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Calculation of Geometrical Structure Factors for Space Groups of Low Symmetry. III

BY E. W. RADOSLOVICH

Division of Soils, Commonwealth Scientific and Industrial Research Organization, Adelaide, Australia

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This paper describes a simple calculator for functions such as $\cos(hx+ky).\cos lz$. Values of these functions may be readily read off from suitably arranged tables of $\cos hx.\cos lz$, after a simple mechanical shift of origin by an amount ky.

Introduction

A simple mechanical device has previously been described (Radoslovich & Megaw, 1955) which allows values of $\begin{Bmatrix}\sin\\\cos\end{Bmatrix}(hx+ky+lz)$* to be read directly from tables of $\begin{Bmatrix}\sin\\\cos\end{Bmatrix}(hx)$. This is useful for space groups $P1$ and $P\bar{1}$, and for certain two-dimensional projections of the monoclinic space groups. The device has also been extended (Radoslovich, 1955) to compute $\Sigma\cos(hx+ky+lz)$. It would, however, be more useful when studying monoclinic crystals to be able to tabulate directly quantities of the kind

$$\begin{Bmatrix}\sin\\\cos\end{Bmatrix}(hx+ky)\cdot\begin{Bmatrix}\sin\\\cos\end{Bmatrix}(lz)\,.$$

This is the form assumed by both A and B in the structure factor expression $F = A+iB$ for the space groups nos. 3 to 15 in the *International Tables* (1952).

* i.e. either $\sin(hx+ky+lz)$ or $\cos(hx+ky+lz)$, as required.

The earlier device has been redesigned to permit such calculations. The tables have been enlarged to read $\begin{Bmatrix}\sin\\\cos\end{Bmatrix}(hx)\cdot\begin{Bmatrix}\sin\\\cos\end{Bmatrix}(lz)$ directly, at suitable intervals of lz and for integral values of h. These tables can still be moved mechanically, however, to include the term ky in the form $\begin{Bmatrix}\sin\\\cos\end{Bmatrix}(hx+ky)\cdot\begin{Bmatrix}\sin\\\cos\end{Bmatrix}(lz)$.

Description

The three angles to be specified (viz. hx, ky and lz) are given as decimal fractions of a cycle, at intervals of 0·01 (i.e. 3·6°); values of cosines are given at the same angular intervals. There are 26 different tables of $K\cos hx$, where K has values $K=\cos lz$, and $lz =$ 0·00, 0·01 . . . 0·25, for successive tables.

