i.e.

$$3{\cdot}62\Delta\{1+(0{\cdot}4u_0/\Delta)^2\}^{\frac{1}{2}} \leqslant U\times\bar{\eta} = 0{\cdot}5\pm0{\cdot}1 \quad (0{\cdot}15 < \bar{\eta} < 0{\cdot}75)\,,$$

whence

$$U=2\pi\Delta/d_{\text{min.}} \leqslant (2\pi/d_{\text{min.}})(0{\cdot}5/3{\cdot}62)/\{1+(0{\cdot}4u_0/\Delta)^2\}^{\frac{1}{2}} \simeq 0{\cdot}8/d_{\text{min.}}\,,$$

so that

$$\bar{\eta} = \exp\,[-0{\cdot}7U] \geqslant \exp\,[-0{\cdot}56/d_{\text{min.}}] \simeq 0{\cdot}5\,,$$

for the reflections within the limiting sphere of Cu $K\alpha$ radiation. Now, this limit on $\bar{\eta}$ corresponds to $R_I \leqslant 45\%$, and provides some justification for the usual bias against attempting the refinement of an approximation with a reliability index greater than 50%. This is to be contrasted with the properly weighted syntheses, for which the useful upper limit of R_I is considerably higher. Similarly the upper limit of u_0 (and Δ) increases progressively as we go from case (*c*) to case (*a*) above.

Finally, we must note that the value of the fluctuation $\Delta\eta$ is not the same for all three coordinates of any one atom. This follows from the fact that only corresponding coordinates of neighbouring (or overlapping) atoms are involved in the equations for the separate shifts (cf. Qurashi & Vand, 1953, equation (9)). However, it appears that the fluctuation $(\Delta\eta)_1$ is the same for all three coordinates. Thus we get

$$\eta_x = \bar{\eta}+(\Delta\eta)_1+(\Delta\eta)_{2,x}\,,$$
$$\eta_y = \bar{\eta}+(\Delta\eta)_1+(\Delta\eta)_{2,y}\,,$$
$$\eta_z = \bar{\eta}+(\Delta\eta)_1+(\Delta\eta)_{2,z}\,.$$

Since $(\delta x)_{\text{calc.}} = \eta_x(\delta x)_{\text{obs.}}$, etc., it is readily seen that when $\{\overline{(\Delta\eta)_2^2}\}^{\frac{1}{2}}$ is comparable with $\bar{\eta}$, the calculated vector shifts can differ very considerably in direction from the actual shifts required. Since $\overline{(\Delta\eta)_2^2} \sim \overline{(\Delta\eta)_1^2}$, this effect is small within the limits of useful $\bar{\eta}$ calculated earlier, because $\{\overline{(\Delta\eta)_2^2}\}^{\frac{1}{2}} < \bar{\eta}/\sqrt{2}$.

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

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This instrument (called SUMCOS) assists in the calculation of $\sum_j \cos(hx_j+ky_j+lz_j)$ by hand. It does this by forming $\cos(hx_j+ky_j+lz_j)$ separately for ten atoms, and simultaneously presenting the values of these ten cosines ready for addition for any given (h, k, l). The final addition must be done by hand.

The values of $\cos(hx_j+ky_j+lz_j)$ are derived from a table of $\cos hx_j$ by using a simple mechanical arrangement to shift the origin of this table by (ky_j+lz_j). The values are presented for addition by switching on a small light behind the particular value of $\cos hx_j$ on the table, which is written on translucent material. New values of $\cos(hx_j+ky_j+lz_j)$ are presented for successive h simply by turning to the next position of a 24-position switch.

1. Introduction

Part I of this paper (Radoslovich & Megaw, 1955) described a device for moving the origin of a table of cosines by any arbitrary amount $(ky+lz)$ in order to read $\cos(hx+ky+lz)$ from a table of $\cos hx$. It consisted of a box carrying a fixed scale and two tables on a movable chart, so that shifts of origin could be made easily and rapidly. The usefulness of this box in calculations for triclinic and monoclinic space groups was pointed out.

Such a box speeds up calculations dealing with one atom at a time. In most calculations, however, we are concerned with several chemically identical but crystallographically distinct atoms, and we are therefore interested in the quantity

$$\sum_{j=0}^{N} \cos(hx_j+ky_j+lz_j)\,,$$

where the summation is over N chemically similar atoms. This could be computed rapidly if the values of cos $(hx_j+ky_j+lz_j)$ presented separately on N such boxes could be easily picked out simultaneously, ready for immediate addition. To achieve this it was necessary to re-design the box so that a convenient number of identical units would stack together in one instrument. A description of *one* of these units is given first; the method of combining them follows.

