who found that the binding energy in complexes of *s*-trinitrobenzene with various hydrocarbons depends in a marked way on the structure of the hydrocarbon, and these binding energies are greater the greater the optical exaltation shown by the hydrocarbon. The binding energy of the complex is high if the hydrocarbon system is completely conjugated, but decreases as soon as the conjugation is interrupted.

When considering the question of the polarizability of the aromatic hydrocarbon it is interesting to note that, in general, complexes with nitro compounds are apparently more stable if electron-repelling groups are introduced into the hydrocarbon and less stable if electron-attracting groups are introduced; indeed, in the latter case it is generally impossible to isolate a crystalline complex. It is tempting to suggest that the introduction of an electron-repelling group into the hydrocarbon leads to a greater availability of electrons in the aromatic nucleus, implying a greater polarizability of the molecule. Considerable care must, however, be exercised in interpreting the effect of substituents on the stability of these complexes, since geometrical effects depending on the size of these substituents will undoubtedly be of importance in determining the approach of the molecules to one another.

The authors wish to express their thanks to Dr W. S. Rapson and Dr E. Theal Stewart for the preparation of the materials used in this work.

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The Accurate Determination of Cell Dimensions from Single-Crystal X-ray Photographs

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The accurate determination of cell dimensions by a graphical extrapolation method from single-crystal X-ray photographs has been discussed by Farquhar & Lipson and applied by them to an orthorhombic crystal, thallium hydrogen tartrate. In the present paper an alternative method of lower accuracy but greater simplicity is described. An account is also given of the application of extrapolation methods, both graphical and analytical, to the determination of the cell dimensions of a monoclinic crystal, a heat-treated orthoclase felspar. Procedures for determining accurate cell dimensions of orthorhombic, monoclinic and triclinic crystals are outlined.

1. Introduction

Cell dimensions may be determined approximately from measurements of layer-line separations in single-crystal rotation photographs, and accurately either with the help of a special goniometer of the Weissenberg type (Buerger, 1937) or by a graphical extrapolation method using a slightly modified ordinary goniometer (Farquhar & Lipson, 1945). In § 2 of the present paper a description is given of a new technique, based on observations of the angular setting of the crystal at which reflexion occurs, and of its application to a monoclinic orthoclase felspar and other crystals. In § 3 analytical and graphical extrapolation methods are applied to the same felspar crystal and in § 4 the relative accuracies of the two methods are discussed. Finally, in § 5 a combined technique is described which has great advantages for triclinic crystals.

2. θ-Method

Theory. Both linear and angular constants are obtained from reflexions of the type ($h00$), ($0k0$), ($00l$) occurring on zero layer-line photographs. The goniometer circle is used to observe the angular settings of the crystal when these planes are reflecting with maximum intensity on either side of the X-ray beam. The mean of the two positions gives the location of a reciprocal-cell axis and the angular constants of the reciprocal cell are then given by the following differences

$$b^* \wedge c^* = \alpha^*, \quad a^* \wedge c^* = \beta^*, \quad a^* \wedge b^* = \gamma^*. \qquad (1)$$

The angular difference of the two positions gives twice the Bragg angle, which is related to the linear constants of the reciprocal cell by the equations

$$ha^* = 2 \sin \theta_{h00}, \quad kb^* = 2 \sin \theta_{0k0}, \quad lc^* = 2 \sin \theta_{00l}. \qquad (2)$$

Experimental. The position of the desired reflexion is found to within 5° by ordinary oscillation methods. The crystal is then moved by steps of $\frac{1}{2}°$ within this range and the reflected beam is recorded on a strip of film loosely held in position on the outer surface of a cylinder which has a slot cut so as to isolate zero layer-line reflexions. The procedure is repeated with the crystal turned through twice the Bragg angle as calculated from approximate cell dimensions. Finally, the apparatus is adjusted so that the collimator makes as small an angle as possible with the face of the target and the positions of maximum reflexion located accurately by taking a series of exposures between each of which the crystal is turned through 3′.

