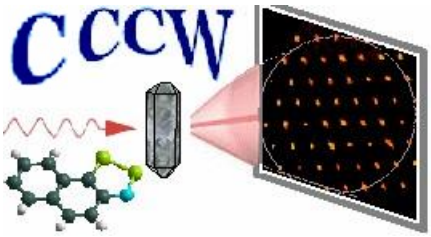

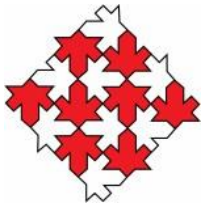

Canadian National Committee for Crystallography
http://xtallography.ca/

2021 Canadian Chemical Crystallography Workshop

August 8th – 11th, 2021

Program (Version 11 – Aug. 11, 2021)

Thank you to our sponsors!

The Canadian National Committee for Crystallography

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CCCW2021 Pre-Workshop Activities

Download and install:

1. Zoom: https://zoom.us/

For security purposes, my institutional Zoom license will not run through a browser; all participants must sign-in to their Zoom accounts to connect.

2. Cambridge Structural Database and Software: Instructions will be distributed by email.

This page consolidates all the free CSD resources in one place:
https://www.ccdc.cam.ac.uk/Community/csd-community/

3. OLEX2: https://www.olexsys.org/

You will have to register in order to download the software (for free).

4. SHELX suite of programs: http://shelx.uni-goettingen.de/register.php

You will have to register before you can go to "Downloads" to obtain the appropriate folder of programs for your operating system. Let Louise know if you need help with the answer to the skill testing question.

5. PLATON (and PLATON Windows Taskbar): https://www.chem.gla.ac.uk/~louis/software/platon/

Scroll down to near the bottom of the page where you will find two download links (Download the PLATON for Windows Taskbar and Download the PLATON executable). You will need to download both.

6. MAC users: Here is a helpful set of instructions for how to build a crystal structure analysis environment on a mac: https://mitsudo.net/en/building-a-crystal-structure-analysis-environment-on-a-mac/

Getting PLATON to work on macs is notoriously difficult. If you are unable to get this to work, we recommend following these parts of the workshop by taking notes and attempting the examples on a Windows-based lab computer later. Our instructors will still be available for questions and help after the workshop.

Recommended for review:

1. The Royal Society of Chemistry's Maths for Chemists booklet: https://edu.rsc.org/resources/maths-for-chemists-booklet/2103.article

While there will be no formal testing, there is an expectation that participants will have a working knowledge of geometric relations, trigonometry, imaginary numbers and linear algebra.

2. OLEX2 has a YouTube channel with curated playlists, including "Modeling Disorder" and "Twinning": https://www.youtube.com/channel/UCV6B2W8zlmXqkU2DbIviQow/about

While it is not required that anyone review this material ahead of time, it is very useful to anyone who wants to get a head start.

3. Louise's All-Time Favorite Crystallography Notes: Interpretation of crystal structure determinations by Huub Kooijman, available from http://www.cryst.chem.uu.nl/huub/notesweb.pdf

4. Notes on OLEX2 by Ilia A. Guzei

These are extremely practical for getting the OLEX2 software running on your laptop, especially if you are a mac user.

Program – Version 2021-08-06 (Program may be updated regularly)

All times are in EDT

Saturday, Aug. 7: Technical check-in from 12pm – 2pm EDT. Instructions will be sent by email.

	Aug. 8	Aug. 9	Aug. 10	Aug. 11	Aug. 12
10am – 11am	Last minute technical check-in (by appointment only)	One-on-one or small group discussions by appointment	One-on-one or small group discussions by appointment	One-on-one or small group discussions by appointment	No scheduled activities
11am – 12pm	L1. Introduction and What are crystals? **(J. Ritch)**	L4. Point Symmetry **(P. Boyle)**	L7. Structure Factors: Part II **(J. Ferrara)**	L10. Crystal Growth **(P. Boyle)**	One-on-one or small group discussions by appointment Drop-in office hours may be possible depending on instructor availability
12pm – 1pm	L2. Bragg's Law **(M. Katz)**	L5. Space Groups **(A. Decken)**	L8. Data collection and reduction **(B. Patrick, with comments from the gallery - P. Boyle & L. Dawe)**	L11. Absolute structure / absolute configuration determination **(T. Maris)**	
1pm – 2pm	L3. Reciprocal Space and Precession Images **(P. Boyle)**	L6. Structure Factors: Part I **(J. Ferrara)**	L9. Twinning **(J. Britten)**	L12. Crystallographic Information Framework and Validation: The cif file and checkCIF **(B. Patrick)**	
2pm - 3pm	Break/Discussions	Break/Discussions	Break/Discussions	Break/Discussions	
3-4:30pm	T1. Introduction to OLEX2 **(J. Ritch L. Dawe J. Britten)**	T3. Introduction to the CSD **(Y. Olatunji-Ojo)**	T6. Data analysis using the CSD **(Y. Olatunji-Ojo)**	T9. Laboratory Demonstration **(D. Chartrand)** (Any remaining time can be used by participants to finalize their presentations)	One-on-one or small group discussions by appointment Drop-in office hours may be possible depending on instructor availability
4:30-6pm	T2. SHELX and the SHELX .ins file structure **(F.H. Schaper)**	T4. Modeling disorder: Fixed positions **(Jamie Ritch Louise Dawe)**	T7. Twinning example 1 and review of basic structure refinement **(J. Britten P. LeMaguerès)**		
6pm – 7pm	End of Day 1	Break/Discussions	Break/Discussions	Break/Discussions	
7pm – 8pm	No scheduled activities	T5. Modeling disorder: Solvent masks **(B. Patrick)**	T8. Modeling disorder in *CRYSTALS:* Rotational disorder **(M. Katz)**	Participant Presentations	End of CCCW21

