

17.5-02 EFFECTS OF HEAVY ATOMS AND SYMMETRY ON THE CUMULATIVE DISTRIBUTION FUNCTION OF NORMALIZED STRUCTURE AMPLITUDES. By G.D. Nigam and Sikha Ghosh, Department of Physics, Indian Institute of Technology, Kharagpur, India.

Expansions for the probability density function of the normalised structure amplitude $|E|$, which account for the known contribution of heavy atoms in the unit-cell have been derived. The expressions for the cumulative distribution function $N(|E|)$ for Edgeworth expansion have been derived by Mitra and Belgaumkar (Proc. Ind. Acad. Sci. (1973), 31,45), and for Gram-Charlier expansion by Shmueli (Acta Cryst., (1979), A35, 282), Shmueli and Wilson (Acta Cryst. (1981) under print). In the present investigation the expressions for $N(|E|)$, using the above modified probability density function, have been obtained. The expressions are composition and symmetry dependent and lead to those obtained by Shmueli if the heavy atom contribution is absent. The polynomial series distribution is also used to derive an expression for $N(|E|)$ in case of a hypercentric crystal. The asymptotic form of the distribution has been used to calculate the effect of heavy atoms on two phase structure seminvariants in $P\bar{1}$. Numerical computation has been carried out to study the effect of composition and symmetry on $N(|E|)$. The results have been compared with those of Shmueli and Wilson and also tested on a few known crystal structures.

17.6-01 CONFORMATIONAL ENERGY ANALYSIS OF BENICE JONES PROTEIN RHE. By A. Chatterjee, B.C. Wang, W. Furey, Jr., C.S. Yoo and M. Sax Biocrystallography Laboratory, VA Medical Center, Pittsburgh, PA 15240 and the Department of Crystallography, University of Pittsburgh, Pittsburgh, PA 15260.

Conformational energy analysis of Bence Jones Protein Rhe starting with coordinates refined to 1.6 Å resolution is carried out by using a suitably chosen empirical conformational energy function and a set of derived energy parameters. In this process the atoms are moved so as to reduce the molecular potential energy in response to perturbation introduced in the system. The energy minimization makes use of the conjugate gradient method by searching along directions corresponding to the current local quadratic approximation to the energy function. The required computer programmes have recently been developed in this laboratory and results will be presented.

17.6-02 CRYSTAL STRUCTURE PREDICTION BY ENERGY MINIMISATION. By C.R.A. Catlow, A.N. Cormack, University College London, and F. Theobald, Laboratoire de Chimie Physique, Besançon, France.

This paper will show that calculations of crystal energetics for ionic solids coupled with efficient minimisation routines are capable of predicting the structure of complex inorganic solids, thereby promising to provide a valuable guide in structure refinements. The calculations we discuss are based on exact summations of both Coulomb and short-range components of the lattice energy. Energy minimisation may be performed with respect to all structural parameters. We illustrate the power of our method with two examples. The first concerns the recently discovered 'B' phases of VO_2 and TiO_2 (Marchand et al., Mat. Res. Bull. 15, 1129 (1980)). Energy minimisations were performed starting from an ideal model based on regular octahedra. The minimised structure shows distortions close to those observed in the X-ray refined model for VO_2 . A predicted structure for the analogous 'B' phase of TiO_2 is also presented; no experimental structure is yet available for this phase. Our second example is the mineral forsterite (Mg_2SiO_4) where again we show that distortions from idealised models are correctly predicted. We conclude with a discussion of potential future application of the technique to complex transition metal compounds and to minerals.

17.6-03 ADAPTION OF THE POTENTIAL ENERGY OF MOLECULAR AND CRYSTAL STRUCTURES TO POWDER DIAGRAMS. By H. Bradaczek, G. Barnickel and H. Labischinski, Institute of Crystallography, Free University Berlin, West Germany.

Recently a method has been developed to carry out potential energy calculations in Fourier space. Using reciprocal sphere potential functions the energy can be described by

$$P_{TOT} = \int_{\text{sphere1}} FF_1^* dV + \int_{\text{sphere2}} FF_2^* dV + \dots$$

where $K = 1, 2, \dots$ corresponds to the kind of interaction in a structure. The radii of the spheres are reciprocal to the interaction width and can be adapted to the first minimum of the potential functions. FF_K^* are the structure factors corresponding either to interactions of the same atom type or of various ones. (Partial structures). The above equation allows the integration over spherical shells, the result of which is proportional to powder or amorphous structure diffractograms. The comparison opens possibilities to adapt parameters of the potential energy to experimental data. The method is usable for crystals as well as for amorphous structures.