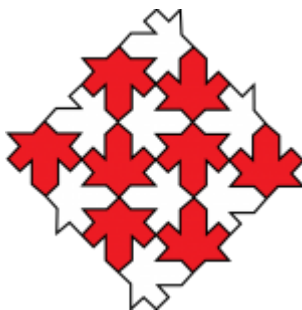


Canadian National
Committee
for Crystallography
<http://xtallography.ca/>

2020 Canadian Chemical Crystallography Workshop – May 19th to MAY 22nd, 2020

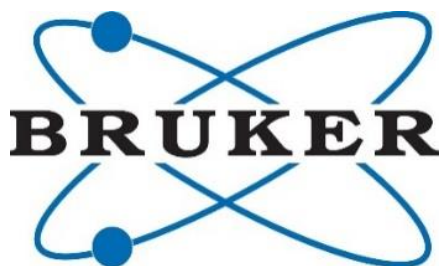
Final Program (Rev. 6 – May 22)

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CCCW2020 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 have been 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/Software>

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. The answer to the skill testing question is: P212121

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.

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.

Draft Program – Version 15.05.20

All times are in EST

	May 19	May 20	May 21	May 22
10am – 11am		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
11am – 12pm	L1. Introduction and What are crystals?	L4. Point Symmetry	L7. Structure Factors	L10. Crystal Growth
12pm – 1pm	L2. Bragg's Law	L5. Space Groups	L8. Data collection and processing	L11. Structural finalization
1pm – 2pm	L3. Reciprocal Space	L6. Precession Images	L9. Twinning	L12. Crystallographic Information Framework and Validation: The cif file and checkCIF
2pm - 3pm	Break/Discussions	Break/Discussions	Break/Discussions	Break/Discussions
3-4:30pm	T1. Introduction to OLEX2	T3. Introduction to the CSD	T6. Modeling disorder in Crystals: Rotational disorder	T8. Twinning example 2
4:30-6pm	T2. SHELX .ins structure	T4. Modeling disorder: Fixed positions	T7. Twinning example 1 and review of basic structure refinement	T9. Data analysis using the CSD
6pm – 7pm	End of Day 1	Break/Discussions	Break/Discussions	Break/Discussions
7pm – 8pm		T5. Modeling disorder: Solvent masks	Alternative Solutions with Mike Katz!	Student 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.

Topic	Session instructor/leader	Additional Resources
L1. What are crystals?	Jamie Ritch	The Mystery of the Giant Crystals
L2. Bragg's Law	Bruce Noll	http://xtallography.ca/wp-content/uploads/2020/05/CCC_W20_Braggs_Law_BNoll.pdf
L3. Reciprocal Space	Paul Boyle	http://xtallography.ca/wp-content/uploads/2020/05/Intro_to_Reciprocal_Space_1.pdf
L4. Point Symmetry	Paul Boyle	http://xtallography.ca/wp-content/uploads/2020/05/Point_Group_Symmetry_and_Crystal_Systems.pdf
L5. Space Groups	Andreas Decken	Symmetry and Space Group Tutorial by Jerry P. Jasinski and Bruce M. Foxman
L6. Precession Images and what they tell us	Jim Britten	http://www.chemistry.mcmaster.ca/~xman/Louise/L6_Precession_Images.pptx
L7. Structure Factors	Joe Ferrara	http://xtallography.ca/wp-content/uploads/2020/05/FT-and-Diffraction-CCCW2020.pdf
L8. Data collection and processing	Jim Britten	http://www.chemistry.mcmaster.ca/~xman/Louise/L8_Basic_Crystallography_-_Data_collection_and_processing.pptx http://www.chemistry.mcmaster.ca/~xman/Louise/L8_decisions_decisions_decisions.pptx
L9. Twinning	Jim Britten	Some PowerPoints on Twinning written by Regine Herbst-Irmer Data for 2020
L10. Crystal Growth	Paul Boyle	Crystal Growing Guides

		http://xtallography.ca/wp-content/uploads/2020/05/crystal_growing_presentation.pdf
L11. Structural finalization	Louise Dawe	http://xtallography.ca/wp-content/uploads/2020/05/Structure_Finalization.pdf
L12. Crystallographic Information Framework and Validation: The cif file and checkCIF	Brian Patrick	IUCr Crystallographic Information Framework Ton Spek's Powerpoint presentations 2020 Lecture Slides
T1. Introduction to OLEX2	Brian Patrick Jamie Ritch	Working with Olex2 Playlist Notes on OLEX2 by Ilia A. Guzei http://xtallography.ca/wp-content/uploads/2018/05/OLEX2_Getting_Started_May_22.pptx http://xtallography.ca/wp-content/uploads/2018/05/n18060.zip 2020 Tutorial Data
T2. SHELX .ins structure	Jim Britten Bruce Noll	The stepwise SHELXL / XP refinement process Alphabetical list of SHELXL instructions Instructional materials for 2020 http://xtallography.ca/wp-content/uploads/2020/05/Hein-Schaper-02-Refinement-2.pdf
T3. Introduction to the CSD	Lee Daniels	CCDC Introduction Videos Playlist

