

Poster Presentation

MS103.P04

XAS at the Canadian Macromolecular Crystallography Facility

J. Cotelesage¹, P. Grochulski¹, M. Fodje¹, J. Gorin¹, K. Janzen¹, S. Labiuk¹, G. George², I. Pickering²

¹Canadian Light Source, Canadian Macromolecular Crystallography Facility, Saskatoon, Canada, ²University of Saskatchewan, Geological Sciences, Saskatoon, Canada

Recent additions to the Canadian Macromolecular Crystallography Facility have expanded the capabilities of its bending magnet beamline. It is now possible to perform x-ray absorption spectroscopy (XAS) on crystals. A wide range of biologically relevant metals can be further studied, supplementing diffraction data. XAS can be used to determine if metalloproteins are photoreducing during diffraction data collection. The geometries of metal complexes can also be inferred with near-edge and EXAFS data, often more accurately than crystallography. CMCF-BM can be employed to do the abovementioned techniques on powder and solution samples that contain a metal of interest. One XAS-based technique that shows promise is single crystal plane polarized EXAFS. This technique combines crystallographic data with the findings from XAS to yield a high resolution three dimensional atomic model. More recently a number of the procedural steps required for the acquisition of XAS-based data have been automated in the MxDC software suite. These changes to data collection make it easier for users new to these disciplines to run the XAS-based experiments. By having the necessary equipment to do XAS at a protein crystallography facility, researchers who may not have had the opportunity delve into the field of XAS now can do so with minimal risk in terms of materials, funds and time.

Keywords: X-ray Absorption Spectroscopy, Canadian Macromolecular Crystallography Facility, metalloproteins