Synchrotron Chemical Crystallography at Pohang Light Source II.

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Single crystal X-ray crystallography is very powerful technique for defining the atomic or molecular structure of crystalline material. This technique determines the atomic positions, and the corresponding bond distances and angles within materials as well as the correlation between structural features and chemical or physical properties.

The supramolecular crystallography beamline (BL2D-SMC) is the unique dedicated chemical crystallography beamline for the structure solution of crystalline materials both small and supramolecule using synchrotron radiation in Korea. The beamline is located at the 2D bending magnet port in the 3GeV storage ring (400mA, top-up mode) of Pohang Light Source II. The optics are consist of two mirrors and a Si (111) double crystal monochromator to operate in the tunable energy range between 8 and 20 keV (1.5 and 0.6 A). Diffraction data are collected by a Rayonix MX225HS CCD area detector (installed in Mar. 2018). It will give a chance to get the structural change of the single crystals or to get the high resolution image data. The beamline control and data collection is controlled by custom-made BL2D-supramolecular data collection software (BL2D-SMDC) with an interactive GUI and is designed to run on a Windows operating system. HKL3000sm is used for cell refinement and data reduction.

BL2D is performing not only general single crystal data collection such as hollow molecular structure (MOFs, cage structure, and very tiny size crystal (< 10 μm3)) but also non-ambient crystallography experiment with variable temperature, gas sorption and photo-excitation to the crystal.

The instruments, status and various application using BL2D will be introduced in this presentation.