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Rubidium 3-carboxy-4-hydroxybenzenesulfonate monohydrate

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The title compound, poly[[rubidium-μ-5-sulfonosalicylic acid] monohydrate], $Rb^+ \cdot C_7H_5O_6S^- \cdot H_2O$, the 5-sulfosalicylic acid anion (3-carboxy-4-hydroxybenzenesulfonate) has lost the proton of $-SO_3H$ group, but retains the usual intermolecular hydrogen bond between the phenolic and carboxylic O atoms. The Rb^+ cation is surrounded by eight O atoms. The crystal packing is stabilized by intermolecular $O-H\cdots O$ hydrogen bonds.

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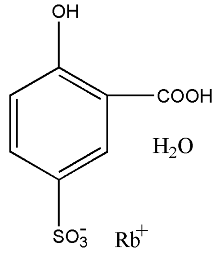
Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.007 Å
R factor = 0.045
wR factor = 0.141
Data-to-parameter ratio = 11.5

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

Comment

5-Sulfosalicylic acid (H_3Ssal) has been known for a long time to possess anti-inflammatory activity. When it forms complexes with metals, its biological activity is greatly enhanced (Marzotto *et al.*, 2001). However, only a few metal complexes of 5-sulfosalicylic acid have been reported (Icbudak *et al.*, 2003; Marzotto *et al.*, 2001; Nothenberg *et al.*, 2000; Wang *et al.*, 1992, 2004; Chen *et al.*, 2003). The heavy alkali metal rubidium has biological activity and affects the health of humans (Qin, 2000). We present here the synthesis and structure of the new compound poly[[rubidium-μ-5-sulfonosalicylic acid] monohydrate], Rb[(H_2Ssal)(H_2O)], (I).



(I)

The molecular structure of (I) is shown in Fig. 1. Selected geometric parameters are given in Table 1. The Rb^+ cations are eight-coordinated by the O atoms of carboxyl, sulfonate and water. The compound is isomorphous with Na[(H_2Ssal)(H_2O)$_2$] (Marzotto *et al.*, 2001). The crystal packing is stabilized by intermolecular $O-H\cdots O$ hydrogen bonds (Table 2 and Fig. 2).

Experimental

5-Sulfosalicylic acid dihydrate (8 mmol) was added to a solution of rubidium carbonate (4 mmol) in water (10 ml). The mixture was stirred for 15 min at 333 K. The solution was then filtered under reduced pressure and set aside for crystallization. After two weeks, pure white crystals of the title compound had formed in the filtered

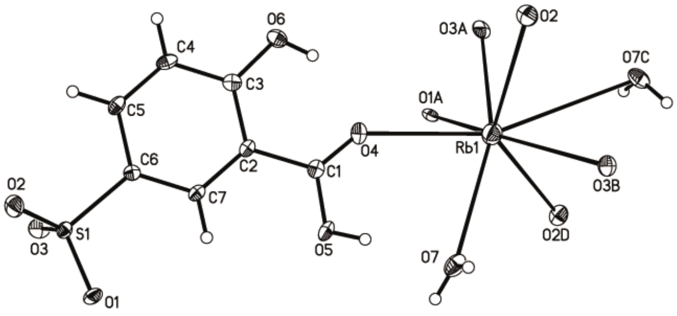


Figure 1
The eight-coordinated rubidium cation of the title compound. Displacement ellipsoids are drawn at the 50% probability level. Atoms labelled with *A*, *B*, *C* and *D* are at the symmetry positions $(-x + 1, y - \frac{1}{2}, -z + \frac{3}{2})$, $(x + 1, y, z)$, $(-x + 2, y - \frac{1}{2}, -z + \frac{3}{2})$ and $(-x + 2, y + \frac{1}{2}, -z + \frac{3}{2})$, respectively.

