MS1-P14 The macromolecular crystallography beamlines BioMAX and MicroMAX at the MAX IV laboratory

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The MAX IV storage ring facility at the MAX IV Laboratory, Lund, Sweden, will come in operation in mid 2016. Due to a multibend achromats approach, the 3 GeV ring will have exceptionally low emittance which will lead to an unprecedented brilliance for a synchrotron radiation source. The BioMAX beamline is one of the first phase beamlines and is dedicated to macromolecular crystallography. Thanks to the low emittance of the storage ring, the focused beam will both be small, 20 x 5 μ m², have a low divergence, 0.1 x 0.1 mrad² with a flux at the sample >10¹³ photons/s. The optics of the beamline are relatively simple with a fixed offset double crystal monochromator and a pair of KB mirrors. This design allows work with both small crystals and large biomolecular complexes with concomitantly large unit cells. BioMAX is designed to be flexible and serve a broad range of needs for the life science community. The experimental setup will be equipped with an MD3 diffractometer with a vertical main rotation axis and two additional axes in a mini-kappa geometry. The setup will include state-of-the-art area detector, sample changer, beam conditioning equipment and auxiliary equipment such as sample cryo and fluorescence detector. The beamline will be controlled using MXCuBE version 3 being developed in collaboration with six other facilities in Europe. The beamline will offer remote access and will use ISPyB for sample management.

MicroMAX, a microfocus station, macromolecular crystallography beamline, is proposed as a state of-the-art exploratory beam line . MicroMAX will deliver a $0.7 \ \mu m^2$ focal spot beam diameter with an X-ray flux $> 10^{13}$ photons/sec in monochromatic mode, and approaching 10^{15} photons/sec in polychromatic mode. of these state-of-the-art specifications, Because MicroMAX will allow very large data sets to be rapidly collected from thousands of micron sized macromolecular crystals cooled to cryogenic temperatures using sample mounting and freezing technologies familiar to any protein crystallographer. In parallel, MicroMAX will develop novel sample delivery environments that will allow the pursuit of serial data collection strategies both at room temperature and using cryo-technologies. This beamline will allow new structures to be solved from very small crystals; and will accelerate the rate of progress towards structures of extremely challenging crystallization targets.

Keywords: Synchrotrons, protein crystallography, automation, serial crystallography

MS1-P15 Facilities for macromolecular crystallography at the HZB

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The Macromolecular Crystallography (MX) group at the Helmholtz-Zentrum Berlin (HZB) has been in operation since 2003. Since then, three state-of-the-art synchrotron beam lines (BL14.1-3) for MX have been built up on a 7T-wavelength shifter source [1,2]. Currently, the three beam lines represent the most productive MX-stations in Germany, with close to 1400 PDB depositions (Status 03/2015). BLs14.1 and 14.2 are energy tuneable in the range 5.5-15.5 keV, while beam line 14.3 is a fixed-energy side station operated at 13.8 keV. All beam lines are equipped with state-of-the-art detectors: BL14.1 with a PILATUS 6M detector and BL14.3 with a large CCD-detector. The HZB-MX beamlines are in regular user operation providing close to 200 beam days per year and about 600 user shifts to approximately 70 research groups across Europe. During the first half of 2015 the endstation of BL14.2 is completely rebuilt. After the re-opening it will feature a DESY-type nanodiffractometer, a G-ROB sample changer and a PILATUS 2M detector. BL14.3 has been equipped with a HC1 crystal dehydration device since 2011. In addition to serving the user community mainly as a screening beam line, it is currently the only MX beamline in Europe with a HC1 device permanently installed [3]. Additional user facilities include office space adjacent to the beam lines, a sample preparation laboratory, a biology laboratory (safety level 1) and high-end computing resources. On the poster, a summary on the experimental possibilities of the beam lines and the ancillary equipment provided to the user community will be given.

- [1] U. Heinemann, K. Büssow, U. Mueller & P. Umbach (2003). Acc. Chem. Res. **36**, 157-163.
- [2] U. Mueller, N. Darowski, M. R. Fuchs, R. Förster, M. Hellmig, K. S. Paithankar, S. Pühringer, M. Steffien, G. Zocher & M. S. Weiss (2012). J. Synchr. Rad. 19, 442-449.
- [3] M. W. Bowler, U. Mueller, M. S. Weiss, J. Sanchez-Weatherby, T. L.-M. Sorensen, M. M. G. M. Thunnissen, T. Ursby, A. Gobbo, S. Russi, M. G. Bowler, S. Brockhauser, O. Svensson & F. Cipriani (2015). Cryst. Growth Des. **15**, 1043-1054.

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