Crystal data for \( \text{Rb}_2\text{CoCl}_4\cdot2\text{H}_2\text{O} \)

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Crystal data for Rb$_2$CoCl$_4$·2H$_2$O

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Abstract

This compound is triclinic, probably isostructural with Rb$_2$MnCl$_4$·2H$_2$O, the space group is P1 or P1, a=6.50±0.04, b=6.99±0.04, c=5.58±0.03 Å, α=92.8±0.1°, β=97.2±0.1°, γ=65.4±0.1°, V=228.76±0.06 Å$^3$, Z=1, D$_m$=2.94±0.03 g·cm$^{-3}$, D$_x$=2.96 g·cm$^{-3}$. The precession method and Zr-filtered MoKα radiation (λ=0.7107 Å) were used. The description of the specimen preparation, chemical analysis, morphology and comparison with similar substances are deposited.

Origin of the specimen

The aggregates of crystals were prepared by the slow evaporation of an aqueous solution at room temperature. The Merck's reagents RbCl Suprapur and CoCl$_2$·6H$_2$O were solved in the molar ratio 2:1 in the redistilled water.

Chemical characterisation

The results of the quantitative chemical analysis (14.76 wt% Co, 34.11 % Cl and 9.38 % H$_2$O) correspond well to the
formula $\text{Rb}_2\text{CoCl}_4\cdot 2\text{H}_2\text{O}$. Theoretical values are: 14.75 wt% Co, 37.77% Cl, 6.82% H$_2$O.

The thermal analysis was also performed. The heating rate was 10 degrees/min. The DTG and TG curves indicated slow decrease of the weight at 80–100°C caused probably by the small inclusions of the solution in crystals. The sharp peaks of the DTA and DTG curves at 115°C and 140°C correspond to the consecutive lost of two water molecules. The peak at 495°C on the DTA curve indicate the phase transition (Amit et al 1972). At 535°C the specimen melts.

Crystal geometry,

The $h00$, $h01$, and $0k1$ precession photographs were performed and the reciprocal angles as well as the row spacings were measured. The reciprocal unit cell edges were obtained from the values $a^*\sin \theta^*$, $b^*\sin \theta^*$ etc., calculated from the row spacings. The reciprocal parameters were inverted into the direct ones.

Crystal morphology

Crystals are violet, irregularly formed, mostly elongated along [110] or tabular along (001). Cleavage parallel with (001). Many crystals are curved. The existence of (110) twins was proved on the precession photograph of one of the specimens. The crystals are stable at the room temperature.
Comparison with other results.

\( \text{Rb}_2\text{CoCl}_4 \cdot 2\text{H}_2\text{O} \) is probably isostructural with \( \text{Rb}_2\text{MnCl}_4 \cdot 2\text{H}_2\text{O} \) \( [a=6.48, b=7.01, c=5.66 \text{ Å}, \alpha=92.3^\circ, \beta=95.2^\circ, \gamma=66.7^\circ] \) or, less probably with \( \text{Ca}_2\text{MnCl}_4 \cdot 2\text{H}_2\text{O} \) \( [a=5.66, b=7.27, c=5.74 \text{ Å}, \alpha=92.2^\circ, \beta=95.7^\circ, \gamma=67.0^\circ] \) (Jensen 1964). Both compounds differing in the mutual positions of the water molecules exhibit also the (110) twinning. The lattice constants from the Jensen's paper were transformed by using the matrix (010/001/100) to be consistent with our data.

The anhydrous \( \text{Rb}_2\text{CoCl}_4 \) is orthorhombic, \( \text{Pnma}, a=9.272, b=7.283, c=12.273 \text{ Å}, Z=4 \) (Amit et al. 1972).

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References:
