and used in the next iteration in place of the original right-hand sides. When successive normalised solutions agree to a sufficient number of figures the answers can be accepted.

The 15 scale factors listed below were obtained (i) by finding the latent root and vector and (ii) by setting $K_{a0}=1{\cdot}0$ and solving for the other 14 values. It can be seen that the primary effect of method (ii) is to exaggerate K_{a0} in relation to the others, but that variations of several percent also occur between the remaining ratios.

When it is desired to extend the method to the case in which more than two layers on independent arbitrary scales intersect at the same h the observational equations can be derived in the following way. Let F_h^2 be the weighted average of the scaled F_h^2 occurring on all the layers. Then the observational equation for F_{hi}^2 will be:

$$(F_{hi}^2)K_i - F_h^2 = 0 ,$$

where

$$F_h^2 = \sum_j (W_{hj}K_jF_{hj}^2)/\sum_j W_{hj} ,$$

hence

$$(F_{hi}^2)K_i - \sum_j W_{hj}(F_{hj}^2)K_j/\sum_j W_{hj} = 0 . \qquad (2)$$

The weight to be given to equations (2) is W_{hi}.* Where m layers intersect at h, all m of the equation (2) must be included to weight the observations correctly, although one equation is dependent on the other $m-1$. When only two layers intersect at h a pair of equations (2) can be reduced to the form of equation (1) with weight $W_h = W_{ha}W_{hb}/(W_{ha}+W_{hb})$.

The latent vector solution given above is the multidimensional analogue of the methods described by Schomaker, Waser, Marsh & Bergman (1959) for the similar problem of fitting least-squares lines and planes to given sets of points.

* It has been pointed out by the referee that the use of equations (2) is equivalent to the minimisation of

$$\sum_{hi} W_{hi}(K_iF_{hi}^2 - F_h^2)^2,$$

where the summation includes one term for each observation of any reflection appearing on more than one layer. The minimisation is, of course, subject to the restriction that

$$\sum_i K_i^2 = 1 .$$

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Extension of the *M* function tables for a hindered rotator of Lipscomb and King.

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(*Received* 18 *August* 1959)

King & Lipscomb (1950) have derived an expression for the structure amplitude from a crystal containing rotating groups for the particular case of the hindered rotator. Under the assumptions made by these authors they have derived a modifying function such that the scattering amplitude is written

$$F = \sum_i f_i \exp[2\pi i\mathbf{h}\cdot\mathbf{k}_i] M_{n_i}^{\gamma_i}(a_i, b_i)$$

where

$$M_n^{\gamma}(a, b) = \sum_{p=0}^{\infty} \varepsilon_p i^{pn} J_{pn}(a) I_p(b) \cos pn\gamma / I_0(b) ,$$

where

n = the number of potential minima,
γ = the rotation angle corresponding to a potential minimum,
a = $2\pi|\mathbf{h}||\mathbf{v}|\sin\psi$,
b = $V_0/2kT$,
V_0 = the height above the minimum of the barrier to rotation,
$\mathbf{v}$ = the vector from the center of rotation to the instantaneous position of the atom,
$\mathbf{h}$ = the reciprocal lattice vector
ψ = the angle between $\mathbf{h}$ and the normal to the plane of rotation of the atom.

We have evaluated the M function for the following values:

(1) a = 0 to 4 in intervals of 0·1,
(2) b = 0·5 to 6 in intervals of 0·5 and ∞,
(3) n = 2, 3, 4, 6,
(4) γ = 0, $\pi/16$, $\pi/8$, $3\pi/16$, $\pi/4$ when n = 2, 4,
γ = 0, $\pi/12$, $\pi/6$ when n = 3, 6.

For the case $n=3$ the M function will have real and imaginary parts and writing

$$M_3^{\gamma}(a, b) = x + iy .$$

The tabular values are listed as $(x^2+y^2)^{\frac{1}{2}}$ with the sign of x.

The evaluation of the M function was accomplished on the IBM type 650 digital computer. The computation time required for one value of the M function was between 0·5 sec. and 10 sec. depending on the number of terms required for convergence.

A few minor changes in the present computer program would allow it to be used as a subroutine in another program which requires the M function. This subroutine is available for the IBM 650 only.

Reference

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The tables can be obtained from the American Documentary Inst.; microfilm copies of the tables and copies of the program for computing the M function on an IBM 650 can be obtained, upon request, from the authors.