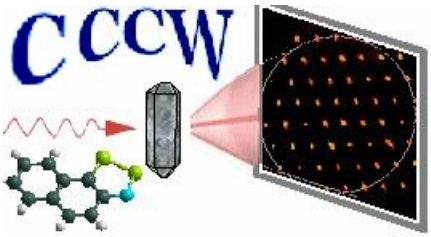
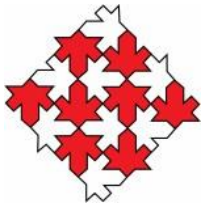




Canadian National Committee for Crystallography
http://xtallography.ca/

2023 Canadian Chemical Crystallography Workshop

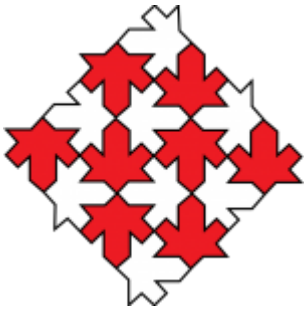
May 30th – June 3rd, 2023

Program

(Version 14 – 2023-06-19)

Contents

Thank you to our sponsors!



The Canadian National Committee for Crystallography

BRUKER

CCDC
advancing structural science

Rigaku

MERCK

Supporting Institutions

Campus Map

★ Indicates **Room D300** in Chemistry

Indicates where an ambassador will be waiting on the first morning.

Practical Considerations

1. Website: Our website is updated regularly, so please keep checking back for program updates and answers to questions.

2. Location: Our workshop room is D300 of the Chemistry Building. This is indicated on the map on the previous page, and is also marked on this Google map: https://goo.gl/maps/yUahfjWiNSs1N33s8

> A CCCW23 "ambassador" will be waiting outside the Chemistry Building on the Main Mall side from 8:30 – 8:55 am on May 30 to help you find your way to our workshop room. If you get lost, please call the UBC X-ray lab at (604) 822-4865.

3. COVID-19 and Masking: Masks are no longer required on UBC campuses. If you are unwell after the workshop has started, please contact the organizers for possible alternative arrangements. It is important that we continue to ensure that other instructors and attendees can fully participate in CCCW23 and subsequent activities (ex. Canadian Society for Chemistry Conference or further travels).

4. Parking and Buses: Due to convocation week at UBC, several parking lots and bus stops are closed. These are indicated with "X" on the previous page. Parking lots that remain open have been circled. More information on parking can be found here. More information on public transit can be found here.

5. Wifi: For academic participants, Eduroam is available. For those affiliated with institutions that do not support Eduroam, a ubcvisitor Wireless Network is available.

6. Meals: Attendees are responsible for their own meals. Local ambassadors will be able to make recommendations for lunch and dinner locations.

7. Networking Night: Thanks to the generous support of Bruker, all attendees and instructors are invited to a group dinner at Gallery Patio & Lounge.

8. Samples: Participants are welcome to bring samples. Please contact Louise and Brian if you would like to schedule time for single crystal data collection.

9. Home-lab problems: Workshop instructors 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 file/folders, so please contact Louise to discuss logistics. Please note that our instructors will treat any shared data with confidentiality.

10. Participant Presentations: All participants are asked to prepare a short (five slides minimum; five minutes maximum) presentation about something that they learned during the workshop. Presentations will take place on Saturday, June 3. Please consider these presentations to be a celebration of knowledge; the intent is for everyone (participants and instructors) to reflect on learning and growth. For participants, a final presentation is required for a letter of completion to be issued.

CCCW2023 Pre-Workshop Activities

Download and install:

1. Cambridge Structural Database and Software: Download instructions were distributed by email.

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

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

You will have to register in order to download the software (for free). Even if you already have OLEX2 installed on your computer, please upgrade to OLEX2-1.5 or Olex2-1.5alpha. Either version will work.

MAC users, please see the bottom of this page for helpful installation resources.

3. 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.

4. 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.

