

Recent Practices on Sulfur SAD Phasing Using Soft X-rays

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A single-crystal x-ray diffraction data set contains critical three-dimensional structural information about the molecules which makeup the crystal. This information is the major direct experimental source for the subsequent elucidation of spatial structures of the crystallized molecules.

In recent years, single wavelength anomalous diffraction (SAD) phasing has become the major method used in macromolecular structure determination. Sulfur atoms are natively present in most protein molecules and their anomalous scattering signal when measured with soft x-rays makes them an ideal phasing probe. With the advances in methodology and diffraction data collection hardware, sulfur SAD phasing has contributed to many *de novo* crystal structure determinations. We have been actively trying this phasing method in routine crystal structure determinations. Several new structures have been determined by the S-SAD method with the data collected using either home lab Cr x-rays or synchrotron x-rays (Photon Factory beamlines 1A and 17A). Details of the data collection, data processing and phasing process will be presented.