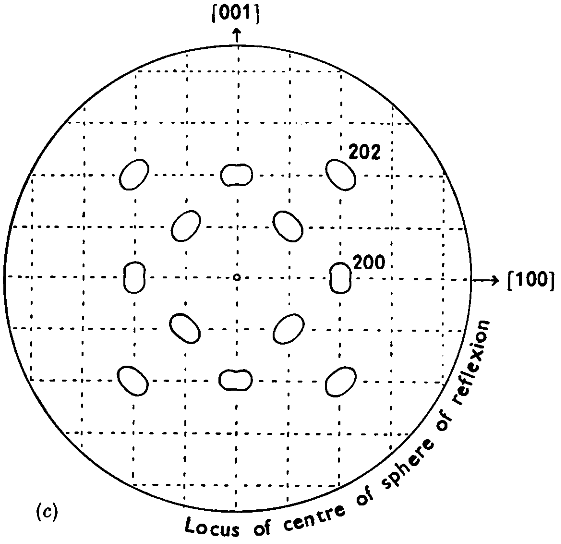

Fig. 8 (*cont.*). (*c*) Equi-reflecting contours in the net $k = 0$, using the elastic constants of hexamine. No correspondence between the Jahn contours and streak directions.

using the elastic constants of hexamine ($c_{11}=1\cdot5$, $c_{12}=0\cdot3$ and $c_{44}=0\cdot7\times10^{11}$ dyne cm.$^{-2}$) given by Ramachandran & Wooster (1951). But, whereas in the case of NaCl-like structures a correspondence was found between the shapes of the Jahn contours and their extension in the form of non-radial streaks, no such correspondence can be observed here (cf. Fig. 8 (*b*) and (*c*)), presumably because the streaks from a molecular crystal are mainly due to vibrations other than purely elastic ones.

4. Discussion

There is a relation between the characteristic shape of the diffuse spot and the associated non-radial streaks, which is obvious in the case of KCl and LiF, and is still valid in the case of the 'diffuse' Laue photographs for $NaClO_3$ (Fig. 3) although the symmetry of the Jahn contour is very much of an approximation in such a case. This relation between the shape of the diffuse spot and the associated non-radial streaks does not hold in the case of the molecular cubic crystal, hexamine. In such a crystal, where the closed molecule is nearly spherical, the molecule vibrates as a unit (this motion may be a rotatory or oscillatory one) and there are also vibrations of the atoms within the molecule. The latter will have frequencies much higher, in general, than those of the elastic vibrations of the lattice as a whole. The acoustical and optical frequencies may differ greatly in such a crystal, and this seems to be confirmed by the independence of diffuse-spot shapes and streak directions on monochromatic photographs of hexamine (Fig. 4).

The author wishes to thank the Egyptian Government for a scholarship which made possible a period of research in England. He is indebted to Prof. Kathleen Lonsdale for help and advice throughout the work.

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Photo-Elastic Properties of Crystals: Some New Results

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(*Received* 29 *March* 1952)

The non-vanishing photo-elastic constants in the C_3, S_6; C_{3h}, C_6, C_{6h}; C_4, S_4, C_{4h} crystal classes are given. Differences between them and those given earlier by Pockels for these classes are pointed out. Some interesting results, which are capable of being verified by experiment, are deduced.

1. Introduction

The author of this paper (Bhagavantam, 1942) gave a method by which group theory can be used for deriving the numbers of independent constants necessary in each of the 32 crystal classes for describing any physical property. The method, at that time, was applied to photo-elasticity in particular, and discrepancies were found and reported in respect of ten crystal classes, namely C_3, S_6, C_{3h}, C_6, C_{6h}, C_4, S_4, C_{4h}, T and T_h, between the results thus obtained and those given earlier by Pockels. It has since been extended by other authors to cover cases of interest and a connected account was published in this journal (Bhagavantam & Suryanarayana, 1949*a*). Jahn (1949) gave an alternative method, also based on group theory, and showed that in all cases the same results may be obtained with his method as well. The subject has attracted the attention of workers in the field of crystal physics on account of some new results that were brought to light, and, amongst other publications, mention may be made of one by Fumi (1951). Such aspects in respect of which the results of Pockels differed from those of the present writer in the T and T_h classes alone were fully discussed and their consequences verified by experiment in potassium alum, ammonium alum, barium nitrate (Bhagavantam & Suryanarayana, 1947, 1948, 1949*a*, *b*) and sodium chlorate (Ramachandran & Chandrasekharan, 1950). It is the purpose of this note to discuss also the other eight crystal classes from this point of view and to draw attention to some outstanding consequences capable of experimental verification.