The values of hx are set out on four strips of paper

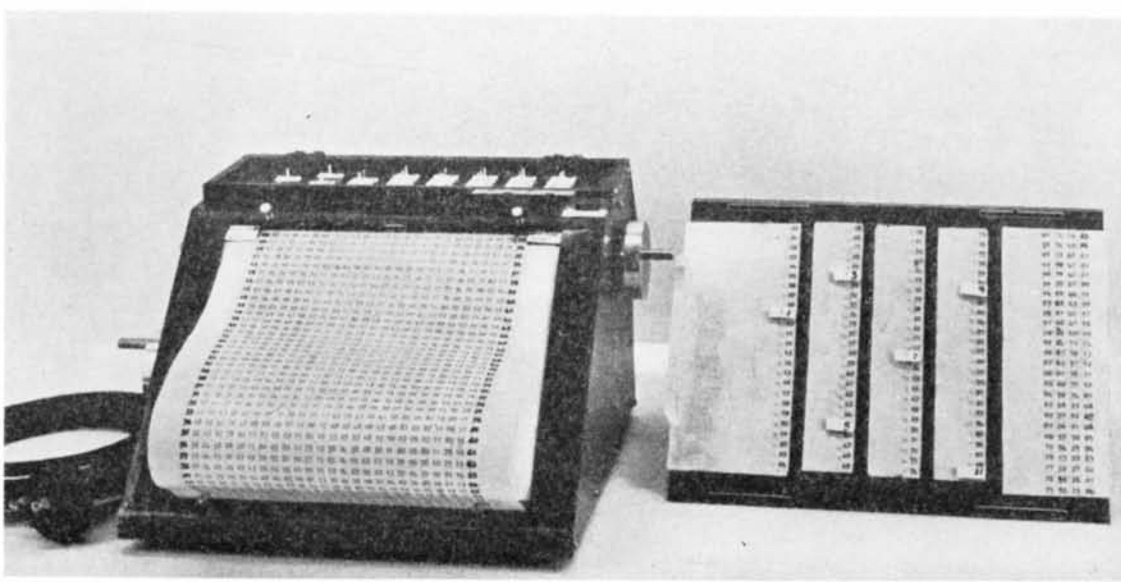

Fig. 1. General view of calculator, with cover removed. This shows the ky scales on the two edges of the chart, and the four columns of the hx scale on the cover, with some 'h' pins in place. (The block of figures on the right of the cover are for use with the $\cos(hx+ky+lz)$ section of the calculator). The markers are conveniently stored in the top compartment.

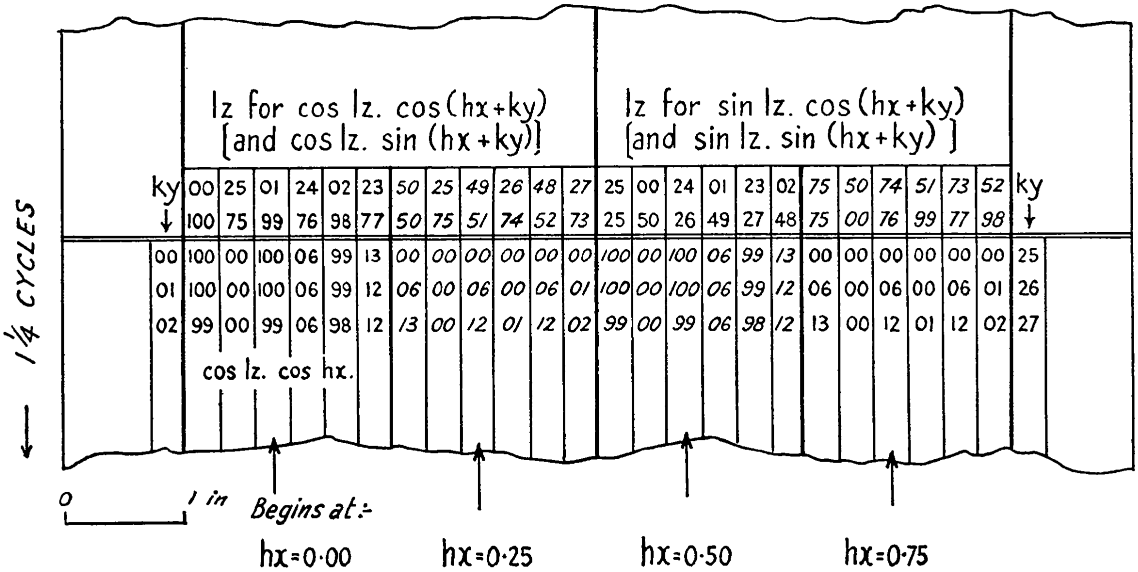

Fig. 2. First section of the movable chart. Arrows point to the table for cos 0·01.cos hx, which is given four times (see text). When lz values are in red (sloping figures here) then cos lz or sin lz is negative.

glued to the lower side of a perspex cover carried on the sloping face of the instrument (Fig. 1). These strips are correctly spaced to reveal, through the remaining transparent sections in the perspex cover, just one at a time of several vertical tables of cosines. The required table on the chart underneath can be chosen by moving the cover sideways, up to about two inches.

Small holes are drilled in the perspex, at the position of each 'hx', into which can be inserted flat markers mounted on a short pin. The markers are numbered 1, 2, 3, ..., corresponding to values of h, and there are two sets, with black and red figures on a white background, for h and $\bar{h}$. The markers are not essential, but are an aid to quick reading.

