

## **EXAFS of the Low Spin Ferric Center of Nitrile Hydratase and Model Complexes**

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Beamline(s): **X9B**

We previously obtained EXAFS spectra of the inactive form of nitrile hydratase obtained from *Rhodococcus* sp. R312 grown in the dark. This "dark form" of nitrile hydratase releases nitric oxide (NO) upon photoactivation of the enzyme. Using EXAFS spectroscopy at beam line X9B, we confirmed the presence of one (and only one) nitrosyl (NO) ligand to the iron, and our multiple scattering analysis allowed us to estimate the Fe-N-O bond angle of  $165^\circ$ , close to that found in most diamagnetic complexes resulting from coordination of NO to low spin Fe(III). The overall coordination of the iron was very similar to that found in a diamagnetic Fe-NO complex also involving a ligand with a  $N_3S_2$  donor set prepared by Prof. Kovacs and co-workers. The University of Washington lab has now prepared new iron and cobalt-containing model complexes with oxidized sulfur ligands (sulfinates and sulfenates) and we will obtain EXAFS spectra of these in the near future for comparison with the enzyme data.