Therefore we conclude that when the ΔF cutoff is relaxed, Karle's rule will give SIR phase information instead of protein phase information. That is:

$$\phi_{hS} + \phi_{kS} + \phi_{(\bar{h}+\bar{k})S} \sim 0 \quad \text{if } (\Delta F_h)(\Delta F_k)(\Delta F_{\bar{h}+\bar{k}}) > 0$$

$$\phi_{hS} + \phi_{kS} + \phi_{(\bar{h}+\bar{k})S} \sim \pi \quad \text{if } (\Delta F_h)(\Delta F_k)(\Delta F_{\bar{h}+\bar{k}}) < 0$$

where S denotes SIR phases. More results and discussion of the above equations will be presented.

01. 2–7 A METHOD FOR RESOLVING PHASE AMBIGUITY IN SIR OR SINGLE-WAVELENGTH ANOMALOUS SCATTERING DATA.

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The use of the gross molecular image, revealed by a new and automated procedure, together with a Fourier "image-enhancement" process has been found to be highly effective for resolving phase ambiguity in single isomorphous replacement (SIR) data or single-wavelength anomalous scattering (SAS) data. When the method was tested using diffraction data for Bence Jones protein Rhe (Wang, et al, JMB 129, 657, 1979) the results were comparable with those obtained by the MIR process. The MIR phases (3Å) obtained previously from two sets of isomorphous and one set of anomalous data had an average phase error of 32.3 degrees. However, the new process using only one set of isomorphous data (no anomalous data), gave an average phase error of 31.8 degrees. The method has been used for the determinations of several previously unknown macromolecular structures, including the crystal structures of two immunoglobulin light chain dimers and a DNA-protein complex.

The method and its applications to known and unknown structures will be presented. In addition, an integrated program package for carrying out the various steps in the method will be introduced. This program package can also be used for extending phase information and improving MIR phases.

01. 3–1 Structural Refinement of a [2Fe-2S] Ferredoxin from Aphanothece sacrum by the Molecular replacement method. By T.Tsukihara, M.Mizushima, K.Fukuyama, and Y.Katsube, Faculty of Engineering, Tottori University, Tottori, 680, JAPAN

A molecular structure of [2Fe-2S] ferredoxin from Spirulina platensis has been determined at 2.5A resolution(Fukuyama et al.,Nature(1980) 286,522). Since the crystal of S. platensis ferredoxin was too thin in thickness to give a good intensity data set, the crystal was not used for a higher resolution analysis. Another [2Fe-2S] ferredoxin from A. sacrum whose amino acid sequence is different from that of S. platensis by about 30% was crystallized in a barnet-shape. We have determined the main chain fold of this ferredoxin by the single isomorphous replacement method at 2.5A resolution (Tsutsui et al.,J.Biochem.(1983)94,299). These ferredoxins are similar to each other in the main chain structure. As four molecules of A. sacrum ferredoxin were in an assymmetric unit, their structures were refined by the molecular replacement method in the present study.

The space group is $P4_1$, and the unit cell dimensions are a=b=92.2 and c=47.6A. Rotational and translational parameters of four independent molecules named A, B, C, and D were determined by a least-squares method on the electron density calculated by the single isomorphous replacement method at 2.5A resolution. Correlation coefficients of the electron density, $C=\sum(\rho-\bar{\rho})(\rho_A-\bar{\rho}_A)/[\sum(\rho-\bar{\rho})^2(\rho_A-\bar{\rho}_A)^2]^{1/2}$, were 0.50, 0.38, and 0.38 for molecules B, C, and D, respectively. Electron density of the solvent region was left unchanged during the first two cycles of the molecular replacement refinement. In the further refinement that of the solvent region was replaced by an averaged electron density of the corresponding region at the previous cycle. The R-value, $R=\Sigma||F_o|-|F_{MR}||/\Sigma|F_o|$, was reduced from 0.45 to 0.36, and the correlation coefficient of structure factors, $C=\Sigma(F_o-F_o)(F_{MR}-F_{MR})/[\Sigma(F_o-F_o)^2\Sigma(F_{MR}-F_{MR})^2]^{1/2}$, was 0.70 after the six cycles of the refinement. Figs.1 a and b show electron density maps of the same section for the first and the final cycles, respectively. The feature of electron density distribution was obviously improved by the refinement. Phase extension from 2.5A to 2.2A resolutions is in progress by the molecular replacement method.

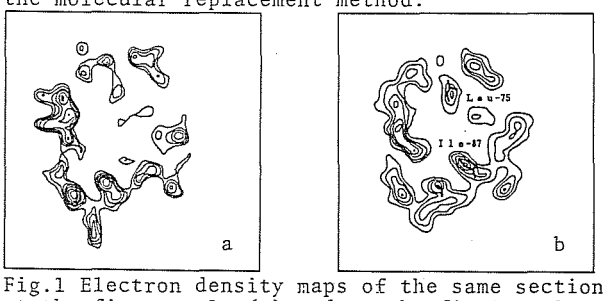

Fig.1 Electron density maps of the same section at the first cycle (a) and at the final cycle (b) of the present refinement. In (b) the side chains of Leu-75 and Ile-87 are drawn on the electron density contours.