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Diaquabis(pyridine-2-sulfonato- κ^2N,O)-cobalt(II)Zong-Sheng Li^a and Seik Weng Ng^{b,c*}

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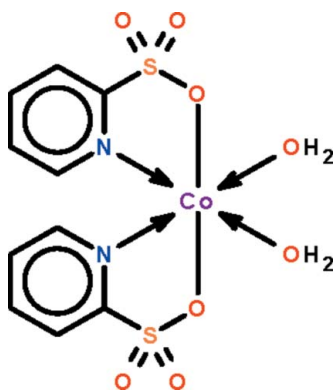
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(C-C) = 0.003$ Å; R factor = 0.024; wR factor = 0.067; data-to-parameter ratio = 15.0.

The title complex, $[Co(C_5H_4NO_3S)_2(H_2O)_2]$, lies on a twofold rotation axis that relates the two water molecules and the two pyridine-2-sulfonate ions. The Co^{II} atom exists in a slightly distorted octahedral environment. The N-donor atoms are *cis* to each other. In the crystal, adjacent molecules are linked by $O-H \cdots O$ hydrogen bonds into a layer motif extending along (001).

Related literature

For the isotypic manganese(II), zinc and cadmium analogs, see: Lobana *et al.* (2004); Xiao (2007); Xiao & Liu (2004).



Experimental

Crystal data

 $[Co(C_5H_4NO_3S)_2(H_2O)_2]$ $M_r = 411.29$

Monoclinic, $C2/c$
 $a = 13.7009$ (9) Å
 $b = 7.1127$ (5) Å
 $c = 16.0180$ (11) Å
 $\beta = 106.734$ (1)°
 $V = 1494.86$ (18) Å³

$Z = 4$
Mo $K\alpha$ radiation
 $\mu = 1.47$ mm⁻¹
 $T = 296$ K
 $0.25 \times 0.20 \times 0.15$ mm

Data collection

Bruker SMART APEX
diffractometer
Absorption correction: multi-scan
(*SADABS*; Sheldrick, 1996)
 $T_{min} = 0.710$, $T_{max} = 0.810$

4331 measured reflections
1695 independent reflections
1590 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.016$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.024$
 $wR(F^2) = 0.067$
 $S = 1.03$
1695 reflections
113 parameters
3 restraints

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{max} = 0.35$ e Å⁻³
 $\Delta\rho_{min} = -0.34$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$O1w-H11 \cdots O2^i$	0.83 (1)	1.90 (1)	2.735 (2)	177 (3)
$O1w-H12 \cdots O3^{ii}$	0.83 (1)	1.88 (1)	2.703 (2)	172 (3)

Symmetry codes: (i) $-x + 1, y + 1, -z + \frac{3}{2}$; (ii) $x + \frac{1}{2}, y + \frac{1}{2}, z$.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINTE* (Bruker, 2007); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *pubCIF* (Westrip, 2010).

We thank Beijing Normal University and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZS2164).

References

- Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Bruker (2007). *APEX2* and *SAINTE*. Bruker AXS Inc., Madison, Wisconsin, USA.
Lobana, T. S., Kinoshita, I., Kimura, K., Nishioka, T., Shiomi, D. & Isobe, K. (2004). *Eur. J. Inorg. Chem.* pp. 356–367.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.
Xiao, Z.-J. (2007). *J. Huaquiao Univ. (Nat. Sci.)*, **28**, 170–173.
Xiao, Z.-J. & Liu, S.-X. (2004). *Chin. J. Struct. Chem.* **23**, 798–802.

supplementary materials

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Diaquabis(pyridine-2-sulfonato- κ^2N,O)cobalt(II)

Z.-S. Li and S. W. Ng

Comment

Diaquabis(pyridine-2-sulfonato)cobalt(II) (Scheme I) is isostructural with the manganese, zinc (Lobana *et al.*, 2004; Xiao & Liu, 2004) and cadmium (Xiao, 2007) analogs. The molecule lies on a twofold rotation axis that relates the two water molecules and the two pyridine-2-sulfonate ions and the Co^{II} atom exist in an slightly distorted octahedral environment. The N donor atoms are *cis* to each other (Fig. 1). Adjacent molecules are linked by water O—H \cdots O_{sulfonate} hydrogen bonds (Table 1) into a layer motif extending along (0 0 1) (Fig. 2).