2. Description of instrument

(a) Outline

The new design incorporates the following changes. The fixed hx scale with its associated marking pins is replaced by a panel of bulbs. The moving scale, which is now translucent, is arranged horizontally in front of these and carries the values of cos hx printed from left to right. The bulb designated hx is required to light up when a multiple switch is at position h; by doing so it clearly marks the required value of cos $(hx+ky+lz)$. For this purpose each pole of the switch is permanently connected to a socket in a panel behind the lights, and likewise each bulb is connected to a socket on this panel. The instrument is set up for calculations with any given set of atomic coordinates by connecting the switch socket h with the bulb socket hx, a process corresponding to placing the marking-pins on the hx scale on the box.

A short subsidiary scale on the chart, reading angular intervals, can be placed so as to label the bulbs with their values of hx for the purpose of making the above connections; it is also used to fix the origin at a position determined by l_1z. By moving k_1y on the main scale up to this new origin we obtain the required displacement (k_1y+l_1z) of the origin, and hence values of cos $(hx+k_1y+l_1z)$. A second subsidiary scale is available for setting up the instrument to read values of sin $(hx+k_1y+l_1z)$.

(b) Tables

The tables of cosines and angular intervals are written on a narrow strip of tracing linen. This is held vertically in a milled channel between two sheets of perspex, and can be moved to the left or right by hand-operated drums at each end. The winding drums move independently, one being used for forward winding and one for backward winding. Small fibre washers prevent them running too freely. The lower disc of each drum, which is of large diameter and knurled, projects through a slot in the perspex, for winding purposes.

The tracing linen is $1\frac{3}{4}$ in. deep, and about 8 ft. long. It contains three blocks of tables, i.e. the main and the two subsidiary tables mentioned above. The main table (Table 1) contains eight rows of figures, i.e. four cosine tables, and four tables of angular intervals labelled ky. The latter are used only in resetting the strip, and so are in light coloured inks, whereas the cosine figures are in heavy Indian ink, since they are finally to be read off for addition. Both

Table 1. *Beginning of main table*

The tables are reproduced approximately actual size. The ky tables are printed in red ink.

$\overline{100}$	$\overline{100}$	$\overline{99}$	$\overline{99}$	$\overline{99}$	$\overline{99}$	$\overline{98}$	$\overline{98}$	...	→ $1\frac{1}{4}$ cycles
00		01		02		03		...	ky
100	**100**	**99**	**99**	**99**	**99**	**98**	**98**	...	
75		76		77		78		...	ky
50		51		52		53		...	ky
	0	$\overline{03}$	$\overline{06}$	$\overline{09}$	$\overline{13}$	$\overline{16}$	$\overline{19}$	...	
25		26		27		28		...	ky
	0	**03**	**06**	**09**	**13**	**16**	**19**	...	

Table 2. *Beginning of setting-up tables*

The tables are reproduced approximately actual size. The tables run for a quarter-cycle each. The lz tables are printed in red ink.

COSINES

50		**51**		**52**		**53**		...	hx
00		99		98		97		...	lz
00		**01**		**02**		**03**		...	hx
25		24		23		22		...	lz
50		49		48		47		...	lz
	25		**26**		**27**		**28**	...	hx
75		74		73		72		...	lz
	75		**76**		**77**		**78**	...	hx

SINES

50		**51**		**52**		**53**		...	hx
25		24		23		22		...	lz
00		**01**		**02**		**03**		...	hx
50		49		48		47		...	lz
75		74		73		72		...	lz
	25		**26**		**27**		**28**	...	hx
00		99		98		97		...	lz
	75		**76**		**77**		**78**	...	hx

tables are at 0·005 cycle intervals, but as ky is linear every second figure only is recorded. The reason for having four rows of cosines (and of ky) is that the cosine cycle has been folded into a quarter-cycle length to keep the width of the box reasonable. Thus the cosine sections begin at $\theta = \pi$, 0, $\pi/2$ and $3\pi/2$ respectively; each section runs through $1\frac{1}{4}$ cycles.

