Direct Methods Resolving the Phase Ambiguity due to One-wavelength Anomalous Scattering or Single Isomorphous Replacement

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Abstract

The direct method [Fan, H.F. and Gu, Y.X. (1985). *Acta Cryst.* A**41**, 280-284] has been used to resolve the phase ambiguity arising from one-wavelength anomalous scattering (OAS) or single isomorphous replacement (SIR) and combined with the solvent flattening method [Wang, B.C. (1981). *Acta Cryst.* A**37**, Suppl. C-11; Wang, B.C. (1985). *Methods in Enzymology*, **115**, 90-112]. This technique has been applied to experimental OAS and SIR data of a number of known proteins. The use of direct methods provided much better phases than the averaged OAS/SIR phases, while the solvent flattening procedure further improved direct-method phases leading to traceable Fourier maps in all cases. Comparison between our method and the solvent flattening technique alone revealed substantial contribution of the direct method.

A new phase extension procedure making use of the SIR information is proposed based on the above technique. The procedure avoids finding unknown phases in the whole range of $0 \sim 2\pi$ by making choice between two equally possible values of SIR doublets and thus is powerful for phase extension. Test with the known protein RNase Sa showed that the method is capable of extending phases from a resolution of 6Å to 2.5Å and resulted in an easily traceable Fourier map. A general purpose program has been written for phasing OAS/SIR data.

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