6. Conclusions and discussion

Only one of the three crystal forms of human haemoglobin is suitable for detailed analysis. This has two molecules related by a screw dyad in a monoclinic unit cell. The two molecules appear to be very nearly parallel to each other and centred approximately at $\pm(x = 0{\cdot}225, y = 0{\cdot}25, z = 0{\cdot}20)$. The peaks near the origin in two of the Patterson projections closely resemble those in corresponding projections of horse haemoglobin and suggest similarities in the molecular structure of the two proteins. The resemblance is particularly striking in the projections on (100), which correspond to the end-on view of the vector chains in the three-dimensional Patterson. An attempt was made to interpret this projection as being due to two identical sets of electron-density peaks, representing close-packed chains viewed end-on, displaced by the intermolecular vector p. Success was only partial: our assumed structure accounted for the positions and relative heights of all the Patterson peaks except one, which remained entirely unexplained. It seems difficult to make further progress with this projection until the electron density is determined directly by the isomorphous-replacement method (Green, Ingram & Perutz, 1954).

Even the very limited interpretation of the Patterson projections presented here involves difficulties which are hard to resolve at this stage. For instance, if the haemoglobin molecule were a completely asymmetric object, parallelism of two such molecules related by screw dyads would have no meaning. In that case the similarity of self-Patterson and cross-Patterson, which appears in two projections of form II, would have a more complex interpretation than the one given. On the other hand, if human reduced haemoglobin had dyad symmetry, as human oxy- and methaemoglobin are known to have, and if the molecular dyads were parallel to the b axes of the crystal, as the similarities of the Patterson projections on (100) of human and horse haemoglobin seem to indicate, then the self- and cross-Pattersons would have to be identical and peak p would be considerably higher than is observed. The fact that this is not so suggests either that in the reduced form the dyad symmetry of the molecule is only approximate, or else that the dyads of the two molecules in the unit cell are not strictly parallel. None of these points can as yet be decided.

So far there is nothing in the results which would explain why reduced haemoglobin crystallizes differently from oxy-, carboxy- and methaemoglobin.

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Short Communications

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 500 words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible; and proofs will not generally be submitted to authors. Publication will be quicker if the contributions are without illustrations.

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The lattice of rhombohedral sulfur. By J. D. H. Donnay, *The Johns Hopkins University, Baltimore* 18, *Maryland, U.S.A.*

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Frondel & Whitfield (1950) established Laue class $\bar{3}$ from a Weissenberg [0001] zero layer. They used the morphology (hexagonal prism $11\bar{2}0$ and rhombohedron $10\bar{1}1$) to rule out point group 3 and establish point group $\bar{3}$ (Groth's 'rhombohedral' crystal class). The lattice mode could not be deduced from the X-ray photographs available to them.

The indices of the crystal forms obey the criterion '$(2h+k+l)$ divisible by 3', so that on purely morphological grounds the lattice is rhombohedral, the space group is uniquely determined as $R\bar{3}$, and the cell given in hexagonal co-ordinates ($a = 10{\cdot}9$, $c = 4{\cdot}26$ kX., $Z = 18$) is a triple cell. The smallest cell is given by $a_{\text{rh.}} = 6{\cdot}45$ kX., $\alpha = 115°\ 18'$, $Z = 6$. In the name 'rhombohedral sulfur', the adjective rhombohedral may well be taken to refer to the lattice mode.

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