The two subsidiary tables (of $\frac{1}{4}$ cycle length) also have eight rows of figures, every row being in angular intervals. The first, third, sixth, and eight rows are labelled hx, and the other four rows lz (Table 2). In order to obtain the double shift of origin (k_1y+l_1z) it is necessary to be able to mark the position of l_1z on the front panel of the instrument, when the subsidiary tables are in position. This is done using thin perspex plates, $\frac{1}{2}$ in. $\times 1\frac{1}{2}$ in., which have a short pin in their upper edge. A row of holes has been drilled at $\frac{1}{4}$ in. intervals (the spacing of the tables) in the perspex face of the instrument, into which the pin can be pushed. Each plate has a small white dot painted on the rear surface at the height of one or other of the lz rows of figures, and a particular value of lz is marked simply by placing the appropriate plate so that the dot lies over it. This dot now becomes the 'origin' of the instrument.

(c) *Bulbs*

There are four rows of small electric bulbs, 25 in each row. These are mounted in standard 'screw-in' holders spaced $\frac{1}{2}$ in. apart and soldered to brass rods fixed immediately behind the perspex panel; this arrangement allows a bulb to be replaced, in case of failure, in three minutes. These rods both support the bulbs and act as the common earth throughout the instrument. The $\frac{1}{2}$ in. spacing means that values on the hx or cosine table can be lit up at 0·01 cycle intervals (though the tables can be set to twice this accuracy). A grid of black paper strips is stuck to the perspex immediately behind the charts, to leave an aperture $\frac{1}{4}$ in. square in front of each bulb. Likewise each bulb is painted black, except for a small area on top; thus any given bulb only lights up one cosine figure on the chart. The bulbs are lit by a small $6V$. transformer.

(d) *Sockets and switches*

The bulbs are connected vertically in pairs (either a 1st- plus 2nd-row bulb, or a 3rd- plus 4th-row bulb) and each pair is connected to one socket on the rear panel. This pairing was done to keep down the number of sockets, but it introduces certain complexities considered in the next paragraph. Since there are four rows of cosines there are two rows of bulb sockets. Two further rows of 23 sockets are connected in sequence to a 48-position switch (two standard 24-pole switches in series); these will be referred to as switch sockets. Pairs of switch sockets in the upper and lower rows correspond to successive values of h, and are wired to successive switch positions, which are therefore called

$$1_a, 1_b;\ 2_a, 2_b;\ 3_a, 3_b;\ \ldots;\ h_a, h_b;\ \ldots.$$

Connections from bulb socket to switch socket are made by a short lead with a wander-plug at each end.

The two switches each have another wafer on which alternate positions are joined together and connected to a panel light, $1_a, 2_a, \ldots, h_a, \ldots$ to a white light, $1_b, 2_b, \ldots, h_b, \ldots$ to a red light, the latter marked with the word 'TOTAL'. The bulbs light up in vertical pairs, giving two values of hx differing by π (i.e. by 0·50 cycle). The top and bottom rows of figures (which begin at $hx = \pi$ and $3\pi/2$ respectively) have strips of red cellophane fixed behind them so that they appear against a red background, while the other two rows are left clear. Thus the two figures illuminated appear against a white and a red background for the first and second half-cycles respectively. If hx lies between 0 and π, the bulb socket hx is connected to the switch socket h_a (see Fig. 1); the *white* light then appears on the panel above the switch to show that the figure against the *white* background is the value required. If hx lies between π and 2π the connection is made to switch socket h_b, and the red panel light indicates the figure against the red background. Fig. 1 shows the

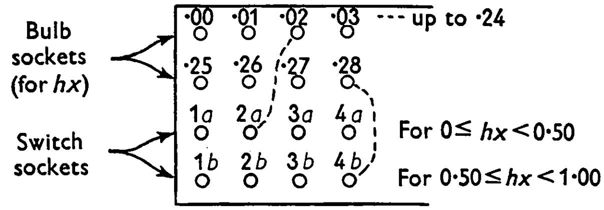

Fig. 1. Rear panel. Scheme of sockets showing connections for $2x = 0{\cdot}02$ and for $4x = 0{\cdot}78$ (i.e. $0{\cdot}28+0{\cdot}50$).

arrangement. For a given h the connection will be made either to switch socket h_a or h_b, but not to both.

Thus the two rows of bulb sockets give half the cycle, and the two switch positions (i.e. two indicating colours) extend this to the full cycle of cosines. Experience suggests that an instrument half a cycle wide would not be too cumbersome, and this would not, of course, require two switch positions for each h.

(e) *Combination of several units into one instrument*

The description so far has been of one basic unit of the main instrument. Ten of these units have been mounted vertically in one frame, as a single device, with all the winding drums at either side on the same shaft (Fig. 2). As mentioned above, for any given h a selection of the ten units will show (white) values of $\cos(hx+k_1y+l_1z)$ at switch position h_a (but not at h_b) and the remainder will show (red) values at the following position h_b. These two sets of cosines are added together, as indicated by the word 'TOTAL' on the red light.

