the structure which eventually led to the identification of the correct unit cell.

It is also a pleasure to acknowledge the benefit of the advice, discussion, and encouragement of Drs David Harker, John P. Howe and John R. Low, all of whom helped so much and are therefore mentioned alphabetically.

References

DICKINS, G. J., DOUGLAS, A. M. B. & TAYLOR, W. H. (1951*a*). *J. Iron Steel Inst.* **167**, 27.

DICKINS, G. J., DOUGLAS, A. M. B. & TAYLOR, W. H. (1951*b*). *Nature, Lond.* **167**, 192.

Internationale Tabellen zur Bestimmung von Kristallstrukturen (1935). Berlin: Borntraeger.

JACOB, C. W. & WARREN, B. E. (1937). *J. Amer. Chem. Soc.* **59**, 2588.

LONSDALE, K. (1936). *Structure Factor Tables.* London: Bell.

SHOEMAKER, D. P. & BERGMAN, B. G. (1951). *J. Amer. Chem. Soc.* (in the Press).

TUCKER, C. W. (1950*a*). *Trans. Amer. Soc. Met.* **42**, 762.

TUCKER, C. W. (1950*b*). U.S. Atomic Energy Commission Declassified Document, no. 2957.

TUCKER, C. W. (1950*c*). *Science*, **112**, 448.

WILSON, A. S. & RUNDLE, R. E. (1949). *Acta Cryst.* **2**, 126.

Acta Cryst. (1951). **4**, 431

Determination of Elastic Constants of Crystals from Diffuse Reflexions of X-rays.
II. Application to some Cubic Crystals

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The formulae required to deduce the elastic constants of cubic crystals from observations of diffuse reflexions are derived from the general theory. The intensities of the diffuse reflexions corresponding to points in reciprocal space distributed along various lines are compared. These lines are always taken in pairs which pass through the same reciprocal-lattice point, e.g. 400, and are parallel to important crystallographic axes, e.g. [110], [111]. Comparisons of these diffuse intensities lead directly to a measurement of ratios of the three elastic constants c_{11}, c_{12}, c_{44}, with an accuracy of about 5 %. Absolute values can be determined from an absolute measurement of the diffuse intensity, though with a lower accuracy. The method was tested using crystals of KCl and KBr and found to give results in agreement with measurements by other methods. It was also applied to $NaClO_3$, galena PbS, and hexamethylenetetramine. The last crystal was chosen as an example of a soft organic crystal which could not easily be studied by other methods, and it is believed to be the first purely organic cubic crystal for which the elastic constants have been determined. The results obtained for these five crystals were as follows:

	c_{11}	c_{12}	c_{44}
KBr	$3{\cdot}8\times10^{11}$	$0{\cdot}60\times10^{11}$	$0{\cdot}64\times10^{11}$ dyne cm.$^{-2}$
KCl	4·3	0·75	0·79
$NaClO_3$	4·9	1·5	1·2
Galena	10·2	3·8	2·5
Hexamethylenetetramine	1·5	0·3	0·7

1. Introduction

In a previous paper (Ramachandran & Wooster, 1951) (hereafter referred to as I) the general principles of a new method were described, in which the elastic constants of crystals are derived from measurements of diffuse reflexion. In this paper it is proposed to describe the results of such measurements for certain cubic crystals. Five crystals have been studied: two alkali halides, KCl and KBr; two inorganic compounds, PbS and $NaClO_3$; and one organic crystal, hexamethylenetetramine, $C_6H_{12}N_4$. Of these, the elastic constants of KCl and KBr are known fairly accurately, and the present experiments with these crystals were performed to test the applicability of the principles described in the earlier paper. The elastic constants of the other three materials were either not known, or different observers had obtained differing results.

2. Some general formulae

We may briefly recapitulate the main definitions and formulae used in calculating the results. Any reciprocal-lattice point of indices *hkl* is known as the 'relp' *hkl*. Starting from this relp a line having direction ratios *A*, *B*, *C* may be drawn, and this is known as the 'rekha' $[ABC]_{hkl}$. The line joining the 'relp', *hkl*, to the origin is known as the corresponding 'rel-vector'. The ratio of the intensity of X-rays diffusely reflected per unit

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cell per unit solid angle in the given direction to that scattered under identical conditions by a single free electron is called the diffuse structure intensity. The diffuse structure intensity of first order, D_1, is given by*

$$D_1=\frac{kT}{\tau}\,|F_T|^2\frac{q^2}{R^2}K[ABC]_{hkl}, \tag{1}$$

where $K[ABC]_{hkl}$ is a function of the elastic constants and of the six indices A, B, C, h, k, l of the rekha $[ABC]_{hkl}$.

The flux of diffusely reflected X-rays, I_d, which is observed by means of a slit subtending a solid angle Ω at the crystal, when a flux I_0 is incident, consists of a number of components. The main part is I_1, due to first-order diffuse reflexions, which varies as $1/R^2$ along a particular rekha. Another part I_2, due to second-order diffuse reflexions, varies as $1/R$; its ratio to I_1 is given by

$$\frac{I_2}{I_1}=\tfrac{1}{2}\pi^3 kTq^2RK'[ABC]_{hkl}/K[ABC]_{hkl}, \tag{2}$$

where $K'[ABC]_{hkl}$ is a function analogous to $K[ABC]_{hkl}$ and is given by equation (7) of I. A third component, I_c, of I_d does not vary with R and is due to Compton scattering, etc. The component I_1 is related to D_1 by the formula

$$\frac{I_1}{I_0}=\frac{\Omega\epsilon^2}{2\mu\tau}D_1. \tag{3}$$

Combining (1) and (3), therefore, $K[ABC]_{hkl}$ can be determined, and hence the elastic constants can be calculated.

To determine I_1, the component due to the first-order diffuse reflexions only, the values of I_d for different R's along a particular rekha are plotted against $1/R^2$, when the intercept on the I_d axis gives I_c which can thus be eliminated. I_2 is eliminated by using equation (2) in which approximate preliminary values of the elastic constants (obtained by neglecting the presence of the second-order diffuse reflexions) are used. Fuller details of the theoretical principles behind this procedure are given in I.

In (1) F_T is the structure amplitude at temperature T and is given in terms of the structure amplitude, F, by

$$F_T=Fe^{-M}. \tag{4}$$

Here
$$M=\frac{8\pi^2}{3}\frac{\sin^2\theta}{\lambda^2}\overline{\xi^2}=\frac{2\pi^2}{3}q^2\overline{\xi^2} \tag{5}$$

(Waller & James, 1927), where $\overline{\xi^2}$ is the mean-square amplitude of vibration. The above formula is strictly true only for a monatomic lattice; for a crystal composed of more than one type of atom, a different value of M applies to each atom. Experiment has shown that the value of M does not vary much from atom to atom (Lonsdale, 1948) so that (4) and (5) can be taken to be true also for a crystal composed of several kinds of atoms, but with $\overline{\xi^2}$ standing for the mean-square amplitude of all the atoms. Values of $\overline{\xi^2}$ at room temperature (293° K.) for a large number of cubic crystals have been given by Lonsdale (1948).

