the x axis is parallel to the hexagonal X axis and the z axis is parallel to the hexagonal Z axis.

3. An example: the magnetoelectric effect

The magnetoelectric effect is represented by the rank 2 c-axial physical-property tensor aeV^2 (Birss, 1964). In the tabulation given by Birss (1964) only the case corresponding to the magnetic point group $\bar{3}(Z)'$ of the magnetic-point-group type $\bar{3}'$ is given. In Table 3 we give the form of the magnetoelectric-effect tensor for all magnetic point groups which are subgroups of $M(Z)\bar{3}(XYZ)M(XY)1'$ (O_h1') and $6(Z)/M(Z)M(X)M(1)1'$ $(D_{6h}1')$ and which belong to the magnetic-point-group type $\bar{3}'$. The complete list of forms of the magnetoelectric-effect tensor invariant under all magnetic point groups is contained within the deposited tabulations.*

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* See deposition footnote.

References

Ascher, E. & Janner, A. (1965). *Acta Cryst.* **18**, 325-330.

Birss, R. R. (1964). *Symmetry and Magnetism.* Amsterdam: North-Holland.

Fumi, F. G. & Ripamonti, C. (1980). *Acta Cryst.* **A28**, 597-601.

Jahn, H. A. (1949). *Acta Cryst.* **2**, 30-33.

Kopsky, V. (1976). *J. Magn. Magn. Mater.* **3**, 201-211.

Kopsky, V. (1979*a*). *Acta Cryst.* **A35**, 83-95.

Kopsky, V. (1979*b*). *Acta Cryst.* **A35**, 95-101.

Litvin, S. Y. & Litvin, D. B. (1990). *Acta Cryst.* **A46** 711-713.

Nye, J. F. (1957). *Physical Properties of Crystals.* Oxford: Clarendon Press.

Sands, D. E. (1982). *Vectors and Tensors in Crystallography.* Reading, MA: Addison-Wesley.

Sirotin, Yu. I. (1962). *Soc. Phys. Crystallogr.* **8**, 195-196.

Sirotin, Yu. I. & Shaskolskaya, M. P. (1975). *Osnovi Kristallogfiziki.* Moscow: Nauka.

Standards on Piezoelectric Crystals. (1949). *Proc. Inst. Radio Eng.* **37**, 1378-1395.

Tenenbaum, J. (1966). *Proc. Indian Acad. Sci.* **64**, 74-83.

Wooster, W. A. (1973). *Tensors and Group Theory for the Physical Property Tensors of Crystals.* Oxford: Clarendon Press.

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A comment on the asymmetric part of the translation function.

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Abstract

The asymmetric part of the translation function is closely related to a unit cell and the symmetry of the multiple implication function. The actual asymmetric part depends on the symmetry of the fragment.

Theory

The translation function is used to locate a correctly oriented molecular fragment in the unit cell with respect to the symmetry elements. The full symmetry translation function can be given, for example, by (Pavelčík, 1988)

$$T(\mathbf{r}) = \min_{i=1}^{F} \min_{j=1}^{F} \min_{m=1}^{S} \min_{n=1}^{S} P\{[\mathbf{R}_n(\mathbf{r}+\mathbf{r}_i)+\mathbf{t}_n] \\ -[\mathbf{R}_m(\mathbf{r}+\mathbf{r}_j)+\mathbf{t}_m]\}, \quad (1)$$

where F is the number of atoms in the fragment, $\mathbf{r}_i$ are vectors to the atoms of the fragment, $\mathbf{r}$ is a search vector, $\mathbf{R}_n$ are rotational and $\mathbf{t}_n$ translational parts of the symmetry operator, respectively. S is the number of space-group operators. A search volume is given by an asymmetric part of the translation function.

In the papers of Egert & Sheldrick (1985) and Rius & Miravitlles (1987) it is stated that the asymmetric unit of the translation function is defined uniquely by the Cheshire groups (Hirshfeld, 1968). It is not clear whether this means an asymmetric unit or a unit cell of the Cheshire group. On the other hand, Wilson & Tollin (1986) state in the *PATMET* program instructions that the unique region is $0-\frac{1}{2}$ on each relevant axis. Both statements are only partially correct. The Cheshire groups have limits in the application to the pure translation problem because of special treatment of chirality.