A standard design of wander-plug is used which allows several plugs to be inserted into the same socket. Thus one double row of switch sockets would suffice for the whole instrument, but only if no value of hx was repeated for two different values of h for a given atom. For triclinic space-groups, values of hx will not recur very often. This possibility is provided for, however, by having four double rows of switch

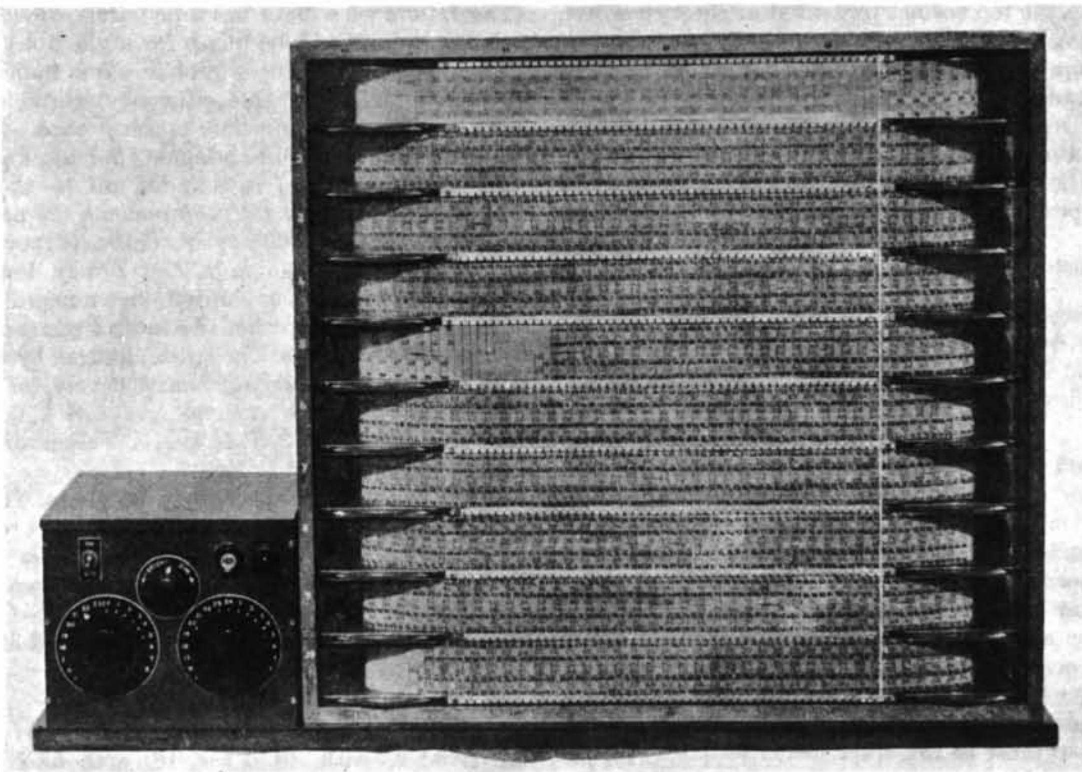

Fig. 2. Front view of SUMCOS. The sine (and part of cosine) setting-up tables are visible in the top unit (the white line on the right is for positioning these).

sockets connected to *separate* wafers of the switches (which have six wafers in all). Thus these four rows have independent circuits (see § 3(c)). To avoid the inconvenience of plugging the remaining six units into one double row of switch sockets a further *four* rows, permanently in parallel, have been connected to another switch wafer. The remaining wafer is required for the indicating lights.

(f) *Dimensions*

The overall height of the instrument is 22 in. and the width 32 in., but the significant area of figures is only 20 in. × 13 in., which is sufficiently compact for rapid reading.

3. Use of the instrument

(a) *Setting up*

The first step is to tabulate hx, ky and lz, for all required positive values of h, k and l, using values of x, y, z, with their maximum known accuracy. (Though this table is the only essential one it is convenient if $\bar{h}x$, $\bar{k}y$, and $\bar{l}z$ are also tabulated.) If the quantity to be calculated is

$$\sum_{j=1}^{N} \cos\,(hx_j+ky_j+lz_j)\ ,$$

then the 'cosine' setting-up tables are moved into position. One unit is assigned to each atom, but this choice cannot be quite arbitrary (see § 3(c)).

