unit cell. It is, however, easily understood *in relation to the dimensions of the unit cell of the parent substance*, the anthracene photo-oxide (now called POA).

The derived A:A has a variable composition but usually consists of a higher proportion of anthraquinone than of anthrone. Its b axis, although very different in length (for POA, $b=5{\cdot}86$ Å) exactly coincides in direction with that of the parent POA. The unit-cell relationships in (010) are as follows

	a	c	β
POA	15·94 Å	11·43 Å	108·2°
A:A	15·82	7·88	102·2

The a of A:A is inclined at about 2° in obtuse β to that of POA.

The consequences of these relationships are that [101], [001] of POA almost coincide in direction with [10$\bar{2}$], [104] of the (001) twin individual A:A, and there are also very close numerical relationships as follows (Fig. 4) between their dimensions.

$$\left\{\begin{array}{ll} OD = 16{\cdot}46\ \text{Å} & OM = 49{\cdot}15 = 3 \times 16{\cdot}38\ \text{Å} \\ \angle DOA_1 = \angle DOA - 2^\circ = 39{\cdot}3^\circ & \angle POM = 38{\cdot}8^\circ \end{array}\right.$$

$$\left\{\begin{array}{ll} OC = 11{\cdot}43\ \text{Å} & ON = 32{\cdot}14 = 3 \times 10{\cdot}71\ \text{Å} \\ \multicolumn{2}{l}{\angle COA = 108{\cdot}2^\circ - 2^\circ = 106{\cdot}2^\circ = 180^\circ - \angle COP} \\ \angle COP = 73{\cdot}8^\circ & \angle A_1ON = 73{\cdot}5^\circ \end{array}\right.$$

These relationships of course involve others, but these are sufficient to prove that the existence of this twin (and of the doubly twinned individual $OC_2D_4A_4$ shown in Fig. 1) is not due to any direct relationship with $OA_1D_1C_1$ or with $OC_2D_2A_2$, but that *it is the consequence of decomposition from the parent substance* $C_{14}H_{10}O_2$. Apart from the coincidence of b-axial directions, which is due to the particular chemical reaction mechanism involved (Lonsdale, Nave & Stephens, 1966), and the near-equality of length of the a axes (POA 15·94, A:A 15·82 Å), there is little resemblance between the two structures; and it is difficult to see why the a axis of the main A:A individual should be displaced from that of POA by 2°. The geometrical relationships of the (001) twin A:A with the parent POA may provide just the reason required. On the other hand the *reorientation of molecules* necessary to form this twin is greater than that required to form the main A:A individual and this, presumably, is the reason for its lesser importance, although it invariably occurs in the same specimen, sometimes in nearly equal strength, sometimes only to about one-eighth of the strength of the main individual.

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A Simple Method of Setting a Single Crystal on One of its Principal Axes

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In order to mount a small single crystal about one of its principal axes it is mounted on a small mount which can be rotated on the top of the goniometer head of an X-ray Weissenberg camera. A series of oscillation photographs with the Weissenberg screens set at 1·0 cm is taken, and by observing the position of the goniometer head when small angle reflexions appear it is possible to set the corresponding planes parallel to the axis of rotation of the camera.

Many small crystals have no outward indication of the position of the unit-cell axes, and even when there are faces visible it is often necessary to cut a small fragment from a larger one or to grind it into a sphere. There are several suggestions in the literature (Wooster, 1964) about how to proceed in order to orientate such a crystal about a principal axis, but we have found the following method much simpler.

The crystal is mounted on a glass fibre which is supported in a small mount as shown in Fig. 1. The larger hole in the stem is filled with plasticine and the fibre is pushed into it through the small hole. All our goniometer heads were modified many years ago to accept such mounts and the top of the goniometer head has marks every 30° around the circumference of the hole into which the mount fits. A set screw through the side of the hole fixes the mount in any desired orientation with respect to the arcs of the goniometer head. With the screens of the Weissenberg camera set at approximately 1·0 cm apart and with the camera stationary and at one end of its travel an oscillation photograph over (say) 25° is taken from a position where one of the arcs is parallel to the X-ray beam. A few minutes' exposure is sufficient since we are only interested in strong reflexions at low values of θ. The camera is then moved 1·5 cm along to expose a new strip of film and a further oscillation, with 1° overlap from the end of the previous one is taken, and so on until one has covered 180° oscillation. It is an easy matter to observe on the film which range of oscillation has a reflexion at the smallest value of θ. Since we know the approximate position of the goniometer head, with respect to the X-ray beam, when this plane was reflecting, one now turns the small crystal mount so that this plane is approximately parallel to one of the arcs. We also know from the photograph the angle and direction through which to turn the arc perpendicular to the plane to set the plane approximately parallel to the axis of rotation of the camera. Thus we have one large-spacing plane parallel to the axis of rotation and parallel to one of the arcs. If the oscillation photographs which correspond to the position where this plane is approximately *perpendicular* to the X-ray beam are now examined, it is possible to set a second large-spacing plane parallel to the axis of rotation and the final accurate setting can be made by any of the standard methods (*e.g.* that of Weisz & Cole, 1948).

The above process takes very little time and is quite straightforward. It does not necessarily find a unit-cell axis, but since we have two of the planes with large spacings parallel to the axis of rotation it must be simply related to the unit-cell axes and a zero layer Weissenberg photograph usually gives all the information necessary to identify it.

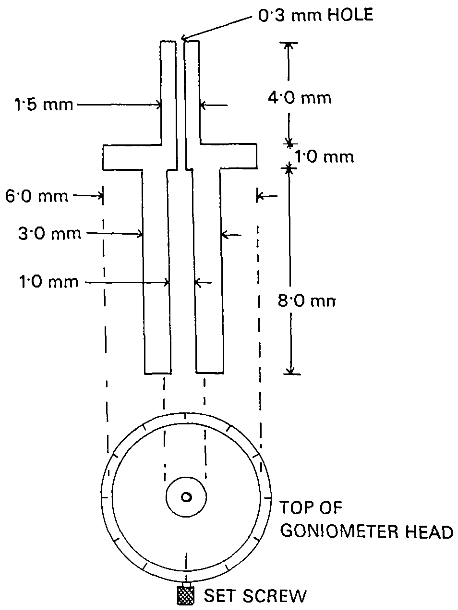

Fig. 1.

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Loi de Distribution des Facteurs de Structure pour une Répartition non Uniforme des Atomes

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To express the fact that atoms cannot overlap, we have used the formalism and the results of the second quantization of a fermion gas. The distribution law of atoms may be written in the form of a square of a probability amplitude. Intervening products of Slater determinants may be expressed as functions of structure factors so that the distribution law becomes a function of structure factors. As an example we have calculated the average of the expression $\langle E_{\mathbf{h}}^2 \,.\, E_{-2\mathbf{h}}\rangle$.

Introduction

La structure d'un cristal est déterminée, dans l'hypothèse des atomes ponctualisés, lorsqu'on connaît les coordonnées ($\mathbf{r}_i$) des atomes à l'intérieur du cristal. S'il y a dans la maille élémentaire N atomes indépendants, la structure dépend de $3N$ paramètres; il revient au même de dire que la structure peut se décrire par les coordonnées d'un point $\mathbf{R}$ dans un espace de configuration à $3N$ dimensions $\{\xi_{3N}\}$ (les coordonnées variant entre 0 et 1, cet espace est un hypercube). La méthode statistique en cristallographie consiste à choisir une loi