The asymmetric part of the translation function depends in general on the space group of the crystal and on the point group of the fragment. Owing to the symmetry of the Patterson function $P(\mathbf{r}) = P(\mathbf{R}_n\mathbf{r})$, (1) can be simplified to*

$$T(\mathbf{r}) = \min_{i=1}^{F} \min_{j=1}^{F} \min_{s=1}^{S} P[(\mathbf{R}_s-\mathbf{I})\mathbf{r}+\mathbf{t}_s+\mathbf{R}_s\mathbf{r}_i-\mathbf{r}_j]. \quad (2)$$

For the extreme case of a single (heavy) atom, the translation function is reduced to

$$T(\mathbf{r}) = \min_{s=1}^{S} P[(\mathbf{R}_s-\mathbf{I})\mathbf{r}+\mathbf{t}_s+(\mathbf{R}_s-\mathbf{I})\mathbf{r}_1]. \quad (3)$$

Equation (3) is equivalent to the multiple implication (symmetry minimum) function, MIF (Ellison & Levy, 1965; Simpson, Dobrott & Lipscomb, 1965), with the origin shifted by an arbitrary vector $\mathbf{r}_1$. The symmetry of the multiple implication function has recently been described by Zimmermann (1988) and Pavelčík (1990). The MIF groups are closely related to the Cheshire groups. In the case of a single atom, the asymmetric part of the translation function is given by the *asymmetric part* of the MIF group.

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* There is an error in equation (9) of Pavelčík (1988). It should read

$$D(\mathbf{r}) = \left[\min_{k=1}^{n} \min_{l\geq k}^{n} \min_{j=2}^{S} \frac{Z_1Z_1}{m_{ij}Z_kZ_l} P(\mathbf{r}-\mathbf{R}_j\mathbf{r}-\mathbf{t}_j+\mathbf{r}_k^o-\mathbf{R}_j\mathbf{r}_l^o)\right]^{1/2}.$$

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For the asymmetric fragment, the unit cell of the translation function is given by

$$T(\mathbf{r}) = T(\mathbf{r}+\mathbf{t}_o) = \min_{i=1}^{F}\min_{j=1}^{F}\min_{s=1}^{S} P[(\mathbf{R}_s-\mathbf{I})(\mathbf{r}+\mathbf{t}_o)+\mathbf{t}_s+\mathbf{R}_s\mathbf{r}_i-\mathbf{r}_j], \quad (4)$$

where $\mathbf{t}_o$ is the new translation period. Equation (4) can only be satisfied if ($\mathbf{t}_c$-centring)

$$(\mathbf{R}_s-\mathbf{I})\mathbf{t}_o-\mathbf{t}_c \equiv \mathbf{0}\,(\mathrm{mod}\ 1), \quad s=1,2,\ldots,S. \quad (5)$$

Equation (5) defines the permissible origin shifts (Giacovazzo, 1974). The translation function has no other symmetry because of general coordinates, $\mathbf{r}_i$, of the fragment. For the asymmetric fragment the unique region of the translation function is given by the *whole cell* of the MIF. These unit cells coincide with those of normalizers of the space groups and are tabulated in *International Tables for Crystallography* (1987). The unique region is equal to 0–$\frac{1}{2}$ for almost all triclinic, monoclinic and orthorhombic space groups.

If the fragment possesses a symmetry, (2) can be rewritten as

$$T(\mathbf{r}) = \min_{i=1}^{F}\min_{j=1}^{F}\min_{k=1}^{H}\min_{l=1}^{H}\min_{s=1}^{S} P[(\mathbf{R}_s-\mathbf{I})\mathbf{r}+\mathbf{t}_s +\mathbf{R}_s\mathbf{G}_p\mathbf{G}_k\mathbf{r}_i-\mathbf{G}_p\mathbf{G}_l\mathbf{r}_j], \quad (6)$$

where H is the order and $\mathbf{G}_k$ are operators of the point group of the fragment and F is now the number of independent atoms in the fragment. If the fragment contains a correctly oriented symmetry element so that $\mathbf{G}_p=\mathbf{R}_p$ then

$$\begin{aligned}T(\mathbf{R}_p\mathbf{r}+\mathbf{t}_p) &= \min_{i=1}^{F}\min_{j=1}^{F}\min_{k=1}^{H}\min_{l=1}^{H}\min_{s=1}^{S} P[(\mathbf{R}_s-\mathbf{I})(\mathbf{R}_p\mathbf{r}+\mathbf{t}_p) +\mathbf{t}_s+\mathbf{R}_s\mathbf{R}_p\mathbf{G}_k\mathbf{r}_i-\mathbf{R}_p\mathbf{G}_l\mathbf{r}_j]\\ &= \min_{i=1}^{F}\min_{j=1}^{F}\min_{k=1}^{H}\min_{l=1}^{H}\min_{m=1}^{S} P[(\mathbf{R}_m-\mathbf{I})\mathbf{r}+\mathbf{t}_m +\mathbf{R}_m\mathbf{G}_k\mathbf{r}_i-\mathbf{G}_l\mathbf{r}_j]=T(\mathbf{r}) \quad (7)\end{aligned}$$

