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Conventional and Synchrotron-based Mössbauer Spectroscopy of Iron Proteins and Spin Crossover Materials

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Mössbauer spectroscopy and synchrotron based nuclear resonance scattering techniques are ideal tools to study electronic and dynamic properties of iron centers in chemical and biological systems. During the last years Nuclear Inelastic Scattering (NIS) has been used by us to detect iron based vibrational modes in powders of iron(II) based spin crossover (SCO) compounds [1]. In order to carry out orientation dependent nuclear resonance scattering experiments on small single crystals of e.g. iron proteins and/or chemical complexes a 2-circle goniometer including sample positioning optics has been installed at beamline P01, PETRA III, DESY, Hamburg. This sample environment has been tested with single crystals of SCO complexes and with hydrogen peroxide treated myoglobin single crystals [2] and is now available for all users of this beamline. Nuclear Forward Scattering (NFS) of SCO microstructures [3] has been applied to monitor the spin switch between the S=0 and S=2 state and quantum chemical calculations based on density functional theory (DFT) have been used to identify spin molecular modes which are responsible for spin marker bands [4]. In order to investigate the dynamic properties of large biomolecules like proteins, DFT methods and molecular mechanics can be coupled for the calculation of the proteins vibrational density of states. Based on our experience with NO transporter proteins [5] we are now studying substrate and inhibitor interactions of Fe-S proteins like the LytB protein [6] which is a potential target enzyme for new antibiotic drugs.

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