Experimental

Pyridine-2-sulfonic acid (0.4 mmol, 0.0641 g) was dissolved in 0.1 M sodium hydroxide (4 ml); cobalt(II) chloride hexahydrate (0.2 mmol, 0.0476 g) and 4,4'-bipyridine-*N,N'*-dioxide (0.2 mmol, 0.0446 g) were added to the solution. The clear solution was allowed to evaporate at ambient conditions, affording red block-shaped crystals after one week, in 40% yield.

Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.93 Å) and were included in the refinement in the riding model approximation, with $U_{\text{iso}}(\text{H})$ set to $1.2U_{\text{eq}}(\text{C})$. The water H-atoms were located in a difference Fourier map and was refined with distance restraints of O—H = 0.83 ± 0.01 and H \cdots H = 1.37 ± 0.01 Å. Their isotropic displacement parameters were refined.

Figures

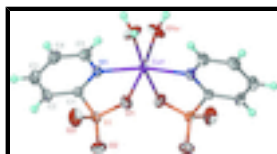


Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of $[\text{Co}(\text{H}_2\text{O})_2(\text{C}_5\text{H}_4\text{NO}_3\text{S})_2]$ at the 50% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius. The unlabeled atoms are related to the labeled ones by twofold rotational symmetry (symmetry code $-x + 1, y, -z + 3/2$).

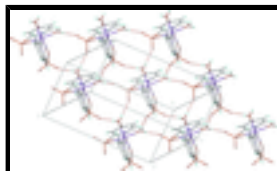


Fig. 2. The hydrogen-bonded layer structure.

supplementary materials

Diaquabis(pyridine-2-sulfonato- κ^2N,O)cobalt(II)

Crystal data

[Co(C ₅ H ₄ NO ₃ S) ₂ (H ₂ O) ₂]	$F(000) = 836$
$M_r = 411.29$	$D_x = 1.827 \text{ Mg m}^{-3}$
Monoclinic, $C2/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Hall symbol: $-C 2yc$	Cell parameters from 3169 reflections
$a = 13.7009 (9) \text{ \AA}$	$\theta = 3.1\text{--}27.6^\circ$
$b = 7.1127 (5) \text{ \AA}$	$\mu = 1.47 \text{ mm}^{-1}$
$c = 16.0180 (11) \text{ \AA}$	$T = 296 \text{ K}$
$\beta = 106.734 (1)^\circ$	Prism, yellow
$V = 1494.86 (18) \text{ \AA}^3$	$0.25 \times 0.20 \times 0.15 \text{ mm}$
$Z = 4$	

Data collection

Bruker SMART APEX diffractometer	1695 independent reflections
Radiation source: fine-focus sealed tube graphite	1590 reflections with $I > 2\sigma(I)$
ω scans	$R_{\text{int}} = 0.016$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$\theta_{\text{max}} = 27.5^\circ$, $\theta_{\text{min}} = 2.7^\circ$
$T_{\text{min}} = 0.710$, $T_{\text{max}} = 0.810$	$h = -17 \rightarrow 11$
4331 measured reflections	$k = -9 \rightarrow 9$
	$l = -13 \rightarrow 20$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.024$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.067$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.03$	$w = 1/[\sigma^2(F_o^2) + (0.0362P)^2 + 1.5779P]$
1695 reflections	where $P = (F_o^2 + 2F_c^2)/3$
113 parameters	$(\Delta/\sigma)_{\text{max}} = 0.001$
3 restraints	$\Delta\rho_{\text{max}} = 0.35 \text{ e \AA}^{-3}$
	$\Delta\rho_{\text{min}} = -0.34 \text{ e \AA}^{-3}$

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.5000	0.69090 (4)	0.7500	0.02354 (11)

