The Crystal Structure of Salicylatotetra-amminecobalt(III) Chloride Monohydrate

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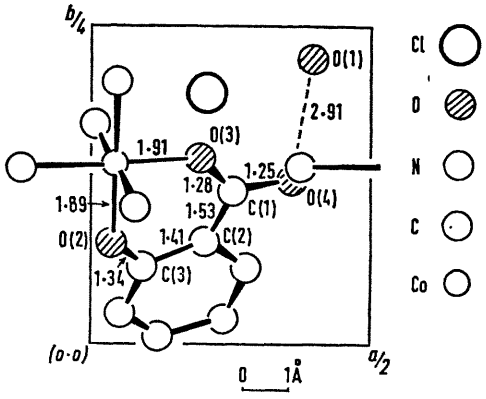
Summary The salicylato-group, $C_6H_4(O^-)CO_2^-$, in the title compound co-ordinates as a bidentate chelate ligand, and forms a non-planar six-membered ring with the cobalt atom.

THOUGH many metal–salicylato-compounds have been studied by the *X*-ray method, little information is yet available on the geometry of the chelated salicylato-group. Salicylatotetra-amminecobalt(III) chloride monohydrate, $[Co(C_7H_4O_3)(NH_3)_4]Cl,H_2O$, seemed to provide a suitable case of a chelated salicylato-group,[1,2] and we therefore determined its structure by *X*-ray techniques.

The compound was prepared by the method of Morgan and Main-Smith,[1] and recrystallized from hot water: deep purple plates, orthorhombic; $a = 12{\cdot}19(2)$, $b = 28{\cdot}01(2)$, $c = 7{\cdot}45(1)$ Å; $U = 2543{\cdot}7$ Å^3; $D_m = 1{\cdot}68 \pm 0{\cdot}02$ g/cm^3 (by flotation); $Z = 8$, $D_c = 1{\cdot}65$ g/cm^3. Space group: *Pbca*: Ni-K_α radiation ($\lambda = 1{\cdot}6591$ Å).

A total of 1231 independent structure amplitudes were obtained from visual estimation. The structure was determined by Patterson and Fourier methods, and refined by isotropic block-diagonal least-squares methods to an *R* value of 0·12. The standard deviations of bond lengths for the six bonds involving cobalt atom were 0·02 Å and for the remaining bonds 0·04 Å.

The crystal structure consists of complex cations, $[Co(C_7H_4O_3)(NH_3)_4]^+$, chloride anions and water molecules as shown in the Figure (projected down the *c*-axis). The cobalt atom is co-ordinated by four ammonia molecules and one salicylato-group which acts as a bidentate ligand (Co–N 1·98—2·00 Å). The cobalt–salicylato six-membered ring is not co-planar. The bond angles in the ring are O(3)–Co–O(2), 94°; Co–O(2)–C(3), 123°; O(2)–C(3)–C(2), 124°; C(3)–C(2)–C(1), 124°; C(2)–C(1)–O(3), 119°; C(1)–O(3)–Co, 129°. Their standard deviations are 2°. The carbon and oxygen atoms of the salicylato-group lie on a plane (within 0·04 Å) except the oxygen atoms of the carboxyl group. The dihedral angle between the plane of the salicylato-group and the plane of the carboxyl group is 18·0°. The water molecules in the crystal are very stable to heat,[1] perhaps because of a short contact between the oxygen atom of the water molecule and that of the carboxyl group [O(1) · · · O(4) 2·91 Å].



FIGURE

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[1] G. T. Morgan and J. D. Main-Smith, *J. Chem. Soc.*, 1924, 1996.
[2] A. G. Beaumont and R. D. Gillard, *J. Chem. Soc.* (*A*), 1968, 2400.