

3rd Workshop on the Simultaneous Combination of Spectroscopies with X-ray Absorption, Scattering and Diffraction Techniques



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Crystallography, Spectroscopy and other Capabilities of the CMCF beamlines at the Canadian Light Source

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The Canadian Macromolecular Crystallography Facility (CMCF) is composed of two beamlines, 08ID-1 and 08B1-1. The 08ID-1 beamline is a highly-specialized protein crystallography beamline suitable for collecting diffraction data from small crystals of macromolecules and crystals with large unit cell dimensions. It is equipped with a Roentec fluorescence detector which allows X-ray absorption near-edge structure (XANES) experiments to identify the electronic states of atoms, as well as facilitate MAD experiments. The 08B1-1 beamline is fully automated and equipped with an MD2 goniometer and mini-KAPPA, allowing routine data collection on crystals of small molecules. Recently, a Vortex ME4 four-element fluorescence detector was installed on this beamline. It allows researchers to perform both XANES- and X-ray absorption fine structure (EXAFS)-based X-ray spectroscopy experiments on metal-containing crystal samples. Structural information from X-ray absorption spectroscopy can be of great benefit to protein crystallographers in cases where it is not possible to obtain easily interpretable data from crystallography alone for regions around metal atoms ($<6\text{\AA}$). Moreover, the metal-ligand distances obtained from EXAFS spectra are determined with about 10 times better accuracy than those obtained from MX structures determined at moderate resolutions ($\sim 2\text{\AA}$). Software controlling the X-ray absorption spectroscopy portion of experiments is fully integrated with the Macromolecular Crystallo

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