The values of ky and lz, and the 26 tables of $K\cos hx$ are set out (Fig. 2) on a moving chart consisting of a strip of tracing linen 8 in. wide and about 15 feet long. The ky values and the cosine tables are arranged vertically, with one space between each two-figure column, whilst values of lz are set out horizontally, as column headings to the cosine tables. Since it is impossible to accommodate all the 26 cosine tables in parallel columns across the chart they have been set out in five sections on the chart, six tables in each section, except the last. There is a blank space of about two inches between sections.

The ky values are set out vertically down the left hand edge of the chart, beginning at $ky = 0·00$ and running through $1\frac{1}{4}$ cycles to $ky = 1·25$ (equivalent to 0·25). This ky column is duplicated on the right-hand edge of the chart, but here the values begin at $ky = 0·25$ and run to $ky = 1·50$ (i.e. 0·50). This set-out of the ky values is repeated in each of the five sections of the chart mentioned above.

Two values of ky are always visible at the top left and right corners of the computer. A small bracket at the upper left corner of the chart area carries the word 'cos' and an arrow. This defines the origin with respect to the left-hand ky scale, to be used when calculating $\cos(hx+ky)\cdot\begin{Bmatrix}\sin\\ \cos\end{Bmatrix}(lz)$. The right-hand bracket defines the origin for calculating $\sin(hx+ky)\begin{Bmatrix}\sin\\ \cos\end{Bmatrix}(lz)$.

Now consider the arrangement of one $K.\cos hx$ table, e.g. when $K = \cos lz$ for $lz = 0·01$. This table lies in the first section of the chart. It is set out vertically, beginning at a value 0·99 corresponding to $\cos 0·01.\cos hx$ for $hx = 0·00$ and running for $1\frac{1}{4}$ cycles through to $hx = 1·25$. The dimensions of the perspex cover of the instrument, however, permit only one quarter of a cycle to be seen at any one time, and therefore this $K.\cos hx$ table is repeated in three further columns, beginning at values corresponding to $hx = 0·25$, 0·50 and 0·75 (Fig. 2). In this way a full cycle of one (and one only) $K\cos hx$ table is always visible through the perspex, no matter how that section of the chart is moved backwards and forwards behind it. Values of $K.\cos hx$ for which $\cos hx$ is negative are in red. The successive columns of $K\cos hx$ tables are not in order of increasing lz, but are arranged so that $\cos l_1z.\cos hx$ and $\sin l_1z.\cos hx\,(=\cos(0·25-l_1z)\times\cos hx)$ are in adjacent columns and hence both values can be read off with only a slight movement of the cover. Values of $\cos l_1z.\cos hx$ and $\cos l_1z.\sin hx$ are obviously related by a chart shift of a quarter cycle.

The value of lz (viz. $lz = 0·01$) to which this table corresponds will appear through the clear sections of the perspex cover at the top of the left-hand $K\cos hx$ column. But this table also represents values of $\cos 0·99\cos hx$, $-\cos 0·51.\cos hx$, $-\cos 0·49\cos hx$, $\sin 0·26\cos hx$, $\sin 0·24\cos hx$, $-\sin 0·76\cos hx$, and

$-\sin 0{\cdot}74 \cos hx$. All eight values of lz, (under the appropriate heading, and in black or red, as the above products have a positive or negative sign) therefore appear at the top of the other three columns of this particular table, $\cos 0{\cdot}01 . \cos hx$. It is by this means that all values of lz from 0·00 to 1·00, and all four combinations $\begin{Bmatrix}\sin lz\\ \cos lz\end{Bmatrix} . \begin{Bmatrix}\sin hx\\ \cos hx\end{Bmatrix}$ can be calculated from the 26 different tables given.

The sign of $\begin{Bmatrix}\sin\\ \cos\end{Bmatrix}(hx+ky) \cdot \begin{Bmatrix}\sin\\ \cos\end{Bmatrix} lz$, which will depend on the sign of both components, is determined from its colour (black or red) on the table. This choice is aided by a simple indicator above the perspex, consisting of a metal bar sliding behind covers. Values of lz for which $\begin{Bmatrix}\sin\\ \cos\end{Bmatrix} lz$ is negative are shown in red; and the metal bar is moved to place 'lz' on it opposite a black or red dot, depending on the colour of lz on the chart. The + and − signs on the bar then show whether all black figures (for the quantity $\begin{Bmatrix}\sin\\ \cos\end{Bmatrix}(hx+ky) \times \begin{Bmatrix}\sin\\ \cos\end{Bmatrix}(lz)$) are to be read as positive and all red figures as negative, or vice versa.