3. Relation between the rekha constant $K[ABC]_{hkl}$ and the elastic constants

For cubic crystals there are only three independent elastic constants c_{11}, c_{12}, c_{44}. Referring all direction cosines to the orthogonal cubic axes, the quantity $K[ABC]_{hkl}$, for which the accurate expressions are (5), and (5a) of I, can be reduced to (Jahn, 1942)

$$\begin{aligned}K[ABC]_{hkl}=[&h^2\{c_{44}^2+c_{44}(c_{11}-c_{44})(v^2+w^2)\\&\qquad+(c_{11}+c_{12})(c_{11}-c_{12}-2c_{44})v^2w^2\}\\&+k^2\{c_{44}^2+c_{44}(c_{11}-c_{44})(w^2+u^2)\\&\qquad+(c_{11}+c_{12})(c_{11}-c_{12}-2c_{44})w^2u^2\}\\&+l^2\{c_{44}^2+c_{44}(c_{11}-c_{44})(u^2+v^2)\\&\qquad+(c_{11}+c_{12})(c_{11}-c_{12}-2c_{44})u^2v^2\}\\&-2hk(c_{12}+c_{44})\{c_{44}+(c_{11}-c_{12}-2c_{44})w^2\}uv\\&-2kl(c_{12}+c_{44})\{c_{44}+(c_{11}-c_{12}-2c_{44})u^2\}vw\\&-2lh(c_{12}+c_{44})\{c_{44}+(c_{11}-c_{12}-2c_{44})v^2\}wu]\\\div(h^2+&k^2+l^2)[c_{11}c_{44}^2+c_{44}(c_{11}+c_{12})\\&\qquad\times(c_{11}-c_{12}-2c_{44})(u^2v^2+v^2w^2+w^2u^2)\\&+(c_{11}+2c_{12}+c_{44})(c_{11}-c_{12}-2c_{44})^2u^2v^2w^2],\end{aligned}$$

where $$(u,v,w)=(A,B,C)/\sqrt{(A^2+B^2+C^2)}. \tag{6}$$

Table 1. *K values in common use for rekhas [ABC] and relps hkl*

	K values for relps having the indices			
$[ABC]$	001	110	111	hkl
[100]	s_2	$\frac{1}{2}(s_1+s_2)$	$\frac{1}{3}(s_1+2s_2)$	$P^2s_1+(Q^2+R^2)\,s_2$
[010]	s_2	$\frac{1}{2}(s_1+s_2)$	$\frac{1}{3}(s_1+2s_2)$	$Q^2s_1+(R^2+P^2)\,s_2$
[001]	s_1	s_2	$\frac{1}{3}(s_1+2s_2)$	$R^2s_1+(P^2+Q^2)\,s_2$
[110]	s_2	$2s_4$	$\frac{1}{3}(s_2+4s_4)$	$(P+Q)^2\,s_4+(P-Q)^2\,s_3+R^2s_2$
[101]	s_3+s_4	$\frac{1}{2}(s_2+s_3+s_4)$	$\frac{1}{3}(s_2+4s_4)$	$(R+P)^2\,s_4+(R-P)^2\,s_3+Q^2s_2$
[011]	s_3+s_4	$\frac{1}{2}(s_2+s_3+s_4)$	$\frac{1}{3}(s_2+4s_4)$	$(Q+R)^2\,s_4+(Q-R)^2\,s_3+P^2s_2$
$[\bar{1}10]$	s_2	$2s_3$	$\frac{1}{3}(s_2+4s_3)$	$(P-Q)^2\,s_4+(P+Q)^2\,s_3+R^2s_2$
$[10\bar{1}]$	s_3+s_4	$\frac{1}{2}(s_2+s_3+s_4)$	$\frac{1}{3}(s_2+4s_3)$	$(R-P)^2\,s_4+(R+P)^2\,s_3+Q^2s_2$
$[0\bar{1}1]$	s_3+s_4	$\frac{1}{2}(s_2+s_3+s_4)$	$\frac{1}{3}(s_2+4s_3)$	$(Q-R)^2\,s_4+(Q+R)^2\,s_3+P^2s_2$
[111]	s_5+2s_6	$2s_5+s_6$	$3s_5$	$(P+Q+R)^2\,s_5+2(1-PQ-QR-RP)\,s_6$
$[\bar{1}11]$	s_5+2s_6	$3s_6$	$\frac{1}{3}(s_5+8s_6)$	$(-P+Q+R)^2\,s_5+2(1+PQ-QR+RP)\,s_6$
$[1\bar{1}1]$	s_5+2s_6	$3s_6$	$\frac{1}{3}(s_5+8s_6)$	$(P-Q+R)^2\,s_5+2(1+PQ+QR-RP)\,s_6$
$[\bar{1}\bar{1}1]$	s_5+2s_6	$2s_5+s_6$	$\frac{1}{3}(s_5+8s_6)$	$(P+Q-R)^2\,s_5+2(1-PQ+QR+RP)\,s_6$

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* For the notation, see I.

Table 2. *K' values in common use for rekhas $[ABC]$ and relps hkl*

$[ABC]$	$K'[ABC]_{hkl}$	$[ABC]$	$K'[ABC]_{hkl}$
$[100]$	$P^4s_1^2+(Q^4+R^4)\ s_2^2$	$[\bar{1}10]$	$(P-Q)^4\ s_4^2+(P+Q)^4\ s_3^2+R^4s_2^2$
$[010]$	$Q^4s_1^2+(R^4+P^4)\ s_2^2$	$[10\bar{1}]$	$(R-P)^4\ s_4^2+(R+P)^4\ s_3^2+Q^4s_2^2$
$[001]$	$R^4s_1^2+(P^4+Q^4)\ s_2^2$	$[01\bar{1}]$	$(Q-R)^4\ s_4^2+(Q+R)^4\ s_3^2+P^3s_2^2$
$[110]$	$(P+Q)^4\ s_4^2+(P-Q)^4\ s_3^2+R^4s_2^2$	$[111]$	$(P+Q+R)^4\ s_5^2+4(1-PQ-QR-RP)^2\ s_6^2$
$[101]$	$(R+P)^4\ s_4^2+(R-P)^4\ s_3^2+Q^4s_2^2$	$[\bar{1}11]$	$(-P+Q+R)^4\ s_5^2+4(1+PQ-QR+RP)^4\ s_6^2$
$[011]$	$(Q+R)^4\ s_4^2+(Q-R)^4\ s_3^2+P^4s_2^2$	$[1\bar{1}1]$	$(P-Q+R)^4\ s_5^2+4(1+PQ+QR-RP)^2\ s_6^2$
		$[11\bar{1}]$	$(P+Q-R)^4\ s_5^2+4(1-PQ+QR+RP)^2\ s_6^2$

This expression further reduces when the rekha is parallel to a cube axis, a face diagonal or a cube diagonal. Following Lonsdale (1948), we give in Table 1 the values of $K[ABC]_{hkl}$ for these special directions. In this table, P, Q, R stand for $h, k, l/\sqrt{(h^2+k^2+l^2)}$ respectively, and the other quantities are

$$s_1=1/c_{11},\qquad s_2=1/c_{44},$$
$$s_3=1/(c_{11}-c_{12}),\qquad s_4=1/(c_{11}+c_{12}+2c_{44}),$$
$$s_5=1/(c_{11}+2c_{12}+4c_{44}),\qquad s_6=1/(c_{11}-c_{12}+c_{44}).$$

From equation (18) of I we derive the values of $K'[ABC]_{hkl}$ given in Table 2.

