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 Å^{-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 axid, 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 Å 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 Å^{-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 Å 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.

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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. 61·5–61·6° 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 Cu $K\alpha$ radiation:

Molecular formula, $C_{16}H_{32}O_2$. Molecular weight, 256·41. The crystal is triclinic with

$$a = 5{\cdot}09,\ b = 5{\cdot}68,\ c = 48{\cdot}1\ \text{Å}\,,$$
$$\alpha = 140{\cdot}0^\circ,\ \beta = 111{\cdot}1^\circ,\ \gamma = 72{\cdot}7^\circ;$$
$$d(001) = 30{\cdot}20\ \text{Å}\,.$$

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

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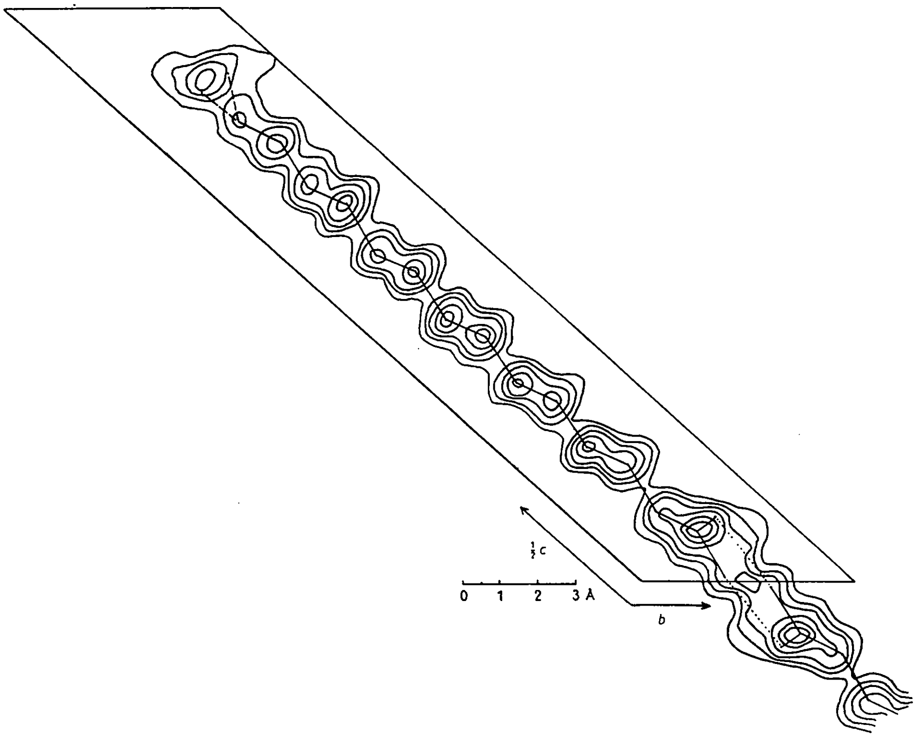

Fig. 1. Isopalmitic acid, projection along the *a* axis.

b c projection. Combining this with the known structure of lauric acid approximate co-ordinates were obtained, and the location of the atoms was helped by the fact that the (0,3,36) reflexion is strong.

A Fourier projection along the *a* axis has been prepared and good resolution of most of the atoms has been obtained. The projection is shown in Fig. 1, and the co-ordinates obtained from it are given in Table 1. The figure of merit based on these co-ordinates is 29%.

Table 1. *Atomic co-ordinates*

Atom	y/b	z/c	Atom	y/b	z/c
OH	0·421	0·0058	C_8	0·453	0·2284
C_1	0·514	0·0450	C_9	0·553	0·2725
O	0·681	0·0583	C_{10}	0·461	0·2858
C_2	0·421	0·0608	C_{11}	0·580	0·3314
C_3	0·540	0·1017	C_{12}	0·481	0·3445
C_4	0·453	0·1182	C_{13}	0·594	0·3845
C_5	0·533	0·1575	C_{14}	0·493	0·4030
C_6	0·461	0·1750	C_{15}	0·487	0·4260
C_7	0·540	0·2143	C_{16}	0·701	0·4430

The terminal branched group is poorly resolved in this projection and therefore the corresponding co-ordinates are uncertain. It will be necessary to use other projections, probably combined with difference syntheses, to obtain more accurate co-ordinates.

The angle of tilt, τ, between the chain axis and (001) has been obtained from the average difference of z co-ordinates between alternate carbon atoms and also from the increment of long spacings, 1·776 Å, calculated by least-squares from powder data of Arosenius *et al.* (1948). The two methods give $\tau = 43°$ and 45° respectively. As the calculation assumes the distance between alternate carbon atoms to be 2·52 Å, as found in lauric acid, and as this might vary from compound to compound, the above figures should be regarded as provisional.

They show, however, sufficiently clearly that the chain of isopalmitic acid is more tilted to the (001) plane than that of any known form of straight-chain fatty acid. The reason for this can readily be understood by considering the comparatively large volume of the terminal branched group; the molecule must find such an angle that the shorter axes of the unit cell expand sufficiently to accommodate the volume of the branched group.

We wish to thank Prof. J. Monteath Robertson for his great interest in this investigation.

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