17.X-07 MEASURABILITY OF BIJVOET DIFFERENCES. By S. Parthasarathy, Department of Crystallography & Biophysics, University of Madras, Guindy Campus, Madras - 600 025, India.

The determination of the absolute configuration of molecules and structure determination of non-centrosymmetric (NC) crystals with heavy atoms are two of the important applications of anomalous scattering with phase shift. A statistical method of selecting the few optimum reflections for Bijvoet difference (BD) measurement (at the stage where the positions of the heavy atoms are known) for the purpose of determining the absolute configuration is pointed out. The success of the anomalous scattering method for determining the structures of NC crystals depends on the possibility of measuring accurately the BDs of a large percentage of reflections. The measurability of BDs can be studied from a knowledge of the probability distribution of normalized BD variables or the Bijvoet ratio. The measurability is expected to be influenced by structural features (e.g., presence of centrosymmetric parts in the molecules, space-group symmetry, the degree of centrosymmetry of the crystal etc.) as well as the non-observability of extremely weak reflections. After dealing with the optimum conditions for observing large BDs in a perfectly NC crystal, the influence of various structural features and of data truncation on the measurability are considered.

17.X-08 WIENER METHODS FOR ELECTRON DENSITY. By D.M. Collins and M.C. Mahar, Department of Chemistry, Texas A&M University, College Station, Texas 77843, USA.

The Wiener formalism here employed is widely used in applications conveniently categorized as smoothing, interpolation, or extrapolation of stationary series. The present application is of the last mentioned type and consists in extrapolation of a set of structure factors (phases and magnitudes) beyond the experimental (2θ) limit of data to increase resolution in the corresponding density function. The application has in view cases for which data are severely curtailed in angular range, but not necessarily in number. Biological macromolecular structure problems, though beyond reach at present, fit the application exactly and, in fact, were the target from the beginning.

Suppose a set of structure factors, spherically complete for some range of $|\underset{\sim}{h}|$ including $|\underset{\sim}{h}|=0$. Now an estimation of electron density at higher-resolution than nominally provided by the original structure factors is found by solving the matrix equation

$$\underset{\approx}{F}\underset{\sim}{C} = \underset{\sim}{\beta}$$

for $\underset{\sim}{C}$ and computing

$$\rho(\underset{\sim}{r}) = \kappa/|\Sigma C(\underset{\sim}{h}) \exp\{-2\pi i \underset{\sim}{h}\cdot\underset{\sim}{r}\}|^2,$$

where κ is a collection of constants, and the summation is over a half-lattice and its origin at which C=1.0. The determinant $|\underset{\approx}{F}|$ is of the general Karle-Hauptman type but with entries restricted by the half-lattice condition. The lead element of $\underset{\sim}{\beta}$ is positive, the others are zero.

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17.X-09 ALTERNATIVES TO R-TESTS. By S.M. Rothstein Department of Chemistry, Brock University, St.Catharines Ontario, Canada. L2S 3A1.

Three alternatives to R-tests are compared in a computer simulation study of power and robustness: RRB's jackknife test on the R-factor ratio(Rothstein, Richardson and Bell, Acta Cryst. (1978),A34,969), Arvesen's jackknife test for the correlation coefficent (Ann. Math. Statist.(1969) 40,2076), and Pitman's test for the correlation coefficient(Biometrika (1939), 31,9) which uses Pearson's statistic.

The RRB jackknife test was found to be robust in the face of considerable Cauchy contamination and to have power at least as good or better than either Arvesen's or Pitman's test, for all distributions considered.

17.X-10 INTENSITY STATISTICS AND PROBABILITY OF VALIDITY OF PHASE RELATIONS. By G.B. Mitra and Sikha Ghosh, School of Research in X-rays and Structure of Matter, Dept. of Physics, Indian Institute of Technology, Kharagpur, India.

A systematic method for applying phase relations in direct methods of structure determination has been developed. N(Z) expressions for Gaussian distribution of structure amplitude components have been derived by Grant, Howells and Rogers (Acta Cryst.(1957) 10, 489) and for Edgeworth distribution by Mitra and Belgaumkar (Proc. Ind. Acad. Sci. (1973) 39, 95), Shmueli (Acta Cryst.(1979) A 35, 282-286) and Wilson (Acta Cryst (1981) under print). Expressions for validity of phase relations based on these probability distributions have been worked out by Cochran and Woolfson (Acta Cryst. (1955) 8, 1) and by Hauptman (Acta Cryst.(1975) A 31, 671) and others respectively. In the present work, expressions for N(Z) and for probability for phase relations based on Cauchy, Rayleigh and several other near Gaussian distributions have been worked out for all space groups as well as for crystals having one or more heavy atoms at known locations. Statistical methods have been applied to hypothetical isomorphous crystals with light atoms occupying all atomic sites including those of heavy atoms. The suggested method consists of determining the statistics involved from comparison of experimental N(Z) values with different theoretical N(Z) curves and then application of the corresponding probability law for phase solutions. Some applications to actual crystal structure solutions have been described.