SAD Phasing at the Presence of Pseudo-translational Symmetry

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Pseudo-translational symmetry results in some reflections group(s) having systematically weak intensities. In the presence of pseudo-translational symmetry, the heavy-atom (anomalous-scatterer) substructure determined by conventional methods from the Bijvoet differences will not be the actual substructure but rather the averaged or approximately, the basic substructure, which will have no or very weak contribution to the systematically weak reflections. SAD phasing based on such averaged heavy-atom substructures will cause abnormally large errors in the phase of systematically weak reflections. To avoid this, special treatment is needed. Direct methods have been developed to solve the phase problem for small structures having pseudo-translational symmetry. The method can be used to obtain the actual heavy-atom substructures from the Bijvoet differences in the presence of pseudo-translational symmetry. Various phasing procedures have been tested and compared using a set of artificial protein SAD data.

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