Triaqua(2,2′-bipyridine)(2-sulfonatobenzoato)cobalt(II)

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In the title compound, $[\text{Co}(C_7H_4O_5S)(C_{10}H_8N_2)(H_2O)_3]$, the Co^{II} atom has a distorted octahedral geometry formed by three aqua O atoms, one carboxylate O atom from a 2-sulfonatobenzoate dianion and two N atoms of a 2,2′-bipyridine ligand. Intermolecular O—H···O hydrogen bonds link the mononuclear units into a two-dimensional network structure.

Comment

Like other sulfobenzoic acids, such as 4-sulfobenzoic acid (Zhang *et al.*, 2005) and 5-sulfoisophthalic acid (Li *et al.*, 2005; Xiao & Morsali, 2005; Yuan *et al.*, 2004), which show diverse coordination modes, 2-sulfobenzoic acid (o-H$_2$sb) is also a versatile ligand and can function variously as a monodentate, bidentate or tridentate ligand; it can also bridge or chelate (Li & Yang, 2004; Su *et al.*, 2005; Xiao *et al.*, 2005). Here, we present the title compound [Co(2,2′-bipy)(o-sb)(H$_2$O)$_3$] (2,2′-bipy is 2,2′-bipyridine), (I), in which the o-sb^{2-} dianion functions in a monodentate coordination mode.

(I)
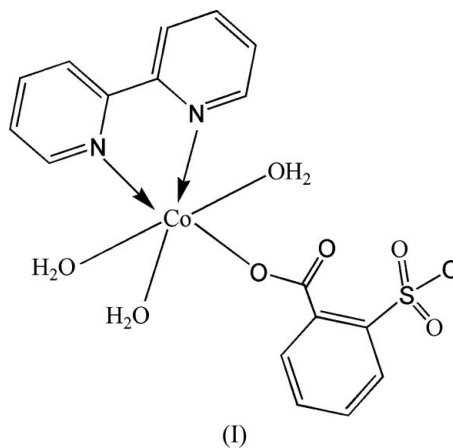
In (I), the Co^{II} atom is in a distorted octahedral environment formed by three aqua O atoms, one carboxylate O atom from an o-sb^{2-} dianion and two N atoms of a 2,2′-bipyridine ligand (Fig. 1 and Table 1). The o-sb^{2-} ligand coordinates to the Co^{II} centre in a monodentate mode, as is the same as observed in the previously reported compound [Mn(phen)$_2$(o-sb)(H$_2$O)]·3H$_2$O (phen is 1,10-phenanthroline; Xiao, 2005). The dihedral angle between the planes of the o-sb^{2-} ring and its carboxylate group is 59.7 (1)°, which is comparable with that in [Mn(phen)$_2$(o-sb)(H$_2$O)]·3H$_2$O and much larger than that in [Ni(o-sb)(bpe)(H$_2$O)$_2$]·0.25H$_2$O (Xiao *et al.*, 2005). The dihedral angle between the o-sb^{2-} ring and the mean plane of the 2,2′-bipyridine rings is 50.6 (2)°.
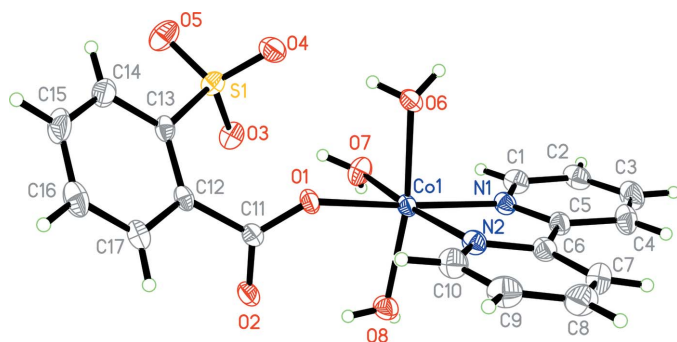
Figure 1
The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

The stability of the crystal structure of (I) is enhanced significantly by hydrogen-bonding interactions (Table 2). There are three intramolecular hydrogen bonds between the coordinated water molecule and the uncoordinated carboxylate O atom (O8—H8B···O2), and between the coordinated water molecule and the uncoordinated sulfonate group (O7—H7A···O3 and O6—H6A···O4). Additional O6—H6B···O2, O8—H8A···O3 and O7—H7B···O5 intermolecular hydrogen bonds link neighbouring mononuclear units into a two-dimensional network structure (Fig. 2).

Experimental

An aqueous solution (10 ml) of $CoCl_2\cdot6H_2O$ (0.20 mmol, 0.047 g) was added slowly to a solution (10 ml) of N,N-dimethylformamide containing 2,2′-bipyridine (0.20 mmol, 0.031 g) and 2-sulfobenzoic acid (0.20 mmol, 0.037 g). Red crystals of (I) suitable for X-ray diffraction analysis were obtained on allowing the solution to stand at room temperature for about two months.

