

17.2-13 PHASING SINGLE ISOMORPHOUS REPLACEMENT DATA WITH DIRECT METHODS. By Marie E. Fraser, Suzanne Fortier and Nancy J. Moore, Department of Chemistry, Queen's University, Kingston, Ontario, Canada, K7L 3N6.

In 1982, Hauptman presented the probabilistic theory of the three-phase structure invariant for a pair of isomorphous structures (H. Hauptman, Acta Cryst. A38, 289 (1982)). Interpretation of these results led to the incorporation of the heavy atom substructure information in the distribution, estimation of the cosine invariants in the full range from -1 to +1 and increased accuracy in the estimation of the three-phase invariants. (S. Fortier et al., Acta Cryst. A41, 571 (1985)).

The heavy atom substructure information used is the phase difference between a reflection from the native and the same reflection from the derivative. This information is available once the positions of the heavy atoms are known. When the heavy atom information is inserted in the probability distribution, the distribution retains an eight-fold ambiguity in the estimation of the three-phase invariant but a four-fold ambiguity in the cosine estimate. The four cosine estimates have slightly different probabilities. The cosine estimates and their weighted mean are being used in the phasing of the native protein.

The theory has been applied to calculated diffraction data from the proteins cytochrome c550 with its platinum derivative and carp calcium-binding parvalbumin with its mercury derivative; and to real data from the latter. The parvalbumin was chosen because SIR data and a refined structure are available from the Protein Data Bank.

17.2-14 THE EFFECTS OF PSEUDOTRANSLATIONS ON RECIPROCAL SPACE. By R. Böhme & W. Gebert, Institut für Mineralogie der RUB, Postfach 102148, D-4630 Bochum, West Germany.

Pseudotranslations in a crystal structure are expected to be recognized by unequal distributions of the normalized structure factors if normalisation has been calculated without taking the pseudotranslations into account (Böhme (1982). Acta Cryst. A38, 318; Casciarano, Giacovazzo & Luic (1985). Acta Cryst. A41, 544).

Here we report on experiences with a structure where the pseudotranslation could not be detected that way: The means of E^2 for each parity class of reflexions were very close to 1.0, in fact they varied only between 0.96 and 1.05 according to SHELXTL (Sheldrick (1983). Version 4.1). Nevertheless a pseudotranslation $(\frac{1}{2}, 0, \frac{1}{2})$ was a priori indicated by the second highest peak of the Patterson function, which could also be verified after solving the structure. The unit cell contained two independent 14-atom-molecules in the asymmetric unit of space group $P-1$ which could be transformed approximately into each other by a centre of symmetry in $(\frac{1}{2}, 0, \frac{1}{2})$. The seven Cl-atoms turned out to be 0.3 - 0.5 Å out of their ideal positions, the remaining lighter ones 0.1 - 0.2 Å only. So the pseudotranslation we are referring to is of type 2 (Böhme (1985). "Crystallographic Computing 3", ed. by Sheldrick et al.).

Results obtained in structure determination procedure by normalizing main and superstructure reflexions separately will be reported as well as those obtained from SHELX and SAPI (Yao, Zheng, Qian, Han, Gu & Fan Beijing 1985).

17.2-15 MAXIMUM ENTROPY ELECTRON DENSITY ESTIMATION. By J. Navaza, C. de Rango and G. Tsoucaris, Lab. de Physique, Centre Pharmaceutique, Chatenay Malabry, France.

The electron density function of a crystal is a physical entity which is at the origin of the diffraction pattern. Because of the limited extension of this pattern accessible to experiment it is not possible to exactly recover the original electron density even if the phases were known. Of course the main difficulty resides in the lack of phase information. The following theory (Navaza, Acta Cryst., 1984, A41 and 1985, A42) establishes a new link between the (unknown) electron density and the diffraction pattern; it is of general validity, applicable both in the ab-initio and phase extension problems. The theory relies upon the modelling of the whole electron density as a random function (i.e. the whole function is considered as a random "variable") denoted by $m(x)$. A probability $P(m)$ is then associated with this random function.

The maximum entropy principle (Jaynes) is used in order to explicitly determine this functional $P(m)$. The entropy

$$H(P) = - \int_A P(m) \ln P(m) \mathcal{D}m \quad (1)$$

is maximized with respect to $P(m)$. The symbol $\int_A \mathcal{D}m$ means integration over all admissible functions. The functional which maximizes (1) and satisfies constraints to be discussed later will be denoted $P_{ME}(m)$. An estimate of the true electron density is provided by the average value of $m(x)$

$$m_{ME}(x) = \int_A m(x) P_{ME}(m) \mathcal{D}m \quad (2)$$

In the process of practical determination of $m_{ME}(x)$ one must take into account all available information:

a) Experimental. For example

$$F_H(m_{ME}) = F_H^{obs}$$

b) Non experimental. For example

$$m(x) \geq 0.$$

An algorithm has been written (about 5000 Fortran instructions) for 3-dimensional structures and all space groups, and tested. Practical applications will be displayed and discussed.