17.2-2 MULTAN87. By T Debaerdemaeker[1], C Tate[2] and M M Woolfson[2].
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The latest version of MULTAN incorporates a number of structure solving algorithms, eg

1. SAYTAN - based on a tangent formula derived from Sayre's equation (Debaerdemaeker, T., Tate, C. and Woolfson, M.M., Acta Cryst., 1985, A41, 286-90).

2. X-Y - based on a parameter-shift approach which maximises a function of phases.

$$\psi_D = \sum_{\underline{h}}\sum_{\underline{k}} |E(\underline{h})E(\underline{k})E(\underline{h}-\underline{k})| \{\cos\Phi_3(\underline{h},\underline{k}) - \sin\Phi_3(\underline{h},\underline{k})\}$$

where $\Phi_3(\underline{h},\underline{k}) = \Phi(\underline{h}) - \Phi(\underline{k}) - \Phi(\underline{h},\underline{k})$.

It has been noted (Debaerdemaeker, T. & Woolfson, M.M., Acta Cryst., 1983, A39, 193-196) that this function is illogical but very effective.

3. YZARC (Declercq, J.P., Germain, G., Woolfson, M.M. and Wright, H., Acta Cryst., 1981, A37, C237).

4. MAGEX (Zhang Shao-hui and Woolfson, M.M., 1982, A38, 683-85).

In the basic SAYTAN mode phase refinement begins with a complete set of random phases and only the 'strongest' path is followed throughout. This is enabled by an efficient algorithm which minimises the computational work at each step.
Examples of the application of MULTAN87 will be given.

17.2-3 PHASE DETERMINATION OF STRUCTURE-FACTOR TRIPLETS AND QUARTETS USING HIGH-ORDER MULTIPLE DIFFRACTION OF X-RAYS. By S.-L. Chang, H.-H. Huang, S.-W. Luh, H.-P. Pan and M.T. Tang Department of Physics, National Tsing Hua University, Taiwan, Rep. of China and J.M. Sasaki, Instituto de Fisica, Universidade Estadual de Campinas, Campinas, S.P. Brazil

The sign relation $S_P = S_L \cdot S_R$ (Chang, Phys. Rev. Lett. 1982, 48, 163-166) is applied to the determination of the signs of structure-factor triplets and quartets involved in high-order multiple diffractions, such as 4-, 5-, 6- and 8-beam cases. S_P is the sign of the cosine of a triplet or quartet phase. S_L and S_R are the signs determined from the diffracted intensity asymmetry and from the relative motion of the reciprocal lattice points to the Ewald sphere, respectively. Experimentally determined S_P's show a good agreement with the theoretical ones.
The applicability of this sign relation for phase determination in high-order multiple diffraction is discussed, based on the Bethe approximation and the dispersion relation of the dynamical theory.

17.2-4 A PSEUDO-RANDOM STARTING SET TENDENCIALLY MAXIMALLY ENTROPICAL. *By M.C. Burla+, G. Cascarano-, C. Giacovazzo-, A. Munzi+, G. Polidori+,*
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In the multisolution procedures several phase sets are developed by applicating the tangent formula or similar techniques to starting sets usually provided by a magic integer sequence or by random generation. The magic integer approach may be considered as an optimized generator of pseudo-random phase values, evenly distributed into the n-dimensional phase space.
Both magic integers (for long sequences) and random starting sets are in general inconsistent with positivity and atomicity of the electron density. This information is normally introduced by tangent formula which may be considered as a procedure for maximizing the entropy under these physical constraints.
It seems therefore of some interest a procedure which generates sets of pseudo random phases tendencially maximally entropical. The starting idea is the following: let $\Phi_{\underline{h}} - \Phi_{\underline{k}} - \Phi_{\underline{h}-\underline{k}}$ be a triplet invariant and $\Phi_{\underline{k}}$, $\Phi_{\underline{h}-\underline{k}}$ known quantities, then $\Phi_{\underline{h}}$ is distributed around $\theta_{\underline{h}}$ ($= \Phi_{\underline{k}} + \Phi_{\underline{h}-\underline{k}}$) according to a Von Mises distribution $M(\Phi_{\underline{h}}, \theta_{\underline{h}}, G)$ where G is the measure of the triplet reliability. If a phase shift A is generated according to the Von Mises distribution $M(\Phi_{\underline{h}}, 0, G)$, the variable $\theta_{\underline{h}} + A$ may be used as a starting estimate of $\Phi_{\underline{h}}$. In practice each trial of a multisolution process may be started by randomly generating N Von Mises phase shifts each one associated to a triplet invariant.
The generated sets of pseudo-random phases, tendencially compatible with positivity and atomicity, can be expanded more easily into the correct solution.
The procedure has proved to be very successful and its results will be shown.

17.2-5 A RECONSIDERATION OF THE ROLE OF TWO-PHASE SEMINVARIANTS. *By M.C. Burla+, G.Cascarano-, C.Giacovazzo-, A. Munzi+, G. Polidori+.*
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According to the representation theory (Giacovazzo, Acta Cryst. A33, 1977) a procedure has been already devised (Giacovazzo et al., Acta Cryst. A35, 1979), which is able to recognize in an automatic way two-phase structure seminvariants of first rank among all pairs of structure factors chosen between the largest reflexions. According to the algebraic results $\Phi = \Phi_{\underline{u}_1} + \Phi_{\underline{u}_2}$ is a two-phase structure seminvariant of first rank if at least two vectors $\underline{h}_1$ and $\underline{h}_2$ and two rotation matrices $\underline{R}_\alpha$ and $\underline{R}_\beta$ exist such that the following system:

$$\Phi_{\underline{u}_1} = \Phi_{\underline{h}_1} - \Phi_{\underline{h}_2\underline{R}_\beta}$$

$$\Phi_{\underline{u}_2} = \Phi_{\underline{h}_2} - \Phi_{\underline{h}_1\underline{R}_\alpha}$$

is satisfied. When $\{\underline{h}_1\}$ and $\{\underline{h}_2\}$ are obtained, the special quartets:

$$\Phi_{\underline{u}_1} + \Phi_{\underline{u}_2\underline{R}_\beta} - \Phi_{\underline{h}_1} + \Phi_{\underline{h}_1\underline{R}_\alpha\underline{R}_\beta}$$

$$\Phi_{\underline{u}_1\underline{R}_\alpha} + \Phi_{\underline{u}_2} - \Phi_{\underline{h}_2} + \Phi_{\underline{h}_2\underline{R}_\alpha\underline{R}_\beta}$$

can be constructed and the probabilistic estimation of Φ via the first representation can be obtained.
The above procedure is quite general and may be applied to any space group, however it is rather time consuming, infact for each pair of reflexions ($\underline{u}_1, \underline{u}_2$) all the possible pairs of matrices ($\underline{R}_\alpha, \underline{R}_\beta$) have to be introduced to search the sets $\{\underline{h}_1\}$ and $\{\underline{h}_2\}$. In order to reduce computing cost, usually a small number of two-phase seminvariants were estimated; furthermore, since two-phase seminvariants are phase relationships of order N^{-1}, the average reliability level of the probabilistic estimates is low.