5. Highly recommended: ORCA 5.0.3 https://orcaforum.kofo.mpg.de/index.php

ORCA is an ab initio quantum chemistry program package. We will be using this during our NoSphereA2 tutorial. NoSphereA2 is part of OLEX2 which comes with a built-in package that will be sufficient for our tutorial, but anyone who is interested using NoSphereA2 after CCCW22 is advised to download and install ORCA. This will first require that you (1) register for an account; (2) log in; and (3) go to "Downloads", found at the top left corner after login.

ORCA users on Windows require OpenMPI (from Microsoft). Very clear instructions are given at:
https://www.olexsys.org/olex2/docs/nosphera2/faq/nosphera2_orca/

MAC users: Our CCCW23 instructor, Andreas Decken, has prepared step-by-step installation instructions for the most recent version of OLEX2! These can be downloaded as a DOCX document here.

Here is a different set of instructions for how to build 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 – (Updated 2023-06-1)

All times are in PDT

	Tuesday, May 30	Wednesday, May 31	Thursday, June 1	Friday, June 2	Saturday, June 3
9 – 10 am	Last minute technical check-in and Welcome **(Decken/Dawe)**	L4. Space Groups **(A. Decken)**	L7. Structure Factors: Part II **(L. Daniels)**	T5. NoSphereA2 **(R. Boeré)**	L12. Absolute structure / absolute configuration determination **(K. Marczenko)**
10 – 11 am	L1. Crystal Growth **(P. Boyle)**	L5. Reciprocal Space and Precession Images **(P. Boyle)**	L8. Data collection and reduction **(B. Patrick)**		L13. High Pressure: Crystallography and Synchrotrons **(C. Beavers)**
11 – 11:15 am	Short Break	Short Break	Short Break	Short Break	Short Break (30 minutes)
11:15 am – 12:15 pm	L2. Bragg's Law and Miller Indices **(K. Marczenko)**	L6. Structure Factors: Part I **(L. Daniels)**	T4. Modeling disorder: Fixed positions and fragment libraries Extended time for extra practice and OLEX2 Q&A **(I. Guzei)**	L10. Twinning **(J. Britten)**	T6. Modeling disorder: Solvent masks **(L. Dawe)** and L11. Crystallographic Information Framework and Validation: The cif file and checkCIF **(B. Patrick)**
12:15 – 1:15 pm	L3. Point Symmetry **(P. Boyle)**	T2. Introduction to the CSD **(Y. Olatunji-Ojo)**		T7. Data analysis using the CSD **(Y. Olatunji-Ojo)**	Break
1:15 – 2:30 pm	Break	Break	Break	Break	Participant Presentations
2:30 – 4pm	T1. Introduction to OLEX2 **(I. Guzei)**	Group work and one-on-one discussions using home or supplied data	L9 (Virtual). SHELX and the SHELX .ins file structure **(F.H. Schaper)**	Group work and one-on-one discussions using home or supplied data	
4 – 5:30pm	Group work and one-on-one discussions using home or supplied data	T3. Data collection and reduction demonstration 1 **(M. Ruf)**		T8. Data collection and reduction demonstration 2 (Twinning) **(Beavers/Daniels)**	Formal End of Workshop
5:30	Formal End of Day	**Networking Night sponsored by Bruker (Start time ~6 pm)**	T5.5 Crystal Growth **(I. Guzei)**	T8.5 Max3D **(J. Britten)**	

Notes:

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

Program Details

Topic	Session instructor/leader	Additional Resources (Will be updated regularly throughout the workshop)
Pre-Workshop Information	Jamie Ritch	*Maybe coming soon!*
L1. Crystal Growth	Paul Boyle	2022 Slides Crystal Growing Guides
L2. Bragg's Law and Miller Indices	Kate Marczenko	2023 Slides Interactive Miller Planes Viewer
L3. Point Symmetry	Paul Boyle	2022 Notes
L4. Space Groups	Andreas Decken	2023 Notes 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
L5. Reciprocal Space and Precession Images	Paul Boyle	2022 Lecture Slides Additional Notes
L6. Structure Factors: Part I	Lee Daniels	2022 Notes
L7. Structure Factors: Part II	Lee Daniels	
L8. Data collection and reduction	Brian Patrick	2022 Slides
L9. SHELX and the SHELX .ins file structure	F. Hein Schaper	2022 Tutorial ins Notes 2022 Tutorial lst Notes 2021 Tutorial Data The stepwise SHELXL / XP refinement process Alphabetical list of SHELXL instructions