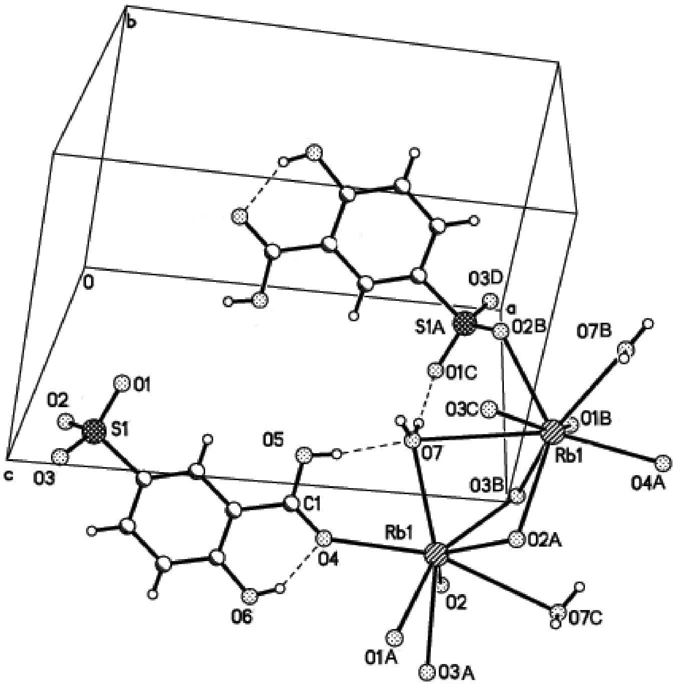


Figure 2
Part of the crystal structure of (I). Dashed lines indicate O—H···O hydrogen bonds.

solution. Analysis calculated for $C_7H_7O_7RbS$: C 26.22, H 2.20, Rb 26.65%; Found: C 26.92, H 1.90, Rb 26.75%. IR (KBr, cm^{-1}): 1670, 1604, 1472, 1444, 1347, 1298, 1200, 1077, 1026, 919, 855, 791, 726, 663. Raman spectra (cm^{-1}): 1659, 1587, 1479, 1435, 1312, 1231, 1197, 1130, 1179, 1030, 886, 783, 713, 660.

Crystal data

$Rb^+\cdot C_7H_5O_6S^-\cdot H_2O$
$M_r = 320.66$
Monoclinic, $P2_1/c$
$a = 11.779$ (11) Å
$b = 7.363$ (7) Å
$c = 12.025$ (11) Å
$\beta = 103.359$ (12)°
$V = 1014.7$ (16) Å^3
$Z = 4$

$D_x = 2.099$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2007 reflections
$\theta = 3.3$–27.7°
$\mu = 5.10$ mm^{-1}
$T = 273$ (2) K
Block, colourless
0.45 × 0.39 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
$T_{min} = 0.116$, $T_{max} = 0.542$
4884 measured reflections

1764 independent reflections
1438 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 25.0°$
$h = -14 \rightarrow 8$
$k = -8 \rightarrow 8$
$l = -13 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.141$
$S = 0.98$
1764 reflections
153 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0973P)^2 + 3.1685P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.07$ e Å^{-3}
$\Delta\rho_{min} = -0.53$ e Å^{-3}

Table 1
Selected bond lengths (Å).

Rb1—O4	2.847 (5)	Rb1—O2	3.005 (4)
Rb1—O3^{i}	2.875 (4)	Rb1—O7	3.014 (5)
Rb1—O2^{ii}	2.907 (4)	Rb1—O1^{iii}	3.110 (5)
Rb1—O3^{iii}	2.945 (5)	Rb1—O7^{iv}	3.466 (5)

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5···O7	0.82	1.92	2.729 (6)	171
O6—H6···O4	0.82	1.89	2.613 (6)	146
O7—H1···O1^{v}	0.84 (4)	1.97 (4)	2.797 (8)	166.0 (4)

Symmetry code: (v) $1 - x, 2 - y, 1 - z$.

H1, attached to O7, was located in a difference Fourier map and refined freely. Other H atoms were placed in calculated positions (O—H = 0.82 Å and C—H = 0.93 Å) and refined as riding, with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}(O)$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2001); software used to prepare material for publication: *SHELXTL*.

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