method proposed by Ito in that the preliminary grouping of planes in this way makes it possible to study more complicated crystals without having especially accurate $\sin^2\theta$ values. It is further of considerable value in cases where space-group extinctions cause the systematic absence of low-order reflexions from the axial planes. When in monoclinic or orthorhombic crystals the plane of largest spacing has a multiplicity higher than two, this is an immediate indication of the existence of such extinctions.

In certain crystal classes, planes of the same form $\{hkl\}$ do not all have the same numerical value of $|F(hkl)|$, and for example $|F(hkl)| \not\equiv |F(\bar{h}kl)|$, say; hence the intensities of spots on the same ring may differ just as though two different forms $\{h_1k_1l_1\}$ and $\{h_2k_2l_2\}$ accidentally had the same spacing. In practice, however, a general consideration of the multiplicities present would indicate the system to which the crystal belonged, and a study of a few planes of low multiplicity and large spacing should give a unit cell from which the remaining rings can be indexed.

A limited application of the use of multiplicities was recorded by Lipson & Steeple (1951), who found that indications of the value of the multiplicity factor on powder photographs on which the lines were 'spotty' is a useful aid to indexing.

When using the method, we have taken two photographs of each crystal, one in a random orientation and a second exposure for which one arc was altered 55° and the other arc 10° with respect to the first photograph, so that a reasonable amount of the limiting sphere was covered in all, and important planes which might be missed on one photograph would probably appear on the other. Quarter-plate films were used, one about 2·5 cm. from the crystal in order to obtain a large number of reflexions, and one approximately 7·5 cm. from the crystal for more accurate measurement of small θ values. Rotation photographs on flat films are more convenient than those on cylindrical films, since circles can then be drawn through equivalent points.

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Acta Cryst. (1952). **5**, 148

Transformation properties of the physical constants of crystals.

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(*Received* 9 *April* 1951)

Material constants connecting physical quantities in crystals, for instance, the elastic constants, are usually given with respect to an orthogonal co-ordinate system the orientation of which is determined by crystal symmetry. Various methods have been developed to express the material constants proper to an arbitrary co-ordinate system in terms of those above, but the procedures are usually involved (see for example Cady, 1946).

We would like to call attention to a compact method making use of the transformation properties of single co-ordinate products. The method is applicable to transformations between orthogonal co-ordinate systems. Here we need not distinguish between co- and contra-variant quantities.

The material constants connecting two tensors of rank m and n transform essentially like the components of a tensor of rank $(m+n)$. These transformation properties are well known. If the co-ordinates of the same point, referred to two co-ordinate systems, are connected by

$$x'_i = \Sigma R_{ij} x_j, \tag{1}$$

where $\Sigma R_{ij} R_{ik} = \delta_{jk}$, an ordinary tensor transforms like

$$T'_{ij}\ldots = \Sigma R_{is} R_{jt} \ldots T_{st} \ldots. \tag{2}$$

Equation (2) is not affected by symmetry in the tensor indices if the summation is carried out over all possible values of the summation indices.

Each of the tensor indices can have three possible values. Hence we can say that a tensor component transforming according to (2) transforms like the co-ordinate product

$$(x_i)_1 (x_j)_2 \ldots, \tag{3}$$

where the numerical subscripts refer to the position of the various indices of the tensor. We can find $T'_{ij}\ldots$ by using (1) on each co-ordinate appearing in (3), and by then identifying each term in the resultant sum of co-ordinate products with the proper tensor component in the original co-ordinate system.

In principle, it is no more difficult to carry out the transformation of the material constants according to (2) than to identify them with co-ordinate products (3) and then carry out the transformation on these co-ordinate products. But the use of co-ordinate products has some practical advantages.

Tensors representing physical quantities are often symmetric in some indices. This symmetry can be incorporated in the co-ordinate products by using the same numerical subscript on the co-ordinates representing interchangeable tensor indices. Thus, the components of the stress-tensor transform like the products

$$x^2, \quad y^2, \quad z^2, \quad yz, \quad zx, \quad xy; \tag{4}$$

that is, no identifying subscripts are needed.

Since material constants transform like the product of the tensor components they connect, they transform like the products of the co-ordinate products representing the tensor components in question. Any symmetry in the tensor indices can thus be carried over directly into the appropriate parts of the total co-ordinate product. This reduces the number of subscripts of (3) and hence the number of products upon expansion after a transformation. Additional symmetry in the material constants, such as index-pair symmetry, is best included after the transformation has been carried out.