because $(\mathbf{R}_s-\mathbf{I})(\mathbf{R}_p\mathbf{r}+\mathbf{t}_p)+\mathbf{t}_s=\mathbf{R}_p[(\mathbf{R}_m-\mathbf{I})\mathbf{r}+\mathbf{t}_m]$, $P(\mathbf{r})=P(\mathbf{R}_p\mathbf{r})$, where $\mathbf{R}_m=\mathbf{R}_p^{-1}\mathbf{R}_s\mathbf{R}_p$, and rearrangement of space-group operators. This means that the translation function has the symmetry of the MIF subgroup. The subgroup contains those symmetry operations which are related to the symmetry operations of the point group of the fragment. The unique region of the translation function is given by the *asymmetric part of the MIF subgroup.*

Example. For a structure with space group $P2_1/c$ and cell dimensions $\mathbf{a}, \mathbf{b}, \mathbf{c}$. The MIF group is $P2/m$ and the MIF unit cell is $\mathbf{a}/2$, $\mathbf{b}/2$, $\mathbf{c}/2$. The search region of the translation function for a single atom is $\mathbf{a}/4$, $\mathbf{b}/4$, $\mathbf{c}/2$ (or $\mathbf{a}/2$, $\mathbf{b}/4$, $\mathbf{c}/4$). For the asymmetric fragment the search region is $\mathbf{a}/2$, $\mathbf{b}/2$, $\mathbf{c}/2$. If the fragment has a twofold axis parallel to $\mathbf{b}$, the MIF subgroup is $P2$ and the search volume is $\mathbf{a}/4$, $\mathbf{b}/2$, $\mathbf{c}/2$ (or $\mathbf{a}/2, \mathbf{b}/2, \mathbf{c}/4$). If the fragment has a plane perpendicular to $\mathbf{b}$, the MIF subgroup is Pm and the search volume is $\mathbf{a}/2$, $\mathbf{b}/4$, $\mathbf{c}/2$. If the fragment has symmetry $2/m$ with twofold axis parallel to $\mathbf{b}$, the search volume of the translation function is the same as that for the single-atom case.

References

EGERT, E. & SHELDRICK, G. M. (1985). *Acta Cryst.* **A41**, 262-268.

ELLISON, R. D. & LEVY, H. A. (1965). *Acta Cryst.* **19**, 260-269.

GIACOVAZZO, C. (1974). *Acta Cryst.* **A30**, 390-395.

HIRSHFELD, F. L. (1968). *Acta Cryst.* **A24**, 301-311.

International Tables for Crystallography (1987). Vol. A. *Space-Group Symmetry*, 2nd ed. Dordrecht: Kluwer.

PAVELČÍK, F. (1988). *Acta Cryst.* **A44**, 724-729.

PAVELČÍK, F. (1990). *J. Appl. Cryst.* **23**, 225-227.

RIUS, J. & MIRAVITLLES, C. (1987). *J. Appl. Cryst.* **20**, 261-264.

SIMPSON, P. G., DOBROTT, R. D. & LIPSCOMB, W. N. (1965). *Acta Cryst.* **18**, 169-179.

WILSON, C. C. & TOLLIN, P. (1986). *J. Appl. Cryst.* **19**, 411-412.

ZIMMERMANN, H. (1988). *Z. Kristallogr.* **183**, 113-122.

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Structure factors, projections, inverse Fourier transforms and crystal symmetry.

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Abstract

The formulae for Fourier and inverse Fourier transforms have been generalized to take into account crystal symmetry using group theory. When the Fourier components (structure factors) are restricted to a given reciprocal plane, the two-dimensional inverse Fourier transform yields the projection of the charge/spin density in the unit cell in direct space, parallel to the axis normal to that plane. The formulae above are further generalized to this two-dimensional case. The latter case is central to a polarized neutron diffraction data analysis using maximum entropy.

Introduction

The recent introduction of new image reconstruction techniques (IRT's) such as maximum entropy (see Bricogne, 1984; Livesey & Skilling, 1985) calls for a reassessment of key formulae in crystallography. Clearly, structure factors, crystal symmetry, projections and Fourier synthesis are not new topics (see Waser, 1955; Bertaut, 1955, 1956, 1959; Bertaut & Waser, 1957; Buerger, 1960; Cornwell, 1969; Lax, 1974, among others). Nevertheless, applying new IRT's entails developing new mathematical tools and it is the aim of the present communication to provide the

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