Notes:

1. L = Lecture; T = Tutorial
2. The following pages include a list of instructors and resources. Resources do not have to be reviewed ahead of time

Topic	Session instructor/leader	Additional Resources
L1. What are crystals?	Jamie Ritch	The Mystery of the Giant Crystals
L2. Bragg's Law	Mike Katz	2021 Slides Interactive Miller Planes Viewer
L3. Reciprocal Space and Precession Images	Paul Boyle	2021 Notes Additional Notes
L4. Point Symmetry	Paul Boyle	2021 Notes
L5. Space Groups	Andreas Decken	2021 Notes and Example Data Examples of Structures in $P2_1/c$ Symmetry and Space Group Tutorial by Jerry P. Jasinski and Bruce M. Foxman
L6. Structure Factors: Part I	Joe Ferrara	2021 Notes
L7. Structure Factors: Part II	Joe Ferrara	
L8. Data collection and reduction	Brian Patrick	2021 Slides
L9. Twinning	Jim Britten	2021_Lecture_Slides Ton Spek's Presentation on TwinRotMat Some PowerPoints on Twinning written by Regine Herbst-Irmer
L10. Crystal Growth	Paul Boyle	2021 Slides Crystal Growing Guides
L11. Absolute structure / absolute configuration determination	Thierry Maris	2021 Slides and Resources
L12. Crystallographic Information Framework and	Brian Patrick	2021 Lecture Slides

Validation: The cif file and checkCIF		IUCr Crystallographic Information Framework Ton Spek's Powerpoint presentations
T1. Introduction to OLEX2	Jamie Ritch Louise Dawe Jim Britten	2021 Tutorial Data_1 2021 Tutorial Data 2 Step-by-Step Example from 2018 Data for Step-by-Step Example from 2018 Working with Olex2 Playlist Notes on OLEX2 by Ilia A. Guzei
T2. SHELX and the SHELX .ins file structure	F. Hein Schaper	2021 Tutorial Data 2021 Tutorial ins Notes 2021 Tutorial lst Notes The stepwise SHELXL / XP refinement process Alphabetical list of SHELXL instructions
T3. Introduction to the CSD	Yinka Olatunji-Ojo	CCDC Introduction Videos Playlist Also Free teaching tutorials for WebCSD
T4. Modeling disorder: Fixed positions	Jamie Ritch Louise Dawe	OLEX2 Modelling Disorder Playlist Toluene across a symmetry element: Fragment instruction in OLEX2

		Data for Disorder Refinement Examples in Olex2 Slides for 2021 Tutorial Data for 2021 Tutorial
T5. Modeling disorder: Solvent masks	Brian Patrick	Using smtbx.mask in OLEX2 OLEX2 disorder across symmetry elements and a Solvent Mask PLATON SQUEEZE by Ton Spek
T6. Data analysis using the CSD	Yinka Olatunji-Ojo	Mercury How-To Videos Mercury 4.0: from visualization to analysis, design and prediction CSD-Community CSD Handouts were sent by email
T7. Twinning example 1 and review of basic structure refinement	Jim Britten Pierre LeMaguerès	OLEX2: A twinning example 2021 Tutorial Data
T8. Modeling disorder in Crystals: Rotational disorder	Mike Katz	Crystals documentation Crystals YouTube Playlist 1 Crystals YouTube Playlist 2 Crystals Program Download
T9. Laboratory Demonstration	Daniel Chartrand	

Reminder: Our instructors are available each morning for drop-in office hours, as well as all day on August 12. In addition to answering questions about the scheduled lectures and tutorials, we would like to help

you with your own problems. We can best do this if you provide us with your data ahead of time, including data collection image frames. We know that these can be large files, so please contact ldawe@wlu.ca to discuss logistics. Please note that our instructors will treat any shared data with confidentiality.

