

and many significant figures are lost when they are combined as indicated in equations (2) and (3). Thus, a double-precision computer program should be used, and  $\pi$  should include the maximum allowed number of significant figures. For a computer allowing a maximum of 16 significant figures,  $\mu R$  may be as high as 5, if a precision of at least four significant figures is desired in  $A^*$ .

Values of the absorption factor are given in Table 1, and these values are compared with those in *International Tables for X-ray Crystallography* (1959), that were obtained by numerical integration. Agreement is good at lower values of  $\mu R$ , but a small amount of error becomes apparent in the values obtained by numerical integration at higher values of  $\mu R$ .

Values of the absorption factor at higher values of  $\mu R$  could be calculated using asymptotic expressions for  $I_v-L_v$ . This was not done because the values of  $\mu R$  used were of sufficient range for most purposes. If a very large value of  $\mu R$  is encountered, it is best either to reduce the radius of the sample or to use shorter wavelength radiation to reduce  $\mu R$ , because the change of the absorption factor with scatter-

ing angle becomes huge near  $0^\circ$  for large  $\mu R$ , and only small deviations of the sample shape from that used for the calculations can produce large errors.

Also, secondary scattering is likely to be quite important for large values of  $\mu R$  when the sample is noncrystalline.

Equations (2) and (3) can be solved at several values of  $z$  without a computer, using values of  $I_v-L_v$  given in the *Handbook of Mathematical Functions* (1964). Interpolation between values obtained will give results of sufficient accuracy for most purposes.

#### References

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**Out-of-zone effects in dynamic electron diffraction intensities from gold. Erratum.** By D. F. LYNCH, *Division of Chemical Physics, CSIRO, P.O.Box 160, Clayton 3168, Australia*

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Corrected labelling is given for Fig. 11 in *Acta Cryst.* (1971) A27, 399.

In Fig. 11 of the article by Lynch (1971) the labelling of the four parts was printed incorrectly. The letters (a), (b), (c), (d) should be (d), (c), (b), (a) respectively, reading from top to bottom of the diagram.

#### Reference

- LYNCH, D. F. (1971). *Acta Cryst.* A27, 399.

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**The mean figure-of-merit for a difference Fourier synthesis.** By EATON E. LATTMAN, *Department of Biophysics, Johns Hopkins University, Baltimore, Maryland 21218, U.S.A.*

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The conventional difference Fourier synthesis has a mean figure-of-merit of  $(2/\pi)$  times that of the native structure, and has coefficients which are incorrectly weighted for the 'best' synthesis of Blow & Crick [*Acta Cryst.* (1959) 12, 794].

Workers in protein structure analysis commonly use difference Fourier syntheses with coefficients:

$$m_P \mathbf{F}_D = m_P (F_H - F_P) \exp(i\varphi_P). \quad (1)$$

Here,  $F_P$  and  $\varphi_P$  are the amplitude and phase of a structure factor of the native crystal, and  $F_H$  is the amplitude of the same structure factor of a slightly modified crystal. The figure-of-merit  $m_P$  is discussed later on. Typically, these syntheses are used not for refinement but to reveal the details of small additions or alterations to the native structure. It may then be useful to calculate the accuracy of such

difference syntheses in the same framework used for assessing conventional protein structure determinations.

Blow & Crick (1959) show that, in a least-squares sense, the 'best' Fourier synthesis has coefficients in which the observed amplitudes are weighted by a figure-of-merit that is given approximately by the cosine of the expected error in the phase angle. The quantity  $m_P$  in equation (1) is, therefore, the cosine of the error in  $\varphi_P$ .

Fig. 1 shows the structure factors  $F_P$  and  $F_H$ , as well as the correct difference structure factor  $\mathbf{f}_D$  to which  $\mathbf{F}_D$  is an approximation. The phase error in the coefficient