Accuracy of the method. The accuracy with which the Bragg angle can be measured depends mainly on the range over which the crystal reflects. This is determined partly by the mosaic structure of the crystal and partly by its dimensions. Most crystals to which the method has been applied reflect over a range not greater than 15′, and for these the position of maximum reflexion can be found to ± 1′. For a range of reflexion of 1° this figure does not exceed ± 3′. Thus, neglecting systematic errors, if $\delta\theta = 1'$ and $\theta > 75°$,

$$\delta a/a = -\cot \theta \delta\theta < 10^{-4}. \qquad (3)$$

Systematic errors may arise from the following three causes:

(*a*) The crystallographic axis makes an angle ψ with the rotation axis. The fractional error due to this cause is proportional to $1 - \cos \psi$, which, with accurate setting, can be made less than 1 part in 50,000.

(*b*) The specimen is not centred on the rotation axis. Error due to this cause can be detected by turning the goniometer circle through 180° and re-determining the positions of maximum reflexion.

(*c*) The specimen has a high absorption coefficient. For a completely absorbing crystal it may be shown (Bradley & Jay, 1932) that

$$\delta a/a = -\cot \theta \delta\theta = -r \cos^2 \theta / AX \sin \theta \approx 10^{-4}, \qquad (4)$$

where $r = 0{\cdot}15$ mm., $AX = 15$ cm., and $\theta = 70°$.

Results. Results of measurements made on crystals of a pyrimidine derivative are given in Table 1 and of a heat-treated orthoclase felspar in Table 2. In addition a small diamond was set up so that the (331) reflexion fell on the equatorial line. The value obtained for the cell-edge, using Cu $K\alpha_1$ radiation, was $3{\cdot}5670 \pm 0{\cdot}0004$ A., which compares well with the accurate value of 3·55974 kX (3·56693 A.) found by Lonsdale (1944).

3. Extrapolation methods applied to a monoclinic crystal

Introduction. In extrapolation methods the positions of reflexions with θ near 90° are determined from the zero layer-line of an oscillation photograph. Suitable reflexions are obtained by oscillating the axis whose repeat distance is being determined symmetrically about the X-ray beam. In the graphical extrapolation method the cell dimension is deduced for each reflexion and the values plotted against some suitable function (Nelson & Riley, 1945); the true value is obtained by extrapolation to $\theta = 90°$. In the analytical extrapolation method the Bragg angle is deduced for each reflexion and these values are used to solve an error equation which takes into account the systematic errors as they affect the Bragg equation (Cohen, 1935).

Theory of the graphical extrapolation method for a monoclinic crystal. By combining the Bragg equation with

$$(\lambda/d)^2 = h^2a^{*2} + k^2b^{*2} + l^2c^{*2} + 2hla^*c^* \cos \beta^*, \qquad (5)$$

we obtain, as set out in Table 3, suitable equations for the determination of cell dimensions of monoclinic crystals by the graphical extrapolation method. These show that for the determination of $a \sin \beta$, $c \sin \beta$, and b, the constants b^{*2}/a^{*2} and b^{*2}/c^{*2} must be known. Similarly, for the determination of β the constants a^* and c^* must be known. In obtaining values of b^{*2}/a^{*2} and b^{*2}/c^{*2} use is made of layer-line spacings and any available data for the axial ratio and β. Values of the constants a^* and c^* are obtained from previous determinations of $a \sin \beta$ and $c \sin \beta$.