4. Expressions for K ratios

We have next to find the K ratio (I, equation (10))

$$\left[\frac{A_1B_1C_1}{A_2B_2C_2}\right]_{hkl}=\frac{K[A_1B_1C_1]_{hkl}}{K[A_2B_2C_2]_{hkl}}.$$

In general, $K[ABC]_{hkl}$ is a homogeneous function (of degree -1) in c_{rs}, as may be seen from (6), so that any ratio of the K's is a function of degree zero in the elastic constants. Consequently, it is not possible to determine the elastic constants absolutely from measurements of K ratios. It is, however, possible to determine all the ratios of elastic constants from such measurements. Thus, if there are n independent elastic constants for a crystal there will be $(n-1)$ independent ratios of elastic constants and in principle, it is possible to determine all these by measuring $(n-1)$ K ratios.

For cubic crystals there are two independent ratios of elastic constants, which may be called 'elastic ratios' for convenience, namely,

$$\chi_1=c_{12}/c_{11}\quad\text{and}\quad\chi_2=c_{44}/c_{11}.$$

The K ratios of cubic crystals should all be expressible in terms of χ_1 and χ_2.

With cubic crystals, it is generally possible to obtain all the necessary data from two or three relps taken from among the various orders of $h00$, $hh0$ and hhh. Therefore, the various K ratios that apply to these relps have been calculated and are given in Table 3. There are, of course, various possible ways of choosing the independent K ratios, but preference has been given to those involving the rekha lying along the rel-vector for each particular relp. This is done because experience has shown that measurements can always be made for this rekha.

In principle, the measurement of two K ratios is sufficient to determine χ_1 and χ_2; but in practice it is advisable to check the observation by additional measurements. The calculation of χ_1 and χ_2 from the values of K ratios requires, in general, the solution of two simultaneous quadratic equations. Since a large number of such equations had to be solved during the investigation, graphical methods were evolved for this purpose. These could be made sufficiently accurate, since the experimental data were accurate only to about 5 %.

Table 3. *The evaluation of K ratios in terms of χ_1 and χ_2*

$$\left[\frac{010}{001}\right]_{00l}=\frac{1}{\chi_2}$$

$$\left[\frac{011}{001}\right]_{00l}=\frac{2(1+\chi_2)}{(1-\chi_1)\ (1+\chi_1+2\chi_2)}$$

$$\left[\frac{001}{110}\right]_{hh0}=\frac{1+\chi_1+2\chi_2}{2\chi_2}$$

$$\left[\frac{010}{110}\right]_{hh0}=\frac{(1+\chi_2)\ (1+\chi_1+2\chi_2)}{4\chi_2}$$

$$\left[\frac{1\bar{1}0}{110}\right]_{hh0}=\frac{1+\chi_1+2\chi_2}{1-\chi_1}$$

$$\left[\frac{111}{110}\right]_{hh0}=\frac{3}{2}\ \frac{(1+\chi_1+2\chi_2)\ (1+2\chi_2)}{(1+2\chi_1+4\chi_2)\ (1-\chi_1+\chi_2)}$$

$$\left[\frac{110}{111}\right]_{hhh}=\frac{(1+2\chi_1+4\chi_2)\ (1+\chi_1+6\chi_2)}{9\chi_2(1+\chi_1+2\chi_2)}$$

$$\left[\frac{11\bar{1}}{111}\right]_{hhh}=\frac{1}{9}+\frac{8}{9}\ \frac{(1+2\chi_1+4\chi_2)}{(1-\chi_1+\chi_2)}$$

$$\left[\frac{001}{111}\right]_{hhh}=\frac{(2+\chi_2)\ (1+2\chi_1+4\chi_2)}{9\chi_2}$$

A set of nine charts, one for each K ratio listed in Table 3, which would give the value of the K ratio corresponding to any combination of χ_1 and χ_2, was prepared. An examination of the literature showed that χ_2 is in general less than 0·6, while χ_1 is theoretically limited to the range $-0{\cdot}5\leqslant\chi_1\leqslant 1{\cdot}0$. Therefore the charts included the range of values $0<\chi_2<1{\cdot}0$ and $-0{\cdot}5<\chi_1<1{\cdot}0$. Two illustrative charts are shown in Figs. 1 and 2.* In these, χ_1 and χ_2 form the x and y coordinates, and curves are drawn at equal intervals of 0·05 for $\log_{10}[A_1B_1C_1/A_2B_2C_2]_{hkl}$. The reason for choosing the logarithm is that, on the logarithmic scale, equal increments correspond to successive multiplications by a constant factor. An increment of 0·05 corresponds to an increase of 12·5 %. Since it is possible to read to a fifth of the distance between successive curves with ease, an accuracy of 2·5 % can be obtained, which is within the limits of experimental error.

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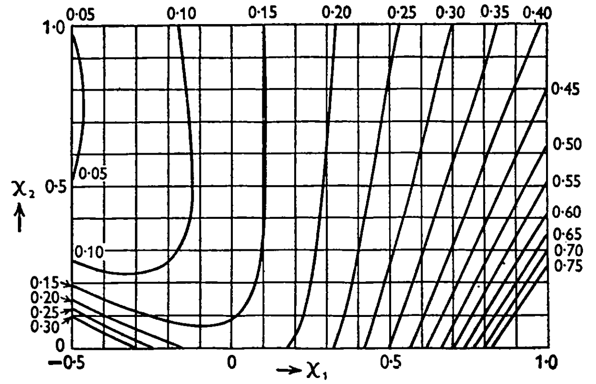
* The authors wish to acknowledge the assistance of the Mathematical Laboratory of this University in computing three of the nine charts.

For actual use the charts are printed on transparent film, so that they can be superposed on one another. Thus, if the values of the K ratios are known, then, by superposing the appropriate charts, the values of χ_1 and χ_2 corresponding to the point of intersection of the two curves can be read off directly. Recalculation of the K-ratios from the values of χ_1 and χ_2 thus found has shown that the method is sufficiently accurate.

