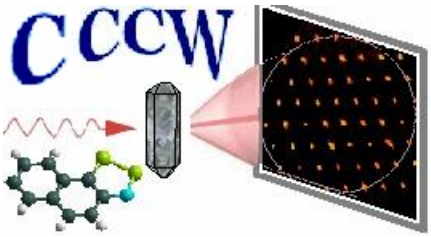

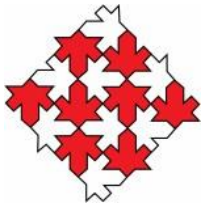

Canadian National Committee for Crystallography
http://xtallography.ca/

2025 Canadian Chemical Crystallography Workshop

June 20th – 24th, 2025

Program

(Version 4 – 2025-06-19)

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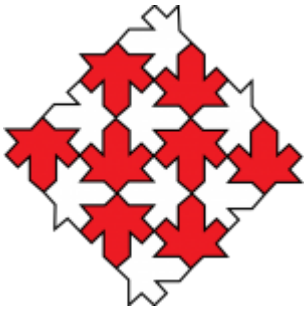
Thank you to our sponsors!



The Canadian National Committee for Crystallography

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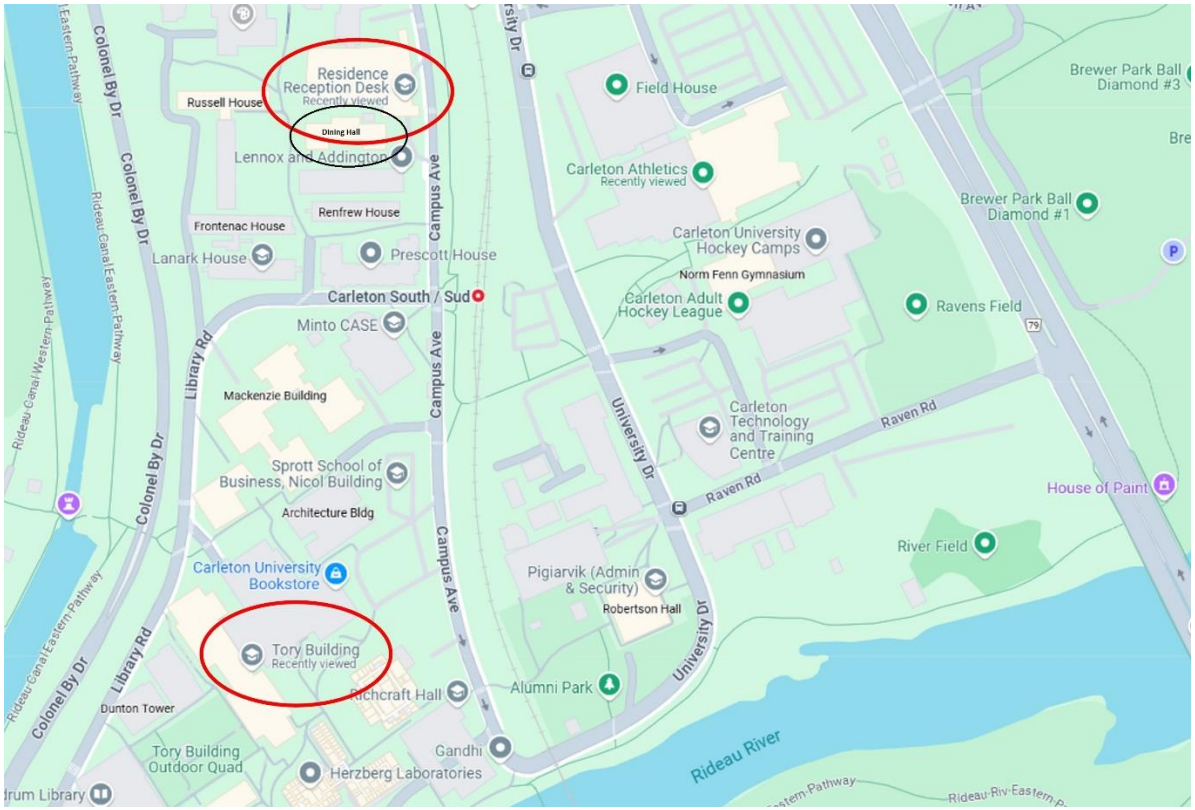
Supporting Institutions

Campus Map



The workshop will be taking place in Tory Building Room 213.

More details about this room can be found here.

Practical Considerations

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

2. Location: The workshop location will be Carleton University's Tory Building Room 213. The Tory Building is searchable on Google Maps.