Theory of the analytical extrapolation method for a monoclinic crystal. For a monoclinic crystal the general basic error equation allowing for systematic errors is given by

$$h^2\lambda^2/(2a \sin \beta)^2 + k^2\lambda^2/(2b)^2 + l^2\lambda^2/(2c \sin \beta)^2 - hl\lambda^2 \times (\cos \beta / 2ac \sin^2 \beta) + D \sin^2 2\theta + E \cos^2 \theta \sin 2\theta = \sin^2 \theta, \qquad (11)$$

where D is the combined experimental-error constant for shrinkage and eccentricity, and E is the experimental-error constant for absorption (Buerger, 1942). By rewriting equation (11) as

$$\mu P + \nu Q + \rho R - \sigma S + D\delta + E\epsilon = \sin^2 \theta, \qquad (12)$$

we obtain, as set out in Table 3, suitable equations for the determination of cell dimensions of monoclinic

Table 1. *Cell dimensions of a pyrimidine derivative as determined by the θ-method.*

(Values obtained from oscillation photographs are enclosed in parentheses; all results expressed in A. units)

Constant	Reflexion	Positions of maximum reflexions	Position of c^*	Position of a^*	θ	$c \sin \beta$	$a \sin \beta$	Mean value of cell constant
c	(002) Cu $K\alpha$	185° 54½′, 55′, 55½′; 167° 45′, 45½′, 45½′	266° 50·2′	—	9° 4·7′	9·77$_0$	—	—
	(0.0.10) Cu $K\alpha_1$	228° 48′; 124° 53′	266° 50·5′	—	51° 57·5′	9·780$_0$	—	11·009$_0$ ± 0·002
	(0.0.10) Cu $K\alpha_2$	228° 58′; 124° 43′	266° 50·5′	—	52° 7·5′	9·782$_2$	—	(10·95)
a	(200) Cu $K\alpha$	251° 42½′, 42½′, 42′; 227° 21′, 20½′, 21′	—	329° 31·6′	12° 10·8′	—	7·30$_8$	—
	(800) Cu $K\alpha_1$	297° 1′; 182° 1½′	—	329° 31·3′	57° 29·8′	—	7·306$_5$	8·223$_6$ ± 0·002
	(800) Cu $K\alpha_2$	297° 15′; 181° 50½′	—	329° 32·7′	57° 42·3′	—	7·308$_0$	(8·13)
β		Mean value of $180° - (a^* - c^*)$ positions						117° 18·2′ ± 1′ (116° 30′)

Table 2. *Comparison of cell dimensions of specimen C, a heat-treated orthoclase felspar, as determined by the θ-method and the graphical and analytical extrapolation methods*

(All results expressed in A. units)

Method	$a \sin \beta$	$c \sin \beta$	a	b	c	β	b^{*2}/a^{*2}	b^{*2}/c^{*2}
θ-method	7·698 ± 0·003 (10.0.$\bar{1}$) plane	6·447 ± 0·002 (008) plane	8·566 ± 0·007 (10.0.$\bar{1}$) plane	13·029 ± 0·004 (0.16.0) plane	7·174 ± 0·005 (008) plane	116° 1½′ ± 3′ (002) ∧ (200)	0·3490 ± 0·0005 $a^2 \sin^2 \beta/b^2$	0·2448 ± 0·0003 $c^2 \sin^2 \beta/b^2$
	7·694 ± 0·005 (600) plane	—	8·562 ± 0·009 (600) plane)	—	—	—	0·3493 ± 0·0014 tan² [(600) ∧ (660)]	0·2438 ± 0·0011 tan² [(002) ∧ (022)]
Graphical extrapolation	7·6978 ± 0·0002	6·4490 ± 0·0002	8·5642 ± 0·0002	13·0300 ± 0·0004	7·1749 ± 0·0002	115·994° ± 0·005	0·3490 assumed	0·2450 assumed
Analytical extrapolation	7·6979	6·4296	—	13·0924	—	—	—	—

Table 3. *Suitable equations for the determination of cell dimensions of monoclinic crystals by extrapolation methods*

