Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Tetraaquabis[2-(4-pyridyl)ethanesulfonato-κN]-cobalt(II)

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Received 23 March 2007
Accepted 28 March 2007

Key indicators

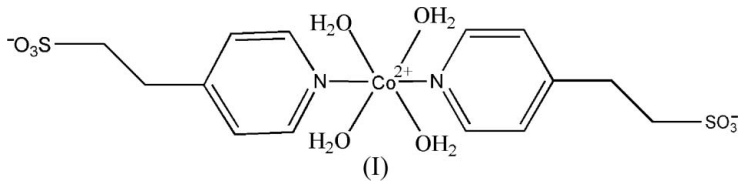
Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.003 Å
R factor = 0.024
wR factor = 0.066
Data-to-parameter ratio = 12.8

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title complex, $[Co(C_7H_8O_3S)_2(H_2O)_4]$, is isostructural with the Zn and Cu analogues. The Co atom (site symmetry $\overline{1}$) adopts a regular *trans*-CoN_2O_4 octahedral geometry.

Comment

The title compound, (I), is isostructural with the known $M^{II}(C_7H_8O_3S)_2(H_2O)_4$ compounds, where M = Zn (Zeng *et al.*, 2000) and Cu (Zhang & Wen, 2006), but it represents the first 2-(4-pyridyl)ethanesulfonate (PES) coordination complex of cobalt(II).



(I)

The molecule of (I) is centrosymmetric (Fig. 1), with a regular *trans*-CoN_2O_4 octahedron (Table 1), including the O atoms of water molecules. Adjacent complex molecules interact by way of O_w—H···O_s (w = water, s = sulfonate) hydrogen bonds (Table 2), leading to a three-dimensional network.

Experimental

$Co(CH_3COO)_2{\cdot}4H_2O$ (0.249 g, 1 mmol) and 4-pyridineethanesulfonic acid (0.0936 g, 0.5 mmol) were dissolved in water (20 ml) and the pH was adjusted to about 4.5 with dilute NaOH

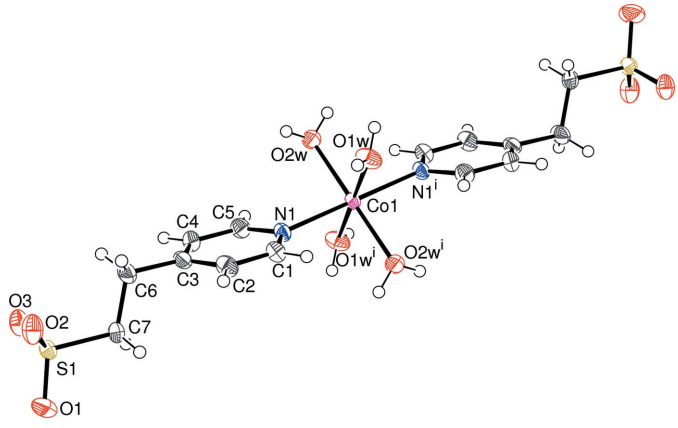


Figure 1
View of the molecular structure of (I), showing 30% displacement ellipsoids (arbitrary spheres for the H atoms). [Symmetry code: (i) $1-x$, $1-y$, $1-z$.]

solution. The resulting clear red solution was allowed to stand in air for two weeks. Orange plate-shaped crystals of (I) formed in a yield of approximately 40% (based on cobalt).

Crystal data

$[Co(C_7H_8O_3S)_2(H_2O)_4]$
M_r = 503.40
Monoclinic, $P2_1/c$
a = 9.1469 (8) Å
b = 8.7961 (7) Å
c = 12.491 (1) Å
β = 94.965 (1)°
V = 1001.20 (14) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.12 mm^{-1}
T = 173 (2) K
0.46 × 0.42 × 0.16 mm

Data collection

Bruker SMART 1K CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.631, T_{max} = 0.836
5462 measured reflections
1900 independent reflections
1695 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.066
S = 1.12
1900 reflections
149 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Table 1
Selected bond lengths (Å).

Co1—O2*W*	2.0897 (14)	Co1—N1	2.1363 (15)
Co1—O1*W*	2.1151 (14)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H9···O3^{i}	0.832 (16)	1.962 (16)	2.7906 (19)	174 (3)
O1*W*—H8···O2^{ii}	0.819 (16)	1.992 (16)	2.806 (2)	172 (2)
O2*W*—H11···O1^{iii}	0.838 (16)	1.957 (17)	2.794 (2)	176 (2)
O2*W*—H10···O3^{ii}	0.852 (16)	1.896 (17)	2.7408 (19)	171 (3)

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

The water H atoms were located in difference maps and refined with the restraints O—H = 0.85 (1) Å and H···H = 1.39 (1) Å. Their U_{iso} values were freely refined. The C-bound H atoms were located in idealized positions (C—H = 0.95 Å) and refined as riding, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97* (Sheldrick, 1997).

This work was supported financially by the Science Foundation of Jilin Province (No. 20030505–4).

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