L10. Twinning	Jim Britten	2023_Lecture_Slides Twin_introduction_Regine_Herbst-Irmer Twinpseudomero_Regine_Herbst-Irmer Ton Spek's Presentation on TwinRotMat
L11. Crystallographic Information Framework and Validation: The CIF file and checkCIF	Brian Patrick	2023 Lecture Slides IUCr Crystallographic Information Framework Ton Spek's Powerpoint presentations
L12. Absolute structure / absolute configuration determination	Kate Marczenko	2023 Slides
L13. High Pressure: Crystallography and Synchrotrons	Christine Beavers	A night at the beamline | Careers | Chemistry World Dropbox link to talk slides
T1. Introduction to OLEX2	Ilia Guzei	Notes on OLEX2 by Ilia A. Guzei Crystallographic problems
T2. Introduction to the CSD	Yinka Olatunji-Ojo	2023 Slides and Worksheets will be sent by email CCDC Introduction Videos Playlist Also Free teaching tutorials for WebCSD
T3. Data collection and reduction demonstration 1	Michael Ruf	
T4. Modeling disorder: Fixed positions	Ilia Guzei	Notes on OLEX2 by Ilia A. Guzei Crystallographic problems

T5. NoSphereA2	René Boeré	2023 Slides 2023 Tutorial Data
T5.5 Crystal Growth	Ilia Guzei	
T6. Modeling disorder: Solvent masks	Louise Dawe	2023 Slides 2023 Data Using smtbx.mask in OLEX2 OLEX2 disorder across symmetry elements and a Solvent Mask PLATON SQUEEZE by Ton Spek
T7. Data analysis using the CSD	Yinka Olatunji-Ojo	2023 Slides and Worksheets will be sent by email The Cambridge Crystallographic Data Centre's YouTube channel for teaching resources and Webinars. Mercury 4.0: from visualization to analysis, design and prediction CSD-Community DECOR (online resource for borrowing and sharing educational resources on crystallography)
T8. Data collection and reduction demonstration 2 (Twinning)	Christine Beavers/Lee Daniels	2023 Slides For access to 2023 data, please contact the presenters or the workshop organizer (file size is very large, so logistics will need to be discussed!)
T8.5 Max3D	Jim Britten	Max3D Slides (PDF; for PPTX, please contact Jim Britten) Max3D software for academic users

Instructors and Organizers

Christine Beavers, Rigaku Americas Corporation
Biography to be added soon!

René Boeré, University of Lethbridge

René Boeré was educated in Canada first at Dalhousie University in Halifax (BSc Hon) where an inspirational professor of inorganic chemistry was Stan Cameron, also a passionate crystallographer. Continuing to the PhD at University of Western Ontario, he learned crystallography painstakingly under the tutelage of Prof. Nick Payne (Picker serial diffractometer; Control Data Corp. mainframe refinement…) As a PDF at University of Guelph, he continued some crystallography with George Fergusson, although most of his structures were determined by the incomparable Wally Cordes at the U. of Arkansas. His academic career has been at the University of Lethbridge in Alberta (1988-) where he is currently Professor of Chemistry. He co-manages the Rigaku SuperNova/Pilatus instrument, trains small molecule crystallographers on the instrument, and regularly teaches an advanced course in Chemical Crystallography including hands-on tutorials on theory and practice of small molecule crystal structure determination.

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.

Mohammad T. Chaudhry, Merck

Mohammad (Mo) Chaudhry is a post-doctoral fellow at Merck & Co (2023). Currently he is exploring the use of metal-organic frameworks and other systems to encapsulate bioactive compounds to determine their structure though small molecule crystallography and microcrystal electron diffraction. Prior to Merck, Mo completed his PhD at the University of British Columbia (2022) under the supervision of Mark MacLachlan. He learned crystallography from Brian Patrick (UBC) and was a previous participant in the CCCW.