Crystal data

$[Co(C_7H_4O_5S)(C_{10}H_8N_2)(H_2O)_3]$	$D_x = 1.610$ Mg m^{-3}
$M_r = 469.32$	Mo $K\alpha$ radiation
Monoclinic, Pc	Cell parameters from 1079
$a = 7.4546 (7)$ Å	reflections
$b = 12.3272 (11)$ Å	$\theta = 2.5$–$25.2°$
$c = 10.5333 (9)$ Å	$\mu = 1.04$ mm^{-1}
$\beta = 90.142 (11)°$	$T = 298 (2)$ K
$V = 967.95 (15)$ Å^3	Block, red
$Z = 2$	$0.32 \times 0.25 \times 0.17$ mm

Data collection

Bruker SMART CCD area-detector diffractometer	2602 independent reflections
	2565 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.021$
Absorption correction: multi-scan (SADABS; Bruker, 2002)	$\theta_{max} = 26.0°$
	$h = -8 \rightarrow 9$
$T_{min} = 0.731$, $T_{max} = 0.843$	$k = -15 \rightarrow 15$
5336 measured reflections	$l = -12 \rightarrow 10$

Refinement

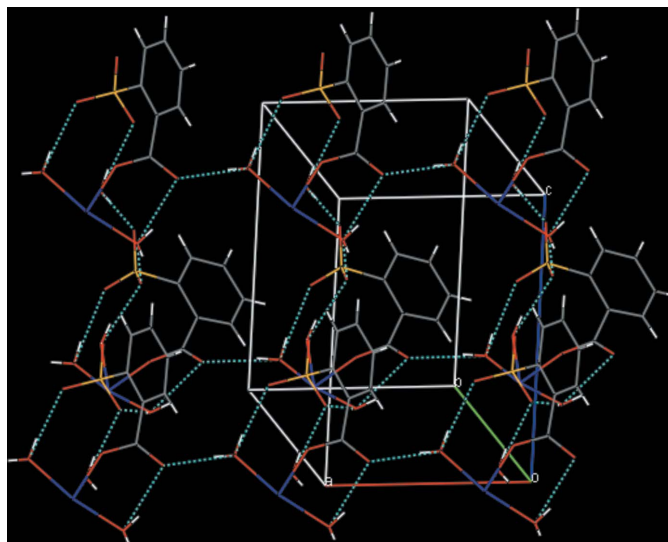|	
Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0228P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.023$	$+ 0.0468P]$
$wR(F^2) = 0.057$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	$(\Delta/\sigma)_{max} = 0.001$
2602 reflections	$\Delta\rho_{max} = 0.21$ e Å^{-3}
262 parameters	$\Delta\rho_{min} = -0.24$ e Å^{-3}
H-atom parameters constrained	Absolute structure: Flack (1983), with 1897 Friedel pairs
	Flack parameter: 0.015 (10)

Figure 2
A view of the two-dimensional network structure formed by hydrogen bonding interactions (shown as dashed lines). For clarity, the 2,2′-bipyridine ligands have been omitted.

Table 1
Selected geometric parameters (Å, °).

Co1—O7	2.085 (2)	Co1—O8	2.112 (2)
Co1—O1	2.092 (2)	Co1—N1	2.115 (2)
Co1—O6	2.094 (2)	Co1—N2	2.118 (2)
O7—Co1—O1	90.00 (8)	O6—Co1—N1	94.57 (8)
O7—Co1—O6	88.49 (8)	O8—Co1—N1	95.25 (8)
O1—Co1—O6	80.58 (7)	O7—Co1—N2	171.44 (9)
O7—Co1—O8	90.41 (8)	O1—Co1—N2	98.51 (8)
O1—Co1—O8	89.66 (7)	O6—Co1—N2	92.05 (8)
O6—Co1—O8	170.18 (8)	O8—Co1—N2	90.49 (8)
O7—Co1—N1	94.23 (8)	N1—Co1—N2	77.21 (8)
O1—Co1—N1	173.49 (7)		

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

$D—H\cdots A$	$D—H$	$H\cdots A$	$D\cdots A$	$D—H\cdots A$
O8—H8B···O2	0.82	2.02	2.780 (3)	155
O8—H8A···O3^i	0.82	2.08	2.873 (3)	164
O7—H7B···O5^i	0.82	1.90	2.717 (3)	178
O7—H7A···O3	0.82	1.89	2.692 (3)	167
O6—H6B···O2^{ii}	0.82	1.93	2.741 (3)	173
O6—H6A···O4	0.82	2.03	2.842 (3)	172

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

Water H atoms were located in a difference map and refined with the distance restraint O—H = 0.82 (1) Å and with $U_{iso}(H)$ = $1.5U_{eq}(O)$. Other H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

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: *XP* (Bruker, 2002); software used to prepare material for publication: *SHELXL97*.

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