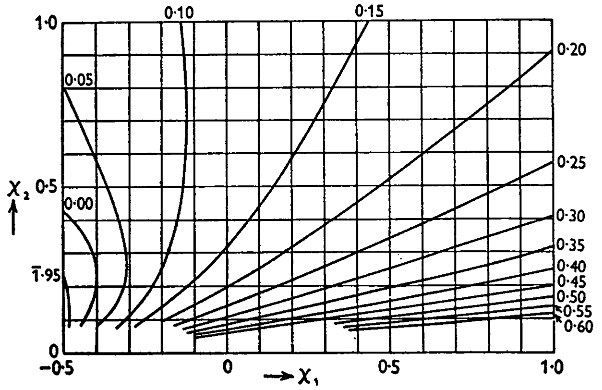
5. Elastic constants of KBr and KCl

The crystals of KBr and KCl studied were synthetic and were made available to the authors through the kindness of Dr E. Burstein of the Naval Research Laboratory, Washington. They were in the form of cleavage blocks and faces were ground on them parallel to (110); consequently, the relps $h00$ and $hh0$ could be studied. Measurements with these crystals were made



$$\log_{10}\left[\frac{111}{01\bar{1}}\right]_{011} = \log_{10}\frac{3}{2}\,\frac{(1+\chi_1+2\chi_2)(1+2\chi_2)}{(1+2\chi_1+4\chi_2)(1-\chi_1+\chi_2)}$$

Fig. 1.



$$\log_{10}\left[\frac{110}{111}\right]_{111} = \log_{10}\frac{(1+2\chi_1+4\chi_2)(1+\chi_1+6\chi_2)}{9\chi_2(1+\chi_1+2\chi_2)}$$

Fig. 2.

Figs. 1, 2. Curves showing the variation of K ratios with χ_1 and χ_2.

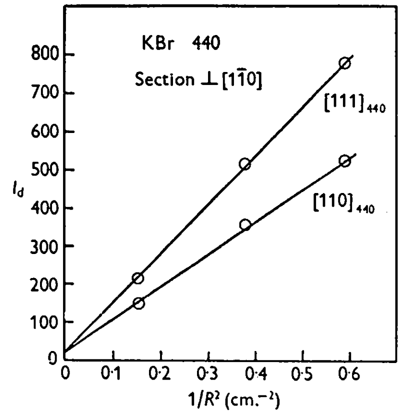


Fig. 3.

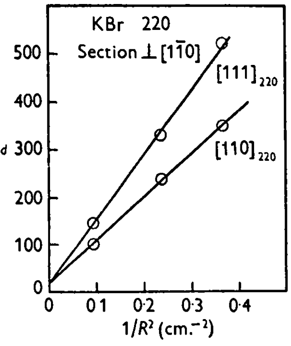


Fig. 4.

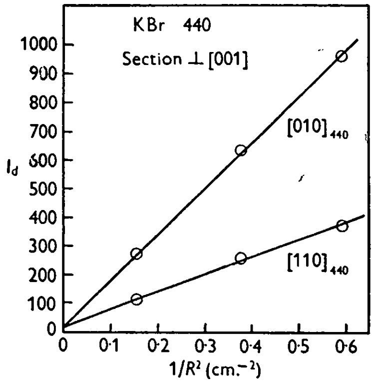


Fig. 5.

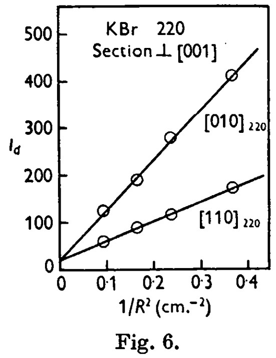


Fig. 6.

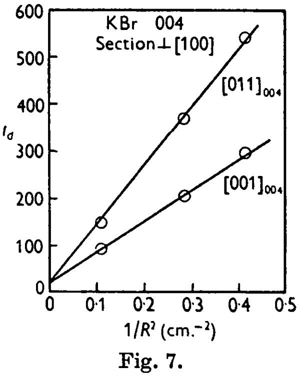


Fig. 7.

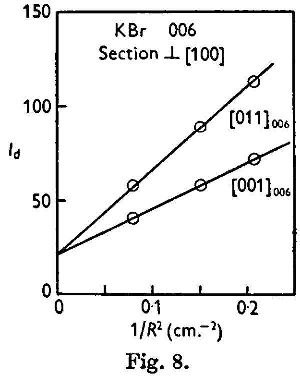


Fig. 8.

Figs. 3–8. Variation of intensity of diffuse flux with distance from the nearest reciprocal-lattice point for various rekhas in potassium bromide.

with the idea of verifying the validity of the method; the details of the analysis are therefore given.

Elastic constants of KBr

Of the two crystals, KBr is more suited for the purpose of testing the method, since it gives more intense diffuse reflexions. The following sections of the various relps were investigated for this crystal:

004: section ⊥ [100]
220: (*a*) section ⊥ [1$\bar{1}$0]
(*b*) section ⊥ [001]
006: section ⊥ [100]
440: (*a*) section ⊥ [1$\bar{1}$0]
(*b*) section ⊥ [001]

Although the crystal was reasonably good, it was not sufficiently perfect for rekhas at right angles to the rel-vector to be studied satisfactorily. The results of the experiments are shown in Figs. 3–8. In these, the values of the diffuse flux I_d (after making the divergence and other corrections) are plotted against $1/R^2$. In making these measurements, the methods described in I were adopted, including the technique of varying slit-heights described in §5·3; but all the measurements have been reduced to a standard size of 5 mm.^{2} for the observing slit and are given in counts per minute. Since the distance of the slit from the crystal is 7·2 mm., the solid angle Ω is $9{\cdot}65\times10^{-4}$. The distance R is measured in cm. on the i–ϕ charts described in I, which have been drawn to the scale of $1/\lambda=50$ cm. Since Cu$K\alpha$ has been invariably used in the investigation this gives 1 A.$^{-1}=76{\cdot}95$ cm. on the charts.

It will be noticed that in all the figures the experimental points lie on straight lines passing through a common point on the axis of ordinates, as required by theory. Subtracting the value I_c (corresponding to the intercept on the axis of ordinates, we have the values of I_1+I_2 given in Table 4. The second-order corrections (I_2) are calculated by using equation (2) with the following elastic constants:

$$c_{11}=3{\cdot}46\times10^{11},\quad c_{12}=0{\cdot}56\times10^{11},$$
$$c_{44}=0{\cdot}505\times10^{11}\text{ dyne cm.}^{-2},$$

which are the mean of the published data due to Huntington (1947) and Galt (1948).