A mechanical drive* for moving the chart smoothly either forwards or backwards is included, though it is not essential. A small non-reversing electric motor is mounted on a pivot so that it can be placed in three positions determined by a standard radio switch. In the first of these the rubber driving wheel from the motor engages a knurled wheel on one winding drum, for forward motion of the chart. The middle position is neutral; and in the third position the knurled wheel on the other chart drum is engaged, for reverse motion. Spring-mounted fibre washers on both winding drums ensure that the chart is always taut. The chart may also be moved manually.

The device is used as follows. Coordinates (x, y, z) known to any desired accuracy can be used as a starting point, and the integral multiples hx, ky and lz are formed to the same accuracy. These quantities are *then* rounded off to the nearest 0·01. The value of lz for some particular calculation (involving either $\cos lz$ or $\sin lz$) is then located at the head of one of the five sections and its colour is set on the sign indicator. The perspex cover is placed so that this lz is visible through one of the transparent strips in the cover. The chart is now moved within that section so that the required value of ky lines up with the arrow, for calculating either $\cos(hx+ky)$ or $\sin(hx+ky)$. The h markers are placed at the tabulated values of hx, and are left in these positions until a further atom is being considered. The values on the chart opposite the markers are values for

$$h = \pm 1, 2 \ldots, \quad \text{of} \begin{Bmatrix}\sin\\ \cos\end{Bmatrix}(hx+ky) \cdot \begin{Bmatrix}\sin\\ \cos\end{Bmatrix}(lz),$$

depending on the position of the cover and on which ky scale is used.

Cos $(hx+ky+lz)$ section

In order to make one device as useful as possible two further sections of chart, both for calculating $\begin{Bmatrix}\sin\\ \cos\end{Bmatrix}(hx+ky+lz)$, are included. One of these is an exact copy of that described previously (Radoslovich & Megaw, 1955), but the tables have been more widely spaced to match the transparent strips on the new perspex cover. The other section has the same layout, but the interval used for all the tables is now 0·005 cycles, so that the accuracy is doubled. This requires twice as many values of hx, and to accommodate these the tables are set out in eight columns rather than four. The perspex cover is replaced by one carrying the hx table in eight columns, at 0·005 cycle intervals.

Discussion

The present computer retains the several advantages of the earlier device, which were discussed in detail by Radoslovich & Megaw (1955). It is, however, worth emphasizing that it is now possible to compute geometrical structure-factors for all of the triclinic and monoclinic space groups directly from the formulae in the *International Tables* (1952), so taking advantage of any symmetry relations for these space groups. Contributions of the separate atoms to the geometrical structure factor can be read off immediately by unskilled computers, using no more than a table of hx, ky and lz values to set up the device. The rounding-off errors are kept to the minimum which is possible when using trigonometrical tables at 0·01 cycle intervals.

The following example shows the speed of this device. Values of $\cos(hx+ky) . \cos lz$ were calculated for an atom for which $x=0{\cdot}938$, $y=0{\cdot}417$ and $z=0{\cdot}055$, the indices being given values $h=\overline{20}, \overline{18}, \ldots, 18, 20$; $k = 0, 1, \ldots, 6$; and $l = 3$ and 4. Eight minutes were needed to set up the h markers, and thereafter 300 values of $\cos(hx+ky) . \cos lz$ were tabulated in 23 minutes, i.e. as fast as they could be written down. It was not tiring to use the computer at this speed, which is considerably faster than can be achieved by other simple methods of calculating trigonometric products of this form.

* The computer was constructed (and in part designed) by Messrs. K. Barrow and A. Palm in the workshops of this Division.

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