		<p>Also Free teaching tutorials for WebCSD</p> <p>2020 Workshop Slides</p>
T4. Modeling disorder: Fixed positions	Jamie Ritch Louise Dawe	<p>OLEX2 Modelling Disorder Playlist</p> <p>Toluene across a symmetry element: Fragment instruction in OLEX2</p> <p>Data for Disorder Refinement Examples in Olex2</p> <p>Slides for 2020 Tutorial</p> <p>Data for 2020 Tutorial</p>
T5. Modeling disorder: Solvent masks	Brian Patrick	<p>Using smtbx.mask in OLEX2</p> <p>OLEX2 disorder across symmetry elements and a Solvent Mask</p> <p>http://xtallography.ca/wp-content/uploads/2019/05/OLEX2_Disorder.pptx</p> <p>http://xtallography.ca/wp-content/uploads/2019/05/Squeeze.zip</p>
T6. Modeling disorder in Crystals: Rotational disorder	Mike Katz	<p>http://www.xtl.ox.ac.uk/tag/crystals-release.1.html</p> <p>http://xtallography.ca/wp-content/uploads/2019/05/Examples_May28_2019_9am.zip</p> <p>http://www.ccp14.ac.uk/ccp/web-mirrors/crystals/crystworkshop-gettingstarted.html</p> <p>http://www.xtl.ox.ac.uk/crystals/documentation.html</p>

T7. Twinning example 1 and review of basic structure refinement	Jim Britten Joe Ferrara	OLEX2: A twinning example Instructional materials for 2020 Instructional materials for 2020 Part 2
T8. Twinning example 2	Bruce Noll Amy Sarjeant	http://xtallography.ca/wp-content/uploads/2019/05/TwinSqueezeExample.zip http://xtallography.ca/wp-content/uploads/2020/05/Non-merohedral-twinning-from-minerals-to-proteins-Sheldrick-Herbst-Irmer.pdf Data for this tutorial (2020) was sent via email.
T9. Data analysis using the CSD	Lee Daniels	Mercury How-To Videos Mercury 4.0: from visualization to analysis, design and prediction CSD-Community

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.

Lee Daniels, [Cambridge Crystallographic Data Centre](#)

Lee is the North-American representative for CCDC, who compile and distribute the Cambridge Structural Database (CSD). Following several years in academic roles at Iowa State University and Texas A&M, Lee took two tours with Rigaku, as an account manager and as the Director of Small-Molecule Products, separated by a brief tenure with Agilent's crystallography division. He holds a PhD in Chemistry from Texas A&M and a BS from Abilene Christian University. He is active in the American Crystallographic Association and the American Chemical Society, and spent several years as a co-editor for Acta Crystallographica. He enjoys working out the details of a complicated crystal structure and the joy of finally finding the twin law that halves the R-factor. He attempts to balance his nerdiness with hiking, cycling, and playing a couple of musical instruments.

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 American 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.

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.

Bruce Noll, [Bruker AXS Inc.](#)

Bruce studied at the Metropolitan State College of Denver where he received his B.S. in Chemistry and later went on to the University of California, Davis where he received his Ph.D. in Inorganic Chemistry. He has more than 20 years experience in crystallography, and worked for 14 years in academia, starting as staff crystallographer at the University of Colorado at Boulder. In 2003, he was appointed Research Associate Professor at the University of Notre Dame. In 2008, Bruce joined Bruker AXS inc. as Senior Applications Scientist. Bruce has experience in all aspects of small-molecule crystallography, from experimental design

to facility maintenance and repair. At Bruker his responsibilities include customer demonstrations and training, as well as scientific support, and he has been a key member of the product development team for both software and hardware.

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.

Amy Sarjeant, [Bristol Myers Squibb](#)

Amy Sarjeant is a Principal Scientist at Bristol Myers Squibb using single-crystal X-ray diffraction to elucidate the structures of small pharmaceutical molecules. She is fascinated by structure packing, intermolecular interactions, and structure-property relationships. When not diffracting, she can be found knitting, kayaking, gardening, baking pies or teaching people about crystallography.

Acknowledgement: Special thank you to **Professor Dean Johnston**, [Otterbein University](#), for providing guidance on PLATON installation for macs. Prof. Johnston maintains an exceptional [Symmetry Resource](#) that may be interest to you!

Thank you to **Shane Liesegang, SJ**, for writing [the scripts](#) that enabled the smooth installation of PLATON for macs.