Constant	Graphical extrapolation		Analytical extrapolation		Rotation axis	Spectra used
$a \sin \beta = \lambda/a^*$	$2 \sin \theta = a^* (h^2 + k^2 b^{*2}/a^{*2})^{\frac{1}{2}}$	(6)	$\mu P = \sin^2 \theta - \nu Q - D\delta - E\epsilon$	(13)	c	$hk0$; h high
$c \sin \beta = \lambda/c^*$	$2 \sin \theta = c^* (k^2 b^{*2}/c^{*2} + l^2)^{\frac{1}{2}}$	(7)	$\rho R = \sin^2 \theta - \nu Q - D\delta - E\epsilon$	(14)	a	$0kl$; l high
$b = \lambda/b^*$	$2 \sin \theta = b^* (k^2 + l^2 c^{*2}/b^{*2})^{\frac{1}{2}}$	(8)	$\nu Q = \sin^2 \theta - \rho R - D\delta - E\epsilon$	(15)	a	$0kl$; k high
	$2 \sin \theta = b^* (h^2 a^{*2}/b^{*2} + k^2)^{\frac{1}{2}}$	(9)	$\nu Q = \sin^2 \theta - \mu P - D\delta - E\epsilon$	(16)	c	$hk0$; k high
$\beta = 180° - \beta^*$	$-\cos \beta^* = ha^*/2lc^* + lc^*/2ha^* - 2 \sin^2 \theta/hla^*c^*$	(10)	$-\sigma S = \sin^2 \theta - \mu P - \rho R - D\delta - E\epsilon$	(17)	b	$h0l$; h and l even

crystals by the analytical extrapolation method. These may be solved directly by considering sufficient reflexions to cover the number of unknown coefficients, or else they may be modified by the method of least squares so as to include all reflexions, and thus take into account the random errors of measurement (Buerger, 1942).

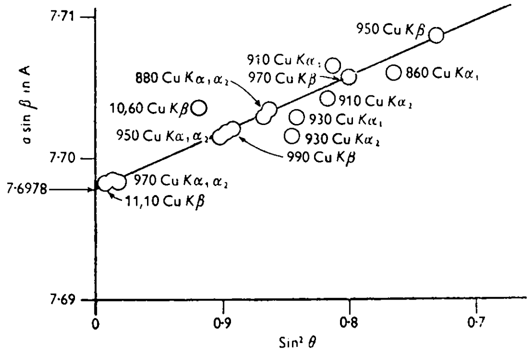

Fig. 1. Extrapolation curve of $a \sin \beta$ *v.* $\sin^2 \theta$ for specimen C, a heat-treated orthoclase felspar.

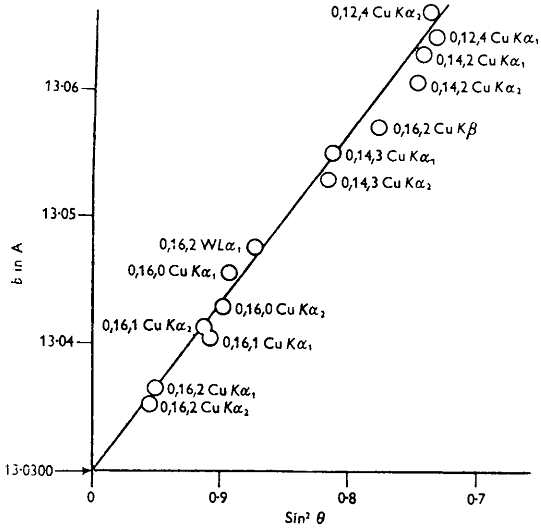

Fig. 2. Extrapolation curve of b *v.* $\sin^2 \theta$ for specimen C, a heat-treated orthoclase felspar.

