17.2-08 THE ESTIMATION OF SIGMA|E(h)| AND ITS APPLICATION IN PHASING PROCEDURES. S.R.Hall and V.Subramanian, Crystallography Centre, University of Western Australia, Nedlands 6009, Australia.

The importance of reliable |E(h)| values to structure invariant phasing procedures has been examined by Subramanian and Hall (paper ##). Their comparison of estimated |E(h)| values and calculated quasi-normalised structure factors |ℰ(h)| for 11 test structures provides a basis for analysing the esd's of individual |E(h)| values. An analysis of the differences between |ℰ(h)| ans |E(h)|, as a function of s^2, |ℰ(h)|, and |F(h)|, is provided.

An expression for calculating the esd of |E(h)| from Wilson plot parameters is proposed. The calculated esd's agree well with rmsd values obtained from the |ℰ(h)| and |E(h)| differences. For reflections with |E(h)| >1.0 the esd's tend to be large so that their inclusion is important to a proper treatment of noise propagation in phasing procedures.

Details on the application of sigma|E(h)| in the direct methods routines GENEV, GENSIN, and GENTAN, available in the XTAL System (Hall et al., Acta Cryst. A36, 979), are to be given.

See preceding abstract.

17.2-09 INTEGRATING TECHNIQUES OF DIRECT METHODS WITH ANOMALOUS DISPERSION. Herbert Hauptman, Medical Foundation of Buffalo, Inc., 73 High Street, Buffalo, New York 14203, U.S.A.

Recent advances in direct methods are here generalized to include the case that the atomic scattering factors may be complex numbers, in particular that anomalous scatterers may be present. Only the probabilistic theory of the two-phase structure invariant is treated here but the method is clearly applicable to the higher order structure invariants as well. The neighborhood principle again plays the central role. Denoting the (complex) atomic scattering factors by

$$f_j = |f_j|\exp(i\delta_j),\ j=1,\ 2,\ \ldots,\ N, \qquad (1)$$

the normalized structure factor E_H is defined by

$$E_H = |E_H|\exp(i\phi_H) = \frac{1}{\alpha_2^{1/2}}\sum_{j=1}^{N} f_j\exp(2\pi i H\cdot r_j), \qquad (2)$$

where

$$\alpha_2 = \sum_{j=1}^{N} |f_j|^2. \qquad (3)$$

The first neighborhood of the two phase structure invariant

$$\psi = \phi_H + \phi_{\bar{H}} \qquad (4)$$

is defined to consist of the two magnitudes

$$|E_H|,\ |E_{\bar{H}}|. \qquad (5)$$

The joint probability distribution of the Friedel pair E_H, $E_{\bar{H}}$ has been found and leads to the conditional probability distribution of the two-phase structure invariant ψ, given the two magnitudes (5) in its first neighborhood. The latter in turn yields an estimate for ψ which is particularly good in the favorable case that $|E_H E_{\bar{H}}|$ is large:

$$\psi = \phi_H + \phi_{\bar{H}} \approx -\eta \qquad (6)$$

where η is defined by

$$Y\cos\eta = c,\quad Y\sin\eta = -s,\quad Y = (c^2+s^2)^{1/2}, \qquad (7)$$

$$c = \sum_{j=1}^{N}|f_j|^2\cos 2\delta_j,\quad s = \sum_{j=1}^{N}|f_j|^2\sin 2\delta_j. \qquad (8)$$

The probabilistic theory of the Friedel pair E_H, $E_{\bar{H}}$ leads also to a formula for the correlation coefficient r of the pair $|E_H|^2$, $|E_{\bar{H}}|^2$:

$$r = \frac{\left\langle(|E_H|^2-1)\,(|E_{\bar{H}}|^2-1)\right\rangle_H}{\left\langle(|E_H|^2-1)^2\right\rangle_H^{1/2}\left\langle(|E_{\bar{H}}|^2-1)^2\right\rangle_H^{1/2}} = 1 - \frac{a_2^2}{\alpha_2^2}, \qquad (9)$$

where

$$a_2^2 = \alpha_2^2 - c^2 - s^2, \qquad (10)$$

and the averages in (9) are taken over all reciprocal lattice vectors H having a fixed value of |H|, i.e. over a spherical shell in reciprocal space. Thus, by employing three or more crystals having only a single kind of anomalous scatterer, (9) is seen to form the basis of a method for the experimental determination of the anomalous scattering factors. Research supported by NSF Grant No. CHE79-11282 and DHHS Grant No. GM-26195.

17.2-10 THE RELIABILITY OF THE Σ_2 RELATION FROM A DYNAMICAL POINT OF VIEW. By J.D.Schagen and H.Schenk, Laboratory for Crystallography, University of Amsterdam, Nieuwe Achtergracht 166, 1018 WV Amsterdam, the Netherlands; B.Post, Polytechnic Institute of New York, 333 Jay Street, Brooklyn, New York 11201, USA.

The reliability of the Σ_2 relation in the centrosymmetric case is given by:

$P+(E_H E_K E_{H-K}) = \frac{1}{2} + \frac{1}{2}\tanh \sigma_3\sigma_2^{-3/2}\,|E_H E_K E_{H-K}|$

(Cochran, Woolfson, Acta Cryst.(1955)8,1). Empirically it has been shown for several centrosymmetric monoclinic structures that the percentages of failures of the Σ_2 relation as function of the triple-product do not agree with the theoretical values based on the probability formula. (Schenk, Acta Cryst. (1973)A29,503; Schenk, Krieger, Acta Cryst.(1973)A29,720

Recently it appeared to be possible to determine the sign of the triple-product from the intensity of the reflections at the three beam point. (Post, Acta Cryst. (1979)A35,17). This suggests that the roots of the dynamical diffraction equation for three beams could be used as measures of the reliability of the Σ_2 relation. The solution of the dynamical diffraction equation at the three beam point gives three roots:

$X_{0,1,2} = (\pm 2\sqrt{A}/3)(\cos(\phi/3 + N.120)\qquad N = 0,1,2$

The largest root is X_0, the other two have values whose sum is equal in magnitude, but is opposite in sign to the X_0 root. It will be shown that for the above mentioned structures the use of the largest root gives measures of comparable reliability as the triple-product. Also for combinations of the three roots, like $X_1.(X_0+X_2)$ and $X_1.(X_0)^2$,the results are of equal reliability.