)-Co(2)-N(3)	94.70(17)
O(1)-Co(1)-N(4)#1	88.63(18)	O(4)-Co(2)-N(3)	178.12(17)
O(1)#1-Co(1)-N(4)#1	88.20(17)	O(6)-Co(2)-O(5)#2	170.73(15)
O(2)-Co(1)-N(4)	90.97(18)	O(4)-Co(2)-O(5)#2	89.54(14)
O(2)#1-Co(1)-N(4)	92.45(17)	N(3)-Co(2)-O(5)#2	89.23(17)
O(1)-Co(1)-N(4)	88.20(17)	O(6)-Co(2)-N(1)	92.52(16)
O(1)#1-Co(1)-N(4)	88.63(18)	O(4)-Co(2)-N(1)	93.64(14)
N(4)#1-Co(1)-N(4)	173.6(3)	N(3)-Co(2)-N(1)	87.90(16)
O(2)-Co(1)-C(1)	30.56(17)	O(5)#2-Co(2)-N(1)	96.01(16)
O(2)#1-Co(1)-C(1)	145.7(2)	O(6)-Co(2)-N(2)#3	87.86(16)
O(1)-Co(1)-C(1)	31.64(17)	O(4)-Co(2)-N(2)#3	89.65(16)
O(1)#1-Co(1)-C(1)	152.1(2)	N(3)-Co(2)-N(2)#3	88.81(17)

N(4)#1-Co(1)-C(1)	89.34(19)	O(5)#2-Co(2)-N(2)#3	83.83(16)
N(4)-Co(1)-C(1)	90.86(19)	N(1)-Co(2)-N(2)#3	176.71(17)
O(2)-Co(1)-C(1)#1	145.7(2)		

Symmetry transformations used to generate equivalent atoms:

Compound 1: #1 = -x + 1, -y, -z + 2; #2 = -x, -y + 1, -z + 1.

Compound 2: #1 = -x, -y, -z + 1; #2 = -x, -y, -z; #3 = x, y, z + 1; #4 = -x + 1, -y + 1, -z + 1; #5 = x, y, z – 1.

Compound 3: #1 = -x + 2, y, -z + 1/2; #2 = -x, -y + 1, -z; #3 = x, -y + 1, z - 1/2; #4 = -x + 1, -y, -z; #5 = -x + 2, -y + 2,-z; #6 = x, -y + 1, z + 1/2.

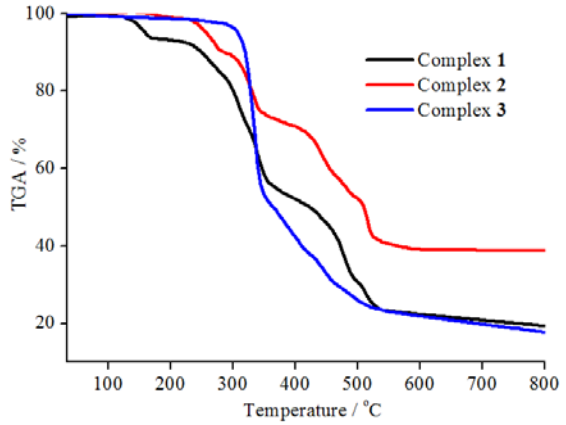

Figure S1. The TG analyses of the compound **1** − **3**.

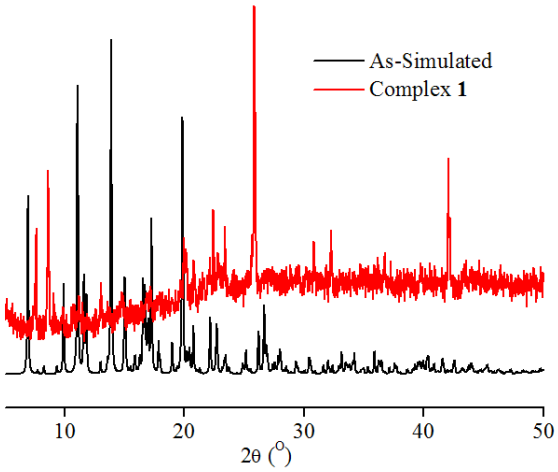

Figure S2. The Powder X-ray diffraction (PXRD) patterns of **1.**

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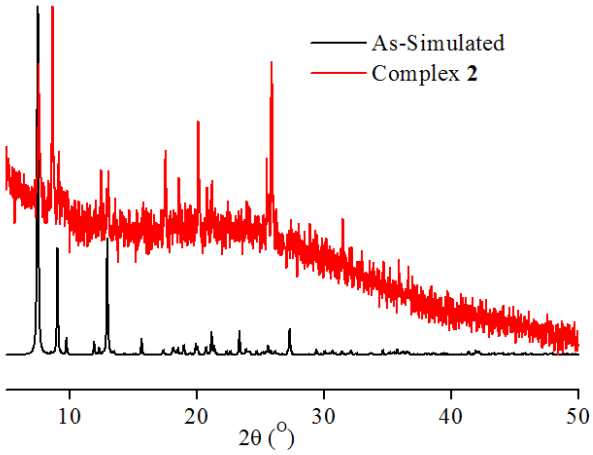