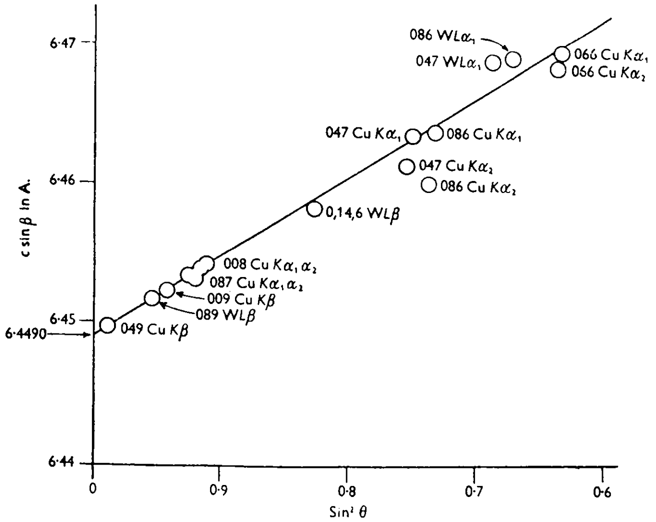

Fig. 3. Extrapolation curve of $c \sin \beta$ *v.* $\sin^2 \theta$ for specimen C, a heat-treated orthoclase felspar.

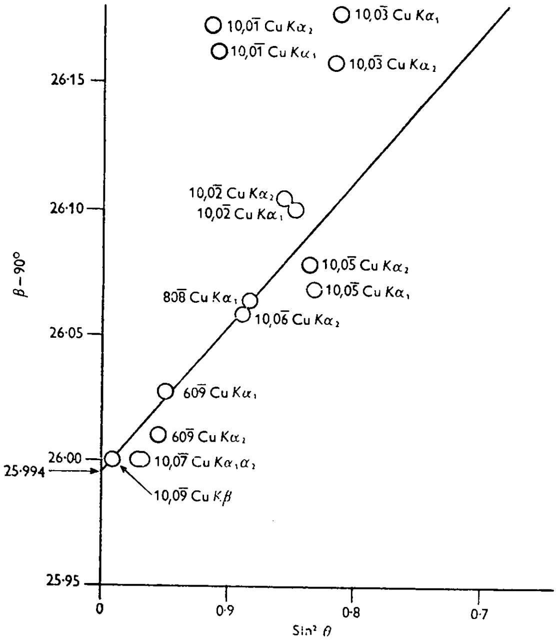

Fig. 4. Extrapolation curve of β–90° *v.* $\sin^2 \theta$ for specimen C, a heat-treated orthoclase felspar.

Experimental. The camera used was the one modified by Farquhar & Lipson (1945) for which a radius of 2·991 ± 0·004 cm. was found by calibration with a quartz powder, using the data for quartz of Wilson & Lipson (1941).

In order to obtain reflexions on the films in the region of $\theta = 85°$ use was made of unfiltered copper radiation. Reflexions were obtained from Cu $K\alpha_1$, Cu $K\alpha_2$, Cu $K\beta$, W $L\alpha_1$ and W $L\beta$ radiations. In the determination of β the resulting film is unsymmetrical, but little difficulty was experienced in obtaining a number of planes reflecting on either side of the film in an oscillation range of 43°.

Results. The cell dimensions of specimen C, the same felspar crystal as used in § 2, have been determined approximately from rotation photographs by Chao, Smare & Taylor (1939), who give $a=8{\cdot}60$ kX ($8{\cdot}62$ A.), $b=13{\cdot}03$ kX ($13{\cdot}06$ A.), $c=7{\cdot}16$ kX ($7{\cdot}17$ A.) and $\beta=116^\circ\ 3'$ (assumed). From these data we have, for graphical extrapolation, $b^{*2}/a^{*2}=0{\cdot}3518$ and $b^{*2}/c^{*2}=0{\cdot}2438$. Good extrapolation was not obtained until a new value of $0{\cdot}3490$ was assumed for the former, and of $0{\cdot}2449$ for the latter. The final extrapolation curves are illustrated in Figs. 1–4 and the results set out in Table 2.

Data used in the graphical extrapolation method were also treated by the analytical method. The method of least squares was used, but the absorption error term was omitted so as to reduce the amount of computation. The results obtained for $a \sin \beta$, b and $c \sin \beta$ are set out in Table 2.

