Supporting Information

One-Pot Synthesis, Crystal Structures and Thermal Properties of Two Three-Dimensional Cobalt(II) Complexes

Bo Tao, Wen Lei, Feiran Cheng, and Hua Xia*

Faculty of Material Science and Chemistry Engineering, China University of Geosciences, Wuhan 430074, China
**E-mail: caihua223@gmail.com*
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Table S1. Crystal data for complexes **1** and **2**

Empirical formula	$C_{10}H_{12}N_2O_6SCo$	$C_{30}H_{34}N_4O_{16}Co_2$
Formula weight	347.21	824.47
Temperature (K)	293(2)	273(2)
Wavelength (Å)	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic
Space group	*C*2/c	*P*2(1)/n
a (Å)	15.505(4)	12.2701(16)
b (Å)	12.780(3)	7.5808(10)
c (Å)	6.6075(18)	17.899(2)
α (°)	90	90
β (°)	102.514(4)	100.044(2)
γ (°)	90	90
Volume ($Å^3$)	1278.2(6)	1639.4(4)
Z	4	2
Density (calculated)(Mg/m^3)	1.804	1.670
Absorption coefficient (mm^{-1})	1.533	1.096
F(000)	708	848
Crystal size (mm^3)	0.16 × 0.12 × 0.10	0.32 × 0.26 × 0.25
Theta range for data collection (°)	2.09 to 28.53	2.31 to 26.00
Index ranges	$-20 \le h \le 20, -17 \le k \le 16, -8 \le l \le 8$	$-15 \le h \le 12, -9 \le k \le 9, -22 \le l \le 22$
Reflections collected	7657	8761
Independent reflections	1616 [R(int) = 0.0729]	3211 [R(int) = 0.0179]
Absorption correction	None	Semi-empirical from equivalents
Max. and min. transmission	0.8618 and 0.7915	0.7712 and 0.7205
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	1616 / 2 / 99	3211 / 1 / 258
Goodness-of-fit on F^2	1.063	1.044
Final R indices [I>2sigma(I)]	R1 = 0.0280, wR2 = 0.0743	R1 = 0.0237, wR2 = 0.0594
R indices (all data)	R1 = 0.0284, wR2 = 0.0745	R1 = 0.0276, wR2 = 0.0616
Largest diff. peak and hole (e $Å^{-3}$)	0.618 and -0.663	0.278 and -0.204

Table S2. Selected bond lengths (Å) and angles (°) for complexes **1** and **2**

Compound **1**			
Bond lengths			
Co(1)-O(3)#1	2.0923(12)	Co(1)-O(1)	2.1692(12)
Co(1)-O(3)	2.0924(12)	O(1)-S(1)	1.4748(11)
Co(1)-N(1)	2.0980(13)	O(2)-S(1)	1.4757(12)
Co(1)-N(1)#1	2.0980(13)	S(1)-O(1)#2	1.4748(11)
Co(1)-O(1)#1	2.1691(13)	S(1)-O(2)#2	1.4757(12)
Bond angles			
O(3)#1-Co(1)-O(3)	92.94(7)	O(3)-Co(1)-O(1)	87.49(4)
O(3)#1-Co(1)-N(1)	94.81(5)	N(1)-Co(1)-O(1)	88.23(4)
O(3)-Co(1)-N(1)	171.35(5)	N(1)#1-Co(1)-O(1)	90.89(5)
O(3)#1-Co(1)-N(1)#1	171.36(5)	O(1)#1-Co(1)-O(1)	178.87(5)
O(3)-Co(1)-N(1)#1	94.81(5)	S(1)-O(1)-Co(1)	137.72(7)
N(1)-Co(1)-N(1)#1	77.74(7)	O(1)-S(1)-O(1)#2	108.89(9)
O(3)#1-Co(1)-O(1)#1	87.50(4)	O(1)-S(1)-O(2)#2	110.14(8)
O(3)-Co(1)-O(1)#1	93.28(5)	O(1)#2-S(1)-O(2)#2	108.89(7)
N(1)-Co(1)-O(1)#1	90.89(5)	O(1)-S(1)-O(2)	108.89(7)
N(1)#1-Co(1)-O(1)#1	88.23(4)	O(1)#2-S(1)-O(2)	110.14(8)
O(3)#1-Co(1)-O(1)	93.28(5)	O(2)#2-S(1)-O(2)	109.87(10)
Compound **2**			
Bond lengths			
Co(1)-O(1)	2.0626(14)	Co(1)-O(3)	2.1223(12)
Co(1)-N(1)	2.1144(14)	Co(1)-O(4)	2.1360(11)
Co(1)-O(2)	2.1176(12)	Co(1)-N(2)	2.1367(14)
Bond angles			
O(1)-Co(1)-N(1)	95.57(6)	O(2)-Co(1)-O(4)	92.96(5)
O(1)-Co(1)-O(2)	175.49(5)	O(3)-Co(1)-O(4)	93.54(5)
N(1)-Co(1)-O(2)	88.81(5)	O(1)-Co(1)-N(2)	86.40(5)
O(1)-Co(1)-O(3)	90.90(5)	N(1)-Co(1)-N(2)	76.88(5)
N(1)-Co(1)-O(3)	170.39(5)	O(2)-Co(1)-N(2)	93.55(5)
O(2)-Co(1)-O(3)	84.62(5)	O(3)-Co(1)-N(2)	96.50(5)
O(1)-Co(1)-O(4)	87.86(5)	O(4)-Co(1)-N(2)	168.50(5)
N(1)-Co(1)-O(4)	93.80(5)		

Symmetry transformations used to generate equivalent atoms: for complex **1**: #1 −x, y, −z+3/2; #2 −x, y, −z+5/2.

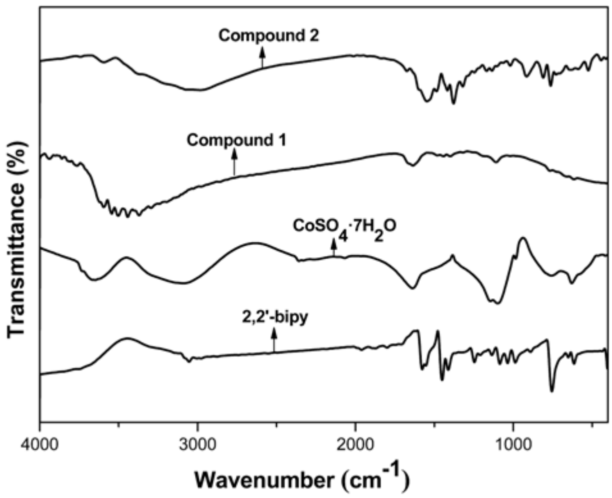

Figure S1. The IR spectra of compounds **1**, **2**, $CoSO_4 \cdot 7H_2O$ and 2,2'-bipy.