3. Wifi: For academic participants, Eduroam is available. If your local institution does not support Eduroam access, guest wifi information will be available on-site.

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

The Teraanga Commons Dining Hall is open for walk-ins!

Breakfast (7 – 9 AM): $12.25 (+ tax)
Lunch (11 AM – 2 PM): $14.95 (+ tax)
Dinner (4:30 – 7 PM): $17.50 (+ tax)

5. Networking Night: Thanks to the generous support of Bruker, all attendees and instructors are invited to a group dinner. This will take place starting at approximately 6 PM on Saturday, June 21. Details about location will be shared during the workshop.

7. 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. Please note that our instructors will treat any shared data with confidentiality.

8. Participant Presentations: All participants are asked to prepare a short (five slides and five minutes maximum) presentation about something that they learned during the workshop. Presentations will take place on Tuesday, June 24. 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.

9. Intellectual Property and Lecture Recording: The educational materials developed for this course, including, but not limited to, lecture notes and slides, handout materials, and any materials linked in the program are the intellectual property of the course instructors or others who have been noted. These materials have been developed for student use only and they are not intended for wider dissemination and/or communication. Posting or providing unauthorized audio, video, or textual material of course content to third-party websites violates instructors' intellectual property rights, and the Canadian Copyright Act. Recording lectures in any way is prohibited in this course unless specific permission has been granted by instructors. (Policies based on guidelines from Wilfrid Laurier University.)

CCCW2025 Pre-Workshop Activities

Download and install:

1. Cambridge Structural Database and Software: Download 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/

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 ensure that you are running the latest version (OLEX2-1.5)

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. Increasingly, these tools are not compatible with MAC systems.

5. CrystalExplorer: https://crystalexplorer.net/download/

The CrystalExplorer tutorial will be done using CrystalExplorer21 on a Windows computer. There are versions available at the above link for Win10 (probably OK on Win11 but I have not yet proven this), MacOS, Ubunto and CentOS (two Unix versions).

The website states 'a license key is no longer required' but that is not the case. Immediately on opening the program, users need to enter the user name and key. These are supplied on their:
https://crystalexplorer.net/licence/

Just type 'user' and copy-paste the license code listed there.

We will only be working with the built-in Tonto software. Further details will be included during the tutorial.

6. Highly recommended: ORCA (latest version is 6.0.1) 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 CCCW 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). Instructions are given at:
https://www.olexsys.org/olex2/docs/nosphera2/faq/nosphera2_orca/

MAC users: Our CCCW25 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. There are also new instructions contained in these notes on how to install ORCA6 and Microsoft MPI.