Lee Daniels, Rigaku Americas Corporation
Biography to be added soon!

Louise Dawe, Wilfrid Laurier University

Louise Dawe is an associate professor in the Department of Chemistry and Biochemistry at Wilfrid Laurier University. She is chair of the Canadian National Committee for Crystallography, a member of the International Union for Crystallography (IUCr) Meeting Sub-Committee, and co-chair of the International Program Committee for the 2026 IUCr Congress and General Assembly. She is also a co-editor with the IUCr journal, Acta Cryst C., and a teaching and education editor with the IUCr Journal of Applied Crystallography. She has been organizing the CCCW since 2019 and has a lot of enthusiasm for teaching and crystallography! She 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.

Ilia Guzei, University of Wisconsin-Madison

Dr. Ilia Guzei has been working in the field of crystallography since 1992 and is currently a Distinguished scientist and Director of X-ray Crystallography at the Department of Chemistry at the University of Wisconsin-Madison. He has been a member of the US National Committee for Crystallography, Treasurer of the American Crystallographic Association (ACA) and of the American Chemical Society Wisconsin Local section, served a poster session chair, session organizer, and meeting co-chair at numerous ACA meetings, and organized workshops at ACA and International Union of Crystallography conferences. He developed an Idealized Molecular Geometry Library for problematic structural refinements, assembled a free collection of teaching structures illustrating various crystallographic challenges, and created Notes on OLEX2, a very popular crystallographic software suite.

Katherine Marczenko, University of Guelph

Katherine (Kate) Marczenko is the manager of the X-ray Facility (X-LAB) in the Department of Chemistry at the University of Guelph. She received her M.Sc. in Noble-Gas Chemistry from McMaster University, and a Ph.D. from Dalhousie University in Main-Group Chemistry. Kate was first exposed to SCXRD on "Molly" (Jim Britten's Bruker Smart Apex II molybdenum source instrument) and has been affectionately naming her instruments ever since. When Kate is not running or maintaining "Panda" (Panalytical Empyrean Powder X-ray Diffractometer), "SuperNova" (Rigaku SuperNova Single-Crystal X-ray Diffractometer), or "Zeus" (Panalytical Zetium X-ray Fluorescence Spectrometer), she is teaching chemistry and looking for new ways to incorporate diffraction techniques into the undergraduate chemistry curriculum. Kate will be starting a new role (mid-workshop!) as Assistant Professor of Chemistry at Carleton University. Her research program will focus on the intersection of energetic materials, main-group chemistry, and crystallography.

Yinka Olatunji-Ojo, Cambridge Crystallographic Data Centre

Yinka is a user support scientist and part of the education and outreach team at the CCDC. She received her Bachelor of Science in Chemistry from Texas Southern University and her Ph.D. in Computational Inorganic Chemistry from the University of North Texas. After a couple of years of being a postdoc and a brief stint at a medical device startup, she joined the CCDC. Yinka is passionate about scientific education and outreach to the broader public.

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.

Jefferson Pells, Simon Fraser University

Jefferson (Jeff) Pells completed his B.Sc. at the University of Calgary, with his undergraduate research focused on organic photovoltaics. He is currently a PhD candidate in the Leznoff group at Simon Fraser University, working on tuning the luminescence originating from gold(I) dithiolate supramolecular complexes. It was during his graduate degree that he was able to gain first-hand experience with X-ray crystallography, and some years later, is now responsible for the maintenance and training of users for the single crystal diffractometer at SFU. His first CCCW experience was in 2018 and is looking forward to returning to it in 2023!

Michael Ruf, Bruker AXS

Michael is a Senior Manager with Bruker and has held various positions in Applications, Engineering and Product Management. He likes interacting with customers even more than crystallography and enjoys teaching and training whenever time allows. Michael received his formal education in Freiburg, Germany where he was introduced to crystallography in the late 80s. After a postdoc in Boulder, Colorado he joined Bruker in Karlsruhe in 1998 and was transferred to the Madison, Wisconsin office in 2000.

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.