Instructors and Organizers

Paul Boyle, University of Western Ontario

Paul Boyle is the manager of the X-ray Crystallography Facility in the Department of Chemistry at University of Western Ontario (Western University). He graduated from Syracuse University where he received his BS in Chemistry. He received his Ph. D. in Inorganic Chemistry from the University of Minnesota which was followed by a post-doctoral position in the lab of Hans-Beat Bürgi at the University of Bern, in Switzerland. His first position as a professional small molecule crystallographer was at the University of New Brunswick, Fredericton. He moved to North Carolina State University to become the Director of the X-ray Crystallography Facility in the Department of Chemistry. Finally, in 2012, relocated to London, ON for his present position. His first involvement in X-ray crystallography comes from his days as an undergraduate and has been enthusiastically putting crystals in X-rays beams since that time.

Jim Britten, McMaster University

Jim Britten is the manager of the McMaster Analytical X-ray (MAX) Diffraction Facility. With the help of Vicky Jarvis, he characterizes single crystal, powder, polycrystalline solid, polymer, thin film, mineral, pharmaceutical, etc. samples for scientists and engineers. He teaches several graduate courses in X-ray diffraction and helps out with the Canadian Chemical Crystallography / Powder Diffraction / Materials Diffraction Workshops. Jim is a former Chair of the Canadian National Committee for Crystallography, former member of the Executive Council of the American Crystallographic Association, and was Program Chair for the 2014 Congress of the IUCr in Montreal. He is co-author (with Weiguang Guan) of the MAX3D reciprocal space visualization software.

Daniel Chartrand, Université de Montréal

Daniel Chartrand is a research advisor working for the of Université de Montréal's X-Ray Diffraction Laboratory since 2019. He got his first taste of crystallography during his bachelor's degree at UdeM with prof. André Beauchamp introductory course. He did his actual first measurement in Daniel Leznoff's group in 2006 where he met Michael J. Katz. Later he joined Prof Garry Hanan group at UdeM for his PhD in coordination chemistry and photocatalysis where he acted as the group crystallographer. Before joining the X-ray service team, he worked on a special project from 2015 to 2019 robotizing solar device fabrication and characterization.

Louise Dawe, Wilfrid Laurier University

Louise Dawe is an associate professor in the Department of Chemistry and Biochemistry at Wilfrid Laurier University. She is vice-chair of the Canadian National Committee for Crystallography, an elected member of the American Crystallographic Association's Communication Committee and is a member of the International Union for Crystallography Calendar Sub-Committee. She has a lot of enthusiasm for teaching and crystallography and looks forward to meeting this year's participants!

Andreas Decken, University of New Brunswick

Andreas attended the UGH Duisburg in Germany for his undergraduate degree. In 1987 he came to McMaster University for a one-year exchange but never left! First introduced to X-ray crystallography by Jim Britten during his Ph.D., also at McMaster, he went on to do a post doc at UT Texas in Austin with Allan Cowley and took over the group's diffractometer. In 1995 Andreas took up his current position at UNB as a lab instructor and crystallographer.

Joseph Ferrara, Rigaku Americas Corporation

Dr. Ferrara received both his Bachelor of Science and Doctorate degrees from Case Western Reserve University in Cleveland, Ohio. His graduate research focused on physical organometallic chemistry under Prof. Wiley C. Youngs. Upon completing his doctorate in 1988, he joined Molecular Structure Corporation, which became a subsidiary of Rigaku Corporation in 1996.

Dr. Ferrara is currently Chief Science Officer, Rigaku Americas Corp. and Vice President, X-ray Research Laboratory, Rigaku Corp. He is a member and past chair of the Scientific Advisory Board for the BioTech Institute of the Lone Star Community College System. He is the Immediate Past President of the America Crystallographic Association and the Books Editor for ACA RefleXions. He is also Secretary-Treasurer of the US National Committee for Crystallography and Treasurer of the Council of Scientific Society Presidents. He spent the last 34 years developing hardware and software tools for X-ray crystallography and X-ray imaging for the research community.

Dr. Ferrara is also a Texas State Firefighters' and Fire Marshals' Association certified firefighter and National Registry Emergency Medical Responder.

Ben Gelfand, University of Calgary

To be added soon!

