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Note on the Crystal Structure of $MoO_3 \cdot 2H_2O$

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The main features of the crystal structure of the yellow molybdic acid $MoO_3 \cdot 2H_2O$ were reported in 1950 by Lindqvist.[1] It was stated that the structure is built up of MoO_6 octahedra which are joined by corners to form approximately square nets of composition MoO_4. The layers are stacked on top of each other, the remaining oxygen atoms occupying positions between the layers. In a later X-ray study [2] systems of weak reflections were observed which correspond to a much larger unit cell than the one of the structure described above. No attempt was made at that time to solve the details of the superstructure.

The present investigation, suggested by Professor Lindqvist, was undertaken in order to elucidate the role of the hydrogen atoms in the bonding system of the structure. Three-dimensional X-ray data have been collected with a PALLRED diffractometer in equi-inclination setting using LiF monochromatized Mo$K\alpha$ radiation ($2\theta \leq 100°$).

It was observed that reflections hkl ($h+l \neq 2n$) (in the notation of Ref. 2) of significant intensities were very few and also of very low intensities. Special investigations of these reflections by slight missetting of the inclination angle (μ) demonstrated that these are actually caused by accidental multiple diffraction. Systematically occurring multiple diffraction was avoided by rotating the crystal around an axis parallel to [100] (in the notation of Ref. 2). The actual unit cell is thus half the one reported in Ref. 2. The relations between the new unit-cell vectors and those of the larger unit cell, the latter being primed, is:

$$\mathbf{a} = \tfrac{1}{2}(\mathbf{a}' + \mathbf{c}')$$
$$\mathbf{b} = \mathbf{b}'$$
$$\mathbf{c} = \tfrac{1}{2}(-\mathbf{a}' + \mathbf{c}')$$

The values of the cell parameters as obtained from Guinier-Hägg powder photographs taken with Cu$K\alpha_1$ radiation and potassium chloride ($a = 6.2919$ Å)[3] added to the specimen as an internal standard are (20°C):

$$a = 10.474 \pm 1 \text{ Å}$$
$$b = 13.825 \pm 2 \text{ Å}$$
$$c = 10.608 \pm 1 \text{ Å}$$
$$\beta = 91.59 \pm .01°$$

The analysis of the superstructure is in progress.

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