Program

All times are Ottawa (EDT) local time

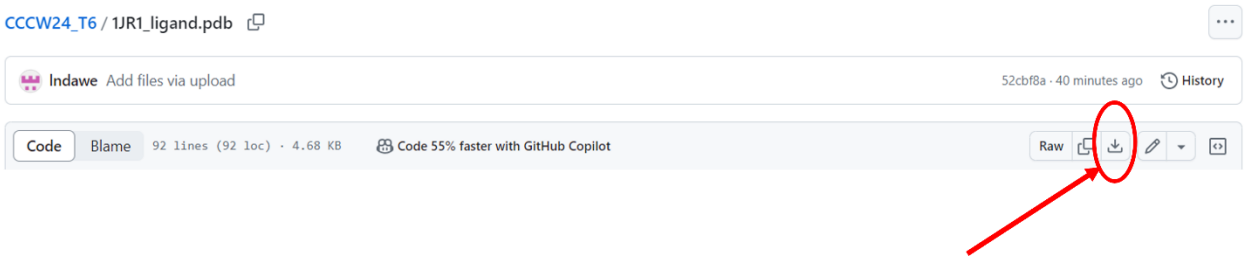
	Friday, June 20	Saturday, June 21	Sunday, June 22	Monday, June 23	Tuesday, June 24
8:15 – 9 am	Technical check-in **(L. Dawe and A. Decken)**	One-on-one discussions	One-on-one discussions	One-on-one discussions	One-on-one discussions
9 – 10 am	L1. Introduction to Crystals, Crystallography, and Crystal Growth **(L. Dawe)**	T1. Introduction to OLEX2 and Modeling disorder: Solvent masks **(L. Watanabe and L. Dawe)**	L8. Absolute structure / absolute configuration determination **(C. Beavers)**	T4. Introduction to CrystalExplorer and Hirshfeld surface analysis **(R. Boeré)**	L11. Crystallographic Information Framework and Validation: The cif file and checkCIF **(B. Patrick)**
10 – 11 am	L2. Bragg's Law, Miller Indices, Point Symmetry and Space Groups – Part 1 **(A. Decken with support from B. Patrick)**		L9. Twinning **(A. Schmidt)**		Group work and one-on-one discussions using home or supplied data
11 – 11:15 am	Short Break	Short Break	Short Break	Short Break	
11:15 am – 12:15 pm	L3. Bragg's Law, Miller Indices, Point Symmetry and Space Groups – Part 1 **(A. Decken with support from B. Patrick)**	L6. Reciprocal Space and Precession Images **(A. Schmidt)**	T3. Modeling disorder: Fixed positions and fragment libraries; and Extended time for extra practice and OLEX2 Q&A **(L. Watanabe + Other Instructors)** **Recommended end time is 1:15 PM**	T5. Introduction to the CSD and Data analysis using the CSD **(Y. Olatunji-Ojo)** **Recommended end time is 1:15 PM**	
12:15 – 1:30 pm	Break	Break			Break
1:30 – 2:30 pm	L4. Structure Factors **(C. Beavers)**	L7. Data collection and reduction **(B. Patrick)**	Break	Break	L12. High Pressure: Crystallography and Synchrotrons **(C. Beavers)**
2:30 – 4pm	L5 (Virtual). SHELX and the SHELX .ins file structure - **(2 hours; F.H. Schaper)**	T2. NoSphereA2 **(R. Boeré)**	L10. Introduction to Crystal Structure Prediction **(A. Mayo)**	Group work and one-on-one discussions using home or supplied data	Participant Presentations (2:30 – 4:30 pm)
4 – 5:30pm	D1. Data collection and reduction demonstration 1 **(1 hour; A. Schmidt)**		D2: ShelxLe Demonstration **(A. Schmidt)**	D3. Data collection and reduction demonstration 2 (Twinning) **(C. Beavers)**	Formal End of Workshop
	Formal End of Day	Short Break	Formal End of Day	Formal End of Day	
		Networking Night sponsored by Bruker (Start time ~6 pm)			

Notes:

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

Program Details – Links will be updated throughout the workshop

- Some links will require an extra step for you to initiate the download. To do this, click on the download button, as shown below.



Topic	Session instructor/leader	Additional Resources (Will be updated regularly throughout the workshop)
L1. Introduction to Crystals, Crystallography, and Crystal Growth	Louise Dawe	2024 Crystal Growing Slides 2022 Slides Crystal Growing Guides
L2. Bragg's Law, Miller Indices, Point Symmetry and Space Groups – Part 1	Andreas Decken	2024 Slides Interactive Miller Planes Viewer
L3. Bragg's Law, Miller Indices, Point Symmetry and Space Groups – Part 2	Andreas Decken	2024 Slides 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
L4. Structure Factors	Christine Beavers	2024 Slides
L5. 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
L6. Reciprocal Space and Precession Images	Ashley Schmidt	2022 Lecture Slides Additional Notes
L7. Data collection and reduction	Brian Patrick	2022 Slides
L8. Absolute structure / absolute configuration determination	Christine Beavers	2023 Slides
L9. Twinning	Ashley Schmidt	2024 Lecture Slides 2024 Twinning Data Twin_introduction_Regine_Herbst-Irmer Twinpseudomero_Regine_Herbst-Irmer Ton Spek's Presentation on TwinRotMat
L10. Introduction to Crystal Structure Prediction	Alex Mayo	
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. High Pressure: Crystallography and Synchrotrons	Christine Beavers	A night at the beamline | Careers | Chemistry World Dropbox link to talk slides
T1. Introduction to OLEX2 and Modeling disorder: Solvent masks	Louise Dawe and Lara Watanabe	2024 Tutorial Slides – Part 1 2024 Tutorial Data – Part 1 2024 Tutorial Slides – Part 2

		2024 Tutorial Data – Part 2 Using smtbx.mask in OLEX2 OLEX2 disorder across symmetry elements and a Solvent Mask PLATON SQUEEZE by Ton Spek Notes on OLEX2 by Ilia A. Guzei Crystallographic problems
T2. NoSphereA2	René Boeré	2024 Slides 2024 Tutorial Data
T3. Modeling disorder: Fixed positions and fragment libraries	Lara Watanabe	2024 Tutorial Slides 2024 Tutorial Data Notes on OLEX2 by Ilia A. Guzei Crystallographic problems
T4. Introduction to CrystalExplorer and Hirshfeld surface analysis	René Boeré	
T5. Introduction to the CSD and Data analysis using the CSD	Yinka Olatunji-Ojo	2025 worksheets were sent by email. Other resources: CCDC Introduction Videos Playlist Free teaching tutorials for WebCSD This is a link to a ligand structure for use in the tutorial. Workshop materials for ConQuest and Mercury: CSD-Core workshop materials Other resources:

