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A method for rapidly relocating misplaced molecules.

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Abstract

A recurrence relationship allows structure factors to be rapidly calculated for a trial structure translated to alternative sites in the unit cell.

Occasionally, when direct or more rarely when heavy-atom methods are used for crystal structure analysis, recognizable molecular fragments emerge from a Fourier synthesis, but cannot be refined. Under these conditions, if nothing else is wrong, it is likely that the interatomic vectors are correct and that the fragment is correctly oriented, but that it is misplaced in the cell. For some centrosymmetric space groups the problem may be resolved by calculating a Fourier synthesis in a corresponding non-centrosymmetric space group, and then locating the symmetry elements. An alternative method is to superpose the Fourier synthesis on the Patterson synthesis. A third possibility is to compute structure factors, placing the model at each point of a grid in the unit cell, and find the site of best agreement between $|F_o|$ and $|F_c|$. The problem of computing so many structure factors seems enormous, but Rae (1977) has given one solution to the problem. We give here an alternative, as implemented in the *CRYSTALS* package (Carruthers, 1975).

The real part of the structure factor may be written as:

$$A_h = \sum_i \{f'_h \sum_j [\cos 2\pi(\mathbf{h}^T.S.\mathbf{x} + \mathbf{h}^T.\mathbf{t})]\},$$

where the subscript h refers to the vector $\mathbf{h}$ and $\mathbf{x}$ are the atom coordinates. The inner summation is over j symmetry operators S and $\mathbf{t}$ for the space group, and the outer summation is over the i atoms in the asymmetric unit, f' being the temperature-corrected form factor for the current atom. A similar expression can be written for the imaginary part.

The order of summation can be rearranged, so that totals are accumulated for all atoms at each symmetry position:

$$A_h = \sum_j \sum_i [f'_h \cos 2\pi(\mathbf{h}^T.S.\mathbf{x} + \mathbf{h}^T.\mathbf{t})]. \quad (1)$$

The recurrence relationships:

$$P_{n+1} = 2P_n \cos y - P_{n-1}, P_n = \cos(x + ny)$$

and

$$Q_{n+1} = 2Q_n \cos y - Q_{n-1}, Q_n = \sin(x + ny)$$

can be used to represent the positional parts of (1) and the corresponding sine formulae:

$$P_{h,S,n+1} = P_{h,S,n}\, 2 \cos 2\pi(\mathbf{h}^T.S.\Delta\mathbf{x}) - P_{h,S,n-1}$$

and

$$Q_{h,S,n+1} = Q_{h,S,n}\, 2 \cos 2\pi(\mathbf{h}^T.S.\Delta\mathbf{x}) - Q_{h,S,n-1}.$$

$P_{h,S,0}$ is the value of P with the initial set of coordinates, for the reflexion $\mathbf{h}$ and the symmetry position S. $P_{h,S,n}$ is the value of P after the structure has been displaced $n\Delta\mathbf{x}$. Once the initial set of sines and cosines has been calculated, the structure can be moved from point to point in the cell without calculating further trigonometric functions.

The cost of this time saving is of course in increased storage requirements. For each reflexion and each symmetry position it is necessary to store the starting values of the eight sines and cosines, and the three step vector cosines as well as $|F_o|$. However, since it is the large structure amplitudes that must be in agreement when the molecule is correctly placed, only the strongest 5 to 10% of the data need be used.

The function computed in *CRYSTALS* as a measure of agreement between $|F_o|$ and $|F_c|$ is:

$$R = G \sum (|F_o|/|F_c|),$$

where G is a scale factor for the output figure-field. This function is used because it assumes no knowledge of the scale of the observations. Our use of this function confirms Rae's (1977) observation that a search grid of 0·25 Å is suitable.

We remark in conclusion that a similar procedure will facilitate the calculation of generalized Fourier sections, for which the usual Beevers–Lipson expansion cannot be used. Details can be found in the *CRYSTALS* user manual.

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