MS20 Rating and improving data quality: instrumentation, analysis and postprocessing

Chairs: Dr. Karine Röwer, Dr. Loes Kroon-Batenburg

MS20-P14

The new chemical crystallography beamline at PETRA III

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I will present the new beamline for chemical crystallography P24, which recwently started user operation at the high brilliance PETRA III synchrotron light source at DESY. The beamline is optimized for diffraction experiments with single crystals of small molecules. Measurements can be conducted at low and high temperatures in a large variety of sample environments including user supplied setups.

For highest flexibility two diffractometers with different geometries (heavy load Kappa and four circle Euler) are available in two endstations.

Besides classical crystal structure determination it is possible to investigate phase transitions, disordered an modulated structures at ambient and non-ambient conditions and dynamics

Keywords: Chemical crystallography, synchrotron radiation

MS23- Advances in electron crystallography methods

Chairs: Dr. Mariana Klementova, Dr. Enrico Mugaioli

MS23-P12

Experimental and computational reduction of dynamical electron scattering allows visualizing individual hydrogen atoms

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Electron crystallography allows structure solution of beam-sensitive organic pharmaceuticals and macromolecules when only nanometre-sized crystals are available. Compared to X-rays, electron diffraction faces a crucial challenge: dynamical electron scattering compromises structure solution and its effects can only be modelled in specific cases. Dynamical scattering can be reduced experimentally by decreasing crystal size – but not without a penalty, as it also reduces the overall diffracting intensity. To boost the very weak diffraction data, the crystals were cryo-cooled and we employed a fast and highly sensitive hybrid pixel detector. Here we show that nanometre-sized crystals from organic pharmaceuticals allow visualization and unconstrained positional refinement of the hydrogen atoms, even whilst ignoring the effects of dynamical scattering during refinement. Furthermore, we introduce a general likelihood-based computational approach for further reducing the adverse effects of dynamic scattering, which significantly improved model accuracy – even for protein crystal data at substantially lower resolution.

Keywords: electron diffraction, hydrogen atoms, dynamical scattering