



2011 Chemical Crystallography Workshop



Université de Montréal



Pavillon J-Armand Bombardier

Lectures: Room 1035 (2074 on the 14th)



Tentative program (rev. 11.JUNE.11). Start times and lunch times are fixed. Everything else will depend on the students needs.

Friday, June 10

8:00	Les Studios Hôtel residents meet Thierry in lobby Others meet Francine at PJAB Breakfast (ATRIUM)
10:00	PJAB – Welcome, introductions (Hein, Jim)
10:15	WinGX (SHELXTL)check-in – make sure everyone has a working copy
10:30	Coffee Break
11:00	Chemical Crystallography – 12 Steps / Example a1 (Jim)
12:30	Lunch (ATRIUM)
1:30	Basic Crystallography - Theory and Practice of X-ray Crystal Structure Determination: Part 1 (Chuck)
3:00	Space Group Symmetry – Using Mercury to study structure (Jim)
3:30	Juice Break
4:00	Divide up: Practice structures / crystal mounting / collection
6:00	Dinner

Saturday, June 11

8:00	Breakfast (ATRIUM)
9:00	Basic Crystallography - Theory and Practice of X-ray Crystal Structure Determination: Part 2 (Chuck)
10:30	Coffee Break
11:00	Structure Factors and Reciprocal Space (Jim)
12:00	And now for something completely different . . . (Adrien)
12:30	Lunch (ATRIUM)
1:30	WinGX analyses– supplied data / more data collections
3:30	Juice Break
4:00	WinGX analyses – supplied data / student data
6:00	Dinner

Sunday, June 12

8:00	Breakfast (ATRIUM)
9:00	Absolute Configuration (Thierry)
10:00	Diagnosis and Treatment of Problem Crystal Structures (Chuck)
10:30	Coffee Break
11:00	Modelling Disorder (Hein)
12:00	The Intelligent Squeeze (Adrien)
12:30	Lunch (ATRIUM)
1:30	WinGX analyses – Solve and refine your own data
3:30	Juice Break
4:00	WinGX analyses – student data
6:00	Dinner

Monday, June 13

8:00	Breakfast (ATRIUM)
9:00	Twins (Andreas)
9:30	Using 'cell_now' (Andreas)
10:00	Crystallographic Information File (CIF) (Hein)
10:30	Coffee Break
11:00	Typical CHECKCIF alerts (Hein)
12:00	And now for something completely different . . . (Chuck, Jim)
12:30	Lunch (ATRIUM)
1:30	WinGX analyses – student data
3:30	Juice Break
4:00	WinGX – finish your refinements / presentation
5:00	Graphics options – Ortep, Mercury, etc
6:00	Dinner

Tuesday, June 14, (PJAB-2074)

8:00	Breakfast (PJAB-2074)
9:00	OLEX2 and Student presentations - ~ 10min each (Chair: Thierry)
10:30	Coffee Break
11:00	Student presentations - ~ 10min each (Chair: Francine)
12:30	Lunch (PJAB-2074)
1:30	Student presentations - ~ 10min each (Chair: Michel)
3:30	Juice Break - Workshop wrap-up – please fill out survey sheet
4:00	Workshop ends

Instructors: Francine Bélanger, Jim Britten, Chuck Campana, Adrien Côté, Andreas Decken, Thierry Maris, Hein Schaper, Michel Simard. Discussion during the presentations is encouraged.

Note: Breakfast, coffee, lunch, and juice breaks are included in the registration fee. We will organize informal dinners, but the cost is not covered in the registration fee.