As the magnitude of I_2 is small, the actual values of the elastic constants used to evaluate them are not important. In fact, in the other crystals that were studied, the preliminary values for calculating I_2 were themselves obtained from the measured data. Plots were made of I_1 against $1/R^2$, and the ratios of the slopes of the various lines give the magnitudes of the K ratios, which are:

$$\left.\begin{array}{l}\left[\dfrac{011}{001}\right]_{00l}\left.\begin{array}{l}=1{\cdot}86\text{ for }004\\=1{\cdot}87\text{ for }006\end{array}\right\}\text{mean}=1{\cdot}865,\\[2ex]\qquad\log_{10}\left[\dfrac{011}{001}\right]_{00l}=0{\cdot}270;\end{array}\right\}\quad(\text{A})$$

$$\left.\begin{array}{l}\left[\dfrac{111}{110}\right]_{hh0}\left.\begin{array}{l}=1{\cdot}49\text{ for }220\\=1{\cdot}51\text{ for }440\end{array}\right\}\text{mean}=1{\cdot}50,\\[2ex]\qquad\log_{10}\left[\dfrac{111}{110}\right]_{hh0}=0{\cdot}175;\end{array}\right\}\quad(\text{B})$$

$$\left.\begin{array}{l}\left[\dfrac{010}{110}\right]_{hh0}\left.\begin{array}{l}=2{\cdot}54\text{ for }220\\=2{\cdot}57\text{ for }440\end{array}\right\}\text{mean}=2{\cdot}555,\\[2ex]\qquad\log_{10}\left[\dfrac{010}{110}\right]_{hh0}=0{\cdot}410.\end{array}\right\}\quad(\text{C})$$

Using the charts of χ_1 and χ_2, we have

	χ_1	χ_2
From (A) and (C)	0·16	0·17
From (B) and (C)	0·16	0·17
Mean	0·16	0·17

Having thus determined the elastic ratios, the elastic constants may be determined absolutely, using (1) and (3). The relevant constants are taken from standard tables, while the temperature factor M is calculated from (5) with the value of $\overline{\xi^2}$ from Lonsdale (1948). Table 5 gives the values of the various quantities used in the calculation, as well as that of $K[ABC]_{hkl}$ calculated from it. Combining these with the values of χ_1 and χ_2, the values of c_{11} in the last column are obtained.

The mean value of c_{11} is $3{\cdot}77\times10^{11}$ dyne cm.$^{-2}$, so that we have finally for KBr

$$c_{11}=3{\cdot}8\times10^{11},\quad c_{12}=0{\cdot}60\times10^{11},$$
$$c_{44}=0{\cdot}64\times10^{11}\text{ dyne cm.}^{-2}.$$

Elastic constants of KCl

With KCl the elastic constants were deduced purely from measurements of diffuse reflexions. Since the experiments with KBr showed that relps which belonged to different orders of reflexion from the same lattice places gave concordant results, only one relp of each type was studied in the case of KCl. The most convenient ones to study were 004 and 440. In neither case was the surface good enough for rekhas at right angles to the rel-vector to be investigated. However, the following rekhas were studied in each section:

Rekhas $[001]_{004}$ and $[011]_{004}$ in section ⊥ [100] of relp 004;

Rekhas $[110]_{440}$ and $[111]_{440}$ in section ⊥ [1$\bar{1}$0] of relp 440;

Rekhas $[110]_{440}$ and $[010]_{440}$ in section ⊥ [001] of relp 440.

Without correcting for the second-order diffuse scattering, the following preliminary values were found for the elastic constants:

$$c_{11}=3{\cdot}85\times10^{11},\quad c_{12}=0{\cdot}72\times10^{11},$$
$$c_{44}=0{\cdot}67\times10^{11}\text{ dyne cm.}^{-2}.$$

The second-order corrections calculated using these preliminary values, as well as the corrected values of

Table 4. *Experimental results for* KBr *giving the diffuse flux as a function of the distance from the relp*

Relp 440; section ⊥ $[1\bar{1}0]$; $I_c=20$

	$[ABC]_{hkl}=[110]_{440}$				$[111]_{440}$			
$1/R^2$	I_1+I_2	I_2	I_1	I_1R^2	I_1+I_2	I_2	I_1	I_1R^2
0·155	130	8·0	122	790	197	9·0	188	1210
0·380	336	12·0	324	850	496	14·0	482	1270
0·592	503	15·0	488	825	757	17·5	739·5	1250
				820 (mean)				1240 (mean)

Relp 220; section ⊥ $[1\bar{1}0]$; $I_c=18$

	$[ABC]_{hkl}=[110]_{220}$				$[111]_{220}$			
$1/R^2$	I_1+I_2	I_2	I_1	I_1R^2	I_1+I_2	I_2	I_1	I_1R^2
0·093	82	1·5	80·5	865	122	2·0	120	1290
0·238	218	2·5	215·5	905	313	3·0	310	1300
0·368	327	3·0	324	880	501	3·5	497·5	1350
				885 (mean)				1315 (mean)

Relp 440; section ⊥ [001]; $I_c=20$

	$[ABC]_{hkl}=[110]_{440}$				$[010]_{440}$			
$1/R^2$	I_1+I_2	I_2	I_1	I_1R^2	I_1+I_2	I_2	I_1	I_1R^2
0·155	93	5·5	87·5	565	254	30	224	1445
0·380	231	8·5	222·5	585	611	48	563	1490
0·592	351	10·5	340·5	575	938	58	880	1490
				575 (mean)				1475 (mean)

Relp 220; section ⊥ [001]; $I_c=20$

	$[ABC]_{hkl}=[110]_{220}$				$[010]_{220}$			
$1/R^2$	I_1+I_2	I_2	I_1	I_1R^2	I_1+I_2	I_2	I_1	I_1R^2
0·093	39	1·0	38	410	103	4	99	1035
0·163	68	1·0	67	410	170	5	165	1015
0·238	98	1·0	97	405	258	6	252	1060
0·368	151	1·5	149·5	410	391	8	383	1040
				410 (mean)				1040 (mean)

Relp 004; section ⊥ [100]; $I_c=20$

	$[ABC]_{hkl}=[001]_{004}$				$[011]_{004}$			
$1/R^2$	I_1+I_2	I_2	I_1	I_1R^2	I_1+I_2	I_2	I_1	I_1R^2
0·111	72	2	70	630	127·5	3	124·5	1120
0·285	185	3	182	640	349	4·5	344·5	1210
0·415	277	3·5	273·5	660	518	7	511	1260
				645 (mean)				1195 (mean)

Relp 006; section ⊥ [100]; $I_c=22$

	$[ABC]_{hkl}=[001]_{006}$				$[011]_{006}$			
$1/R^2$	I_1+I_2	I_2	I_1	I_1R^2	I_1+I_2	I_2	I_1	I_1R^2
0·080	19	1	18	225	36	2·5	33·5	420
0·151	36	1·5	34·5	230	67	3·5	63·5	420
0·208	49·5	2	47·5	225	91	3·5	87·5	420
				227 (mean)				420 (mean)

Table 5. *Data involved in the absolute calculation of* c_{11} *for* KBr

$[ABC]_{hkl}$	I_1R^2	$I_0\times10^{-6}$	F_T	q	$\epsilon^2\times10^{26}$	$K[ABC]_{hkl}$ $\times10^{12}$	$c_{11}\times10^{-11}$ (dyne cm.$^{-2}$)
$[001]_{004}$	645	185	115·2	46·7	5·54	2·80	3·57
$[001]_{006}$	225	100	73·2	70·0	4·42	2·53	3·95
$[110]_{220}$	410	110	138·0	33·1	6·56	3·49	3·80
$[110]_{440}$	575	165	80·3	66·2	4·48	3·52	3·77

I_1, are shown in Table 6. Again, it will be noticed that I_1R^2 is nearly constant for each rekha. In particular, for the rekha $[110]_{440}$, the two independent measurements made in different sections agree within the limits of accuracy of the determinations.

