tetragonal transition of NH_4NO_3, where maxima of about 2° C. occurred. It was noted that the transition toward the high-energy form provides a more reliable temperature point than does the transition in the opposite direction. The transition points of these crystals as determined by other investigators are listed in Table 2.

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Length of central bond in thiophthen.

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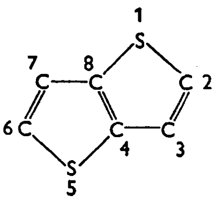
Calculations by Evans & de Heer (1949) on the bond lengths in thiophthen, assuming that the σ-bond system is free from strain, lead to a length for the bond 4–8 which is greater than the experimental value (Cox, Gillot & Jeffrey, 1949) by $\sim 0{\cdot}05$ A. The experimental X-ray study of thiophthen, carried out by Cox *et al.* (1949), shows, however, that the angles 1–8–7 and 3–4–5 are about 135°; and this means that it cannot be correct to neglect strain in the σ skeleton when calculating the equilibrium bond lengths. We shall here calculate the effect of this strain on the length of bond 4–8, assuming that the natural values of angles 1–8–7 and 3–4–5 are 120°.



To a first approximation the bond 4–8 bisects externally both the angles 1–8–7 and 3–4–5, and the bond lengths 4–8, 1–8, 8–7, 3–4 and 4–5 may be assigned the common value l_0.

Consider the system of bonds at atom 8. Then if g denotes the mean force constant for distortion of the angles at this atom, and if ϕ denotes the angle 1–8–7, the potential energy due to angular strain at atom 8 is given by

$$\begin{aligned} V_{\text{strain}} &= \tfrac{1}{2}g\{(\phi-\tfrac{2}{3}\pi)^2+(\tfrac{1}{3}\pi-\tfrac{1}{2}\phi)^2+(\tfrac{1}{3}\pi-\tfrac{1}{2}\phi)^2\} \\ &= \tfrac{3}{4}g(\phi-\tfrac{2}{3}\pi)^2. \end{aligned}$$

Denote by $2G$ the force in the central bond required to keep the angle 1–8–7 at its value ϕ. Then the work done by this force when 1–8–7 increases by $\delta\phi$ is

$$2G\delta(l_0\cos\tfrac{1}{2}\phi) = -Gl_0\sin\tfrac{1}{2}\phi\,\delta\phi.$$

Therefore in equilibrium

$$Gl_0\sin\tfrac{1}{2}\phi\,\delta\phi = \delta V_{\text{strain}} = \tfrac{3}{2}g(\phi-\tfrac{2}{3}\pi)\,\delta\phi,$$

so that

$$G = \frac{3g(\phi-\tfrac{2}{3}\pi)}{2l_0\sin\tfrac{1}{2}\phi}.$$

Now denote by f the force constant of the bond 4–8. Then, if l is the equilibrium length of this bond, we have

$$f(l-l_0) = -2G.$$

Therefore, eliminating G, we obtain

$$(l-l_0) = -\frac{3g(\phi-\tfrac{2}{3}\pi)}{fl_0\sin\tfrac{1}{2}\phi}.$$

A reasonable choice of values for f and g is

$$g = 0{\cdot}7\times10^{-11}\ \text{dyne/radian},\quad f = 7{\cdot}0\times10^{5}\ \text{dynes/cm.};$$

and from the X-ray study $\phi \doteqdot \tfrac{3}{4}\pi$, $l_0 \doteqdot 1{\cdot}4\times10^{-8}$ cm. Therefore

$$l-l_0 = -\frac{3\times0{\cdot}7\times10^{-11}\times\tfrac{1}{12}\pi}{7{\cdot}0\times10^{5}\times1{\cdot}4\times10^{-8}\times\sin\tfrac{3}{8}\pi} = -0{\cdot}06\times10^{-8}\ \text{cm.}$$

We conclude that the effect of strain in the angles 1–8–7 and 3–4–5 is to shorten the central bond 4–8 by about 0·06 A.; and this brings the calculated bond lengths into line with those determined experimentally by Cox *et al.*

The author is much indebted to Professor M. G. Evans and Dr Jeffrey for drawing his attention to the present problem.

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A note on the diffraction patterns of crystalline proteins.

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Certain structures, C_n, have been proposed as models for the skeletons of native protein molecules (Wrinch, 1937). Before this hypothesis can be tested against X-ray diffraction data, the transforms of such structures into reciprocal space S^* must be investigated. In this note we take a preliminary step in this direction and demonstrate that all the C_n structures have certain common properties in S^*, whether or not some or all the residues in the tetrapeptides are deleted (Wrinch, 1948*a*).

All the skeletons place the N, C, C atoms of their amino-acid backbones at points of a diamond network, typified by points with cubic co-ordinates $\bar{1}\bar{1}\bar{1}$, $00\bar{2}$, in the scale k: a reasonable value of the metric of the network, $a = k\sqrt{3}$, is *c.* $1\frac{1}{2}$ A. First we replace the atoms by point atoms; there result sets of 'weights' on the diamond network. As previous studies have shown (Wrinch, 1946), for any set of weights on a lattice L in 'atomic' space S, the transform T in S^* is periodic; its lattice is L^*, the lattice reciprocal to L. Choose for L the coarsest possible lattice, the body-centered cubic lattice (000, 111), and the finest possible lattice for T results; it is the face-centered cubic lattice (000, $\frac{1}{2}\frac{1}{2}0$) in the scale $k^* = 1/k$.

