

fourth-order tensor pq ($p, q = 1, 2, 3, 4, 5, 6$) in all trigonal and hexagonal groups: an higher order tensor is treated elsewhere (Fumi, 1952*b*). The equations of invariance for symmetry C_3 are obtained in Table 2: for instance, the equation for the z^2yz component reads $z^2yz = -\frac{1}{2}\sqrt{3}z^2xz - \frac{1}{2}z^2yz$. Direct inspection of the common scheme for symmetry C_3 (Table 3) gives the schemes of the polar and of the axial tensor pq for symmetries $C_{3v}(\sigma_v, x \rightarrow -x, y \rightarrow y, z \rightarrow z)$ and $C_{3h}(\sigma_h, x \rightarrow x, y \rightarrow y, z \rightarrow -z)$; for the polar tensor, the independent components for symmetry C_3 which are odd in x or in z vanish in C_{3v} and in C_{3h} respectively, while for the axial tensor these components are the only non-vanishing ones. Direct inspection of the common scheme for symmetry C_6 yields in a similar fashion the schemes for symmetry C_{6v} , and direct inspection of the common scheme for symmetry D_3 provides the scheme of the axial tensor for symmetry D_{3h} . The independent components of the axial tensor coincide with those of the polar tensor for symmetry D_6 , as for the other groups which do

not contain improper rotations (Fumi, 1952*a*). The independent components of the polar tensor are the same in symmetry groups which differ by the inversion (Fumi, 1952*a*).

The results for the polar tensor pq can be compared with the schemes of photoelastic constants (Szivessy, 1929; Bond, 1943; Mason, 1950; for C_3, C_{3i}, C_{3h}, C_6 and C_{6h} see, however, Bhagavantam, 1942).

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Globulite units in protein crystals?* By DOROTHY WRINCH, *Department of Physics, Smith College, Northampton, Mass., U. S. A.*

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It has recently been remarked (Wrinch, 1952*a*) that certain findings regarding residue numbers favor the possibility that the horse hemoglobin and myoglobin structures and the insulin and ribonuclease structures are particles made up of various complements of molecules in various arrays, all the molecules having skeletons of NCC polymers of similar type. In this note we study this hypothesis in the light of certain intensity data obtained in X-ray crystal studies which are recorded in the literature (Perutz, 1949; Boyes-Watson, Davidson & Perutz, 1947; Kendrew, 1950). In particular we look for evidence for or against the hypothesis (Wrinch, 1937) that such skeletons, if present, are globulite (and indeed cage-like) in character, not differing grossly in dimensions in various directions.

For the monoclinic horse methemoglobin crystal, the mean intensity curve as a function of distance from the origin (Perutz, 1949) and the $(h0l)$ intensities (Boyes-Watson *et al.*, 1947) are recorded. To test the globulite hypothesis, or any other hypothesis as to shape, it is of course fruitless to study the mean intensity curve in isolation. However the $(h0l)$ intensities throw light on the situation, when studied in conjunction with it. Perutz's (1949) mean intensity curve (small curve in Fig. 1) represents the *spherical smoothing* of all the intensities. Let us then construct, from the $(h0l)$ intensities, the mean intensity curve as a function of distance from the origin, thus *circularly smoothing* these co-planar intensities (last curve of Fig. 1). We remark that sufficiently far from the origin there is a general resemblance between the two curves. Both descend from relatively high values to a minimum at $c. 0.17 \text{ \AA}^{-1}$ and both subsequently develop a maximum at $c. 0.22 \text{ \AA}^{-1}$. So far as it goes, this situation is in accord with the hypothesis that the

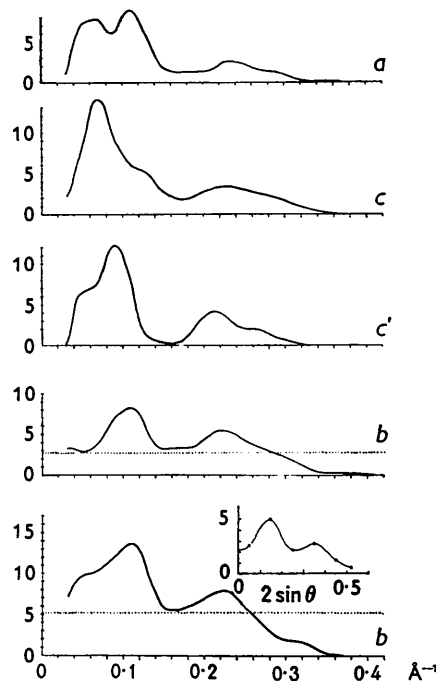


Fig. 1. Inset curve: Perutz's mean intensity curve for the horse methemoglobin crystal as a function of distance from the center (Perutz, 1949). Lowest curve: the circularly smoothed intensity function for the same crystal, calculated from the given $(h0l)$ intensities (Boyes-Watson *et al.*, 1947). Upper four curves: the circularly smoothed intensity functions for the horse myoglobin crystal calculated from the given intensities on central planes normal to a , c , c' and b respectively (Kendrew, 1950).

