

### ABSTRACT

The investigations reported in this thesis deal mainly with the refinement of the crystal structure of the room temperature phase of cubic aquopentamminecobalt (111) perchlorate -  $[\text{Co}(\text{NH}_3)_5\text{H}_2\text{O}] (\text{ClO}_4)_3$  - and with an investigation into the role of the structural units, the cations and anions, in the phenomena exhibited by these crystals.

Crystals of this compound have previously been reported as exhibiting dimorphism, the dimorphs not being related by a temperature-dependent displacive transition. One dimorph is orthorhombic and of symmetry that of space group  $\text{Pmn}2_1$ , while the other is cubic and of symmetry that of space group  $\text{Pn}3n$ .

Further it was reported that the cubic dimorph exhibited pseudo-symmetry with the true unit of repeat having a cell length twice that of the pseudo-cell and that the symmetry of the latter cell was that of space group  $\text{Fm}3m$ .

The existence of a temperature-dependent phase transition in crystals of the cubic dimorph has now been established. This transition takes place at about  $36^\circ\text{C}$  and involves a change in symmetry to that of the pseudo-unit cell.

An analysis of the diffuse scattering of X-rays by crystals of the room temperature phase of cubic aquopentamminecobalt (111) perchlorate not only revealed information about the shapes and

orientations of the structural units but also established that the interionic forces between these units are weak.

These units have also been shown to exhibit disorder involving orientational disorder on the part of both sets of units.

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## EXPERIMENTAL INVESTIGATION INTO THE OCCURRENCE OF BIXYMERISM

### IN CRYSTALS OF AQUENTAMINE-CORALY (III) PERCHLORATE

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