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Unit cell and space group of the carbide Fe_2MoC.

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The carbide described by Kuo (1953) as M_aC_b is probably identical with an iron–molybdenum carbide referred to by Lashko & Nesterova (1951) and by Habraken (1954). Kuo (1956) gave interplanar spacings but otherwise there are no previously published crystallographic data. It has now been established by the analysis of residues separated by electrolysis from suitably treated steels that the chemical composition is Fe_2MoC.

The carbide is obtainable only as a finely divided powder, and the unit-cell and lattice parameters have been determined from interplanar spacings using photographs from quadruple focusing and cylindrical powder cameras. An internal standard was used to correct the spacings and on the basis of these measurements it was established that an orthorhombic unit cell would account for all the spacings. The following lattice parameters were determined:

$$a_0 = 16{\cdot}27_6 \pm 0{\cdot}02,\quad b_0 = 10{\cdot}03_4 \pm 0{\cdot}01,\quad c_0 = 11{\cdot}32_3 \pm 0{\cdot}01\ \text{Å}\,.$$

The only systematic absences are odd values of l for $00l$ spacings. This indicates the space group $P222_1$ (D_2^2 — No. 17).

The process of indexing was materially assisted by recognition of certain similarities with the powder pattern of cementite. The b cell dimensions of the two structures appear to be related and this cell dimension in the new carbide is almost exactly double that of cementite. An explanation of the relationship between the cementite lattice and α iron has been proposed elsewhere (Andrews, 1963), and it may be that the new carbide is similarly related in a manner which involves close-packed straight or zigzag rows of atoms parallel to the cube diagonal or the carbide b axis respectively. Further work will aim to establish the mutual orientation of the two carbides completely and this should provide information which will assist the determination of atomic positions.

Confirmation of the unit cell of Fe_2MoC has been obtained from electron-diffraction patterns. Some of these patterns show systematic absences which might be taken to indicate a body-centred lattice. The effect has also been noted for cementite by Beattie (1961) who used the term ‘spurious extinctions’ since they do not occur in every orientation. Although two modifications of each structure are not entirely ruled out, it appears more likely that this is an electron-diffraction phenomenon.

A table of interplanar spacings is being submitted for inclusion in the X-ray Powder Data File and further details of the metallurgical aspects will be published elsewhere.

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Comment on three proposed hydrate structures.

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In the course of preparing a review of hydrate structures (Clark, 1963), some anomalies in three proposed structures were discovered. The present note records these features, but no further study of the structures is planned by the present author. The three structures are those for potassium sodium DL-tartrate tetrahydrate, $KNaC_4H_4O_6.4H_2O$ (Sadanaga, 1950), strontium formate dihydrate, $Sr(HCOO)_2.2H_2O$ (Galigné & Falgueirettes, 1961), and lithium acetate dihydrate, $LiCH_3COO.2H_2O$ (Amirthalingam & Padmanabhan, 1958).

The potassium sodium DL-tartrate tetrahydrate crystals are triclinic $P\bar{1}$, with two formula units per cell. In general the reported structural characteristics are reasonable. The tartrate molecules are joined in pairs by two hydrogen bonds parallel to the **b** direction, one bond between adjacent carboxyl oxygen atoms (2·52 Å) and one between tartrate hydroxyl groups (2·73 Å).

There are two abnormally short distances involving tartrate oxygen atoms that are not noted by Sadanaga. The first is a separation of 2·11 Å between carboxyl oxygen atoms O(1) and O(2) of one tartrate molecule, and the second is a 1·93 Å distance between a carboxyl oxygen atom O(2) of one molecule and a hydroxyl group OH(6) of a paired molecule.

The sodium cation is described as six-coordinated by three water molecules, one carboxyl oxygen atom plus one hydroxyl group from a tartrate group, and one carboxyl oxygen atom from a second tartrate group. Two additional somewhat distant neighbors were not mentioned by Sadanaga. One of these is oxygen atom O(2)

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