2. Non-vanishing photo-elastic constants

The individual non-vanishing constants were also arrived at (Bhagavantam, 1942) by the direct method in all crystal classes, and the resulting numbers were found to agree with the numbers predicted by the application of group-theoretical methods. Cases in which there are differences between our results and those of Pockels, with the exception of T and T_h, are given below:

C_3, S_6

$$\begin{array}{cccccc}
q_{11} & q_{12} & q_{13} & q_{14} & q_{15} & -2q_{61} \\
q_{12} & q_{11} & q_{13} & -q_{14} & -q_{15} & 2q_{61} \\
q_{31} & q_{31} & q_{33} & 0 & 0 & 0 \\
q_{41} & -q_{41} & 0 & q_{44} & q_{45} & -2q_{51} \\
q_{51} & -q_{51} & 0 & -q_{45} & q_{44} & 2q_{41} \\
q_{61} & -q_{61} & 0 & -q_{15} & q_{14} & q_{11}-q_{12}
\end{array}$$

C_{3h}, C_6, C_{6h}

$$\begin{array}{cccccc}
q_{11} & q_{12} & q_{13} & 0 & 0 & -2q_{61} \\
q_{12} & q_{11} & q_{13} & 0 & 0 & 2q_{61} \\
q_{31} & q_{31} & q_{33} & 0 & 0 & 0 \\
0 & 0 & 0 & q_{44} & q_{45} & 0 \\
0 & 0 & 0 & -q_{45} & q_{44} & 0 \\
q_{61} & -q_{61} & 0 & 0 & 0 & q_{11}-q_{12}
\end{array}$$

C_4, S_4, C_{4h}

$$\begin{array}{cccccc}
q_{11} & q_{12} & q_{13} & 0 & 0 & q_{16} \\
q_{12} & q_{11} & q_{13} & 0 & 0 & -q_{16} \\
q_{31} & q_{31} & q_{33} & 0 & 0 & 0 \\
0 & 0 & 0 & q_{44} & q_{45} & 0 \\
0 & 0 & 0 & -q_{45} & q_{44} & 0 \\
q_{61} & -q_{61} & 0 & 0 & 0 & q_{66}
\end{array}$$

They fall into three groups. The scheme for the first group differs from the corresponding one given by Pockels in showing q_{61} as non-vanishing. Similarly, q_{61} and q_{45} in the second group and q_{45} alone in the third group are extra non-vanishing constants according to the present writer. Fumi (1952) has reported identical schemes for these classes in a recent note.*

3. Some new results

If a crystal belonging to one of the classes under the first two groups is chosen and a prism cut out of it with the length (X axis) and breadth (Y axis) constituting its base, as equal and lying in the symmetry plane; and the Z axis, the height of the prism, as parallel to the optic axis which is also the axis of crystallographic symmetry; we can obtain the following results with it.

Let a stress of the simple linear compressional type (all the components except XX are zero) be applied along the X axis of the prism. The index ellipsoid in the usual notation may be represented by the equations (1) and (2), respectively, before and after the application of the stress.

$$B^0_{11}x^2+B^0_{11}y^2+B^0_{33}z^2 = 1\,. \tag{1}$$

$$B_{11}x^2+B_{22}y^2+B_{33}z^2+2B_{23}yz+2B_{31}zx+2B_{12}xy=1\,. \tag{2}$$

In these equations

$$B_{11}-B^0_{11}=-q_{11}.XX;\; B_{22}-B^0_{11}=-q_{12}.XX;$$
$$B_{33}-B^0_{33}=-q_{31}.XX;\; B_{23}=-q_{41}.XX;$$
$$B_{31}=-q_{51}.XX;\; B_{12}=-q_{61}.XX\,.$$

If the crystal belongs to either C_{3h} or C_6 or C_{6h} class, then B_{23} and B_{31} will vanish, but this is of no important consequence. It may, however, be noted that a section of the ellipsoid by the $X\,Y$ plane which was a circle before the application of the stress becomes an ellipse after the application of the stress, with the equation

$$B_{11}x^2+B_{22}y^2+2B_{12}xy = 1\,,$$

showing that X and Y, the directions of longitudinal contraction and lateral expansion, are not the principal axes in this section. They would have been so in Pockels's scheme because $q_{16}=0$ and therefore $B_{12}=0$. If the new principal axes are designated by X' and Y' making an angle θ with X and Y respectively, we can transform the ellipse by substituting $x = x'\cos\theta-y'\sin\theta$; $y=x'\sin\theta+y'\cos\theta$ into the dashed system. By equating the coefficient of the $x'y'$ term in the transformed equation to zero, we obtain the condition that x' and y' may be the principal directions as

$$\tan 2\theta = \frac{2q_{61}}{q_{11}-q_{12}}\,.$$

This is an important condition and shows, as is to be expected, that if $q_{61} = 0$, $\theta = 0$ and the axis of stress

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* There are small differences arising out of differences in notation but a careful comparison will show that they are not of material consequence.

