

( $=1/A$ ) for given values of  $\mu R$  and  $\theta$ , where  $R$  is the radius of the crystal and  $\theta$  is the Bragg angle. Values of the absorption factor for equatorial reflexions from a cylindrical crystal have been tabulated, with an accuracy of better than  $10^{-3}$ , at intervals in  $\theta$  of  $5^\circ$  and in  $\mu R$  of 0.1 from 0 to 10.0 and of 0.5 from 10.0 to 31.5 (Weber, 1967). A tabulation for a spherical crystal, terminating at  $\mu R=10.0$ , has been given by Bond in *International Tables for X-ray Crystallography* (1959), based on interpolation of a tabulation at intervals of 1 in  $\mu R$  and  $15^\circ$  in  $\theta$ . A further tabulation for a spherical crystal, with an accuracy of better than  $10^{-3}$  has recently been given by Weber (1969) at the same intervals as his earlier values for a cylindrical crystal. In both cases further interpolation is necessary for values of  $\mu R$  and  $\theta$  between those for which  $A^*$  is given. For neutron diffraction the value of  $\mu R$  is normally within the range 0 to 1.0, for which interpolation from existing tables is unsatisfactory if accurate corrections are required. We have therefore evaluated the transmission factor [equation (1)] for these two crystal shapes at intervals of 0.01 in  $\mu R$  within this range.

The integral for equatorial reflexions from a cylinder was evaluated using Simpson's rule and the accuracy of the integration was determined from the difference between evaluations using two intervals, one twice the other. The integral for a sphere was obtained by appropriate further integration of the results for a cylinder, the required integrand values being obtained by Aitken interpolation. In both cases the results obtained are accurate to four places of decimals.

Although absorption corrections have previously been tabulated as a function of  $\theta$ , we find that interpolation can be carried out much more conveniently if they are tabulated as a function of  $\sin^2\theta$ . The intervals of  $\sin^2\theta$  used in the present tables are such that linear interpolation is acceptable. Table 1(a) and (b) list the values of  $A_{hkl}$  for equatorial reflexions from a cylindrical crystal at intervals of 0.1 in  $\sin^2\theta$  from 0 to 0.7 and intervals of 0.05 in  $\sin^2\theta$  from 0.65

to 1.00 respectively. Table 2(a) and (b) gives the corresponding values for a spherical crystal. In all cases the interval in  $\mu R$  is 0.01.

If the high accuracy of the tabulated values is not required it may be more convenient to use an analytical expression for the transmission factor. In this case one of the following approximations may be used.

(a) Error not exceeding 0.004:

$$A_{hkl} = \exp \{ -(a_1 + b_1 \sin^2\theta)\mu R - (a_2 + b_2 \sin^2\theta)(\mu R)^2 \}, \quad (2)$$

with the following values for the coefficients.

	Cylinder	Sphere
$a_1$	1.7133	1.5108
$b_1$	-0.0368	-0.0315
$a_2$	-0.0927	-0.0951
$b_2$	-0.0375	-0.2898
Max error	0.0035	0.0024

(b) Error not exceeding 0.04:

$$A_{hkl} = \exp \{ -(a_1 + b_1 \sin^2\theta)\mu R \}, \quad (3)$$

with the following values for the coefficients.

	Cylinder	Sphere
$a_1$	1.6598	1.4523
$b_1$	-0.2832	-0.2252

### References

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**The R-factor ratio test in crystallography; an approximation.** By G.S. PAWLEY,\* *Kemisk Institut, Aarhus Universitet, DK-8000 Aarhus, Denmark*

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The range of validity of an approximation for the  $F$  distribution is investigated. The  $R$  factor ratio as used by crystallographers is calculated and compared with tabulated values. This is done for the range of degrees of freedom generally encountered in crystallographic problems.

Familiarity with the  $R$ -factor ratio test as developed by Hamilton (1964, 1965) is assumed. If we have a crystallographic problem with  $n$  observations, we usually fit to them an unconstrained model of the structure involving  $m$  parameters. Typically  $n \sim 1000$ ,  $m \sim 100$ . If we now perform a refinement where we constrain the range of the  $m$  parameters so that they are determined by a smaller set of  $m-b$  different parameters, we say we are applying  $b$  constraints. When all refinements are complete we then need to test for any significance in the resulting difference.

Let the unconstrained refinement yield an  $R$ -factor  $R_0$  and the constrained refinement  $R_Q$  [for definitions of  $R$  see Hamilton (1964) or (1965)]. We then calculate

$$\mathcal{R} = R_Q/R_0$$

for our significance test. Hamilton shows that  $\mathcal{R}$  is distributed as

$$\left[ \frac{b}{n-m} \cdot F + 1 \right]^{1/2}$$

where  $F$  is  $F$ -distributed with  $b$  and  $n-m$  degrees of freedom. We therefore require the significance points of this distribution.

