Nuclear Resonant Vibrational Spectroscopy of *Pyrococcus furiosus* Rubredoxin and Ferredoxin

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Iron-sulfur proteins, which are found in all life forms, have been a continuing focus of biological studies because of their important role in electron transfer and in catalysis. Rubredoxins are small electron-transfer proteins that contain a single $Fe(S\text{-}cys)_4$ redox center. The *Pyrococcus furiosus* ferredoxin contains a single $[Fe_4S_4]$ cluster.

Nuclear resonant vibrational spectroscopy (NRVS) is a relatively new technique with valuable characteristics for probing iron metalloproteins through their vibrational spectra. The NRVS method offers less restrictive selection rules than infrared or resonance Raman spectroscopy. The primary requirement for NRVS intensity is motion of the resonant nucleus (in our case ^{57}Fe) along the direction of the incident X-ray beam in a given normal mode.

Detailed NRVS spectra have been obtained for oxidized and reduced rubredoxin and *P.f.* ferredoxin. The ^{57}Fe partial vibrational density of states (PVDOS) spectra were extracted from the raw spectra using PHOENIX program and interpreted by normal mode analysis with optimization of Urey-Bradley force fields.