Michael J. Katz, Memorial University of Newfoundland

Originally from Haifa Israel, Mike moved to Canada when he was 7 years old, and after roughly 20 years got his PhD from Simon Fraser University in Burnaby BC under the supervision of Daniel Leznoff. As an undergraduate and graduate student, Mike worked on coordination polymers. The first diffractometer that he used was a Nonius diffractometer with a point detector. It took a week to collect his first data set, but by the time that week was over, Mike was sold on crystallography. It was during this time that he met Brian Patrick, Joseph Ferrara, and Lee Daniels (yes, it is a very small world). Mike was a postdoc at Northwestern University just outside of Chicago Illinois (Go Cubs!), which is where he first met Amy Sarjeant, who introduced Mike to Louise Dawe. Mike worked for Professors Hupp and Farha on Metal-Organic Frameworks, and solar energy conversion. In 2015, Mike moved back to Canada to start his independent career at Memorial University working on Metal-Organic Frameworks. Mike has always maintained his crystallography skills during these times. X-ray diffraction is a logical puzzle, and, as Fred Einstein once told him, if the data was worth collecting, then the structure is worth solving.

Pierre LeMaguerès, Rigaku Americas Corporation

Dr. Pierre Le Magueres obtained a Ph.D. in physical chemistry and small molecule crystallography at the University of Rennes (France) in 1995, working under Dr. Lahcene Ouahab on the synthesis and analysis of molecular materials combining inorganic polyoxometalates and organic cation radicals based on tetrathiofulvalene derivatives. From 1996 to 2000, Dr. Le Magueres worked as a postdoctoral researcher with renowned Prof. Jay Kochi at the University of Houston, where he pursued his work on the synthesis and X-ray characterization of air-sensitive cation radicals and charge transfer complexes. In 2000, deciding to broaden his horizons and learn protein crystallography, Dr. Le Magueres joined the biochemistry department at the University of Houston and worked as a postdoctoral researcher with Prof. Kurt Krause on the design and X-ray characterization of potential new inhibitors for alanine racemase, a protein essential for the growth of infectious diseases such as tuberculosis.

Dr. Le Magueres was hired in 2004 as a protein crystallographer in the Life Sciences department at Rigaku. After 14 years in protein crystallography, he shifted to a position as a small molecule crystallographer at Rigaku Americas Corporation in The Woodlands, TX. While still helping with protein crystallography if needed, Dr Le Magueres' duties are now centered on the analysis of small molecule samples and the development of hardware and software products at Rigaku for small molecule crystallography.

Thierry Maris, Université de Montréal

Thierry Maris was born in France and received his Ph.D. in Physical Chemistry at the Université de Bordeaux in 1996. After a short period at the University of Amsterdam to perform some molecular modelling simulations, he spent two year as a Marie Skłodowska-Curie Postdoctoral Fellow at the Chemical Crystallography Laboratory of Oxford University to study inclusion complexes. Then in 2000, he moved to the Université de Montréal as a post-doctoral fellow to study complex molecular porous materials in Prof. James D. Wuest group, before being hired as a research assistant and manager of the X-ray diffraction facilities.

Yinka Olatunji-Ojo, Cambridge Crystallographic Data Centre

To be added soon!

Brian Patrick, University of British Columbia

I am originally from St. Eustache, QC, just outside of Montreal. I attended the University of Waterloo for my undergraduate degree (B.Sc. '92), then moved west to do my Ph.D. under Jim Trotter at UBC. After graduating in '97, I post-doc'd for Carol Brock for a year at the University of Kentucky before returning to UBC in 1999 when I became the manager of the Chemistry department's Structural Chemistry Facility.

Jamie Ritch, University of Winnipeg

Jamie Ritch received his B.Sc. (Hons) and Ph.D. degrees from the University of Calgary. After a post-doctoral position at the University of Lethbridge, he joined the University of Winnipeg as an Assistant Professor in 2011. Since 2015 he is an Associate Professor. His research focuses on the synthetic main group chemistry and the coordination of heavy chalcogen ligands to transition metals. He has a long-standing interest in small molecule crystallography, having solved his own structures since 2005. He is also the MB/SK regional judge for the Chemical Institute of Canada's annual Crystal Growing Competition.

Frank Hein Schaper, Université de Montréal

Frank (Hein) Schaper is Associate Professor in Inorganic Chemistry at the Université de Montréal. Like many inorganic chemists, he started doing X-ray crystallography doing his Ph. D. with H.-H. Brintzinger in Germany, where he determined X-ray structures for his and his group mates research projects. Since then single crystal X-ray crystallography is by far his most favourite analytic technique. He is teaching B. Sc. level and graduate level crystallography classes at UdeM.