S1	0.33529 (3)	0.39913 (6)	0.66183 (2)	0.02716 (12)
O1	0.38590 (11)	0.4900 (2)	0.74481 (7)	0.0379 (3)
O2	0.37681 (13)	0.21672 (19)	0.65256 (10)	0.0474 (4)
O3	0.22560 (11)	0.3995 (3)	0.64164 (10)	0.0504 (4)
O1W	0.59993 (12)	0.9037 (2)	0.74438 (11)	0.0467 (4)
H11	0.6059 (18)	1.001 (2)	0.7743 (14)	0.055 (7)*
H12	0.6431 (16)	0.902 (3)	0.7169 (15)	0.060 (8)*
N1	0.44352 (10)	0.6597 (2)	0.61055 (9)	0.0255 (3)
C1	0.36597 (12)	0.5407 (2)	0.58114 (9)	0.0237 (3)
C2	0.31435 (14)	0.5162 (3)	0.49417 (11)	0.0339 (4)
H2	0.2589	0.4352	0.4769	0.041*
C3	0.34772 (16)	0.6160 (3)	0.43366 (11)	0.0398 (4)
H3	0.3149	0.6034	0.3744	0.048*
C4	0.43020 (15)	0.7344 (3)	0.46221 (12)	0.0384 (4)
H4	0.4551	0.7998	0.4224	0.046*
C5	0.47534 (14)	0.7548 (3)	0.55036 (12)	0.0344 (4)
H5	0.5299	0.8374	0.5691	0.041*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.02474 (17)	0.02440 (17)	0.02083 (16)	0.000	0.00555 (11)	0.000
S1	0.0294 (2)	0.0293 (2)	0.0240 (2)	-0.00801 (15)	0.00954 (16)	0.00137 (14)
O1	0.0506 (8)	0.0432 (7)	0.0214 (5)	-0.0189 (6)	0.0125 (5)	-0.0010 (5)
O2	0.0711 (11)	0.0282 (7)	0.0465 (8)	0.0001 (7)	0.0228 (7)	0.0063 (6)
O3	0.0306 (7)	0.0803 (12)	0.0433 (8)	-0.0137 (7)	0.0154 (6)	0.0049 (7)
O1W	0.0496 (9)	0.0409 (8)	0.0625 (9)	-0.0211 (7)	0.0367 (8)	-0.0254 (8)
N1	0.0268 (7)	0.0279 (7)	0.0218 (6)	-0.0028 (5)	0.0068 (5)	0.0036 (5)
C1	0.0262 (7)	0.0245 (7)	0.0216 (7)	0.0003 (6)	0.0088 (6)	0.0013 (6)
C2	0.0371 (9)	0.0382 (9)	0.0246 (8)	-0.0068 (8)	0.0060 (7)	-0.0044 (7)
C3	0.0489 (11)	0.0493 (11)	0.0201 (7)	0.0006 (9)	0.0081 (7)	0.0008 (7)
C4	0.0488 (11)	0.0418 (10)	0.0291 (8)	0.0012 (9)	0.0184 (8)	0.0109 (8)
C5	0.0364 (9)	0.0346 (9)	0.0335 (9)	-0.0077 (8)	0.0119 (7)	0.0070 (7)

Geometric parameters (\AA , $^\circ$)

Co1—O1W	2.0601 (14)	O1W—H12	0.832 (9)
Co1—O1W ⁱ	2.0601 (13)	N1—C1	1.334 (2)
Co1—O1	2.1018 (13)	N1—C5	1.349 (2)
Co1—O1 ⁱ	2.1018 (13)	C1—C2	1.380 (2)
Co1—N1	2.1545 (13)	C2—C3	1.381 (3)
Co1—N1 ⁱ	2.1545 (13)	C2—H2	0.9300
S1—O2	1.4414 (15)	C3—C4	1.378 (3)
S1—O3	1.4432 (14)	C3—H3	0.9300
S1—O1	1.4612 (13)	C4—C5	1.376 (3)
S1—C1	1.7814 (15)	C4—H4	0.9300
O1W—H11	0.833 (9)	C5—H5	0.9300
O1W—Co1—O1W ⁱ	85.45 (9)	Co1—O1W—H11	122.9 (16)