Within each unit the bulb sockets are now connected to the switch sockets, this being done so that when the switch is at position h_a (or h_b) the value of hx, rounded off to two figures, is lit up on the table. This procedure is quite straightforward. (If the hx table is copied out and permanently fixed above the sockets on the rear panel, it considerably speeds up the wiring process.) After the connections are made, the successive values of hx are lit up simply by rotating the switch, and the correctness of the connections can therefore be promptly checked. These connections are not altered until all calculations with that atom have been completed.

(b) *Use of main table*

With the setting-up tables in place the small perspex plates are attached so that the origin is placed at lz for $l = l_1$ in each unit. The charts are now set so that ky for $k = k_1$ is brought up to the origin in each unit, thus giving values of $\cos\,(hx+k_1y+l_1z)$ (§ 2(a)). The indices (h, k_1, l_1) are the same in all units and hence we obtain

$$\sum_{j=1}^{10} \cos\,(hx_j+ky_j+lz_j)$$

by adding the ten cosines presented at the two switch positions h_a and h_b.

This sum is therefore computed for all (h, k_1, l_1) as h runs through a sequence of values, and the charts are then reset for the next value of k, e.g. (k_1+1). After computing all (h, k, l_1) the charts are moved back to the cosine setting-up tables, in order to place the perspex origin markers at new positions, e.g. $(l_1+1)z$.

Obviously we could get $\sum_j \sin(hx_j+ky_j+lz_j)$ by subtracting 0·25 from all values of lz. The 'sine' setting-up table does this conveniently; otherwise the ky, cosine and hx tables (and hence rear connections) are used as described.

(c) *Problem of independent circuits and choice of atoms*

Because of the limited number of wafers on the switches, only four rows of switch sockets have independent circuits, so that a preliminary sorting-out of the coordinates is necessary.

When hx has been tabulated for the ten atoms the values for any atom must be looked over to see if some hx occur twice for the same atom. If so, then one of the four independent rows of switch sockets must be used for that atom. If N atoms are considered then $(N-4)$ must be found for which hx has no repeat values; but this is not a very stringent condition for triclinic space groups, where x is rarely a simple fraction. In any case the tables on the instrument have been called hx, ky and lz for convenience, and ky or lz can equally well be the quantity connected up to the switches (for all atoms) if hx proves inconvenient to use.

4. Discussion*

This machine attempts to fill a gap in the considerable range of computational aids and machines for structure factors now available. It is, by contrast with many techniques, relatively more efficient for the space groups of lowest symmetry.

The basic design is simple. It is not an analogue machine and therefore does not demand high precision in its construction. The few different components used are very reliable, so that little maintenance is needed. (The failure of a bulb is immediately obvious, since too few cosines will be lit up for a given h.) The cost of making the machine is probably less than for other machines (of comparable efficiency) suitable for use with triclinic or monoclinic space groups.

The accuracy is quite adequate for most problems. One component (hx) is rounded off to the nearest 0·01 cycle; the other two components (ky and lz) are set to the nearest 0·005 cycle. This accuracy is maintained however large h, k and l may become. In practice one index is limited instrumentally to 23 values in all, but the other two indices can run through any number of values. The index changed by switching (i.e. h) may be wired up consecutively, or in some convenient sequence such as $\ldots, \bar{6}, \bar{4}, \bar{2}, 0, 2, 4, \ldots$ followed by $\ldots, \bar{5}, \bar{3}, \bar{1}, 1, 3, \ldots$. Values of k and l can be taken in any order.

Some estimate of speed may be given. Tabulating hx, ky and lz (20 values of each) for ten atoms took 50 min., and checking for recurring values a further 10 min. The initial connections for a given problem occupied 12–15 min. per atom. An unskilled assistant using SUMCOS for the first time computed 300 values of

$$\sum_{4\text{ atoms}} \cos(hx+ky+lz)$$

for fixed l, with $\overline{18} \leqslant k \leqslant 18$ and $h+k+l$ even, in 5 hr.; an experienced operator would take rather less than this. Many problems, however, would not require such frequent resetting of the charts as this particular one did.

A device of this kind is useful in various exploratory calculations during lengthy structure determinations. It also makes the use of three-dimensional data more feasible for laboratories without ready access to the considerably more efficient electronic computers, such as EDSAC.

The writer acknowledges with sincere thanks his indebtedness to Dr W. H. Taylor and Dr H. D. Megaw, and to the workshop staff of the Crystallographic Laboratory for their ready cooperation. The work was done during the tenure of a C.S.I.R.O. Overseas Studentship.

* See also the discussion in Part I (Radoslovich & Megaw, 1955).

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