From the K ratios obtained from these measurements, the mean values of χ_1 and χ_2 deduced were $\chi_1=0{\cdot}175$, $\chi_2=0{\cdot}185$. Using these and the other data shown in Table 7, the values of $K[ABC]_{hkl}$ and c_{11} were calculated. Thus, the final values of the elastic constants of KCl are:

$$c_{11}=4{\cdot}3\times10^{11},\quad c_{12}=0{\cdot}75\times10^{11},$$
$$c_{44}=0{\cdot}79\times10^{11}\,\text{dyne cm.}^{-2}.$$

Reviewing the experimental results for KBr and KCl, the following remarks may be made. Measurements made with different relps in the case of KBr lead to values of K ratios in reasonable agreement with one another. Similarly, with both KCl and KBr, the absolute values of c_{11} calculated from different relps agree to within 10 %, which is within the limits of experimental error. The values of elastic constants determined here are compared with those obtained by other methods in Tables 8 and 9, from which it will be seen that they are in reasonable agreement. In fact, the difference between the new values and those obtained by ultrasonic methods is less than that between static and ultrasonic measurements.

6. Elastic constants of sodium chlorate

The elastic constants of sodium chlorate were first measured by Voigt (1910), who obtained a negative value for c_{12}. However, recent measurements of Mason (1946) and of Bhagavantam & Suryanarayana (1947) do not confirm the results of Voigt, although they are in fair agreement with each other. The elastic constants of sodium chlorate were therefore measured by the new

Table 6. *Experimental results for* KCl *giving the diffuse flux as a function of the distance from the relp*

Relp 004; section ⊥ [100]; $I_c=16$

		$[ABC]_{hkl}=[001]_{004}$			$[011]_{004}$		
R	$1/R^2$	I_2	I_1	I_1R^2	I_2	I_1	I_1R^2
3·00	0·111	0·5	19·5	175	1·0	37·0	335
2·25	0·197	0·5	33·0	170	1·5	63·5	320
1·80	0·308	1·0	53·5	170	1·5	99·5	320
				172 (mean)			325 (mean)

Relp 440; section ⊥ $[1\bar{1}0]$; $I_c=12$

		$[ABC]_{hkl}=[110]_{440}$			$[111]_{440}$		
R	$1/R^2$	I_2	I_1	I_1R^2	I_2	I_1	I_1R^2
3·60	0·077	1·0	13·0	175	1·0	20·0	260
2·71	0·136	1·5	22·5	165	1·5	32·5	240
2·18	0·211	1·5	34·0	160	2·0	52·0	245
				165 (mean)			250 (mean)

Relp 440; section ⊥ [001]; $I_c=12$

		$[ABC]_{hkl}=[110]_{440}$			$[010]_{440}$		
R	$1/R^2$	I_2	I_1	I_1R^2	I_2	I_1	I_1R^2
3·60	0·077	1·0	12·0	155	5·5	29·5	385
2·71	0·136	1·5	20·0	150	6·5	51·5	380
2·18	0·211	2·0	36·0	170	8·5	83·5	395
				160 (mean)			385 (mean)

Table 7. *Data involved in the absolute calculation of* c_{11} *for* KCl

$[ABC]_{hkl}$	I_1R^2	$I_0\times10^{-6}$	q	F_T	$\epsilon^2\times10^{26}$	$K[ABC]_{hkl}$ $\times10^{12}$	$c_{11}\times10^{-11}$ (dyne cm.$^{-2}$)
$[001]_{004}$	172	110	49·1	64·7	5·36	2·28	4·39
$[110]_{440}$	163	97	69·4	44·3	4·42	3·09	4·18

Table 8. *Elastic constants of* KBr

(Dyne cm.$^{-2}$)	Diffuse reflexion (Ramachandran & Wooster)	Static (Bridgman, 1924)	Ultrasonic (Galt, 1948)
$c_{11}\times10^{-11}$	3·8	3·33	3·46
$c_{12}\times10^{-11}$	0·60	0·58	0·58
$c_{44}\times10^{-11}$	0·64	0·62	0·505

Table 9. *Elastic constants of* KCl

(Dyne cm.$^{-2}$)	Diffuse reflexion (Ramachandran & Wooster)	Static (Bridgman, 1924)	Ultrasonic (Galt, 1948)
$c_{11}\times10^{-11}$	4·3	3·70	3·98
$c_{12}\times10^{-11}$	0·75	0·81	0·62
$c_{44}\times10^{-11}$	0·79	0·79	0·625

method, so as to decide between the two sets of discrepant values. Garrido (1948) has described the results of a photographic investigation of the diffuse reflexions given by $NaClO_3$. Measurements made by the authors do not confirm the shapes of isodiffusion surfaces plotted by Garrido, but they are in agreement with the calculations from the elastic constants of Mason or of Bhagavantam & Suryanarayana (Ramachandran & Wooster, 1950).

The crystals studied were grown from a saturated solution in water. A large number of crystals of size more than 1 cm. were obtained. They were found to be exceedingly good, the mosaic spread being very small. In fact, this was the only substance for which rekhas at right angles to the rel-vectors could be measured with accuracy.

The structure of $NaClO_3$ has been determined by Zachariasen (1929). The best relps to study are 006 and 333. For the former a natural (001) face was used, and for the latter a ground and etched (111) face was employed. The calculations follow the procedure in the previous cases, except for the value of F_T. In this case it was obtained using the tables of Zachariasen (1929), who has given the values of the atomic structure factor f_T at room temperature for Na^+, Cl^{+5} and O^{-2}. The second-order corrections were calculated with the preliminary values

$$c_{11}=4\cdot3\times10^{11},\quad c_{12}=1\cdot5\times10^{11},$$
$$c_{44}=1\cdot0\times10^{11}\,\text{dynes cm.}^{-2},$$

deduced from the measurements directly. The values of I_1R^2 for the different rekhas and the corresponding K ratios are summarized in Table 10. The K ratios are, therefore,

$$\left[\frac{011}{001}\right]_{006}=2\cdot10,\quad \left[\frac{010}{001}\right]_{006}=3\cdot68,\quad \left[\frac{110}{111}\right]_{333}=1\cdot88,$$
$$\left[\frac{001}{111}\right]_{333}=2\cdot58\quad\text{and}\quad \left[\frac{11\bar{1}}{111}\right]_{333}=2\cdot37.$$

From these, the mean values of χ_1 and χ_2 are deduced to be $\chi_1=0\cdot31$, $\chi_2=0\cdot25$.