4. Comparison of results

In Table 2 a comparison is made between the values of the cell dimensions obtained for specimen C by extrapolation methods and the θ-method. It will be seen in the first place that although the analytical extrapolation has the advantage that no constants have to be known, the results are not reliable. They are not improved by the insertion of the absorption term. Buerger (1942) has pointed out that it is dangerous to use reflexions from different planes if the absorption is high, and if the crystal shape departs appreciably from cylindrical. The crystal of specimen C, although not highly absorbing, had the shape of a cube so that a single absorption-error coefficient could not hold for all sets of planes of which the reflexions were used.

In the second place results obtained by the θ-method are not as accurate as those from the graphical extrapolation method, but they are in good agreement with them. They supply good values for the constants b^{*2}/a^{*2} and b^{*2}/c^{*2} which are in general not very well known in the graphical extrapolation method. Values for these constants can also be obtained by the θ-method from the following angular relationships

$$\tan (100) \wedge (110) = b^*/a^*,$$
$$\tan (001) \wedge (011) = b^*/c^*. \qquad (18)$$

Higher orders of these planes may also be used. In Table 2 some values are given for the planes (600) ∧ (660) and (002) ∧ (022) but the results are not very accurate.

5. The θ-method and graphical extrapolation method combined

From the work on specimen C it appears to us that the best method of determining accurate cell dimensions of orthorhombic, monoclinic and triclinic crystals from single-crystal X-ray photographs is by a combination of the θ-method and the graphical extrapolation method.

In all three crystal classes the θ-method can be used to give

$$a^* = \lambda/d_{100}, \quad b^* = \lambda/d_{010}, \quad c^* = \lambda/d_{001}. \qquad (19)$$

For both orthorhombic and monoclinic crystals the constants b^{*2}/a^{*2} and b^{*2}/c^{*2} are formed and used in the graphical extrapolation method to give accurate values of a, b and c for orthorhombic, and $a \sin \beta$, b and $c \sin \beta$ for monoclinic crystals. In the case of monoclinic crystals new values of a^* and c^* are formed from the accurate values of $a \sin \beta$ and $c \sin \beta$ respectively and the angle β determined by extrapolation.

For triclinic crystals the procedure is a little more lengthy. By combining the Bragg equation with

$$(\lambda/d)^2 = h^2a^{*2} + k^2b^{*2} + l^2c^{*2} + 2hka^*b^* \cos \gamma^* + 2hla^*c^* \cos \beta^* + 2klb^*c^* \cos \alpha^*, \qquad (20)$$

we obtain, as set out in Table 4, suitable equations for the determination of cell dimensions of triclinic crystals by the graphical extrapolation method. The θ-method is used to obtain values of a^*, b^* and c^* which are then used as constants in equations (27)–(29) for the determination of α^*, β^* and γ^* by graphical extrapolation. Having now values for all six constants, a^*, b^* and c^* are refined by extrapolation. This involves solving the quadratic equations (21)–(26). It is possible to obtain initial values of α^*, β^* and γ^* by the θ-method using equation (1).

In the case of triclinic crystals there seems to be no difficulty that has not already been met with in the case of a monoclinic crystal. In the graphical extrapolation method it is preferable to mount the film in

Table 4. *Suitable equations for the determination of cell dimensions of triclinic crystals by the graphical extrapolation method*