Figure S3. The Powder X-ray diffraction (PXRD) patterns of **2.**

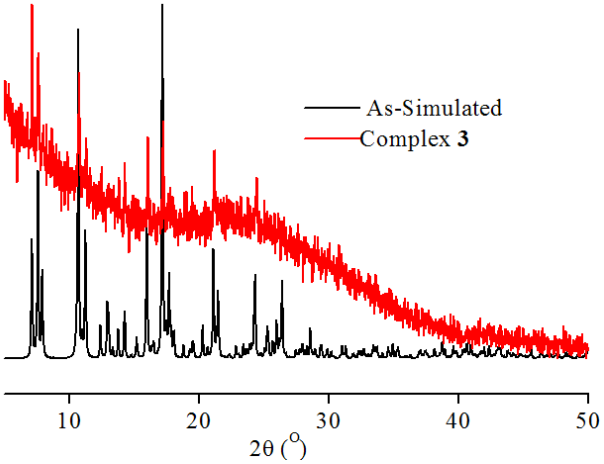

Figure S4. The Powder X-ray diffraction (PXRD) patterns of **3.**

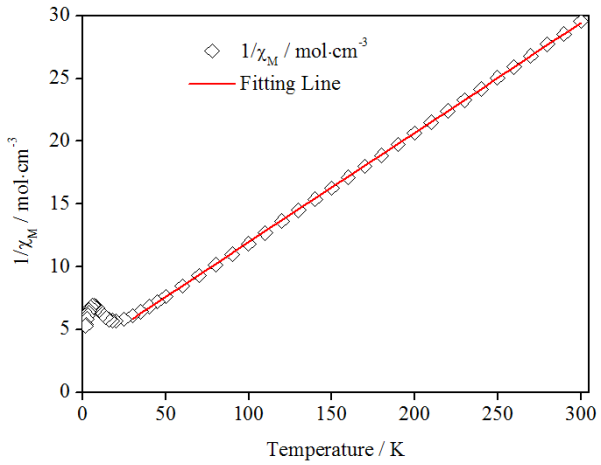

Figure S5. Temperature dependence of χ_M^{-1} for **1** (open squares and red line represent experimental data and fits). C = 11.99 cm^3 K mol^{-1}.

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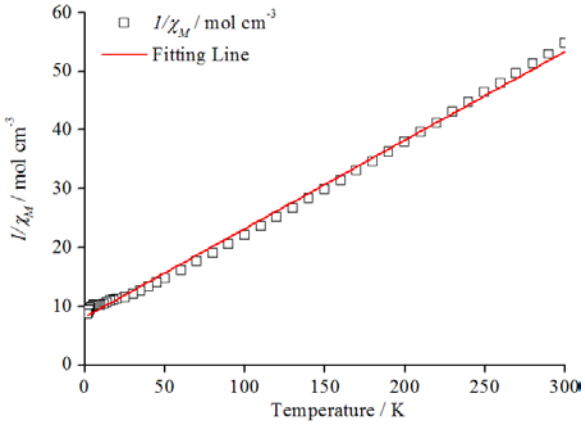

Figure S6. Temperature dependence of χ_M^{-1} for **2** (open squares and red line represent experimental data and fits). C = 6.63 cm^3 K mol^{-1}.

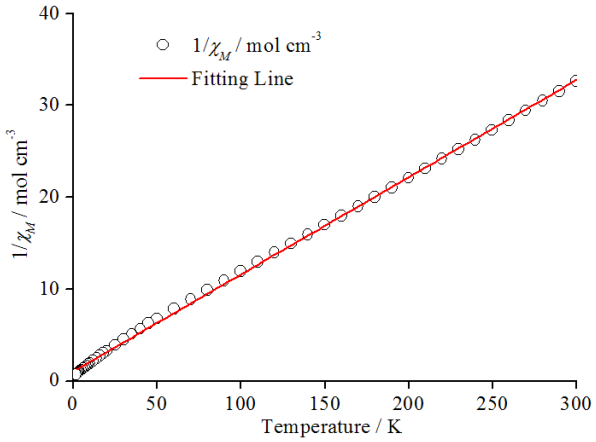

Figure S7. Temperature dependence of χ_M^{-1} for **3** (open circles and red line represent experimental data and fits). C = 9.45 cm^3 K mol^{-1}.