

X-ray Absorption Spectroscopy of Biological Molecules in Single Crystals

Britt Hedman,¹ Mary C. Corbett,² Matthew J. Latimer,¹ Keith O. Hodgson^{1,2}

¹Stanford Synchrotron Radiation Laboratory and ²Department of Chemistry,
Stanford University, Stanford, CA 94305; hedman@ssrl.slac.stanford.edu

X-ray absorption near-edge structure is sensitive to the electronic structure and geometric arrangement around an absorbing atom site. For non-oriented powder or solution samples, an averaged isotropic edge spectrum is obtained, which contains a superposition of polarized spectral features of all molecular dipoles averaged over all possible orientations. By using polarized single-crystal x-ray absorption spectroscopy, and aligning a molecular vector in the sample with the direction of the incident radiation polarization vector, one can selectively excite transitions into the orbitals along that molecular orientation and thereby obtain enhanced information about the electronic structure. The same approach can also be used for EXAFS to maximize or minimize the contribution of a particular backscattering vector and thereby obtain selected bond distance determinations to higher accuracy and an improved model of the structure of active sites. The sensitivity of the near-edge spectrum to electronic structure, combined with the accuracy of the EXAFS-derived bond-lengths makes the combination of single crystal x-ray absorption spectroscopy and protein crystallography a particularly powerful one. Instrumentation for such studies, at SSRL beam line 9-3, will be described, and examples of applications to biological systems will be presented.

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