(X) and a line perpendicular thereto (Y) will remain the principal directions. This result is new, and if we measure θ and $q_{11}-q_{12}$ experimentally, we can evaluate q_{61} for a chosen crystal.

If to the same prism, a tangential stress XY is applied, we have again $B_{11}x^2+B_{22}y^2+2B_{12}xy = 1$ as the equation of the elliptic section in the $X\ Y$ plane, where $B_{11}-B^0_{11} = B^0_{11}-B_{22} = 2q_{61}.XY$ and $B_{12} = -(q_{11}-q_{12})XY$. The existence of B_{12} shows that birefringence is caused by the $X\ Y$ plane being sheared, a result which persists even when the coefficients of x and y remain unchanged. In this case, q_{61} causes a different kind of birefringence in that n_x-n_y, which is zero before the application of stress, becomes equal to $4q_{61}.XY.\frac{1}{2}n_0^3$ as a result of the stress XY. This again is a new result and has been visualized by Fumi (1952) in his recent note. n_x-n_y would be zero even in the stressed crystal if $q_{61} = 0$.

If, from the class of crystals C_4, S_4 and C_{4h}, we choose one and cut a prism of the same type as above (axis of crystallographic symmetry is Z, and X and Y are in the plane perpendicular thereto) and subject it to a tangential stress ZX, according to the scheme of q's given in this paper, we have amongst other things, $B_{23} = -q_{45}.ZX$, indicating a tilt of the principal axes in the YZ plane. This is capable of being experimentally observed. On the other hand, the same amount of stress applied as ZY will cause an equal tilt of the principal axes in the XZ plane but in the *opposite sense.*

In an actual experiment, choice of crystals belonging to the classes C_3, C_6, C_4 and S_4 will cause complications as they are optically active, making the observations more difficult, and may therefore be avoided.

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Acta Cryst. (1952). **5**, 593

The Crystal Structure of Naphthalene Tetrachloride, $C_{10}H_8Cl_4$

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(*Received* 15 *February* 1952)

The values of the diamagnetic anisotropy in the monoclinic crystal of naphthalene tetrachloride were found to be

$$\chi_1-\chi_2 = 56{\cdot}2\times10^{-6}\ \text{c.g.s.e.m.u.}\quad \theta = +23{\cdot}2^\circ\ (\chi_2 \frown [100])$$
$$\chi_1-\chi_3 = 2{\cdot}6\times10^{-6}\quad \psi = -\ 0{\cdot}5^\circ\ (\chi_1 \frown [001])$$
$$\chi_3-\chi_2 = 53{\cdot}5\times10^{-6}\quad (\chi_3\ \text{along}\ [010])$$

These results show that the (100) plane is the plane of the molecule. The dimensions of the unit cell, which contains four molecules, each having a diad axis of symmetry, are $a = 7{\cdot}92_5\pm0{\cdot}03$, $b = 10{\cdot}25\pm0{\cdot}04$, $c = 14{\cdot}25\pm0{\cdot}05$ Å, $\beta = 112{\cdot}6\pm0{\cdot}5$. The space group is $I2/c$ and Patterson projections confirm the molecular orientation deduced from the magnetic measurements. The C–Cl bonds have the configuration 1ε, 2κ, 3κ, 4ε (deduced from electron-density projections on (100), (010) and (001)), and interatomic Cl $\cdots$ Cl distances agree closely with those derived from other chlorinated cyclohexane compounds. The aromatic ring has the normal C–C distances of 1·39–1·40 Å and is undistorted. Eight of the carbon atoms appear to be closely co-planar.

Introduction

The results of previous crystallographic investigations on naphthalene tetrachloride crystals are summarised by Groth (1906–19, vol. 5, p. 368). Sir W. H. Bragg (1927) studied this substance by the X-ray method and found its lattice to be monoclinic body-centred, with four molecules per unit cell. The cell dimensions he reported, $a = 7{\cdot}88$, $b = 10{\cdot}30$, $c = 14{\cdot}20$ Å, $\beta = 112^\circ 40'$, agree with the data recorded by Groth except in the doubling of the c-axis length. Bragg adopted the space group C_s^4 and suggested that the molecules

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