How then is it indicated in S^* that the atomic nuclei of the skeletons are further restricted, to the diamond network? The answer to the question emerges (Wrinch, 1946) when we remark the values of T at the *non-lattice points* $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{3}{4}, \frac{3}{4}, \frac{3}{4}$, namely, $\bar{p}_0 + ip_1$, $p_0 - p_1$, $\bar{p}_0 - ip_1$, where p_0 and p_1 are the proportions in which the total weight is divided between the two face-centered lattices with the common translation 220, L_0 with origin at, say, $00\bar{2}$, L_1 with origin at, say, $\bar{1}\bar{1}\bar{1}$. Such points are on the body-centered cubic lattice reciprocal to the face-centred cubic lattice (000, 220); hence the par values of the amplitudes of the p_0 and p_1 terms: the origins of L_0 and L_1 lie on submultiple lattice points with one-half and one-quarter the displacements; hence the periodicity of the phases of these terms only in larger cells, with displacements two and four times as large.

As p_0/p_1 varies, there is nothing distinctive about the point $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$. But at the other points characteristic features emerge, namely values of $|T|$ at least as large as $\frac{1}{2}\sqrt{2}$. For the C_n point sets, with or without their tetrapeptides, $p_0 = p_1$ and $|T|$ has maxima of height $\frac{1}{2}\sqrt{2}$ at such points. For intermediate cases, when some of the residues in the tetrapeptides are absent, there are only negligible changes in the positions and heights of the maxima. Distinctive characteristics in S^* for all such structures have therefore been found. Whether T is T_C, the transform of the carbon point atoms, or T_N, the transform of the nitrogen point atoms, or $T_C + T_N$, T is a periodic function with par values at a lattice of 'primary' peaks, and there are also 'secondary' peaks at which $|T| \sim \frac{1}{2}\sqrt{2}$. For the first, reciprocals of the distances from the origin are *c.* $\frac{1}{2}$A. $\sqrt{6}(1, \frac{1}{2}\sqrt{2}, \frac{1}{3}\sqrt{3}, \frac{1}{2}, \ldots)$, for the second *c.* 2A. $(1, \frac{1}{11}\sqrt{(33)}, \frac{1}{19}\sqrt{(57)}, \frac{1}{3}, \ldots)$.

We now reinstate the atoms. The transform is $T_C f_C + T_N f_N$. Despite the atomic scattering factors, which destroy the periodicity of the transform, the primary and secondary peaks persist at points little displaced in position, though their heights are 'damped'. Thus for the peaks nearest to the origin, $|T|$ is now *c.* $\frac{1}{5}\sqrt{2}$.

The entries on the intensity map of a crystalline protein are made up of contributions from the skeletons, the R-substituents and the waters. Subject to the discussion of possible small systematic deviations of atoms from network positions, it is here predicted that the contributions of the molecular skeletons have maxima at certain points far out from the origin. It seems unlikely that the R-groups or waters make appreciable contributions at these points. If this is the case, the prediction would say that the intensity maps of the crystals should show the maxima described, always of course taking into account the contributions of all the atoms to the intensity at the origin. So far no published studies record intensities so far out as any of the points. It may be emphasized that the prediction specifies not only the distances of the points from the origin, but also the directions relative to the postulated C_n skeletons. The crystal classes of the various crystalline proteins suggest the probable orientations therein of structures associated with diamond networks if present (Wrinch, 1948*b*), and so also the directions in which the search for the predicted intensity maxima may be begun.

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Notes and News

Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. Copy should be sent direct to the British Co-editor (R. C. Evans, Crystallographic Laboratory, Cavendish Laboratory, Cambridge, England).

International Union of Crystallography

The Executive Committee has accepted a kind invitation from the Swedish National Committee of Crystallography to hold the Second General Assembly and International Congress in Stockholm from 27 June to 3 July 1951. These dates have been chosen in consultation with the Swedish National Committee and with the National Committee of all the Adhering Bodies. It is hoped that this early notice will make it possible for crystallographers throughout the world to arrange to attend.

Further particulars of the meeting will be given from time to time in these columns and elsewhere.

International Tables: offprints in quantity

The *International Tables* Commission announces that it is hoped that arrangements can be made with the printer of the *International Tables* for the supply of offprints of sets of separate tables likely to be useful for class work or for continuous laboratory reference. These would be sold in quantities of not less than 25 at a time and would vary in size from 3 to 127 pages. The price for a 7-page offprint ($8\frac{1}{4} \times 11$ in.), with title-page extra but no cover, would be of the order of $2 post free for 25, and *pro rata* for larger quantities. A grey board cover would add about $1.50 per 25.