In table 1 we have listed the co-ordinate products corresponding to the most important material constants. In some cases numerical factors (2) enter because of the definition of the strain tensor (Voigt). Of course, the usual index of the material constants which refers to a second-rank symmetric tensor assigns the numbers 1–6 to the six products (4), in the order indicated.

Table 1. *Co-ordinate products*

Dielectric constant (ε)	$(x_i x_j)$
Piezoelectric constant (e)	$(x_i)_1 (x_j x_k)_2$
Piezoelectric modulus (d)	$(2-\delta_{jk})\,(x_i)_1\,(x_j x_k)_2$
Elastic constant (c)	$(x_i x_j)_1\,(x_k x_m)_2$
Elastic modulus (s)	$(2-\delta_{ij})\,(2-\delta_{km})\,(x_i x_j)_1\,(x_k x_m)_2$
Photoelastic constant (p)	$(x_i x_j)_1\,(x_k x_m)_2$
Photoelastic modulus (π)	$(2-\delta_{km})\,(x_i x_j)_1\,(x_k x_m)_2$

The alternate definition of the strain tensor (Love, Wooster) leads to products without any numerical factors.

The rule for the transformation (2) also holds under inversion provided one supplies an extra change of sign for the material constants that do not truly transform like products of polar vector components.

The correspondence between the transformation properties of the material constants and the co-ordinate products (3) is also of great value in determining the symmetry of the scheme of material constants required by crystal symmetry.

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Acta Cryst. (1952). **5**, 149

The crystal structure of decamethylenediamine.

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(*Received* 10 *September* 1951)

As a continuation of the study of bond-length alternation in long-chain aliphatic compounds we have examined the structure of decamethylenediamine. Being a homologue of hexamethylenediamine (Binnie & Robertson, 1950) this compound also would be expected to exhibit an alternation of carbon–carbon bond lengths. The investigation has encountered experimental difficulties. The diamine reacts with carbon dioxide and must be protected from the atmosphere. The crystals available were extremely thin plates, and as a result only a small fraction of the possible reflexions could be observed. The incompleteness of the data thus prevented any accurate determination of bond lengths. However, the approximate shape and orientation of the molecule have been found.

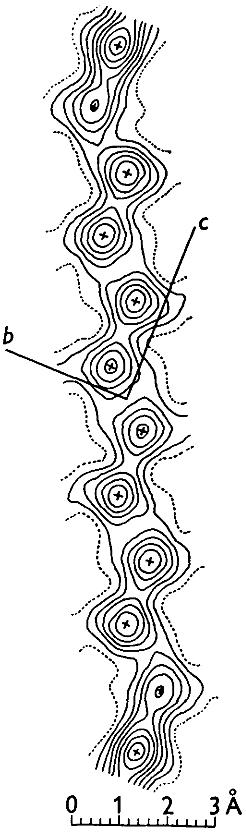

Fig. 1. Molecule of decamethylenediamine projected on (100). Contours at intervals of 1 e.Å^{-2}, the one-electron line being broken.

Decamethylenediamine is orthorhombic with

$$a = 7\cdot25 \pm 0\cdot05,\quad b = 5\cdot72 \pm 0\cdot03,\quad c = 29\cdot4 \pm 0\cdot2\,\text{Å}.$$

The space group is D_{2h}^{15}-*Pbca*. The density lies between 0·88 and 1·04 g.cm.$^{-3}$, requiring four chemical molecules per unit cell.

The cell dimensions and space group indicate that the molecular arrangement in decamethylenediamine is similar to that of hexamethylenediamine (Binnie & Robertson, 1950). The similarity permitted a reasonable trial structure to be found for the (0*kl*) zone. When the Fourier projection on (100) was calculated all the carbon and nitrogen atoms were clearly resolved (Fig. 1). The new co-ordinates gave a reduced discrepancy but none of the structure factors changed sign. With the crystals available it was not possible to extend the range of measured intensities. As a result refinement could not be continued by Fourier syntheses. Nevertheless, the projection confirms the similarity to the hexamethylenediamine orientation.

No intensity data were obtained for the (*h*0*l*) zone, but it was noted that, as in the case of hexamethylenediamine, the (200) reflexion was unusually strong.

When additional attempts at obtaining larger crystals did not succeed, work was transferred to the analogous decamethylene glycol which proved more suited to the accurate measurement of bond lengths. The completion of the study of decamethylenediamine is dependent upon better methods of growing crystals.

We wish to thank Imperial Chemical Industries Ltd. for the sample of decamethylenediamine used in the investigation.

Reference

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