supplementary materials

O1W—Co1—O1	173.62 (6)	Co1—O1W—H12	126.6 (16)
O1W ⁱ —Co1—O1	90.29 (6)	H11—O1W—H12	110.3 (15)
O1W—Co1—O1 ⁱ	90.29 (6)	C1—N1—C5	117.02 (14)
O1W ⁱ —Co1—O1 ⁱ	173.61 (6)	C1—N1—Co1	116.31 (10)
O1—Co1—O1 ⁱ	94.34 (8)	C5—N1—Co1	126.58 (12)
O1W—Co1—N1	94.31 (6)	N1—C1—C2	124.14 (15)
O1W ⁱ —Co1—N1	94.36 (6)	N1—C1—S1	115.65 (11)
O1—Co1—N1	81.26 (5)	C2—C1—S1	120.12 (13)
O1 ⁱ —Co1—N1	90.69 (5)	C1—C2—C3	117.83 (17)
O1W—Co1—N1 ⁱ	94.36 (6)	C1—C2—H2	121.1
O1W ⁱ —Co1—N1 ⁱ	94.31 (6)	C3—C2—H2	121.1
O1—Co1—N1 ⁱ	90.69 (5)	C4—C3—C2	119.14 (16)
O1 ⁱ —Co1—N1 ⁱ	81.26 (5)	C4—C3—H3	120.4
N1—Co1—N1 ⁱ	168.19 (8)	C2—C3—H3	120.4
O2—S1—O3	113.26 (10)	C3—C4—C5	119.23 (17)
O2—S1—O1	113.20 (9)	C3—C4—H4	120.4
O3—S1—O1	113.19 (9)	C5—C4—H4	120.4
O2—S1—C1	104.56 (8)	N1—C5—C4	122.56 (17)
O3—S1—C1	106.52 (8)	N1—C5—H5	118.7
O1—S1—C1	105.11 (7)	C4—C5—H5	118.7
S1—O1—Co1	119.31 (7)		
O2—S1—O1—Co1	98.03 (11)	C5—N1—C1—C2	-3.1 (3)
O3—S1—O1—Co1	-131.35 (10)	Co1—N1—C1—C2	173.84 (14)
C1—S1—O1—Co1	-15.48 (11)	C5—N1—C1—S1	173.39 (13)
O1W ⁱ —Co1—O1—S1	104.28 (10)	Co1—N1—C1—S1	-9.71 (16)
O1 ⁱ —Co1—O1—S1	-80.13 (9)	O2—S1—C1—N1	-103.32 (14)
N1—Co1—O1—S1	9.91 (10)	O3—S1—C1—N1	136.50 (14)
N1 ⁱ —Co1—O1—S1	-161.41 (10)	O1—S1—C1—N1	16.13 (15)
O1W—Co1—N1—C1	-174.23 (12)	O2—S1—C1—C2	73.28 (16)
O1W ⁱ —Co1—N1—C1	-88.48 (12)	O3—S1—C1—C2	-46.89 (17)
O1—Co1—N1—C1	1.14 (12)	O1—S1—C1—C2	-167.27 (15)
O1 ⁱ —Co1—N1—C1	95.43 (12)	N1—C1—C2—C3	2.6 (3)
N1 ⁱ —Co1—N1—C1	48.64 (11)	S1—C1—C2—C3	-173.66 (14)
O1W—Co1—N1—C5	2.33 (15)	C1—C2—C3—C4	0.0 (3)
O1W ⁱ —Co1—N1—C5	88.09 (15)	C2—C3—C4—C5	-2.0 (3)
O1—Co1—N1—C5	177.71 (16)	C1—N1—C5—C4	0.9 (3)
O1 ⁱ —Co1—N1—C5	-88.01 (15)	Co1—N1—C5—C4	-175.65 (14)
N1 ⁱ —Co1—N1—C5	-134.79 (15)	C3—C4—C5—N1	1.6 (3)

Symmetry codes: (i) $-x+1, y, -z+3/2$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1w—H11 \cdots O2 ⁱⁱ	0.83 (1)	1.90 (1)	2.735 (2)	177 (3)

O1w—H12...O3ⁱⁱⁱ 0.83 (1) 1.88 (1) 2.703 (2) 172 (3)
 Symmetry codes: (ii) $-x+1, y+1, -z+3/2$; (iii) $x+1/2, y+1/2, z$.

Fig. 1

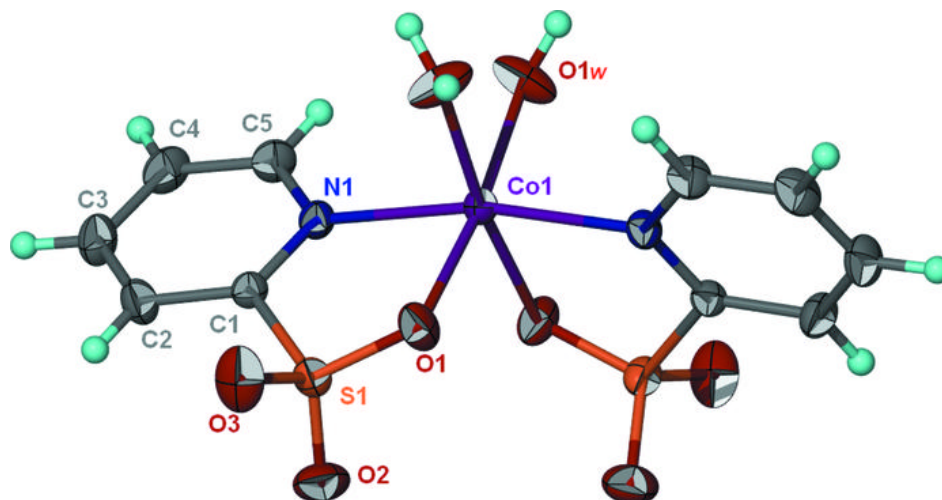


Fig. 2