\* On leave from Department of Physics, Edinburgh University, Edinburgh, Scotland (now returned).

Table 1.  $\mathcal{R}_{b,n-m,\alpha}$  and the differences  $1000(\mathcal{R}^{\text{approx}} - \mathcal{R})$ 

$b$	$n-m$	$\alpha=0.50$		$\alpha=0.25$		$\alpha=0.10$		$\alpha=0.025$		$\alpha=0.01$	
2	480	1.001	0	1.003	-1	1.005	-2	1.008	-3	1.010	-3
3	480	1.002	0	1.004	0	1.007	-1	1.010	-1	1.012	-2
5	480	1.005	-1*	1.007	0	1.010	-1	1.013	0	1.016	-1
10	480	1.010	0	1.013	0	1.017	0	1.021	0	1.024	0
2	240	1.003	-1	1.006	-2	1.010	-3	1.015	-4	1.019	-6
3	240	1.005	-1	1.009	-1	1.013	-1	1.020	-3	1.024	-3
5	240	1.009	0	1.014	0	1.019	0	1.027	-1	1.032	-1
10	240	1.019	0	1.026	0	1.033	0	1.043	0	1.049	-1
15	240	1.030	-1*	1.038	0	1.046	0	1.057	0	1.064	0
2	120	1.006	-2	1.012	-3	1.019	-5	1.031	-10	1.039	-12
3	120	1.010	-1	1.017	-1	1.026	-2	1.040	-5	1.048	-5
5	120	1.018	0	1.028	-1	1.039	-1	1.054	-1	1.064	-2
10	120	1.038	0	1.052	0	1.067	-1	1.086	0	1.098	-1
20	120	1.078	0	1.097	0	1.117	0	1.142	0	1.157	0
2	40	1.017	-4	1.035	-9	1.059	-17	1.097	-31	1.122	-38
3	40	1.030	-3	1.052	-4	1.080	-7	1.122	-13	1.150	-16
5	40	1.054	-2	1.083	-2	1.118	-3	1.167	-5	1.200	-7
10	40	1.112	0	1.154	-1	1.200	-1	1.264	-2	1.304	-2
20	40	1.221	0	1.280	0	1.343	-1	1.426	0	1.478	-1

\* These differences do not indicate growing trends in variation, but are caused by smaller differences being rounded off in different directions.

Most tables of the  $F$  distribution do not cover adequately the region where  $n-m$  is large, and interpolation is necessary. To avoid this we can make use of an approximation for  $F$  given by Lindley & Miller (1953). To calculate  $\mathcal{R}$  at the  $\alpha$  probability level we require  $x_\alpha$ , the  $\alpha$ -probability point of the normal distribution (one tail):

$$\begin{array}{ccccccc} \alpha & 0.50 & 0.25 & 0.10 & 0.05 & 0.01 & 0.005 & 0.001 \\ x_\alpha & 0.0000 & 0.6745 & 1.2816 & 1.6449 & 2.3263 & 2.5758 & 3.0902 \end{array} .$$

Defining

$$\lambda = (x_\alpha^2 - 3)/6$$

and

$$h = 2/(b-1)^{-1} + (n-m-1)^{-1},$$

$$F = \exp\{2[x_\alpha(h+\lambda)^{1/2}/h - ((b-1)^{-1} - (n-m-1)^{-1})(\lambda+5/6)]\} .$$

Then

$$\mathcal{R}_{b,n-m,\alpha}^{\text{approx}} = \left[ \frac{b}{n-m} \cdot F + 1 \right]^{1/2} .$$

This is obviously very easy to calculate in any constrained refinement program, and if we do use it we should know its range of validity.

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**Application of Patterson methods to the solution of molecular crystal structures containing a known rigid group.** By H.R. HARRISON, *Chemical Crystallography Laboratory, South Parks Road, Oxford, England* and M.A. JOYNSON, *Laboratory of Molecular Biophysics, Dept. of Zoology, Parks Road, Oxford, England*

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The rotational and translational parameters of a known molecular rigid group in an unknown crystal structure have been determined using reciprocal-space methods based on the Patterson function. Various refinements of the rotation function have been introduced in order to increase the speed and sensitivity of this method.

A number of methods have been proposed for interpreting the Patterson function of crystals containing a molecular

fragment of known internal geometry, *e.g.* Hoppe (1957) and Nordman & Nakatsu (1963). The rotation function

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