



Canadian National  
Committee  
for Crystallography  
<http://xtallography.ca/>

## **2019 Canadian Chemical Crystallography Workshop – May 26<sup>th</sup> to MAY 29<sup>th</sup>, 2019**

**Concordia University, Montreal, QC**

Hall Building, 1455 Maisonneuve Blvd W

### **Tentative Program (Rev. 4 – May 26)**

Daily start times are fixed. Everything else will depend on the students' requests, and so the schedule may be subject to regular updates.

# Thank you to our sponsors!



The Canadian National Committee for Crystallography



**Rigaku**



## Sunday May 26<sup>th</sup>: Hall Building 423

10:00	Welcome, introductions (Louise)
10:15	Olex2, SHELX, Platon, Mercury, CSD, MAX3D check-in – make sure everyone has working software
10:30	Coffee Break
11:00	Basic Crystallography – Crystals, Bragg's Law (Bruce)
11:30	Basic Crystallography – $\lambda$ Symmetry (Paul)
1:05	Break for Lunch
2:05	Basic Crystallography – Data collection and processing (Jim)
3:00	Basic Crystallography – Reciprocal Space (Paul)
4:00	Juice Break
4:15	Olex2 – Getting started (Louise)
6:00	Break for Dinner

**Monday May 27<sup>th</sup> : Hall Building 1011**

9:00	Structure Factors (Joe)
10:30	Coffee/Tea Break
11:00	Problem Crystal Structures (Bruce)
12:30	Break for Lunch
1:30	Olex2 – Disorder and Solvent Masks (Louise)
2:30	Analyses – supplied and student data (All instructors present)
3:30	Juice Break
4:00	Introduction to ConQuest and Mercury (Louise)
5:00	Analyses – supplied and student data (All instructors present)
6:00	Break for Dinner

**Tuesday May 28<sup>th</sup>: Hall Building 1011**

9:00	Refinement using Crystals vs. Shelx (Mike and Louise)
10:30	Crystal Growth (Paul)
11:00	Coffee Break
11:30	Panel Discussion: Crystallography and Career Paths (All instructors present)
12:15	A moment to reflect - extinction (Jim)
12:30	Break for Lunch
1:30	HKLF 5 for non-Merohedral twins and Dealing with Merohedral Twins in Olex2 (Jim)
3:30	Juice Break
4:00	Analyses – supplied and student data (All instructors present)
6:00	<b>Group Dinner Sponsored by Bruker</b> Location: Sir Winston Churchill Pub (1455 Crescent St., Montreal)

**Wednesday May 29<sup>th</sup> : Hall Building 1011**

9:00	The Power and Pitfalls of Sharing Crystallographic Data (Amy)
9:45	cif Finalization and Scandal (Louise)
10:30	Coffee Break
11:00	Cambridge Structural Database Software Hands-on Demo and Q&A (Amy)
12:30	Break for Lunch
1:30	Analyses – supplied and student data (All instructors present) \\ Prepare short presentations
3:30	Juice Break
4:00	Student presentations - ~ 10min per student, with 5 minutes for discussion and questions during and after presentations
9pm	Wrap-up. Workshop ends.

## **Instructors and Organizers**

Paul Boyle, [University of Western Ontario](#)

Jim Britten, [McMaster University](#)

Louise Dawe, [Wilfrid Laurier University](#)

Joseph Ferrara, [Rigaku Americas Corporation](#)

Ashlee Howarth, [Concordia University](#)

Michael J. Katz, [Memorial University of Newfoundland](#)

Bruce Noll, [Bruker AXS Inc.](#)

Amy Sarjeant, [Cambridge Crystallographic Data Centre](#)