packing. In particular, they can be irrational, in which case the plane parallel to the bases of the prisms is not a lattice plane.

For given $(\mathbf{o}_1\mathbf{o}_2\mathbf{o}_3)$ and α, ξ, the basis $(\mathbf{e}_1\mathbf{e}_2\mathbf{e}_3)$ can be determined and from it the type of Bravais lattice can be identified (for example, using the method of reduced cells). Conversely, given a vector basis $(\mathbf{e}_1\mathbf{e}_2\mathbf{e}_3)$ defining any type of Bravais lattice, there are always solutions for $(\mathbf{o}_1\mathbf{o}_2\mathbf{o}_3)$ and α, ξ compatible with each type of packing.

Fig. 7(*a*) shows an *I* packing with a simple cubic lattice, in which $\mathbf{o}_1 = \mathbf{u}_1 - 1/2\mathbf{u}_3$; $\mathbf{o}_2 = \mathbf{u}_2 - 3/4\mathbf{u}_3$; $\mathbf{o}_3 = \mathbf{u}_3$, where $\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3$ define a cubic unit cell. The angle of $\mathbf{o}_3$ with the normal to the plane of the bases is 42·03°. Fig. 7(*b*) shows an *E* packing with a body-centred tetragonal lattice; the lattice of hexagons is quadrangular and $\mathbf{o}_3$ is perpendicular to the plane of the bases (straight prisms).

6. The shape of space fillers

The polyhedra considered so far were derived from prisms by introducing additional edges and faces, and therefore have dihedral angles of 180° between pairs of lateral faces. This geometric feature is of course not essential and completely convex space-filling polyhedra can be derived from the 'prismatic' polyhedra. For example, the regular truncated octahedron can be obtained by a suitable deformation of the topologically isomorphic *I* packing of prisms described above. In general, a 'prismatic' packing in which, as we have seen, the prisms need not be straight or regular, may be deformed into another space-filling packing of the same periodicity and topological type, provided the deformation is the same at lattice equivalent points. Furthermore, this deformation preserves the type of packing, in the sense that an *E* packing, for example, remains an *E* packing upon deformation.

We have used this procedure to obtain a model of an *E* packing consisting of truly convex polyhedra with planar faces. The complete description of this polyhedron will not be given since it is not specially relevant, but we show in Fig. 8 a perspective line diagram of the polyhedron obtained (point group 222).

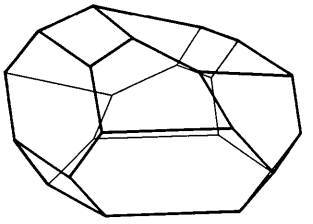

Fig. 8. Perspective view of a type II polyhedron that fills space with its enantiomorph.

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SHORT COMMUNICATIONS

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible.*

Acta Cryst. (1986). A**42**, 286-287

A peak interpolation formula for Fourier map interpretation. By F. PAVELČÍK, *Department of Analytical Chemistry, Faculty of Pharmacy, Komensky University, CS* 832 32 *Bratislava, Czechoslovakia*

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Abstract

A weighted 19-point parabolic interpolation formula applicable to computer interpretation of Fourier maps is derived.

In the course of programming and testing a peak-picking routine for automatic interpretation of Patterson, superposition and symmetry maps (Pavelčík, 1986), we found that in some cases, where peak shapes are poor, the peak interpolation formula due to Rollett (1965) gave some corrections greater than half of the grid spacing. Instead of using a simple three-point parabolic 1D interpolation a weighted 19-point 3D parabolic interpolation was derived. The peak coordinates are given by minimizing the sum

$$\sum_{i=1}^{27} w_i \left[F_i - \left(A_0 + \sum_{j=1}^{3} A_j x_j + \sum_{j=1}^{3} A A_j x_j^2 \right) \right]^2,$$

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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).

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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

(*Received* 22 *April* 1986)

In the paper by Mathieson [*Acta Cryst.* (1985), A**41**, 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

Acta Cryst. (1986). A**42**, 287

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

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