where $w_i = 4$ for $i = 5, 11, 13, 14, 15, 17, 23$ (the central and six nearest grid points),

$w_i = 0$ for $i = 1, 3, 7, 9, 19, 21, 25, 27$ (the furthest points),

$w_i = 1$ for the rest (the intermediate points).

The i values for points with $x_1, x_2, x_3 = -1, 0, 1$ are $i = 14 + x_1 + 3x_2 + 9x_3$ so that the origin is at $i = 14$. The origin is placed at the point which is locally highest. The nearest points are given higher weights than the more distant points. In extreme cases, when these weights are high enough this formula would reduce to 1D parabolic three-point formula (seven points altogether), so that the proposed formula is some sort of compromise between a 19-point interpolation and a well bounded seven-point interpolation.

Because the derivation follows closely that of Rollett (1965) only the final formulae are given:

$$A_0 = (-F_2 - F_4 - F_6 - F_8 - F_{10} - F_{12} - F_{16} - F_{18} - F_{20}$$
$$- F_{22} - F_{24} - F_{26} + 4F_5 + 4F_{11} + 4F_{13} + 4F_{15}$$
$$+ 4F_{17} + 4F_{23} + 12F_{14})/24$$

$$A_1 = [F_6 - F_4 + F_{12} - F_{10} + 4(F_{15} - F_{13})$$
$$+ F_{18} - F_{16} + F_{24} - F_{22}]/16$$

$$A_2 = [F_8 - F_2 + F_{16} - F_{10} + 4(F_{17} - F_{11})$$
$$+ F_{18} - F_{12} + F_{26} - F_{20}]/16$$

$$A_3 = [F_{22} - F_4 + F_{20} - F_2 + 4(F_{23} - F_5)$$
$$+ F_{26} - F_8 + F_{24} - F_6]/16$$

$$AA_1 = (F_4 + F_6 + F_{10} + F_{12} + F_{16} + F_{18} + F_{22} + F_{24} - 2F_5$$
$$- 2F_{11} - 2F_{17} - 2F_{23} + 2F_{15} + 2F_{13} - 4F_{14})/12$$

$$AA_2 = (F_2 + F_8 + F_{10} + F_{16} + F_{12} + F_{18} + F_{20} + F_{26} - 2F_5$$
$$- 2F_{13} - 2F_{15} - 2F_{23} + 2F_{11} + 2F_{17} - 4F_{14})/12$$

$$AA_3 = (F_2 + F_4 + F_6 + F_8 + F_{20} + F_{22} + F_{24} + F_{26} - 2F_{11}$$
$$- 2F_{13} - 2F_{15} - 2F_{17} + 2F_5 + 2F_{23} - 4F_{14})/12.$$

Calculated corrections (in grid spacing units) are given by

$$x_i = -A_i/2AA_i, \qquad i = 1, 2, 3,$$

and the peak height is

$$F_{max} = A_0 - \sum_{i=1}^{3} A_i^2/4AA_i.$$

For convenience (peaks are not strictly parabolic near maximum), F_{14} can be used instead of A_0 so that $F_{max} = F_{14}$ when corrections are zero (e.g. origin of Patterson synthesis).

References

PAVELČÍK, F. (1986). J. Appl. Cryst. Submitted.
ROLLETT, J. S. (1xt5). Computing Methods in Crystallography, pp. 35-37. Oxford: Pergamon Press.

Small-crystal X-ray diffractometry with a crystal ante-monochromator: erratum.

By A. McL. Mathieson, Division of Chemical Physics, CSIRO, PO Box 160, Clayton, Victoria, Australia 3168

In the paper by Mathieson [Acta Cryst. (1985), A41, 309–316] the definition of k given in the Abstract should read $k = (\Delta\lambda/\lambda)$.

All relevant information is given in the Abstract.

International Union of Crystallography

International Union of Crystallography announces the Ewald Prize

The International Union of Crystallography announces the establishment of the Ewald Prize for outstanding contributions to the science of crystallography. The name of the prize has been chosen with the kind consent of the late Paul Peter Ewald, to recognize Professor Ewald's significant contributions to the foundations of crystallography and to the founding of the International Union of Crystallography, especially his services as the President of the Provisional International Crystallographic Committee from 1946 to 1948, as the first Editor of the Union's publication Acta Crystallographica from 1948 to 1959, and as the President of the Union from 1960 to 1963.

The prize consists of a medal, a certificate and a financial award. It will be presented once every three years during the triennial International Congresses of Crystallography.

The first prize will be presented during the XIV Congress at Perth, Australia, in 1987. This year will be the seventy-fifth anniversary of the discovery of X-ray diffraction in 1912.

Any scientist who has made contributions of exceptional distinction to the science of crystallography is eligible for the Ewald Prize, irrespective of nationality, age or experience. No restrictions are placed on the time or the means of publication of his or her contributions. The prize may be shared by several contributors to the same scientific achievement.

Nominations for the Ewald Prize are invited. They should be submitted in writing, accompanied by supporting documentation, to the Executive Secretary of the International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, United Kingdom. The closing date for nominations is 30 September 1986.

TH. HAHN
President

K. V. J. KURKI-SUONIO
General Secretary