

Noble gas MIR and anomalous dispersion in proteins

Marc Schiltz, William E. Shepard, T. Prange, and Roger Fourme
LURE, Université Paris-Sud, Bat. 209d, Orsay, France

O. Svensson
European Synchrotron Radiation Facility, BP 220, F-38043 Grenoble Cedex, France

Åke V. Kvick
Experimental Division, European Synchrotron Radiation Facility, BP 220, F-38043 Grenoble Cedex, France

Marc Schiltz,
LURE, Université Paris-Sud, Bat. 209d, Orsay, France

Richard Kahn
Institut de Biologie Structurale, 41 Avenue des Martyrs, 38027 Grenoble Cedex, France

Protein complexes with the noble gases xenon and krypton are highly isomorphous with the native structures and can be used as heavy atom derivatives for phase determination. A general method for the preparation of such derivatives is presented. A device has been designed that allows diffraction studies on protein crystals under gas pressure up to 60 bar. Crystal mounting and x-ray data collection do not significantly differ from standard techniques [Schiltz et al. (1994) *J. Appl. Crystallogr.* **27**, 950-960]. The method has been specially adapted for fast data collection schemes using synchrotron radiation, where native and derivative data can be collected on the same crystal, and in the same orientation. This allows for many systematic errors to cancel out in the process of phasing. Extremely accurate electron-density maps have been obtained with the SIRAS (single isomorphous replacement with anomalous scattering) method at the high-energy side of the krypton K-edge (14.32 keV). Similar experiments were also carried out at the xenon K-edge (34.59 keV), and they established the feasibility of protein crystallography at very short wavelengths.