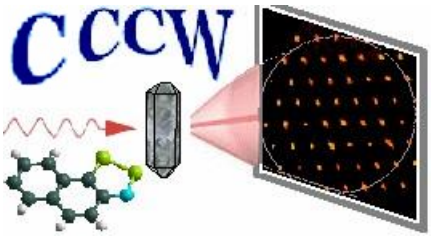

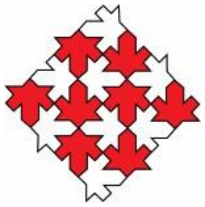

Canadian National Committee for Crystallography
http://xtallography.ca/

2022 Canadian Chemical Crystallography Workshop

June 9th – 12th, 2022

Program (Version 11 – Final)

Contents

Thank you to our sponsors!

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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 EEEL445 (EEEL = Energy Environment Experiential Learning).EEEL is a lone glass building on the north side of the main campus. https://goo.gl/maps/m2YFpBZUS2uh9LSw7

> A CCCW22 "ambassador" will be in Lot 20 from 8 – 8:50 am on June 9 to help you find your way to our workshop room.

3. COVID-19 and Masking: Masks are no longer required on University Calgary campuses, starting May 1. Any updates to venue policy will be found here.

> **Masks are still strongly recommended for use on campus, and we are asking all participants of CCCW22 to please wear a mask while in our workshop room.** Wearing a mask will help ensure that all attendees can fully participate in CCCW22, and subsequent activities (ex. CCCE or further travels).

4. Parking: the EEEL building is located at 750 Campus Drive NW. There are two convenient public parking lots available close to EEEL, one directly beside EEEL building and one just across the street, Lot 21. (Lot 21 may be cheaper.)

5. Wifi: For academic participants, Eduroam is available. For those affiliated with institutions that do not support Eduroam, AirUC-Guest, can be accessed.

6. Meals: Attendees are responsible for their own meals. There is a food court and other services available in MacEwan Student Centre. This is a link to a map from our workshop location to the Student Centre.

7. Pub Night: Thanks to the generous support of Bruker, all attendees and instructors are invited to a group dinner at Last Defence Lounge. Alberta does not currently have any capacity limits, or other COVID restrictions associated with dining, and so space has been reserved inside the pub, adjacent to the door which leads to their patio. The full outdoor patio has also been reserved for our event.

8. Samples: Thanks to the generous support of Rigaku, an XtaLAB mini II benchtop diffractometer will be available for room temperature data collections throughout the workshop. Participants are welcome to bring samples. Please contact Louise 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 minutes maximum) presentation about something that they learned during the workshop. Presentations will take place from 7-8:30pm on Sunday, June 12. Please consider these presentations to be a celebration of knowledge; the intent is for everyone (participants and instructors) to reflect on learning and growth.

CCCW2022 Pre-Workshop Activities

Download and install:

1. 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/

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 version 1.5-alpha.

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.

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 1 (2022-05-27; program may be updated regularly)
All times are in MDT

	June 9	June 10	June 11	June 12
9 – 10 am	Last minute technical check-in	One-on-one or small group discussions	One-on-one or small group discussions	One-on-one or small group discussions
10 – 11 am	L1. Introductions and An Intro to Crystals and Crystallography **(J. Ritch)**	L4. Point Symmetry **(P. Boyle)**	L7. Structure Factors: Part II **(J. Ferrara)**	L10. Crystallographic Information Framework and Validation: The cif file and checkCIF **(B. Patrick)**
11 am – 12 pm	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 **(K. Marczenko)**
12 – 12:15 pm	Short Break/ Catch-Up	Short Break/ Catch-Up	Short Break/ Catch-Up	Short Break/ Catch-Up
12:15 – 1:15 pm	L3. Reciprocal Space and Precession Images **(P. Boyle)**	L6. Structure Factors: Part I **(J. Ferrara)**	L9. Twinning **(J. Britten)**	L12. Crystal Growth **(P. Boyle)**
1:15 – 2:30 pm	Break/Discussions	Break/Discussions	Break/Discussions	Break/Discussions
2:30 – 4pm	T1. Introduction to OLEX2 **(J. Ritch L. Dawe)**	T4. Modeling disorder: Fixed positions **(J. Ritch K. Marczenko)**	T6. Modeling disorder: Solvent masks **(B. Patrick)**	T9. Data collection and reduction demonstration 2 (Twinning) **(E. Rheinheimer)**
4 – 5:30pm	T2 (Virtual). SHELX and the SHELX .ins file structure **(F.H. Schaper)**	T5 (Virtual). Data collection and reduction demonstration 1 **(J. Britten)**	T7. NoSphereA2 **(R. Boeré)**	T10. *CRYSTALS* demonstration*:* Rotational disorder **(M. Katz)**
5:30 – 7pm	Break/Discussions	Break/Discussions	Break/Discussions	Break/Discussions
7 – 8:30 pm	T3 (Virtual). Introduction to the CSD **(Y. Olatunji-Ojo)**	**Bruker Pub Night (The Last Defence Lounge; starts at 6 pm)**	T8 (Virtual). Data analysis using the CSD **(Y. Olatunji-Ojo)**	Participant Presentations

