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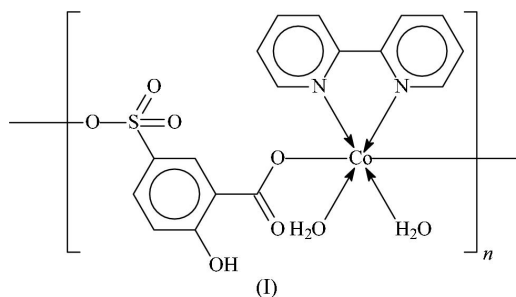
## Key indicators

Single-crystal X-ray study  
*T* = 295 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.010 \text{ \AA}$   
*R* factor = 0.072  
*wR* factor = 0.168  
Data-to-parameter ratio = 12.2For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.**catena-Poly[[*cis*-diaqua(2,2'-bipyridine)cobalt(II)]- $\mu$ -3-carboxylato-4-hydroxybenzenesulfonato]**

The chains of the title compound,  $[\text{Co}(\text{C}_7\text{H}_4\text{O}_6\text{S})(\text{C}_{10}\text{H}_8\text{N}_2)(\text{H}_2\text{O})_2]_n$ , adopt a zigzag conformation as they propagate *via* glide planes. The octahedral coordination of the Co atom comprises the O atoms of two water molecules, the N atoms of the heterocycle, the carboxyl O atom of the dianion and the sulfonyl O atom of a symmetry-related dianion. The water molecules form hydrogen bonds within the chain only.

## Comment

5-Sulfosalicylic (3-carboxy-4-hydroxybenzenesulfonic) acid possesses three sites for binding, *i.e.* the  $-\text{CO}_2\text{H}$ ,  $-\text{OH}$  and  $-\text{SO}_3\text{H}$  groups can coordinate to metal atoms. In some complexes, all the sites are deprotonated, whereas in others, only one is deprotonated. The present study follows on from reports on the N-heterocycle complexes of metal 3-carboxylato-4-hydroxybenzenesulfonates. When the copper derivative is reacted with 2,2'-bipyridine, two of the N-heterocycles bind to the Cu atom; this is bonded to only one monoanion; the other monoanion interacts indirectly through the coordinated water molecule (Gao *et al.*, 2005).



Cobalt(II) 3-carboxylato-4-hydroxybenzenesulfonate exists as a hexaaquacobalt salt in which the cation and anion are linked through hydrogen bonds (Ma *et al.*, 2003). Only one 2,2'-bipyridine is able to chelate to the Co atom in the title hexacoordinate compound. Two other coordination sites that are *cis* to each other are occupied by water molecules, and adjacent cations are linked through the dianion (Fig. 1) to afford a chain motif. The 3-carboxylato-4-hydroxybenzenesulfonate dianion uses the carboxylate  $-\text{CO}_2$  and the sulfonate  $-\text{SO}_3$  portions to bind. The manner of propagation gives rise to a zigzag conformation for the chain; the water molecules are engaged in hydrogen bonding only within each chain (Table 2).

## Experimental

Cobalt(II) acetate tetrahydrate (0.125 g, 0.5 mmol) and 5-sulfosalicylic acid dihydrate (0.126 g, 0.5 mmol) were dissolved in water

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(15 ml) and the solution was mixed with 2,2'-bipyridine (0.078 g, 0.5 mmol) dissolved in methanol (5 ml). Purple block-shaped crystals deposited from the solution after about a week.

Crystal data

[Co(C<sub>7</sub>H<sub>4</sub>O<sub>6</sub>S)(C<sub>10</sub>H<sub>8</sub>N<sub>2</sub>)(H<sub>2</sub>O)<sub>2</sub>]  $D_x = 1.679 \text{ Mg m}^{-3}$   
 $M_r = 467.31$  Mo  $K\alpha$  radiation  
 Monoclinic,  $P2_1/n$  Cell parameters from 2900 reflections  
 $a = 14.425 (1) \text{ \AA}$   $\theta = 2.9\text{--}26.1^\circ$   
 $b = 7.6138 (5) \text{ \AA}$   $\mu = 1.09 \text{ mm}^{-1}$   
 $c = 18.129 (1) \text{ \AA}$   $T = 295 (2) \text{ K}$   
 $\beta = 111.776 (1)^\circ$  Block, purple  
 $V = 1849.0 (2) \text{ \AA}^3$   $Z = 4$   
 $0.23 \times 0.16 \times 0.10 \text{ mm}$

Data collection

Bruker SMART APEX area-detector diffractometer 3233 independent reflections  
 $\varphi$  and  $\omega$  scans 3135 reflections with  $I > 2\sigma(I)$   
 Absorption correction: multi-scan (*SADABS*; Bruker, 2002)  $R_{\text{int}} = 0.030$   
 $T_{\text{min}} = 0.787$ ,  $T_{\text{max}} = 0.899$   $\theta_{\text{max}} = 25.0^\circ$   
 9285 measured reflections  $h = -15 \rightarrow 17$   
 $l = -21 \rightarrow 21$