		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)
D1. Data collection and reduction demonstration 1	Ashley Schmidt	
D2: ShelxLe Demonstration	Ashley Schmidt	A 2025 folder was sent by email
D3. Data collection and reduction demonstration 2 (Twinning)	Christine Beavers	2023 Slides
Group work and one-on-one discussions using home or supplied data	Supplied Data	C4H12NReO3F2 Crystallographic problems Li_2 and Structure Factors

Instructors and Organizers

Christine Beavers, Rigaku Americas Corporation

Christine received both her B.S. in Chemistry and her Ph.D in Analytical Chemistry at the University of California, Davis, with the latter supervised by Professor Marilyn Olmstead and co-supervised by Professor Alan Balch. During her Ph.D., Christine was informed that her weakly diffracting samples would benefit from high-intensity synchrotron X-rays, and since first seeing this light, she has remained heavily involved in synchrotron experimentation. She did her postdoc at the Advanced Light Source on the chemical crystallography beamline 11.3.1 and remained at the ALS to work with COMPRES (the COnsortium for Materials Properties Research in Earth Science) on beamline 12.2.2. In 2018, she accepted a position at Diamond Light Source as the Principal Beamline Scientist on I15, the extreme conditions beamline. After four years abroad, she was excited to join Rigaku Americas and return home to California. After a year and a bit in Sales, she became the Synchrotron Business Development Manager for Rigaku Corporation; her focus lies in reaching out to facilities around the world and discussing the cutting edge of X-ray detector technology. When she isn't sharing her cool toys with beamlines around the world, she enjoys riding her horses, reading, writing, and playing video games.

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 now Professor Emeritus of Chemistry. He co-manages the Rigaku SuperNova/Pilatus instrument, trains small molecule crystallographers on the instrument, and has taught an advanced course in Chemical Crystallography including hands-on tutorials on theory and practice of small molecule crystal structure determination.

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. (Jim is available for remote consultation in 2025.)

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 section (main) editor with the IUCr journal, Acta Cryst B., 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.

Roberto Diaz-Rodriguez, University of Ottawa

To be added

Alex Mayo, XtalPi

Alex is a business development manager for XtalPi, a technology company built on crystal structure prediction that now provides various research services in the materials and pharmaceutical industries. He previously spent 3 years working as a Scientist at SSPI in Halifax, NS, and his academic history includes a post-doc at UOttawa (Prof. Tom Woo), PhD at Dalhousie (Prof. Erin Johnson), and MSc at UofGuelph (Prof. Kathryn Preuss). His research interests are centred around molecular solid state chemistry and using tools such as crystallography and CSP to understand the structure-property relationships of materials.

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.

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.

Ashley Schmidt, Bruker AXS

Dr. Ashley Schmidt received her B.S. in Environmental Chemistry from Duquesne University in Pittsburgh, PA, where she developed a keen interest in crystallography under the guidance of her research advisor Jennifer Aitken. Dr. Schmidt then pursued her Ph.D. in Inorganic Chemistry at the University of Texas at Dallas, where she encountered and solved numerous difficult crystallographic problems while studying rare earth intermetallics with Julia Chan. During her doctoral studies, she spent four months at the Advanced Photon Source, where she worked with Saul Lapidus at the high-resolution powder diffraction beam line, 11-BM. After completing her Ph.D., Dr. Schmidt did her postdoctoral work at Los Alamos National Laboratory, where she worked on Uranium-based superconductors and other low dimensional materials. As an Applications Scientist in the Single Crystal X-Ray Diffraction division at Bruker, Dr. Schmidt is dedicated to sharing her expertise in crystallography to train and educate.

Lara Watanabe, University of Guelph

Dr. Lara Watanabe is originally from Nova Scotia, but obtained her BSc from Mount Allison University in Chemistry working on main group molecules. She then moved to Windsor, ON to pursue graduate studies and began to learn crystallography. She graduated with her PhD in 2022 and then took up a post at Carleton University as a postdoctoral research associate learning atomic layer deposition and synthesizing inorganic precursors. During this time she continued her passion for crystallography by becoming the group crystallographer for the Barry group, until she moved to her current role as at the University of Guelph as Crystallographer and Teaching Lecturer. She has been in this role since May 2024, and looks forward to being part of the CCCW instructors as she was a former participant as a graduate student.