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

Program Details

Topic	Session instructor/leader	Additional Resources
L1. Introductions and An Intro to Crystals and Crystallography	Jamie Ritch	The Mystery of the Giant Crystals Password will be sent by email
L2. Bragg's Law	Mike Katz	2021 Slides Interactive Miller Planes Viewer
L3. Reciprocal Space and Precession Images	Paul Boyle	2022 Lecture Slides Additional Notes
L4. Point Symmetry	Paul Boyle	2022 Notes
L5. Space Groups	Andreas Decken	2022 Lecture Slides 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	2022 Notes
L7. Structure Factors: Part II	Joe Ferrara	
L8. Data collection and reduction	Brian Patrick	2022 Slides
L9. Twinning	Jim Britten	2021_Lecture_Slides 2021 Tutorial Data Ton Spek's Presentation on TwinRotMat Some PowerPoints on Twinning written by Regine Herbst-Irmer

L10. Crystallographic Information Framework and Validation: The cif file and checkCIF	Brian Patrick	2022 Lecture Slides IUCr Crystallographic Information Framework Ton Spek's Powerpoint presentations
L11. Absolute structure / absolute configuration determination	Kate Marczenko	2022 Slides
L12. Crystal Growth	Paul Boyle	2022 Slides Crystal Growing Guides
T1. Introduction to OLEX2	Jamie Ritch Louise Dawe Jim Britten	Step-by-Step Example 2022 Data for Step-by-Step Example 2022 2021 Tutorial Data_1 2021 Tutorial Data 2 Working with Olex2 Playlist Notes on OLEX2 by Ilia A. Guzei
T2. 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
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 Kate Marczenko	OLEX2 Modelling Disorder Playlist Toluene across a symmetry element: Fragment instruction in OLEX2 Slides for 2021 Tutorial Data for 2021 Tutorial
T5. Data collection and reduction demonstration 1	Jim Britten	2022 Sample Data
T6. Modeling disorder: Solvent masks	Brian Patrick	2022 Slides 2022 Data Using smtbx.mask in OLEX2 OLEX2 disorder across symmetry elements and a Solvent Mask PLATON SQUEEZE by Ton Spek
T7. NoSphereA2	René Boeré	2022 Slides 2022 Sample Data
T8. Data analysis using the CSD	Yinka Olatunji-Ojo	2022 Slides and Worksheets were sent by email Mercury How-To Videos Mercury 4.0: from visualization to analysis, design and prediction CSD-Community
T9. Data collection and reduction demonstration 2 (Twinning)	Eric Rheinheimer	OLEX2: A twinning example
T10. Modeling disorder in Crystals: Rotational disorder	Mike Katz	Crystals documentation

		Crystals YouTube Playlist 1 Crystals YouTube Playlist 2 Crystals Program Download

Instructors and Organizers

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.

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, chair of the American Crystallographic Association's Communication Committee, a member of the International Union for Crystallography (IUCr) Calendar 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 their Journal of Applied Crystallography. 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 Vice-Chair of the US National Committee for Crystallography, Chair of the IUCr2026 LLC Board, and Treasurer of the Council of Scientific Society Presidents. He is a Past President of the America Crystallographic Association and current Books Editor for ACA RefleXions. He spent the last 36 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 Technician.

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.

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.

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.

Eric Rheinheimer, Rigaku Americas Corporation

Biography to be added soon!

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.

Michael Ruf, Bruker AXS

Biography to be added soon!

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.

Special thank you to Dr. Ben Gelfand, who served as our local chair until May 2022, but was unable to join us at CCCW22. This workshop has been made possible by his efforts, which are sincerely appreciated!