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Key indicators

Single-crystal X-ray study
 $T = 133\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.002\text{ \AA}$
 R factor = 0.026
 wR factor = 0.074
Data-to-parameter ratio = 19.7For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.*trans*-Diaquabis(2-pyridylethanol-*N,O*)-
cobalt(II) disaccharinate

The title complex, $[\text{Co}(\text{pyet})_2(\text{H}_2\text{O})_2](\text{sac})_2$ (sac^- is the saccharinate anion, $\text{C}_7\text{H}_4\text{NO}_3\text{S}^-$, and pyet is 2-pyridylethanol, $\text{C}_7\text{H}_9\text{NO}$) contains sac^- ions and $[\text{Co}(\text{H}_2\text{O})_2(\text{pyet})_2]^{2+}$ cations, in which the Co^{2+} ion lies on a centre of symmetry and is octahedrally coordinated by two water and two neutral pyet molecules, which act as *N*- and *O*-donor bidentate ligands forming two symmetrically-related six-membered chelate rings. The crystal packing is determined by hydrogen bonding, as well as weak sac^- – sac^- π – π -stacking interactions, resulting in a three-dimensional network.

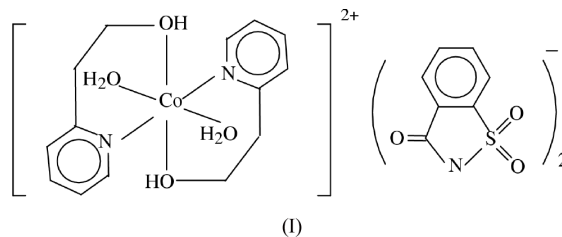
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Comment

Saccharin, chemically known as *o*-sulfobenzimide, is the most widely used artificial sweetener. Its deprotonated form, the saccharinate anion ($\text{C}_7\text{H}_4\text{NO}_3\text{S}^-$) (sac^-), readily coordinates to metal ions, forming stable metal complexes in the solid state. This study is a continuation of our research on the synthesis and structural characterization of complexes of metal saccharinates with other ligands containing hydroxymethyl and hydroxyethyl groups, such as monoethanolamine (Andac *et al.*, 2000, Yilmaz, Andac *et al.*, 2001; Yilmaz, Topcu *et al.*, 2001), monoethanolethylenediamine (Yilmaz *et al.*, 2002), diethanolamine (Yilmaz, Topcu *et al.*, 2001), triethanolamine (Topcu *et al.*, 2001), dimethanolpyridine (Andac *et al.*, 2002) and 2-pyridylethanol (Hamamci *et al.*, 2002*a*). In this paper, we report the structure of the 2-pyridylethanol (pyet) complex of cobalt(II) saccharinate, *viz.* $[\text{Co}(\text{H}_2\text{O})_2(\text{pyet})_2](\text{sac})_2$, (I).



The structure of (I) is shown in Fig. 1, and the chemical unit consists of a complex cation, $[\text{Co}(\text{H}_2\text{O})_2(\text{pyet})_2]^{2+}$, and two sac^- anions. In the complex cation, the Co^{II} ion lies on an inversion centre and is octahedrally coordinated by a pair of neutral pyet ligands and two water molecules, forming a CoN_2O_4 core. The sac^- ions are not in the primary coordination sphere, being separate counter-ions. Each pyet ligand behaves as a bidentate ligand through the *N* and hydroxyl *O*

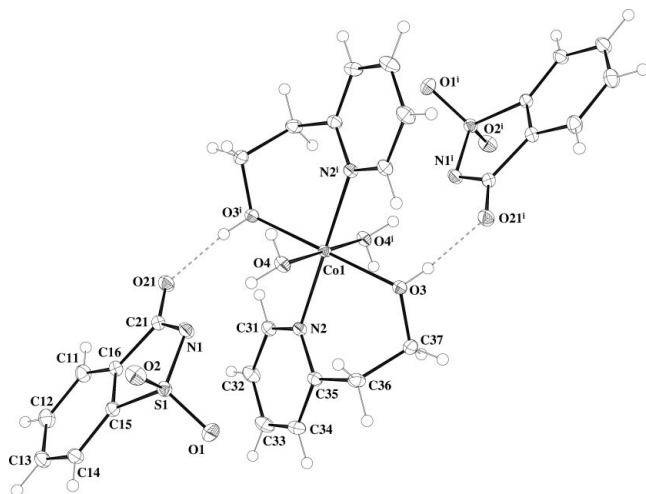


Figure 1
A molecular view of $[\text{Co}(\text{H}_2\text{O})_2(\text{pyet})_2](\text{sac})_2$ (40% displacement ellipsoids). [Symmetry code: (i) $-x, -y, -z$.]

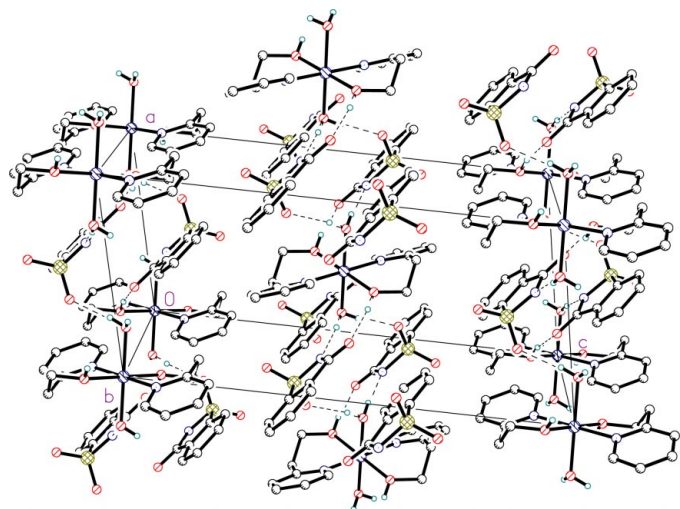


Figure 2
Packing diagram of $[\text{Co}(\text{H}_2\text{O})_2(\text{pyet})_2](\text{sac})_2$, showing the hydrogen-bonding scheme.

