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An X-ray study of Hydroxyl ammonium lithium sulphate hexahydrate

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Abstract. Unit-cell dimensions and space group of hydroxyl ammonium lithium sulphate hexahydrate have been determined. The crystal belongs to the monoclinic system with space group $P2_1 - C_2^2$. The unit-cell dimensions are $a = 15.50 \pm 0.03$ Å, $b = 5.02 \pm 0.01$ Å, $c = 5.67 \pm 0.01$ Å and $\beta = 92°$. There are two molecules in the unit cell.

Single crystals of hydroxyl ammonium lithium sulphate hexahydrate were grown at room temperature by slow evaporation of saturated aqueous solution of $(HONH_3)_2SO_4$ and $Li_2SO_4 \cdot H_2O$ in stoichiometric quantities. Infrared spectra were recorded to confirm the formation of the mixed sulphate. The formula $(HONH_3)LiSO_4 \cdot 6\,H_2O$ is arrived at by thermogravimetric analysis.

Oscillation photographs taken along the long axis of the crystal showed mirror symmetry indicating a minimum possible monoclinic symmetry. Zero-layer, first-layer Weissenberg and precession photographs were taken along the long axis and an axis perpendicular to it. The radiation used is Cu$K\alpha$ of wavelength 1.5418 Å.

The unit cell dimensions obtained from zero-layer Weissenberg and precession photographs are: $a = 15.50 \pm 0.03$ Å, $b = 5.02 \pm 0.01$ Å and $c = 5.67 \pm 0.01$ Å. Zero-layer Weissenberg measurements gave a value of $\beta = 92°$.

From the systematic absences of spots, we arrived at the extinction condition $0k0$ (k odd). The density of the crystal was measured to be 1.825 gm/cm^3 and that calculated assuming two molecules per unit cell was 1.795 gm/cm^3. From the above mentioned observations the space group of the crystal was concluded to be $P2_1 - C_2^2$. The long axis, which is the unique axis was identified as the b-axis.

An ESR study of vanadyl doped $(HONH_3)LiSO_4 \cdot 6H_2O$ crystals confirmed monoclinic symmetry. No structural phase transition was observed during a study of the temperature variation of ESR signals down to 77 K. A detailed report on the ESR measurements will be published elsewhere.

A detailed crystal structure analysis is not planned.

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