



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

2017 Canadian Chemical Crystallography Workshop – May 22nd to MAY 26nd , 2017

McMaster University

Chemistry Department – ABB-163



Tentative program (rev. 4 – May 23).

Daily start times are fixed. Everything else will depend on the students' requests.

Monday Mechanics, May 22

10:00	Welcome, introductions (Jim)
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 (Chuck)
11:30	Basic Crystallography – Symmetry (Chuck)
12:30	Break for Lunch
1:30	Basic Crystallography – Data collection and processing (Chuck)
2:00	Basic Crystallography – Reciprocal Space (Chuck)
2:30	Collecting Accurate Diffraction Data (Lee)
3:30	Juice Break
4:00	Structure Factors and where to put them (Jim)
5:00	Olex2 – Getting started (Louise)
6:00	Break for Dinner

Technique Tuesday, May 23

9:00	Olex2 (Louise)
10:30	Coffee/Tea Break
11:00	More Olex2 (Louise, Jim)
12:30	Break for Lunch
1:30	Analyses – supplied data / record R1
3:30	Juice Break
4:00	Analyses – supplied data / student data/
6:00	Break for Dinner

Wreckage Wednesday, May 24

9:00	Solution and Refinement of Problem Crystal Structures - A Clinical Approach (Chuck)
10:30	Coffee Break
11:00	Solution and Refinement of Problem Crystal Structures - A Clinical Approach cont.(Chuck et al)
12:30	Break for Lunch
1:30	Analyses – Solve and refine your own data \\ disorder group session
3:30	Juice Break
4:00	Analyses – student data \\ Olex2 group session (Jim)
6:00	Group Dinner (Pheonix) Thanks to cash donation from Bruker

Twining Thursday, May 25

9:00	Dealing with Twins
9:45	Working with the CSD databases (Shyam)
10:30	Coffee Break
11:00	More Twining Examples
12:00	Structure Finalization (Louise)
12:30	Break for Lunch
1:30	
2:15	And now for something completely different . . . Materials Characterization at the Canadian Centre for Electron Microscopy (Alison)
2:45	Analyses – student data \\ Disorder refinement
3:30	Juice Break
4:00	ConQuest/Mercury Hands-on Demo (Shyam)
6:00	Break for dinner

Friendly Friday, May 26

	Structure presentations - ~ 10min each
9:10	
9:20	
9:30	
9:40	
9:50	
10:00	
10:10	
10:20	
10:30	Coffee Break
	Student presentations - ~ 10min each
11:00	
11:10	
11:20	
11:30	
11:40	
11:50	
12:00	
12:10	
12:20	
12:30	
12:40	Wrap-up. Workshop ends

Discussion during the presentations is encouraged.

Instructors, Organizers: Jalil Assoud, Jim Britten, Chuck Campana, Lee Daniels, Louise Dawe, Brian Patrick, Alison Mark, Shyam Vyas.