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A Device for Calculating Structure Factors

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A simple device is described for calculating structure factors of the form

$$\Sigma f \cos (\sin) 2\pi hx/a . \cos (\sin) 2\pi ky/b \, .$$

Dials on a pivoted table are set so as to create moments proportional to the terms, and the sum is obtained by restoring the balance with an applied torque. The machine is compact and robust, and experience has shown it to be accurate and convenient to operate.

Structure factor machines, like children, generally seem attractive only to their parents. I venture to describe the present simple device, however, because it has now been in frequent use in the Cavendish Laboratory for a year and has been reported on favourably by those who have employed it. It is primarily designed for organic compounds containing carbon, oxygen and nitrogen atoms. In its present form it adds fifteen terms of the type

$$f \cos (\sin) 2\pi hx/a . \cos (\sin) 2\pi ky/b \, . \qquad (1)$$

There is no drawback, other than that of increasing size, to adding to the number of terms. It reads F in terms of f for a carbon atom, the ratios f_N/f_C and f_O/f_O being assumed to be 1·2 and 1·5 respectively over the usual range of θ. This approximation is sufficiently close for all but the last stages of refining a structure. Readings of F taken without any special precautions repeat to less than $0{\cdot}05f$, which is also amply sufficient for most work. It is best worked by two observers, one calling the values of hx/a, ky/b and booking the answers, the other setting the dials and reading the values of F. Under these conditions it takes less than 1 min. to read a value of F for fifteen sets of coordinates. It is a convenient desk instrument, the base being 20 in.×11 in. and the height 3 in.

The principle was suggested to me by Dr V. Vand, who refers to it at the end of a paper on another type of machine (Vand, 1950). The machine is shown in Fig. 1. Summation is affected by gravity. A rocking table carries a number of dials with off-set weights which create moments proportional to (1) about the centre of each dial, and the total moment is read by restoring the balance of the table. It is locked or released by the handle (opposite 9 on the inch scale) and brought back to level, indicated by a spirit gauge, by turning the micrometer head on the left. This applies the necessary couple by twisting a torsion wire attached to the micrometer head on the left and to the opposite end of the table.

A dial is shown in Fig. 2. Each weight is set to a value of cos (sin) $2\pi ky/b$ by using the central scales, the cos scale being on the right and the sin scale on the left. For instance, if ky/b is 3·63, the weight is set at 63, intergers before the decimal place being of course neglected. Semi-cylindrical perspex lenses attached to the slides facilitate the setting. The weight is on a screw, and a slight turn to left or right locks or unlocks it. Each dial is then turned till the appropriate setting for hx/a comes opposite a cos mark at the bottom or a sin mark on the right (these can be seen in Fig. 1*). The moment of the weight about the centre is then the product $\begin{pmatrix}\cos\\ \sin\end{pmatrix} \times \begin{pmatrix}\cos\\ \sin\end{pmatrix}$. This being done for all the dials, the table is set free and the reading is taken by turning the micrometer head until the bubble is central. Oscillations are damped by a small vane in a pot of heavy oil, seen in Fig. 3. The weights marked C, N, O are adjusted so that the masses of weight plus slides are in the appropriate ratio. The adjustment of zero is made by a levelling screw which can be seen opposite 6 on the inch scale in Fig. 1. The small drawer to the left of it contains a supply of carbon, nitrogen and oxygen weights.

The drill in evaluating a large number of F values is first to set the values of $2\pi ky/b$ for a given value of k on the central scales, this being the more tedious setting. One then runs through the values of h. With a little practice, settings of hx/a on the dials can be made by one reader as fast as the other can read them from a graph or table. When a set of 'h' readings has been made, the weights are reset for the next value of k and the process is repeated. It is a completely mechanical operation, involving no mental arithmetic, which much reduces the tiresome labour of structure-factor calculation.

