electron densities, just as the synthetic vector maps in the reduced form in which they are more readily calculated refer to deviations from the level of medium in S. Since $\bar{g}$ and m may differ, it is necessary to take account of a possible difference in level when comparing synthetic and experimental vector maps as also to bear in mind the scales of the two maps.

The importance of focussing attention on the crystal reduced to the level of the medium is apparent, when synthetic maps are under construction. However, this procedure has a crucial significance in the interpretation of experimental vector maps in general. For suppose a vector map such as B or D, but at the level corresponding to $w_v = 0$, has been obtained by calculation from observed intensities, with $I(000)$ taken to be zero. How will the presence of the 'molecule' be detected? Comparing the vector map with the vector map of the molecule (shown between A and C) we see that not even in the neighborhood of the origin is the experimental map symptomatic of the molecule, however its level be adjusted. Such an experimental vector map is not the vector map of the crystal comprising only the molecule or molecules, since to every entry in S_v, vectors from every point in the unit cell make a contribution. No approximation to the vector map is obtained when the medium is neglected. Correspondingly, if it is claimed that some particular structure in a protein hydrate is detected from an experimental vector map, the claim can only be substantiated in terms of the proposed structure reduced to the level of the medium, not in terms of the proposed structure.

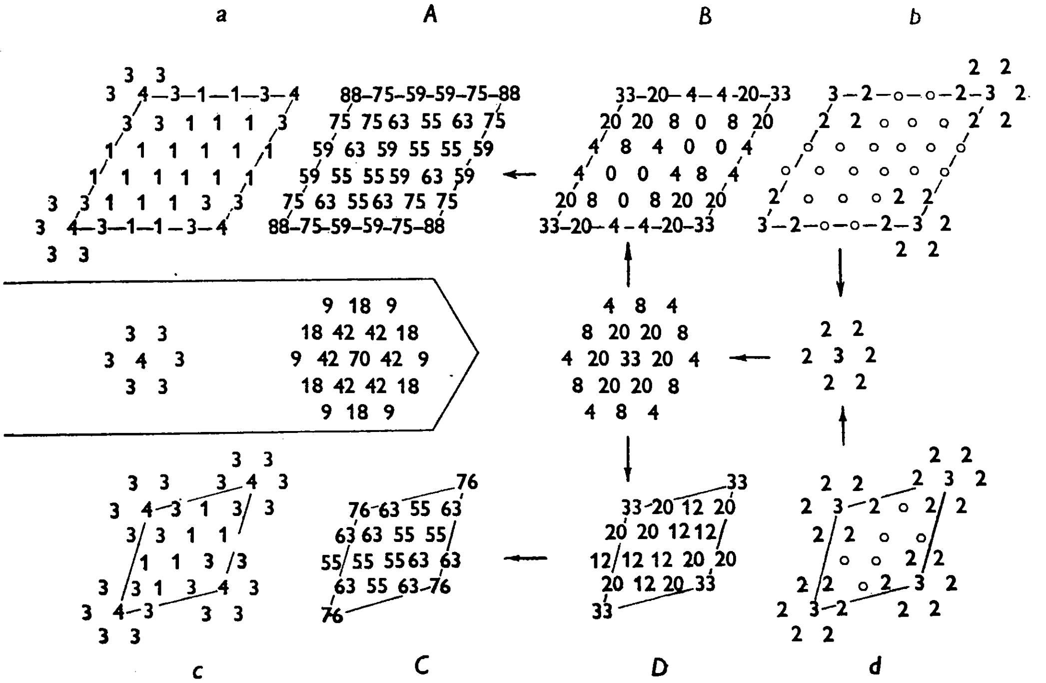

Fig. 1.

There are two practical results of these findings: (1) In the study of the language of vector space, which would seem to be a necessary preliminary to the interpretation of experimental vector maps of proteins, the focus of interest is reduced structures represented by entries of both signs. (2) When the crucially important intensities observed in X-ray studies of proteins are recorded in the form of vector contour maps, the topology of the positive and negative regions forms an integrated whole. It may then be suggested that negative contours, as well as positive contours, be recorded in such maps.

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The unit cell and space group of ammonium metavanadate, NH_4VO_3.

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The crystal chemistry of the vanadates is of interest because of the possibility of the existence of a series of framework structures analogous to those of the silicates. Ketelaar (1936) has shown that the oxide, V_2O_5, is built of vanadium–oxygen tetrahedra which are linked by the sharing of three oxygen atoms of each tetrahedron by two vanadium atoms. This would be the analogue of SiO_2 where the tetrahedra share all four oxygen atoms. Sørum

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(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:

$$a_0=4\cdot96,\quad b_0=11\cdot82,\quad c_0=5\cdot63\,\text{A.};$$
$$a:b:c=0\cdot420:1:0\cdot476.$$

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

Assuming the density to be $2\cdot326\,\text{g.cm.}^{-3}$, as reported by Mellor (1947, p. 758), the number of formula weights per unit cell can be calculated:

$$z=\frac{V\rho}{1\cdot6502\times\text{M.W.}}=\frac{4\cdot96\times11\cdot82\times5\cdot63\times2\cdot326}{1\cdot6502\times116\cdot99}=3\cdot97\sim4.$$

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_{2h}^{11}–$Pbcm$ 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.

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Prismatic cleavage of molybdenite.

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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:

$$\omega=4\cdot336\pm0\cdot007,\quad \epsilon=\pm2\cdot03,\quad B=\pm2\cdot300.$$

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).

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