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catena-Poly[[diaquabis[(4-tolylsulfanyl)acetato-κO]-cobalt(II)]-μ-4,4′-bipyridine-$\kappa^2 N:N'$]

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Key indicators

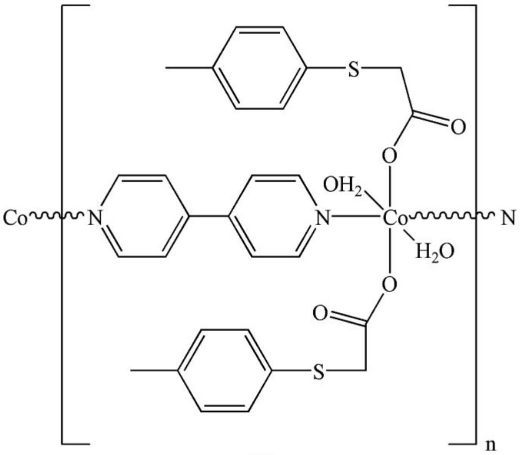
Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.002 Å
R factor = 0.028
wR factor = 0.081
Data-to-parameter ratio = 16.9

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

In the crystal structure of the title complex, $[Co(C_9H_9O_2S)_2(C_{10}H_8N_2)(H_2O)_2]_n$, a one-dimensional chain is formed in which the Co^{II} atoms are in a slightly disorted octahedral environment, coordinated by two water molecules, two (4-tolylsulfanyl)acetate and two bridging 4,4′-bipyridine ligands. The Co atom lies on a twofold rotation axis. These one-dimensional chains are connected into a two dimensional network *via* intermolecular O—H···O hydrogen bonds

Comment

Some related complexes of 4,4′-bipyridine (4,4′-bipy) have been reported recently (Wen *et al.*, 2005; Kryschenko *et al.*, 2003; Lang *et al.*, 2004). The (4-tolylsulfanyl)acetate (tta) ligand can not only coordinate to metal centers through the carboxylate group, but also form π–π interactions through the 4-tolylsulfanyl group (Gao *et al.*, 2005), although none are present in the title structure, (I).



(I)

The structure of (I) (Fig. 1) consists of linear chains formed through 4,4′-bipy ligands linking six-coordinate Co^{II} atoms, which lie on twofold rotation axes. Selected bonds lengths and angles are given in Table 1. Intermolecular O—H···O hydrogen bonds link chains into a two-dimensional network (Table 2). The title complex is isostructural with the nickel analogue (Lin *et al.*, 2006).

Experimental

$Co(NO_3)_2\cdot6H_2O$ (0.145 g, 0.5 mmol), (4-tolylsulfanyl)acetic acid (0.091 g, 0.5 mmol) 4,4′-bipy (0.039 g, 0.25 mmol) and water (18 ml) were sealed in a 25 ml Teflon-lined stainless steel reactor and the solution was heated at 433 K for 72 h and then cooled to room temperature over a period of 72 h. Red crystals suitable for X-ray analysis were obtained.

Crystal data

$[Co(C_9H_9O_2S)_2(C_{10}H_8N_2)(H_2O)_2]$
$M_r = 613.61$
Monoclinic, $C2/c$
$a = 21.684$ (4) Å
$b = 11.376$ (2) Å
$c = 11.032$ (2) Å
$\beta = 92.828$ (3)°
$V = 2718.0$ (9) Å^3

$Z = 4$
$D_x = 1.500$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.83$ mm^{-1}
$T = 273$ (2) K
Prism, red
0.30 × 0.28 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.779$, $T_{max} = 0.861$

8766 measured reflections
3178 independent reflections
2583 reflections with $I > 2\sigma(I)$
$R_{int} = 0.020$
$\theta_{max} = 27.7°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.081$
$S = 1.08$
3178 reflections
188 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0485P)^2 + 0.1764P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O1*W*	2.1077 (12)	Co1—N1	2.1338 (16)
Co1—O2	2.1254 (10)	Co1—N2^{i}	2.1412 (17)
O1*W*—Co1—O1*W*^{ii}	173.77 (6)	O1*W*^{ii}—Co1—N1	93.11 (3)
O1*W*—Co1—O2^{ii}	91.64 (5)	O2—Co1—N1	91.32 (3)
O1*W*^{i}—Co1—O2^{ii}	88.21 (5)	O1*W*^{ii}—Co1—N2^{i}	86.89 (3)
O2—Co1—O2^{ii}	177.36 (5)	O2—Co1—N2^{i}	88.68 (3)

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WA*···O1^{i}	0.82 (1)	1.85 (2)	2.6317 (18)	159 (2)
O1*W*—H1*WB*···O2^{iii}	0.81 (1)	2.07 (2)	2.8470 (16)	161 (2)

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

The methyl groups were allowed to rotate to fit the electron density [C—H = 0.96 Å and $U_{iso}(H) = 1.5U_{eq}(C)$]; the other C-bound H atoms were positioned geometrically [aromatic C—H = 0.93 Å and aliphatic C—H = 0.97 Å, with $U_{iso}(H) = 1.2U_{eq}(C)$]. Water H atoms were located in a difference map and refined with distance restraints of O—H = 0.85 (2) Å and H···H = 1.30 (2) Å; their displacement parameters were set at $1.5U_{eq}(O)$.

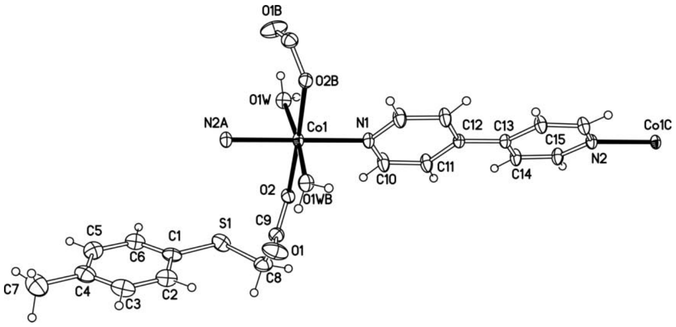


Figure 1
A view of part of the title structure, showing 30% probability displacement ellipsoids [symmetry codes: (A) $x, -1+y, z$; (B) $-x+1, y, \frac{1}{2}-z$; (C) $x, 1+y, z$.].

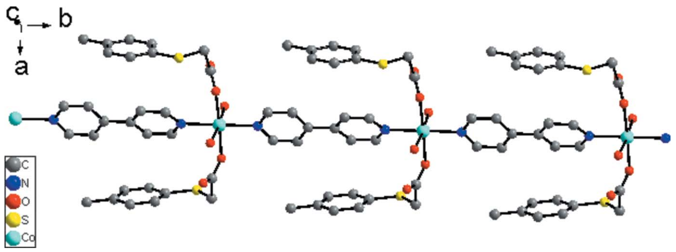


Figure 2
The chain structure of the title compound. All H atoms have been omitted for clarity.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2002); software used to prepare material for publication: *SHELXL97*.

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m1394 Zheng *et al.* • $[Co(C_9H_9O_2S)_2(C_{10}H_8N_2)(H_2O)_2]$ *Acta Cryst.* (2006). E**62**, m1393–m1394