It would be out of place here to describe details of construction. There are points, however, which deserve special mention. The suspension at each end is an important feature, shown in Fig. 3. It is a thin lamina, clamped to the table at the top and to the

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* The setting marks for 'sin' are shown on the left hand side in Fig. 1 in error; they should be on the right hand side to preserve the sign convention.

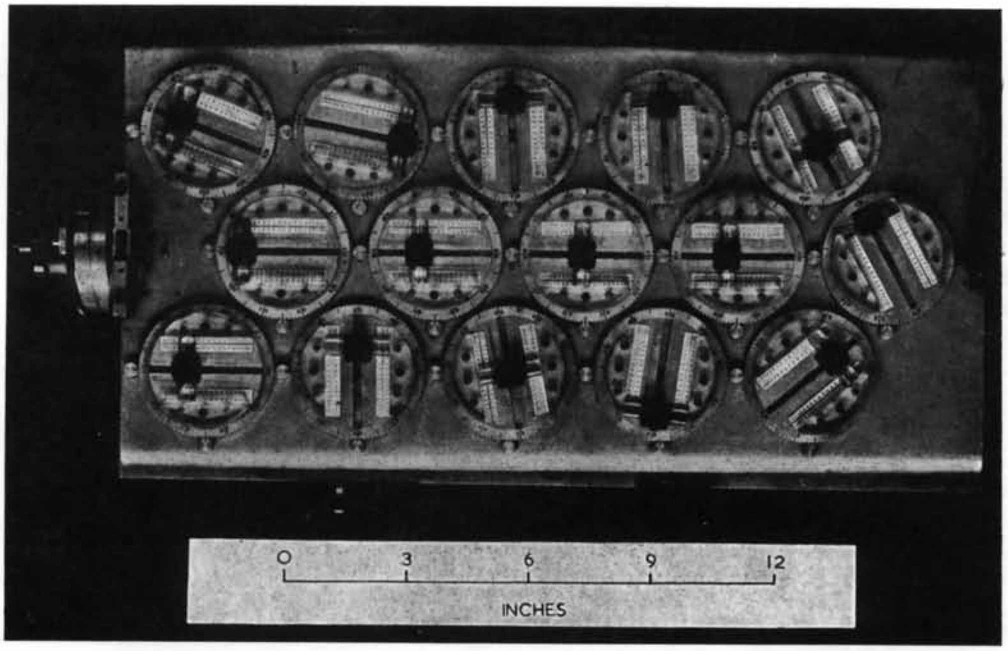

Fig. 1.

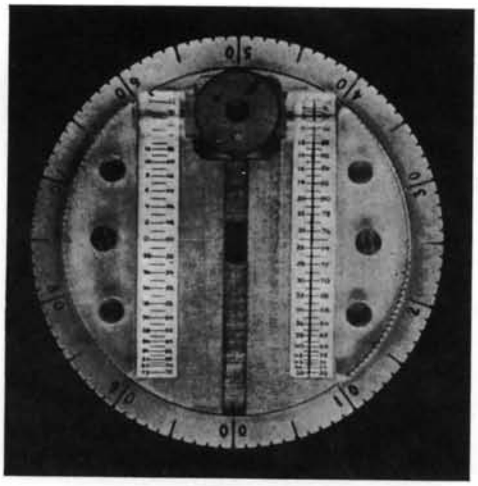

Fig. 2.