Constant	Equation		Rotation axis	Spectra used
a^*	$h^2a^{*2} + 2hkb^* \cos \gamma^* a^* + (k^2b^{*2} - 4 \sin^2 \theta) = 0$	(21)	c	$hk0$; h high
	$h^2a^{*2} + 2hlc^* \cos \beta^* a^* + (l^2c^{*2} - 4 \sin^2 \theta) = 0$	(22)	b	$h0l$; h high
b^*	$k^2b^{*2} + 2hka^* \cos \gamma^* b^* + (h^2a^{*2} - 4 \sin^2 \theta) = 0$	(23)	c	$hk0$; k high
	$k^2b^{*2} + 2klc^* \cos \alpha^* b^* + (l^2c^{*2} - 4 \sin^2 \theta) = 0$	(24)	a	$0kl$; k high
c^*	$l^2c^{*2} + 2hla^* \cos \beta^* c^* + (h^2a^{*2} - 4 \sin^2 \theta) = 0$	(25)	b	$h0l$; l high
	$l^2c^{*2} + 2klb^* \cos \alpha^* c^* + (k^2b^{*2} - 4 \sin^2 \theta) = 0$	(26)	a	$0kl$; l high
α^*	$\cos \alpha^* = (4 \sin^2 \theta - k^2b^{*2} - l^2c^{*2})/2klb^*c^*$	(27)	a	$0kl$; k and l even
β^*	$\cos \beta^* = (4 \sin^2 \theta - h^2a^{*2} - l^2c^{*2})/2hla^*c^*$	(28)	b	$h0l$; h and l even
γ^*	$\cos \gamma^* = (4 \sin^2 \theta - h^2a^{*2} - k^2b^{*2})/2hka^*b^*$	(29)	c	$hk0$; h and k even

the Straumanis manner rather than in that of van Arkel. The use of film techniques for the isolation of reflexions makes the θ-method both lengthy and tedious and considerable improvement could be effected by the introduction of an ionization method.

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The Crystal Structures of Zinc and Magnesium Benzene Sulphonates

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The crystal structures of the isomorphous zinc and magnesium benzene sulphonates have been determined. The crystals are monoclinic, with space group $P2_1/n$ and two molecules in a unit cell with edges $a = 22{\cdot}6$ A., $b = 6{\cdot}32$ A., $c = 6{\cdot}94$ A., $\beta = 93^\circ\,36'$ (magnesium compound).

The signs of the structure amplitudes were fixed by comparison of corresponding reflexions from the isomorphous structures, and Fourier projections along the b and c axes were used to determine the structure.

In the structure, metal atoms are surrounded by regular octahedra of water molecules, which are linked by hydrogen bonds to oxygen atoms of the sulphonate group. These oxygen atoms and a carbon atom of the benzene ring are joined to a sulphur atom by bonds which make angles of approximately 109° with each other. The benzene ring is plane and the minimum distance between neighbouring rings is about 3·5 A. The position and orientation of the molecules in the structure suggest an explanation of the observed twin growth.

Introduction

An investigation on a series of isomorphous benzene and toluene sulphonates was started in Manchester by Hargreaves and one of us (A. D. I. N.) with a view to obtaining a complete structural analysis by X-ray methods. It was hoped that this would provide useful information about the configuration of the sulphonate group. Hargreaves (1946) has described the b axis projection of the isomorphous zinc and magnesium toluene sulphonate structures.

It was found that zinc and magnesium benzene sulphonates were isomorphous, with space group $P2_1/n$, and two molecules in unit cells with the dimensions given in Table 1. In order to conform with the usual convention, the angle β given corresponds to the supplement of that quoted by Hargreaves (1946).

Table 1. *Cell dimensions of* $Mg(C_6H_5SO_3)_2 . 6H_2O$ *and* $Zn(C_6H_5SO_3)_2 . 6H_2O$

Compound	a in A.	b in A.	c in A.	β
Zinc benzene sulphonate	22·5	6·32	6·98	93° 36′
Magnesium benzene sulphonate	22·6	6·32	6·94	93° 36′

As the space group is centrosymmetrical a positive or negative sign is associated with each structure amplitude, and since the metal atoms must be situated at symmetry centres it was decided to fix the signs of the structure amplitudes by comparison of corresponding reflexions from the two isomorphous structures, and then to obtain Fourier projections of the unit cell along the b and c crystallographic axes. From these two projections it was hoped that it would be possible to fix the positions of all the atoms in the unit cell and so to calculate interatomic bond distances.