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Protein Crystallography at Ultra Short Wavelengths : Feasibility Study of Anomalous Dispersion Experiments at the Xenon K-edge

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Abstract

A protein crystallography experiment at the xenon K-edge (λ = 0.358 A) has been successfully carried out at the material science beamline (BL2/IDll) of the ESRF. The samples used in this methodological study were crystals of porcine pancreatic elastase, a 26 kDa protein of known structure. The diffraction data are of excellent quality. The combination of isomorphous replacement and anomalous dispersion of a single xenon heavy-atom derivative allowed accurate phase determination and the computation of a high-quality electron density map of the protein molecule. This is the first fully documented report on a complete protein crystallography experiment - from data collection up to phase determination and calculation of an electron density map - carried out with data obtained at ultra short wavelengths. Experimental considerations as well as possible advantages and drawbacks of protein crystallography at very short and ultra short wavelengths are discussed.

Keywords

Macromolecular crystallography, Short-wavelength X-rays, Data collection, Anomalous dispersion, Isomorphous Replacement, Xenon derivatives