atoms, forming a six-membered chelate ring with the Co^{II} ion. The two pyet ligands form the equatorial plane of the coordination octahedron, while two water molecules occupy the axial positions with a *trans* configuration. Some distortion of the metal coordination sphere from regular octahedral geometry is apparent, especially in the $\text{O}_{\text{water}}-\text{Co}-\text{N}_{\text{pyet}}$ angles (Table 1).

Both sac^- (C11–C16/C21/O21/N1/S1) and pyet (C31–C36/N2) are essentially planar, with an r.m.s. deviation of *ca* 0.01 and 0.04 Å, respectively, but the OH group deviates significantly from the pyet plane by *ca* 1 Å. Furthermore, the Co^{2+} ion lies in the pyet plane. The crystal packing of the title compound is shown in Fig. 2. It exhibits parallel stacking of pairs of the sac^- ions and thus results in weak $\pi-\pi$ interactions (> 4.0 Å; the planes are defined by atoms C11–C16/S1/N1/C21/O21 and Ni/N2/C31–C36 for sac^- and pyet, respectively). The

H atoms of the water molecules (O4) and hydroxyl group (O3) of pyet form $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds with the sulfonyl O (O1) and carbonyl (O21) O atom of neighbouring sac^- anions. Additionally, two weak $\text{C}-\text{H}\cdots\text{O}$ interactions between H atoms of the pyridine ring and the carbonyl and sulfonyl O atoms of the adjacent sac^- ions occur. The hydrogen bonds and weak $\pi-\pi$ interactions stabilize the crystal structure, forming a three-dimensional network.

The title compound is isostructural with the corresponding nickel(II) complex (Hamamci *et al.*, 2002*b*).

Experimental

Previously prepared $[\text{Co}(\text{sac})_2(\text{H}_2\text{O})_4]\cdot 2\text{H}_2\text{O}$ (1.0 mmol, 0.53 g; Haider *et al.*, 1985) was dissolved in methanol (30 ml) at 303 K with stirring. Pyet (0.25 g, 2.0 mmol) was then added to the solution dropwise. The resulting solution was left to stand at room temperature and allowed to evaporate slowly for crystallization. Yellow single crystals, obtained within a week, were collected by suction filtration, washed with acetone and dried in air.

Crystal data

$[\text{Co}(\text{C}_7\text{H}_9\text{NO})_2(\text{H}_2\text{O})_2] \cdot$
 $(\text{C}_7\text{H}_4\text{NO}_3\text{S})_2$
 $M_r = 705.61$
Monoclinic, $P2_1/n$
 $a = 8.8391$ (6) Å
 $b = 8.7910$ (6) Å
 $c = 19.1564$ (12) Å
 $\beta = 100.876$ (3)°
 $V = 1461.80$ (17) Å³
 $Z = 2$

$D_x = 1.603$ Mg m⁻³
Mo $K\alpha$ radiation
Cell parameters from 7972 reflections
 $\theta = 2.2$ – 30.5°
 $\mu = 0.80$ mm⁻¹
 $T = 133$ (2) K
Prism, yellow
 $0.24 \times 0.21 \times 0.16$ mm

Data collection

Bruker SMART 1000 CCD diffractometer
 ω and φ scans
Absorption correction: multi-scan (SADABS; Bruker, 1998)
 $T_{\text{min}} = 0.833$, $T_{\text{max}} = 0.928$
27599 measured reflections

4281 independent reflections
3827 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.024$
 $\theta_{\text{max}} = 30.0^\circ$
 $h = -12 \rightarrow 12$
 $k = -12 \rightarrow 12$
 $l = -26 \rightarrow 26$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.026$
 $wR(F^2) = 0.074$
 $S = 1.04$
4281 reflections
217 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0486P)^2 + 0.2616P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.48$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.26$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Co–O3	2.0855 (8)	Co–N2	2.1303 (9)
Co–O4	2.1087 (8)		
O3 ⁱ –Co–O4	88.28 (3)	O3–Co–N2	89.85 (3)
O3–Co–O4	91.72 (3)	O4 ⁱ –Co–N2	86.98 (3)
O3 ⁱ –Co–N2	90.15 (3)	O4–Co–N2	93.02 (3)

Symmetry code: (i) $-x, -y, -z$.

Table 2

Hydrogen-bonding geometry (Å, °).

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C32—H32···O21 ^{iv}	0.95	2.64	3.3559 (15)	133
C33—H33···O1 ⁱⁱ	0.95	2.44	3.3295 (14)	156
O4—H4A···O2 ⁱⁱⁱ	0.823 (17)	2.010 (18)	2.8270 (12)	172 (1)
O3—H3···O21 ⁱ	0.827 (18)	1.830 (18)	2.6433 (11)	168 (1)

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

The H atoms of the hydroxyl group and water molecules were refined freely, while H atoms bonded to carbon were included using a riding model, starting from calculated positions.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINTE* (Bruker, 1998); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* (Siemens, 1994); software used to prepare material for publication: *SHELXL97*.

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