The relevant data for the absolute calculation of the elastic constants are shown in Table 11.

Table 11. *Data involved in the absolute calculation of* c_{11} *for* $NaClO_3$

$[ABC]_{hkl}$	I_1R^2	$I_0\times10^{-6}$	q	F_T	$\epsilon^2\times10^{26}$	$K[ABC]_{hkl}$ $\times10^{12}$	$c_{11}\times10^{-11}$ (dyne cm.$^{-2}$)
$[001]_{006}$	80	97·5	70·3	30·9	4·42	1·87	5·35
$[111]_{333}$	131	101	60·9	37·5	4·66	2·56	4·46

The mean value of c_{11} is $4\cdot90\times10^{11}$ dyne cm.$^{-2}$, so that the elastic constants of sodium chlorate as measured by the present method are those shown in Table 12, where they are compared with the measurements of the previous workers. The new measurements agree reasonably well with the values of Bhagavantam & Suryanarayana and of Mason, but not with those of Voigt. Thus the new method confirms the determinations of the recent workers.

7. Elastic constants of galena

The elastic constants of galena (PbS) were first measured by Bhagavantam & Bhimasenachar (1944), who obtained the values

$$c_{11}=2\cdot65\times10^{11},\quad c_{12}=6\cdot99\times10^{11},$$
$$c_{44}=4\cdot47\times10^{11}\,\text{dyne cm.}^{-2}.$$

However, as shown by Hearmon (1946), these lead to a negative value for Young's modulus along a cube axis (s_{11}), which is physically not reasonable. Bhagavantam (1946) has more recently published another set of values for the elastic constants, viz.

$$c_{11}=8\cdot69\times10^{11},\quad c_{12}=4\cdot01\times10^{11},$$
$$c_{44}=4\cdot42\times10^{11}\,\text{dyne cm.}^{-2}.$$

As a result of some preliminary experiments designed to test these revised data, it was found that the measurements of diffuse reflexions did not agree with them. Consequently, galena was studied in greater detail.

Two faces were studied, one a cubic cleavage face and the other a natural rhombic dodecahedral face. The former was remarkably good, the half-width of mosaic spread as measured with a plane crystal monochromator of fluorspar being only 5′ of arc. The other crystal had a half-width of about 20′ of arc. The relevant data for this substance, as well as the experimental results, are shown in Tables 13 and 14. Only the final results are shown, the calculations having been made in exactly the same manner as for KBr and KCl. The preliminary values of elastic constants were

$$c_{11}=9\cdot0\times10^{11},\quad c_{12}=3\cdot2\times10^{11},$$
$$c_{44}=2\cdot5\times10^{11}\,\text{dyne cm.}^{-2}.$$

Table 10. *Experimental results for* $NaClO_3$ *giving the diffuse flux* I_1 *as a function of the distance from the relp along certain rekhas*

Relp and section	Rekha	I_1R^2
006, ⊥ [100]	$[001]_{006}$	80
	$[011]_{006}$	168
	$[010]_{006}$	294
333, ⊥ [1$\bar{1}$0]	$[111]_{333}$	131
	$[110]_{333}$	246
	$[001]_{333}$	338
	$[11\bar{1}]_{333}$	300

Table 12. *Elastic constants of* $NaClO_3$

(Dyne cm.$^{-2}$)	R. & W.	B. &. S.	M.	V.
$c_{11}\times10^{-11}$	4·9	5·09	4·90	6·19
$c_{12}\times10^{-11}$	1·5	1·55	1·45	−2·09
$c_{44}\times10^{-11}$	1·2	1·18	1·18	1·20

R. & W. = Ramachandran & Wooster; B. & S. = Bhagavantam & Suryanarayana (1947); M. = Mason (1946); V. = Voigt (1910).

Table 13. *Experimental results for galena giving the diffuse flux I_1 as a function of the distance from the relp along certain rekhas*

Relp and section	Rekha	I_1R^2
004, ⊥ [100]	$[001]_{004}$	191
	$[011]_{004}$	399
440, ⊥ [1$\bar{1}$0]	$[110]_{440}$	196
	$[111]_{440}$	359
440, ⊥ [001]	$[110]_{440}$	198
	$[010]_{440}$	465

$$\left[\frac{011}{001}\right]_{004}=2\cdot09,\quad \left[\frac{111}{110}\right]_{440}=1\cdot82,\quad \left[\frac{010}{110}\right]_{440}=2\cdot36.$$

Table 14. *Data involved in the absolute calculation of c_{11} for galena*

$[ABC]_{hkl}$	I_1R^2	$I_0\times10^{-6}$	q	F_T	$\epsilon^2\times10^{26}$	$K[ABC]_{hkl}$ $\times10^{12}$	$c_{11}\times10^{-11}$ (dyne cm.$^{-2}$)
$[001]_{004}$	191	92	51·5	240	5·23	1·04	9·61
$[110]_{440}$	197	97	72·9	182	4·43	1·00	10·75

It may be noticed that, just as with KCl, the two independent measurements for the rekha $[110]_{440}$ agree in giving very nearly the same value for the slope, viz. 196 and 198. From the data in Table 13 the mean values of χ_1 and χ_2 are found to be

$$\chi_1=0\cdot38,\quad \chi_2=0\cdot25.$$

Thus, the elastic constants of galena are

$$c_{11}=10\cdot2\times10^{11},\quad c_{12}=3\cdot8\times10^{11},$$
$$c_{44}=2\cdot5\times10^{11}\,\text{dyne cm.}^{-2}.$$

It may be remarked that these lead to the value $5\cdot9\times10^{11}$ dyne cm.$^{-2}$ for the bulk modulus, which is in reasonable agreement with the value $5\cdot13\times10^{11}$ dyne cm.$^{-2}$ deduced from the compressibility data of Madelung & Fuchs (1921).

8. Elastic constants of hexamethylenetetramine

As far as is known, elastic constants have not been measured previously for any purely organic cubic crystal. Hexamethylenetetramine is a crystal of this type, whose structure has been investigated in great detail (Wyckoff & Corey, 1934; Brill, Grimm, Hermann & Peters, 1939). Crystals of this substance, which will be called briefly 'hexamine', were grown from a saturated solution in methylated spirit, by gradually lowering its temperature in a thermostat. The crystals, of dimensions of about a centimetre, were of rhombic dodecahedral form {110} and were reasonably perfect, so that they could be used for the present study. The relps investigated were 440 using a natural (110) face and 222 using a ground (111) face.

