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The Macromolecular Neutron Single Crystal Diffractometer BIODIFF for Proteins at the Heinz Maier-Leibnitz Zentrum MLZ

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Neutron single crystal diffraction provides an experimental method for the direct location of hydrogen and deuterium atoms in biological macromolecules. At the FRM II neutron source the neutron single crystal diffractometer BIODIFF, a joint project of the Forschungszentrum Jülich and the FRM II, is mainly dedicated to the structure determination of enzymes. Typical scientific questions address the determination of protonation states of amino acid side chains in the active center, the orientation of individual water molecules essential for the catalytic mechanism and the characterization of the hydrogen bonding network between the enzyme active center and an inhibitor or substrate. This knowledge is often crucial towards understanding the specific function and behavior of an enzyme. BIODIFF is designed as a monochromatic diffractometer and is able to operate in the wavelength range of 2.4 Å to about 5.6 Å. This allows to adapt the wavelength to the size of the unit cell of the sample crystal. Data collection at cryogenic temperatures is possible, allowing studies of cryo-trapped enzymatic intermediates. Recently a hexapod has been installed at BIODIFF which allows an easy online collimator alignment. Some recent examples will be presented to illustrate the potential of neutron macromolecular crystallography. In addition, a potential detector upgrade for BIODIFF will be presented, which will expand the maximum unit cell limits.

Primary author: Dr OSTERMANN, Andreas (Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München)

Co-author: Dr SCHRADER, Tobias (Forschungszentrum Jülich, Jülich Centre for Neutron Science at Heinz Maier-Leibnitz Zentrum (MLZ))

Presenter: Dr OSTERMANN, Andreas (Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München)

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