(1943) found that sodium metavanadate, $NaVO_3$, has a structure similar to diopside with tetrahedra sharing two oxygen atoms to form chains held together by sodium atoms. It was considered of interest to investigate the structure of ammonium metavanadate as another example of a member of the group.

Crystals of ammonium metavanadate were grown from water solution by dissolving powdered material at about 80° C. and allowing the solution to cool. Since the material decomposes in water above 90° C., some question arises as to the composition of the product. Lattice-constant measurements and density, however, are in good agreement with a composition of NH_4VO_3. The precipitated crystals are clear, pale yellow plates or needles. The morphological symmetry appears orthorhombic with no evidence of hemihedry.

Rotation and Weissenberg patterns were taken about the needle axis and precession patterns about the normal to the needle axis. From these, the unit cell was found to be orthorhombic with the following unrefined lattice constants:

$$a_0 = 4{\cdot}96, \quad b_0 = 11{\cdot}82, \quad c_0 = 5{\cdot}63\,\text{A.};$$
$$a : b : c = 0{\cdot}420 : 1 : 0{\cdot}476.$$

The only systematic absences are $h0l$ with l odd and $0kl$ with k odd. Two orthorhombic space groups are possible: C^8_{2v}–Pbc or D^{11}_{2h}–$Pbcm$. The holohedral appearance of the crystals suggests that the latter is more probable.

Assuming the density to be $2{\cdot}326\,\text{g.cm.}^{-3}$, as reported by Mellor (1947, p. 758), the number of formula weights per unit cell can be calculated:

$$z = \frac{V\rho}{1{\cdot}6502 \times \text{M.W.}} = \frac{4{\cdot}96 \times 11{\cdot}82 \times 5{\cdot}63 \times 2{\cdot}326}{1{\cdot}6502 \times 116{\cdot}99} = 3{\cdot}97 \sim 4.$$

The fact that z is a whole number is considered adequate evidence that the material is not a hydrate and is, indeed, NH_4VO_3.

The space group D^{11}_{2h}–$Pbcm$ calls for eight atoms in the general position. Since there are only four formula weights per unit cell, the NH_4VO_3 groups must lie on the mirror plane. If the structure contains VO_4 tetrahedra, as postulated, the orientation of the tetrahedra is fixed by virtue of the fact that only one mirror plane (plus symmetrical equivalents) exists in a tetrahedron. They must lie in such a position that the vanadium and two oxygen atoms lie in the mirror plane. The other symmetry elements develop from this a chain structure with two shared oxygen atoms. Preliminary structure-factor computations are consistent with this tentative arrangement. A complete structure determination is in process.

References

Ketelaar, J. A. A. (1936). *Z. Krystallogr.* **95**, 9.

Mellor, J. W. (1947). *A Comprehensive Treatise on Inorganic and Theoretical Chemistry*, vol. 9 (new impression). London, New York and Toronto: Longmans, Green and Co.

Sørum, H. (1943). *K. norske vidensk. Selsk. Forh.* **15**, 39.

Acta Cryst. (1950). **3**, 477

Prismatic cleavage of molybdenite.

By René Bailly, *Washington University, St Louis, Missouri, U.S.A.*

(*Received* 5 *June* 1950)

Molybdenite (MoS_2) is hexagonal. The basal cleavage (0001) is perfect and the hardness lies between 1 and 1·5, according to the sample. Optically, the mineral is uniaxial, negative:

$$\omega = 4{\cdot}336 \pm 0{\cdot}007, \quad \epsilon = \pm 2{\cdot}03, \quad B = \pm 2{\cdot}300.$$

Although molybdenite is considered opaque in visible light, it is particularly transparent in infra-red and near infra-red light above 7500 A. This property has made possible the complete optical study of the mineral by the use of photoelectric and electronic devices (Bailly, 1938, 1947, 1948*a*, *b*). The use of the infra-red image-converter eyepiece adapted to the polarizing microscope is especially suitable for examination in parallel or convergent light. Molybdenite is so transparent in infra-red light that sections half a millimeter thick can be examined.