The procedure followed was similar to that for the previous substances. The absorption coefficient for Cu $K\alpha$ is obtained from the measurements of Brill *et al.* (1939), the mean value 4·28 being used for μ/ρ. The structure amplitudes F_T for the two reflexions 440 and 222 are obtained from the measurements of the two groups of workers mentioned above. The experimental values are used, as they represent F_T at room temperature. They are

$(F_T)_{440}=22\cdot0$ (mean of 23·1 of Wyckoff & Corey and 21·0 of Brill *et al.*),

$(F_T)_{222}=42\cdot3$ (measurement of Wyckoff & Corey).

Some factors had to be considered for hexamine, which were not important with the other crystals studied. Since the absorption coefficient is low, the X-ray beam penetrated appreciably into the crystal. As a result of this, it was not possible to make measurements as close to the Bragg setting as with other crystals. Thus, there was a greater possibility of dispersion effects coming into the measurements, which were, however, neglected. The second factor was the Compton scattering. As compared with values of 10–20 counts/min. with the previous crystals, the constant contribution I_c to the diffuse flux was of the order of 100 counts/min. with hexamine, because of the fact that it is composed of elements of low atomic number. However, this large 'background' did not stand in the way of the accuracy of the measurements, since the diffuse reflexions due to acoustical waves were also quite large, because of the low elastic constants.

The preliminary values of the elastic constants were

$$c_{11}=1\cdot7\times10^{11},\quad c_{12}=0\cdot1\times10^{11},$$
$$c_{44}=0\cdot6\times10^{11}\,\text{dyne cm.}^{-2}.$$

The experimental results are summarized in Tables 15 and 16.

Table 15. *Experimental results for hexamethylenetetramine giving the diffuse flux I_1 as a function of the distance from the relp along certain rekhas*

Relp and section	Rekha	I_1R^2
440, ⊥ [1$\bar{1}$0]	$[110]_{440}$	1300
	$[111]_{440}$	1940
440, ⊥ [001]	$[110]_{440}$	1280
	$[010]_{440}$	2170
222, ⊥ [1$\bar{1}$0]	$[111]_{222}$	1865
	$[110]_{222}$	2750
	$[001]_{222}$	3845

Table 16. *Data involved in the absolute calculation of c_{11} for hexamethylenetetramine*

$[ABC]_{hkl}$	I_1R^2	$I_0\times10^{-6}$	q	F_T	$\epsilon^2\times10^{26}$	$K[ABC]_{hkl}$ $\times10^{12}$	$c_{11}\times10^{-11}$ (dyne cm.$^{-2}$)
$[110]_{440}$	1290	94	61·8	22·0	4·62	6·54	1·47
$[111]_{222}$	1865	70	38·0	42·3	6·20	6·14	1·54

The mean values of χ_1 and χ_2 from the K ratios obtained from Table 15 are

$$\chi_1 = 0{\cdot}21, \quad \chi_2 = 0{\cdot}44;$$

and hence the elastic constants of hexamine are

$$c_{11} = 1{\cdot}5 \times 10^{11}, \quad c_{12} = 0{\cdot}3 \times 10^{11},$$
$$c_{44} = 0{\cdot}7 \times 10^{11}\ \text{dyne cm.}^{-2}.$$

It may be mentioned that the absolute values of elastic constants are not very reliable, because they depend on the value of μ, the linear absorption coefficient. The value used here for μ/ρ is 4·28, experimentally found by Brill *et al.* (1939), who state that this is appreciably lower than the value 6·23 calculated from the mass absorption coefficients of carbon, hydrogen and nitrogen. If the latter were used, then all the elastic constants would be reduced to about two-thirds of the values given above. The magnitudes χ_1 and χ_2 are, however, expected to be accurate to ± 0·05.

9. Concluding remarks

(*a*) *Application to other cubic and non-cubic crystals*

It is believed that the experimental procedure described in this paper can be employed for most cubic crystals. It is possible in general to find one or two reflexions from among the various orders of $00l$, $hh0$ and hhh which satisfy the requirements mentioned in I, § 10, but if this is not possible, in any particular case, then the general formula, equation (6) of this paper, can be used to calculate rekha constants and K ratios for other relps.

Essentially, no new principles have to be taken into account in extending the method to crystals of lower symmetry. Since the number of independent elastic constants is larger, more measurements are required. The formulae are also more complicated than for cubic crystals; but by considering reflexions with simple indices and also special sections of reciprocal space, it may be possible to study one or two elastic constants at a time and thus simplify the calculations.

(*b*) *Advantages and limitations of the new method*

An advantage of the present method over the usual methods is that the crystal need not be subjected to any strains whatsoever. Consequently, it would be possible to measure elastic constants of crystals for which the yield strength is very low. A second advantage is that only a relatively small crystal is required. Although in the present study the smallest face that could be used was about 5 × 5 mm.^{2} in cross-section, this size could be further reduced by using more intense X-ray sources.

The authors believe that it would be difficult to increase the accuracy of measurement of the elastic constants beyond ± 3 %. The accuracy of ultrasonic methods is greater than this, but that of static methods is generally of the same order. Another limitation is the long time required for the study, and the necessity for having a rather elaborate equipment. However, should occasions arise where the usual methods are not satisfactory, or where a discrepancy has to be investigated, this new method should prove a valuable adjunct to those existing at present.

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References

Bhagavantam, S. (1946). Presidential Address to the Section of Physics, 33rd Indian Science Congress.

Bhagavantam, S. & Bhimasenachar, J. (1944). *Proc. Indian Acad. Sci.* A, **20**, 298.

Bhagavantam, S. & Suryanarayana, D. (1947). *Phys. Rev.* **71**, 553.

Bridgman, P. W. (1924). *Proc. Nat. Acad. Sci., Wash.*, **10**, 411.

Brill, R., Grimm, H. G., Hermann, C. & Peters, C. (1939). *Ann. Phys., Lpz.*, **34**, 393.

Galt, J. K. (1948). *Phys. Rev.* **73**, 1460.

Garrido, J. (1948). *Acta Cryst.* **1**, 1.

Hearmon, R. F. S. (1946). *Rev. Mod. Phys.* **18**, 409.

Huntington, H. B. (1947). *Phys. Rev.* **72**, 321.

Jahn, H. A. (1942). *Proc. Roy. Soc.* A, **179**, 320.

Lonsdale, K. (1948). *Acta Cryst.* **1**, 142.

Madelung, E. & Fuchs, R. (1921). *Ann. Phys., Lpz.*, **65**, 289.

Mason, W. P. (1946). *Phys. Rev.* **70**, 529.

Ramachandran, G. N. & Wooster, W. A. (1950). *Acta Cryst.* **3**, 73.

Voigt, W. (1910). *Lehrbuch der Kristallphysik*. Leipzig: Teubner.

Waller, I. & James, R. W. (1927). *Proc. Roy. Soc.* A, **117**, 214.

Wyckoff, R. W. G. & Corey, R. B. (1934). *Z. Krystallogr.* **89**, 462.

Zachariasen, W. H. (1929). *Z. Krystallogr.* **71**, 517.