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units, if present, are globulite in character. Even more interesting, because of their rather wider scope, are the corresponding curves obtained by circularly smoothing the four sets of intensities on planes through the origin recorded for horse myoglobin. For this monoclinic crystal, intensities in central planes normal to a , to b , to c and to c' $[20\bar{1}]$ are given (Kendrew, 1950). Again we obtain curves with the characteristics mentioned, the curves being arranged with the 'a' curve first in Fig. 1 with the smallest maximum at $c. 0.22 \text{ \AA}^{-1}$ and the 'b' curve fourth in Fig. 1 with the largest such maximum. The general resemblance of the myoglobin curves *inter se*, once a sufficient distance from the origin is reached, certainly favors the idea of globulite units in this protein crystal. The relation of these four curves to the two for the hemoglobin crystal suggests that there may be globulites of the same type in both crystals (Wrinch, 1949). To facilitate the comparison for the two crystals of the circularly smoothed intensities in the central plane normal to the dyad axis, the average value of the intensities is shown by a dotted line.

Actually, however, structures of the classical type have been proposed for both these crystals. Thus, for the hemoglobin parallel polypeptide chains in the a direction are postulated, with a 5 \AA periodicity along their lengths (Boyes-Watson *et al.*, 1947). It is difficult to see how a geometrically polar structure of this type can be reconciled with the circularly smoothed intensity curve which has been calculated, particularly in view of the

fact that the intensities responsible for the maximum at $c. 0.22 \text{ \AA}^{-1}$ lie in various directions from the origin (Boyes-Watson *et al.*, 1947). For the myoglobin crystal parallel polypeptide chains in the c' direction are postulated, again with the 5 \AA periodicity. It seems improbable that the sequence of four curves shown can be reconciled with this structure.

Viewed, however, in the light of the globulite hypothesis, the set of curves seems readily interpretable, at least in outline (Wrinch, 1946, 1952*b*), in terms of a water medium containing protein structures composed of arrays of globulite cage-like skeletons, in different numbers, in different positions and differently substituted in the two crystals. This matter is now under detailed study.

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The crystal structure of isopalmitic acid. By E. STENHAGEN, *Medicinsk-Kemiska Institutionen, The University, Uppsala, Sweden*, V. VAND* and A. SIM, *Chemistry Department, The University, Glasgow W. 2, Scotland*

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The structure of iso-fatty acids is of interest because of their biological importance. Long-spacing measurements for some of these acids are reported by Velick (1947) and Arosenius, Ställberg, Stenhagen & Tägtström-Eketorp (1948). Single-crystal data are given by Clark & Chu (1951).

Crystals of iso-palmitic acid, m.p. $61.5\text{--}61.6^\circ \text{ C.}$, were grown from light petroleum as thin, elongated plates with well developed $\{001\}$ faces. All the crystals were found to be twinned in one way or other on the (001) plane, which suggests that twinning provides an essential mechanism of growth of crystals of this compound.

Some crystals simulated single crystals in their outward shape and also by showing complete extinctions in polarized light, but they also proved to be twins on (001) with one half having an opposite angle of tilt of the molecules. Twinning at first confused the interpretation of the X-ray photographs and an erroneous large unit cell was postulated. By splitting the twins in half parallel to (001), however, true single crystals were finally obtained on which the determination was based.

Caution is therefore needed in interpreting any single-crystal data of long-chain compounds which appear to

show an unduly large unit cell, as twinning might be responsible for misinterpretation of the results.

The following data were obtained from rotation, oscillation, zero- and n -layer Weissenberg photographs, using Ni-filtered $\text{Cu } K\alpha$ radiation:

Molecular formula, $\text{C}_{16}\text{H}_{32}\text{O}_2$. Molecular weight, 256.41. The crystal is triclinic with

$$\begin{aligned} a &= 5.09, \quad b = 5.68, \quad c = 48.1 \text{ \AA}, \\ \alpha &= 140.0^\circ, \quad \beta = 111.1^\circ, \quad \gamma = 72.7^\circ; \\ d(001) &= 30.20 \text{ \AA}. \end{aligned}$$

Two molecules per unit cell. Density calc. = 1.020 g.cm.^{-3} . Density meas. = 1.012 g.cm.^{-3} . No systematic absences. Space group, $P1$ or $P\bar{1}$; Fourier projection indicates $P\bar{1}$.

Intensities of reflexions were measured visually, using the multiple-film technique. Normal Lorentz and polarization factors were applied to obtain structure factors, absolute values being obtained at a later stage by comparison with calculated structure factors. The scattering curve for carbon and oxygen is that used by Vand, Morley & Lomer (1951) for lauric acid. The (010) reflexion is very strong, and the (020) fairly strong, indicating the orientation of the plane of the chain along the c axis in the

* I.C.I. Research Fellow.