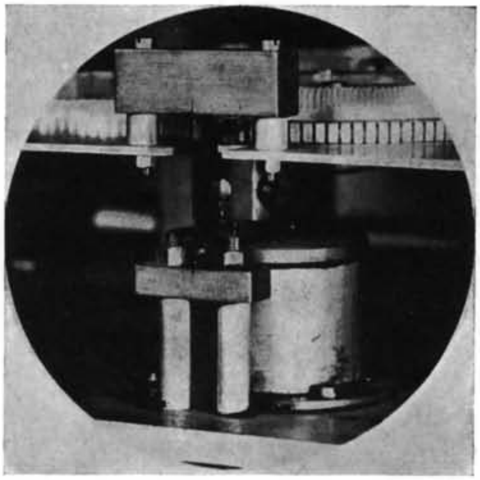

Fig. 3.

base at the bottom. If the table rocks through an angle θ, the height of its centre of gravity alters by $\alpha\theta^2+\beta\theta^4+\ldots$ and it is easy to calculate that α becomes zero when the centre of gravity is one-third of the length of the spring below the upper clamp. It is convenient to place the centre of gravity near this point, finding a position such that the restoring forces of gravity and of the laminar supports combine to make the table only just stable in the central position. The main controlling force is then that of the torsion wire. The advantages of the lamina suspension are its freedom from friction, its high mechanical strength, and its rigidity in the axial direction which enables the torsion wire to be kept taut. This method is far superior to knife edges for a rocking arrangement such as the present. Setting by means of the spirit level is rapid and accurate. I am indebted to the head of the workshop, Mr Fuller, for this and many other suggestions. The setting of a dial is made positive by a small spring which presses into slits around the rim (to be seen in Fig. 3), so that the dial settles into place exactly opposite one of the hundred divisions. Two knurled segments of perspex, seen on either side in Fig. 2, make it easy to grasp the dial whatever its orientation. The weights are of brass, and the rest of the apparatus of aluminium, the table being made of duralumin 2 mm. in thickness. The torsion control is of steel piano wire 18 in. in length and 0·36 in. in diameter (20 s.w.g.). A half turn in either direction balances the moments of six carbon atoms. It would be a simple matter to extend the scale by balancer weights set at definite points on the table when required for a very large value of F, but in practice this has not been found necessary. The lamina supports of the table are of steel tape 1·2 in. × 0·375 in., and 0·15 in. thick. The construction of the calculator required some two to three weeks of workshop time.

I wish to express my warm thanks to Mr Fuller, and to Mr Collins who constructed the apparatus.

Reference

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The Structure of Rubidium Trioxalatochromate (III), $Rb_3[Cr(C_2O_4)_3].xH_2O$, and its Relation to the Corresponding Potassium and Ammonium Structures

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By comparing Weissenberg photographs, Harker sections and Patterson projections it is shown that the compound $Rb_3[Cr(C_2O_4)_3].xH_2O$ and the corresponding potassium compound are isotype. The corresponding ammonium compound has a different structure. It is shown that this difference in structure is not due to the different sizes of the cations, but that it is probably due to the ability of an ammonium ion to form tetrahedrally directed hydrogen bonds.

Introduction

In two recent communications (van Niekerk & Schoening, 1952*a*, *b*) the crystal structures of potassium and ammonium trioxalatochromate (III) have been described. In the latter publication the two different schemes, according to which the complex ions and the cations are arranged in the two structures, were discussed. The question whether this difference in arrangement was due to (1) the difference in size of the cations, or (2) the ability of an ammonium ion to form hydrogen bonds, remained unanswered. To get further information as regards the first point it was decided to investigate the structures of the corresponding rubidium and cesium compounds. Goldschmidt and Pauling give the following data for the effective ionic radii of these ions:

	K^+	NH_4^+	Rb^+	Cs^+
Goldschmidt	1·33 Å	1·43 Å	1·49 Å	1·65 Å
Pauling	1·33	1·48	1·48	1·69

Although it has not been possible so far to crystallize the cesium compound, a structural analysis of the rubidium compound, as described below, seems to give a definite answer to the above question.

Preparation and crystal data

Crystals of $Rb_3[Cr(C_2O_4)_3].xH_2O$ were prepared following the method described by Werner (1912). The crystals are monoclinic and dark blue in colour. They generally crystallize as plates with well developed {010} and {021} faces round the [100] zone. In this respect they resemble the corresponding ammonium rather than the potassium compound.