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

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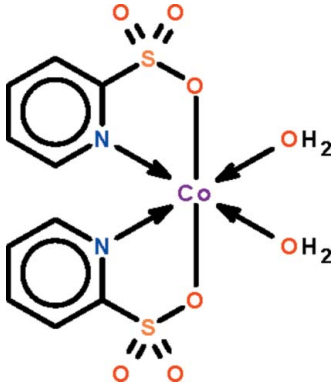
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.024; wR factor = 0.067; data-to-parameter ratio = 15.0.

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 an slightly distorted octahedral environment. The N-donor atoms are *cis* to each other. In the crystal, adjacent molecules are linked by O—H···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
β = 106.734 (1)°
V = 1494.86 (18) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.47 mm^{-1}
T = 296 K
0.25 × 0.20 × 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···A	D—H	H···A	D···A	D—H···A
O1w—H11···O2^{i}	0.83 (1)	1.90 (1)	2.735 (2)	177 (3)
O1w—H12···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: *SAINT* (Bruker, 2007); data reduction: *SAINT*; 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: *publCIF* (Westrip, 2010).

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

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supporting information

Acta Cryst. (2011). E**67**, m1781 [https://doi.org/10.1107/S1600536811048203]

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

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S1. Comment

Diaquabis(pyridine-2-sulfonate)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···$O_{sulfonate}$ hydrogen bonds (Table 1) into a layer motif extending along (0 0 1) (Fig. 2).

S2. 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.

S3. 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_{iso}(H) set to 1.2U_{eq}(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···H = 1.37±0.01 Å. Their isotropic displacement parameters were refined.

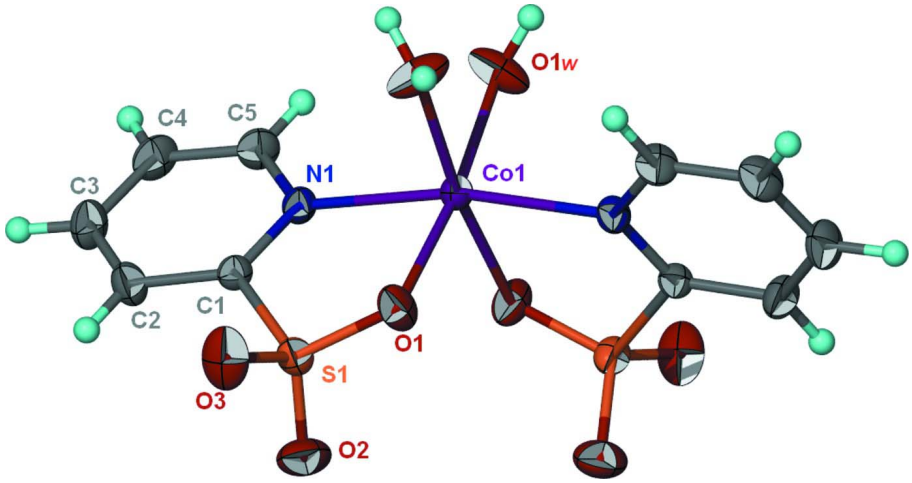

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of $[Co(H_2O)_2(C_5H_4NO_3S)_2]$ 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).

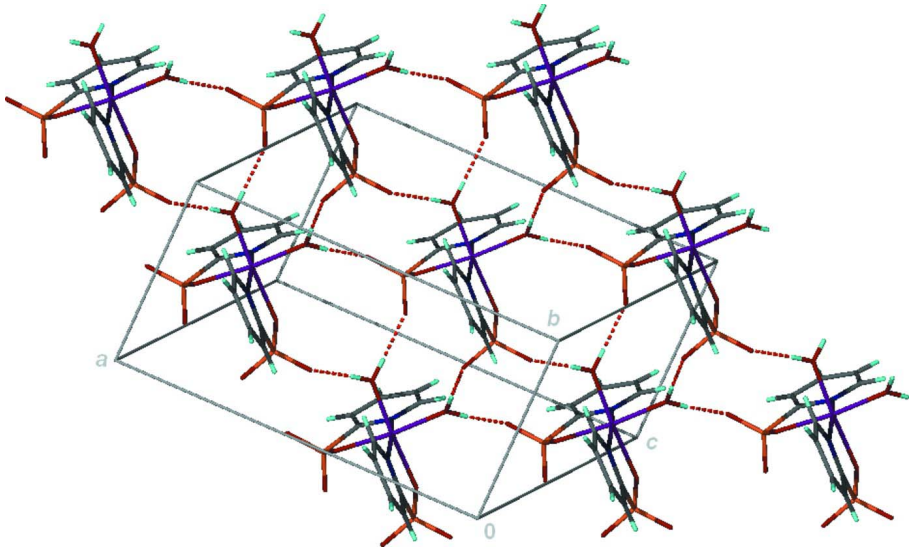

Figure 2

The hydrogen-bonded layer structure.

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

Crystal data

$[Co(C_5H_4NO_3S)_2(H_2O)_2]$
$M_r = 411.29$
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
$a = 13.7009$ (9) Å
$b = 7.1127$ (5) Å
$c = 16.0180$ (11) Å
$\beta = 106.734$ (1)°
$V = 1494.86$ (18) Å^3
$Z = 4$
$F(000) = 836$
$D_x = 1.827$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3169 reflections
$\theta = 3.1$–27.6°
$\mu = 1.47$ mm^{-1}

T = 296 K
Prism, yellow

0.25 × 0.20 × 0.15 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
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
θ_{max} = 27.5°, θ_{min} = 2.7°
h = −17→11
k = −9→9
l = −13→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.067
S = 1.03
1695 reflections
113 parameters
3 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0362P)^2 + 1.5779P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{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 (Å²)

	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 (7)
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 (Å, º)

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)
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 code: (i) −*x*+1, *y*, −*z*+3/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1w—H11···O2^{ii}	0.83 (1)	1.90 (1)	2.735 (2)	177 (3)
O1w—H12···O3^{iii}	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*.