Single Crystal XAS Studies on Metalloprotein Intermediates

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Synchrotron based Metal K-edge XAS and EXAFS spectroscopy is a powerful tool for electronic and geometric structure determination of metalloprotein active sites and is dominantly applied to isotropic samples. The combined single crystal XAS and diffraction technique developed at SSRL on beamline 9-3 can be applied to anisotropic protein crystals to obtain direction specific metrical and electronic information about the active site. In addition, important electronic structure information on unstable, trapped intermediate and transient species can be obtained, which can guide the structure determination process or help develop a strategy for diffraction data collection.

Two recent studies on metalloprotein active sites will be presented. In the first study, Single crystal XAS studies on the Ni containing active site of Methyl Coenzyme M Reductase was combined with solution XAS and EXAFS data. The data were used to determine the redox state of a putative Ni(III)-Me intermediate and coupled to structure determination. In the second study, the electronic structure of oxyhemoglobin was explored using both solution and single crystal Fe K-pre-edge and near-edge XAS studies to differentiate between two putative electronic structure descriptions.

SSRL operations are funded by the Department of Energy, Office of Basic Energy Sciences. The SSRL Structural Molecular Biology program is supported by the National Institutes of Health, National Center for Research Resources, Biomedical Technology Program, and Department of Energy, Office of Biological and Environmental Research.