In parallel infra-red light, without an analyzer, a large number of sections (0001), 0·02–0·5 mm. thick, showed numerous and at first sight unorientated cracks. However, in some carefully cleaved sections, observed under medium magnification, clear and neat hexagonal figures appeared. Some figures showed concentric hexagons (Fig. 1); the non-concentric hexagons had their similar edges parallel (Fig. 2).

In addition to the irregular cracks, some sections presented a lattice of rectilinear cracks which included angles of 60° (Figs. 3, 4) and were parallel to the edges of the hexagonal figures when some of these figures were present (Fig. 5).

A possible explanation of the appearance of the hexagonal cracks is that they are due to a prismatic, vertical cleavage. Since the (0001) cleavage sheets have no elasticity and the hardness of the mineral is very low, the crystals are broken by deformation in numerous irregular fractures which conceal the few prismatic cleavages. Consequently, the prismatic cleavage is observed megascopically with difficulty. Only one specimen among those studied clearly showed the prismatic cleavage in visible reflected light (Fig. 6).

References

Bailly, R. (1938). *Bull. Acad. Belg. Cl. Sci.* **12**, 791.

Bailly, R. (1947). *Bull. Soc. franç. Minér.* **70**, 49.

Bailly, R. (1948*a*). *Amer. Min.* **33**, 519.

Bailly, R. (1948*b*). *Science*, **108**, 143.

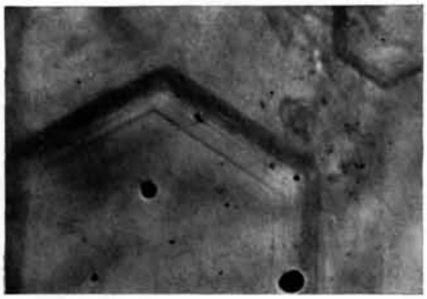

Fig. 1. Concentric hexagonal figures.

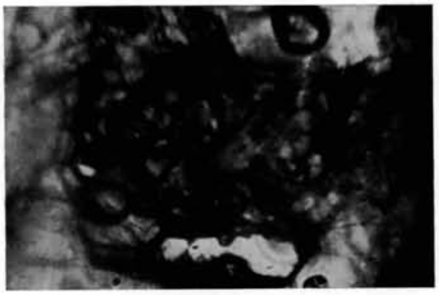

Fig. 2. Hexagonal figures.

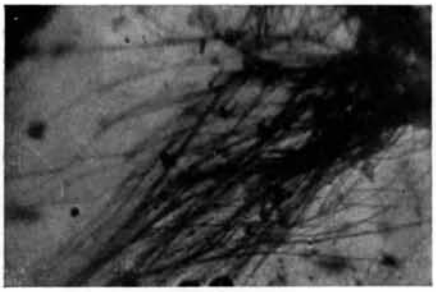

Fig. 3. Cleavages at 60°.

Fig. 4. Cleavages at 60°.

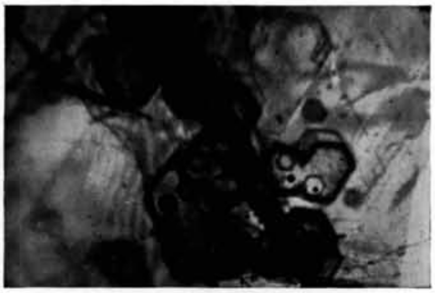

Fig. 5. Cleavages and hexagonal figures.

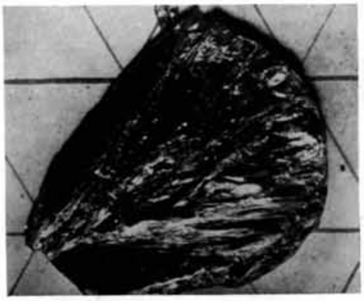

Fig. 6. Megascopic appearance of the prismatic cleavages.