17.4-06 STRUCTURE REFINEMENTS OF MULTIMODAL ATOMIC DENSITY DISTRIBUTIONS IN THE EINSTEIN APPROXIMATION. By W.F. Kuhs, Institut Laue-Langevin, 156X, F-38042 Grenoble, France.

Using the recently developed program system PROMETHEUS /1/ structure refinements of various disordered structures (mainly ionic conductors) have been carried out. The multimodal probability density distributions of the disordered ions can be described as anharmonic modifications of a gaussian probability density function ('pdf'). However terms up to fifth and sixth order are found to be necessary for a correct description. Such higher order modifications can be easily introduced in a Gram-Charlier expansion of the harmonic (gaussian) pdf. The fourier-transform of this expansion is exact and can be introduced in a conventional least-squares refinement procedure. The resulting general pdfs as well as the corresponding mean potentials (=effective one particle potentials) show two (or even more) local extrema (=modes). The activation energy of the transitions between the different modes as well as the ordering schemes of the corresponding low-temperature phases can be derived by an inspection of these multimodal mean potentials. In this way one can avoid the introduction of sophisticated (harmonic) split-models, which moreover yield a significantly worse fit to the data. In the limit of the Einstein-approximation only a multimodal one particle model allows for a direct comparsion of the different disorder locations with respect to their potentials.

/1/ U.H.Zucker, E.Perenthaler, W.F.Kuhs & H.Schulz The PROMETHEUS-System, to be published.

17.4-07 CALCULATION OF THE ELECTRON DENSITY DISTRIBUTION WITH AN ACCOUNT OF STATISTICAL ERRORS IN STRUCTURE AMPLITUDES AND SERIES TERMINATION. By A.A.Shevyrev and V.I.Simonov, Institute of Crystallography, Academy of Sciences of the USSR, Moscow, USSR.

On calculating the electron density distribution in crystals it is desirable to eliminate statistical errors in the observed moduli of structure amplitudes and to smooth out the effect of the Fourier series termination. Of special importance is the location of light atoms in the presence of heavy ones in the structure as well as the calculation of the difference density distribution. Proceeding from the mathematical methods of stable Fourier series summation used when the Fourier series coefficients are not free from statistical errors (Тихонов А.Н., Арсенин В.Я. Методы решения некорректных задач. Изд. "Наука", М., 1974), the following expression has been derived:

$$\rho(\vec{r}) = \frac{1}{V} \sum_{\vec{H}} W_{\vec{H}} F_{\vec{H}} \exp[-2\pi i \vec{H}\vec{r}]$$

where

$$W_{\vec{H}} = \begin{cases} |F_{\vec{H}}|^2 / (|F_{\vec{H}}|^2 + \sigma^2_{|F_{\vec{H}}|}) & , \text{if } |F_{\vec{H}}| > \beta \sigma_{|F_{\vec{H}}|} \\ 0 & , \text{if } |F_{\vec{H}}| \leq \beta \sigma_{|F_{\vec{H}}|} \end{cases}$$

The parameter β depends on the law of errors' distribution in $|F_{\vec{H}}|_{obs}$. If the errors follow the Gaussian distribution, $\beta = 2$ is recommended.

The use of special $\sigma_{\vec{H}}$ -factors was suggested to smooth out the Fourier series termination waves (Ланцош К. Практические методы прикладного анализа. Физматгиз, М., 1961, 230 с.):

$$\rho(\vec{r}) = \frac{1}{V} \sum_{\vec{H}} \sigma_{\vec{H}} F_{\vec{H}} \exp[-2\pi i \vec{H}\vec{r}].$$

In the case of three-dimensional series, the $\sigma_{\vec{H}}$ -factors have the form:

$$\sigma_{hkl} = \frac{\sin \frac{\pi h}{H+1} \sin \frac{\pi k}{K+1} \sin \frac{\pi l}{L+1}}{\pi^3 hkl/[(H+1)(K+1)(L+1)]}$$

where hkl are the usual indices of the corresponding structure amplitudes, whereas the values of HKL depend on the limits of the observed set of F_{hkl} and are determined for each structure amplitude in the following way:

H = max h for the given k,l and h > 0

H = max |h| for the given k,l and h < 0 .

The values of K and L are determined by the same method. Thus, the $\sigma_{\vec{H}}$ -factors are peculiar to each Fourier coefficient and depend on its indices and on the used set of structure amplitudes. The paper gives examples of practical application of the above-mentioned methods.

17.5-01 NON-IDEAL DISTRIBUTIONS AND MOMENTS OF INTENSITY. By U. Shmueli and U. Kaldor, Department of Chemistry, Tel-Aviv University, 69978 Ramat Aviv, Israel and A.J.C. Wilson, Department of Physics, University of Birmingham, Birmingham B15 2TT, England.

Intensity statistics allowing for deviations from the behaviour predicted by the central limit theorem, was recently reinvestigated and extended to all the space groups (Shmueli, U. & Wilson, A.J.C., Acta Cryst.(1981); Shmueli, U. & Kaldor, U., Acta Cryst.(1981)). These deviations concern effects of atomic heterogeneity and space-group symmetry on intensities from non-dispersive crystals with all the atoms in general positions. An outline of the topic is given by one of us (U.S.) in this Congress.

In this poster presentation, probability functions, cumulative distributions and moments of the normalized intensity, based on the above non-ideal statistics, will be summarized and new aspects of their derivations will be outlined. The theory will be illustrated by hypothetical and practical examples and a method whereby these calculations are linked to a standard system of crystallographic programs will be described.