$$\sum X_k Y_l \sin \Phi_{h,k} = \cos \varphi\varphi_h (\sum X_k \cos \varphi\varphi_k \sum Y_l \sin \varphi\varphi_l + \sum X_k \sin \varphi\varphi_k \sum Y_l \cos \varphi\varphi_l) + \sin \varphi\varphi_h (\sum X_k \cos \varphi\varphi_k \sum Y_l \cos \varphi\varphi_l - \sum X_k \sin \varphi\varphi_k \sum Y_l \sin \varphi\varphi_l), \quad (8)$$

where $\varphi\varphi hkl = (\varphi hkl_p + \varphi h\bar{k}l_p)$ and the sums include all terms having a common h and l but different k index. These summations can be performed prior to generating the triples and stored in two-dimensional arrays. The contribution of the full collection of valid triples to the formulae is thus reduced to a two-dimensional permutation over these arrays.

Degeneracies among the refined phases

Since the translation components of (4) and (5) are independent of the value of the k index with regard to $P2_1$ symmetry, (1) and (2) can be rewritten as

$$\cos 4\pi \mathbf{h} \cdot \mathbf{r}_p = \langle (G_k G_l - S_k S_l) \cos \varphi\varphi_{k,l} - (G_k S_l + S_k G_l) \sin \varphi\varphi_{k,l} \rangle_k / \langle A_k A_l \rangle_k, \quad (9)$$

$$\sin 4\pi \mathbf{h} \cdot \mathbf{r}_p = \langle (G_k G_l - S_k S_l) \sin \varphi\varphi_{k,l} + (G_k S_l + S_k G_l) \cos \varphi\varphi_{k,l} \rangle_k / \langle A_k A_l \rangle_k, \quad (10)$$

where $\mathbf{h} \cdot \mathbf{r}_p = hx_p + lz_p$, $\varphi\varphi_{k,l} = \varphi\varphi_k + \varphi\varphi_l$, and the particular vectors $\mathbf{k}$ and $\mathbf{l}$ include all terms with a common h and l index. The refinement result on the right-hand side of the equations is independent of the particular k index of the vector $\mathbf{h}$ since $y_p = 0$. It follows that the calculations need not be performed over the full set of G_h and S_k values, but only over the first unique two-dimensional component of such vectors, as the full set with a common h and l index may readily be obtained by adding the known values of $\varphi\varphi_h$ to the first computed value of $4\pi \mathbf{h} \cdot \mathbf{r}_p$.

The simplified formula

With the following abbreviations to define the particular sums with a common h and l index,

$$B_h = \sum_k (G_{hkl} \cos \varphi\varphi_{hkl} + S_{hkl} \sin \varphi\varphi_{hkl}), \quad (11)$$

$$C_h = \sum_k (G_{hkl} \sin \varphi\varphi_{hkl} - S_{hkl} \cos \varphi\varphi_{hkl}), \quad (12)$$

$$D_h = \sum_k 2 |Ehkl_p Eh\bar{k}l_p|, \quad (13)$$

and with the use of the factoring scheme given by (7) and (8), equations (9) and (10) may be drastically simplified to

$$\cos 4\pi \mathbf{h} \cdot \mathbf{r}_p = \langle B_k B_l - C_k C_l \rangle_k / \langle D_k D_l \rangle_k, \quad (14)$$

$$\sin 4\pi \mathbf{h} \cdot \mathbf{r}_p = \langle B_k C_l + C_k B_l \rangle_k / \langle D_k D_l \rangle_k. \quad (15)$$

Comparison of results

Table 2 in the previous analysis summarized the refinement of the translation-function phases for various-sized misplaced fragments of the crystal structure of tetrahymanol hemihydrate (Langs, Duax, Carrell, Berman & Caspi, 1977), $2(C_{30}H_{52}O).H_2O$, monoclinic, $P2_1$. The degree of refinement convergence towards the known shift value was estimated as $\langle \cos 4\pi \mathbf{h}.[\mathbf{r}_p(\text{obs}) - \mathbf{r}_p(\text{cal})] \rangle$ given in the right-hand column of that Table 2. A fragment of 31 of the 63 non-hydrogen atoms was sufficiently large to permit a phase convergence to $\langle \cos \Delta \rangle \simeq 0{\cdot}99$ for three separate trials in which the basis sets comprised 759, 1499 and 2293 of the largest G_h values among the 5020 measured data. Each of these refined phase sets produced a translation map in which the peak height of the solution vector was ten times larger than the largest spurious peak.

Trials involving a smaller 14-atom fragment which represented 20% of the scattering power of the asymmetric unit were not as encouraging. A basis set of 1392 G_h values refined to $\langle \cos \Delta \rangle = 0{\cdot}373$; a large basis set of 1826 values showed a small improvement with $\langle \cos \Delta \rangle = 0{\cdot}427$ which represented an average phase error of 65° and produced a map in which the solution vector was as large as the two largest spurious peaks. Clearly there may have been a small advantage to further increasing the size of the basis set, but the expense of the calculations did not seem to warrant these efforts. Equations (14) and (15) now permit one to refine the full set of 5020 data in a fraction of the time previously required. This phase refinement converged to $\langle \cos \Delta \rangle = 0{\cdot}860$ and produced a translation map in which the solution vector was 13 times larger than the next spurious peak.

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International Union of Crystallography

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Commission on Crystallographic Apparatus

As a result of an expression of concern by the Commission on Journals with respect to the problem of the underestimation of standard deviations in the lattice constants reported in papers submitted to the journals published by the International Union of Crystallography, the Commission on Crystallographic Apparatus has decided to set up a project to assess the cause of the problem and to determine ways in which the problem may be solved.

This projecy (The Accuracy in Lattice Parameter Measurement Project) is to be organized by Professor Sagrario Martinez-Carrera of the Instituto de Quimica Physica 'Rocasolano'.

Any scientists who wish to participate in or to obtain further details about this project should contact Professor Sagrario Martinez-Carrera, Consejo Superior de Investigaciones Cientificas, Instituto de Quimica Physica 'Rocasolano', Serrano 119, Madrid, Spain.