Refinement

Refinement on  $F^2$   $w = 1/[\sigma^2(F_o^2) + (0.0596P)^2 + 5.6865P]$   
 $R[F^2 > 2\sigma(F^2)] = 0.072$  where  $P = (F_o^2 + 2F_c^2)/3$   
 $wR(F^2) = 0.168$   $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $S = 1.34$   $\Delta\rho_{\text{max}} = 0.55 \text{ e \AA}^{-3}$   
 3233 reflections  $\Delta\rho_{\text{min}} = -0.68 \text{ e \AA}^{-3}$   
 265 parameters  
 H-atom parameters constrained

Table 1

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

Co1—O1	2.036 (4)	Co1—O2w	2.040 (4)
Co1—O4 <sup>i</sup>	2.154 (4)	Co1—N1	2.103 (4)
Co1—O1w	2.168 (4)	Co1—N2	2.125 (5)
O1—Co1—O4 <sup>i</sup>	80.7 (2)	O4 <sup>i</sup> —Co1—N1	91.6 (2)
O1—Co1—O1w	90.7 (2)	O4 <sup>i</sup> —Co1—N2	97.0 (2)
O1—Co1—O2w	93.8 (2)	O1w—Co1—O2w	93.9 (2)
O1—Co1—N1	97.5 (2)	O1w—Co1—N1	89.9 (2)
O1—Co1—N2	174.1 (2)	O1w—Co1—N2	91.6 (2)
O4 <sup>i</sup> —Co1—O1w	171.4 (1)	O2w—Co1—N1	168.0 (2)
O4 <sup>i</sup> —Co1—O2w	86.4 (2)	O2w—Co1—N2	91.4 (2)

Symmetry code: (i)  $x - \frac{1}{2}, \frac{1}{2} - y, z - \frac{1}{2}$ .

Table 2

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

$D\text{--}H\cdots A$	$D\text{--}H$	$H\cdots A$	$D\cdots A$	$D\text{--}H\cdots A$
O3—H3o $\cdots$ O1	0.85	1.84	2.574 (6)	143
O1w—H1w1 $\cdots$ O2	0.85	1.94	2.706 (6)	149
O1w—H1w2 $\cdots$ O5 <sup>ii</sup>	0.85	1.99	2.827 (5)	169
O2w—H2w2 $\cdots$ O6 <sup>ii</sup>	0.85	1.92	2.705 (5)	153
O2w—H2w1 $\cdots$ O6 <sup>iii</sup>	0.85	1.89	2.718 (5)	166

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

The aromatic H atoms were positioned geometrically and were included in the refinement in the riding-model approximation [ $C\text{--}H = 0.93 \text{ \AA}$  and  $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C)$ ]. The water and hydroxyl H atoms were also placed in calculated positions ( $O\text{--}H = 0.85 \text{ \AA}$ ) and these bonds were rotated around the  $\text{Co--O}_{\text{water}}$  or  $\text{C--O}$  axis to fit the electron density;  $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(O)$ . Although the data were

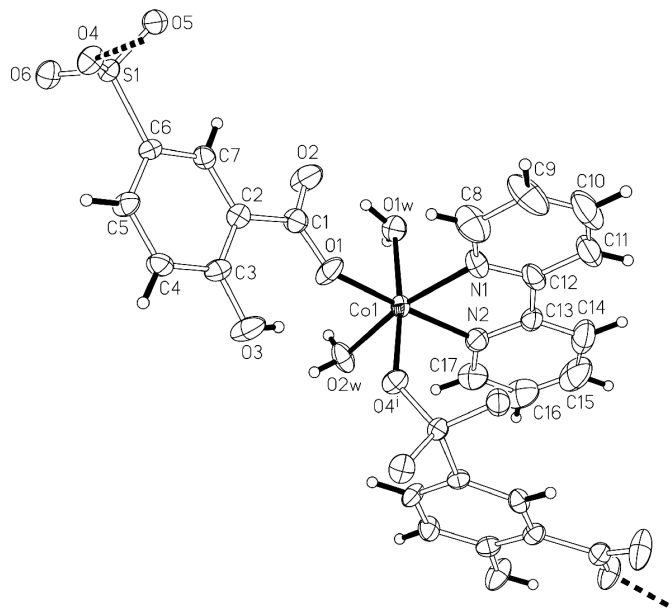


Figure 1

ORTEPII plot (Johnson, 1976) of a portion of the chain of (I). Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (i)  $x - \frac{1}{2}, \frac{1}{2} - y, z - \frac{1}{2}$ ].

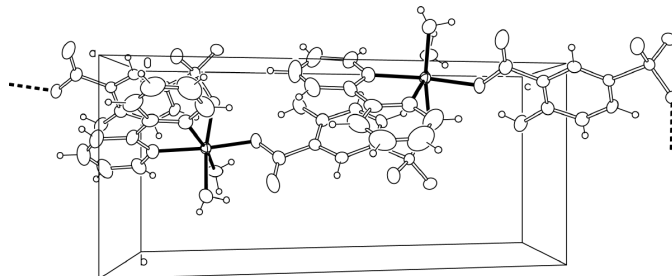


Figure 2

ORTEPII (Johnson, 1976) view of the chain motif.

measured to a  $2\theta$  limit of  $56^\circ$ , only the intensities below  $50^\circ$  were used in the refinement; the use of all reflections gave a much larger residual index.

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: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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