17.2-17 ,SOLUTION OF THE PHASE PROBLEM FOR NON-CENTROSYMMETRIC CASES IN TWO STAGES. By Fan Hai-fu, Gu Yuan-xin, Xu Zhang-bao, Qian Jin-zi and Zheng Chao-de, Institute of Physics, Academia Sinica, Beijin, China.

The phase problem in noncentrosymmetric cases may be solved in such a way that the real and imaginary parts of the structure factors are treated separately and successively. The procedure includes two steps:

1. The structure is first solved on the basis of a pseudo symmetry which is higher than that of the actual one by an additional inversion centre. Signs instead of phases are then obtained for the structure factors. These signs would in fact consist of those of the real parts of the structure factors. Consequently an E-map containing both enantiomorphs can be obtained.

2. From the E-map so obtained, the real parts and the absolute values of the imaginary parts of the structure factors can be calculated approximately. Finally the signs of the imaginary parts can easily be determined and hence the phase problem can be solved with the aid of the component relation

$$B_H = (f/V) \sum_{H'} B_{H'} A_{H-H'}$$

where A denotes the real part and B the imaginary part of the structure factor; f is a function of the atomic form factor and V is the volume of the unit cell (Fan Hai-fu, Acta Physica Sinica, 21 (1965) 1114; see also J. Karle, Acta Cryst., 21 (1966) 273).

In comparison with the other methods, the procedure described above has the following advantages:

1. By executing the first step, the amount of calculation needed for permuting the phases in the starting reflection set can be reduced by a factor of about 4. Alternatively the number of reflections in the starting set can be doubled while the amount of calculation remains about the same as in the usual permutation procedure. This is valuable in the determination of complex structures.

2. The second step can strongly restrict the tendency for the whole set of phases to reduce to a centrosymmetric one. Hence the procedure has the effect of stabilizing the specified enantiomorph. This is important in the determination of structures with polar space groups like $P2_1$.

Crystal structures in space groups $P2_1$ and $P2_12_12_1$ with and without heavy atoms have been used as examples to prove the efficiency of the procedure.

17.2-18 THE PROBLEM OF MULTIPLE SOLUTIONS IN STRUCTURE DETERMINATION AND THE APPLICATIONS OF MODIFIED SAYRE'S EQUATIONS.

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Three types of crystals often lead to multiple solutions in the determination of their structures:
1. Structures composed of light atoms with polar space groups such as $P2_1$, $Pna2_1$, $P4_1$, etc.— Phase determination by direct methods in this type of structures often results in one set of centrosymmetric phases leading to an E-map containing both enantiomorphs.
2. Structures with pseudo-symmetry higher than the actual symmetry by an additional inverse centre and/or sub-periodicity of translation — Two or more structure images related by the additional symmetry would appear simultaneously in the resulting E-map or Fourier map.
3. Structures containing heavy atoms with higher symmetry than that of the whole structure by an additional inverse centre and/or sub-periodicity of translation—Two or more structure images of the light atom portion related by the additional symmetry would appear simultaneously in the resulting E-map or Fourier map.

Multiple solutions can be divided into two categories:
1. The translational multiple solutions— This leads to a systematic undetermination of certain(but not all)types of phases of the structure factors. The problem can be solved with the aid of the modified Sayre's equations (Fan Hai-fu, Acta Physica Sinica, 21(1965)1105; Fan Hai-fu, Acta Physica Sinica, 24(1975)57; Fan Hai-fu et al., Acta Physica Sinica, 27(1978)554), which have the common form of

$$F_H^o = (f/V) \sum_{H'} F_{H'}^o F_{H-H'}$$

where F^o's denote structure factors with phases systematically undetermined, F's denote structure factors with phases derivable from a pseudo structure model containing simultaneously all possible solutions, f is a function of atomic form factor and V is the volume of the unit cell.
2. The enantiomorphic double solutions— This leads to the ambiguity on signs of the imaginary components of all the structure factors (notice that the origin is fixed at the pseudo inverse centre for the reason of simplicity). This problem can be solved by making use of another type of modified Sayre's equation — component relation(Fan Hai-fu, Acta Physica Sinica, 21(1965)1114; Fan Hai-fu & Zheng Qi-tai, Acta Physica Sinica, 27(1978)169; see also J. Karle, Acta Cryst., 21(1966)273.),

$$B_H = (f/V) \sum_{H'} B_{H'} A_{H-H'}$$

where A's denote the real components of the structure factors, which can be derived from a pseudo structure model containing both enantiomorphs, while B's denote the imaginary components, of which the absolute values can be obtained as

$$|B_H| = (|F_H|^2 - A_H^2)^{1/2}$$

where $|F_H|$'s are the observed structure amplitudes.
A number of examples are given to elucidate the efficiency of the procedures in solving structures which had been difficult to solve by ordinary methods.