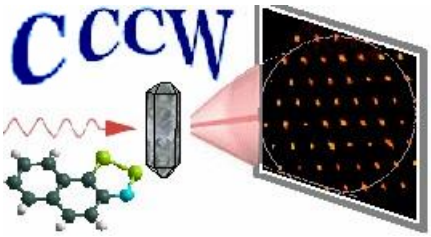
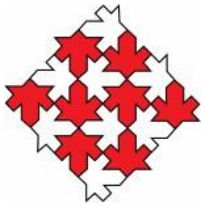




Canadian National Committee for Crystallography
http://xtallography.ca/

2024 Canadian Chemical Crystallography Workshop

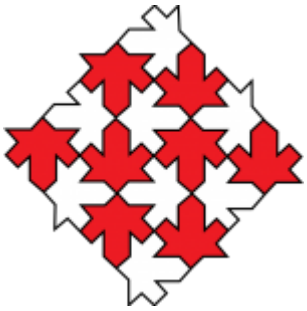
May 28th – June 1st, 2024

Program

(Version 7 – 2024-06-01)

Contents

Thank you to our sponsors!



The Canadian National Committee for Crystallography

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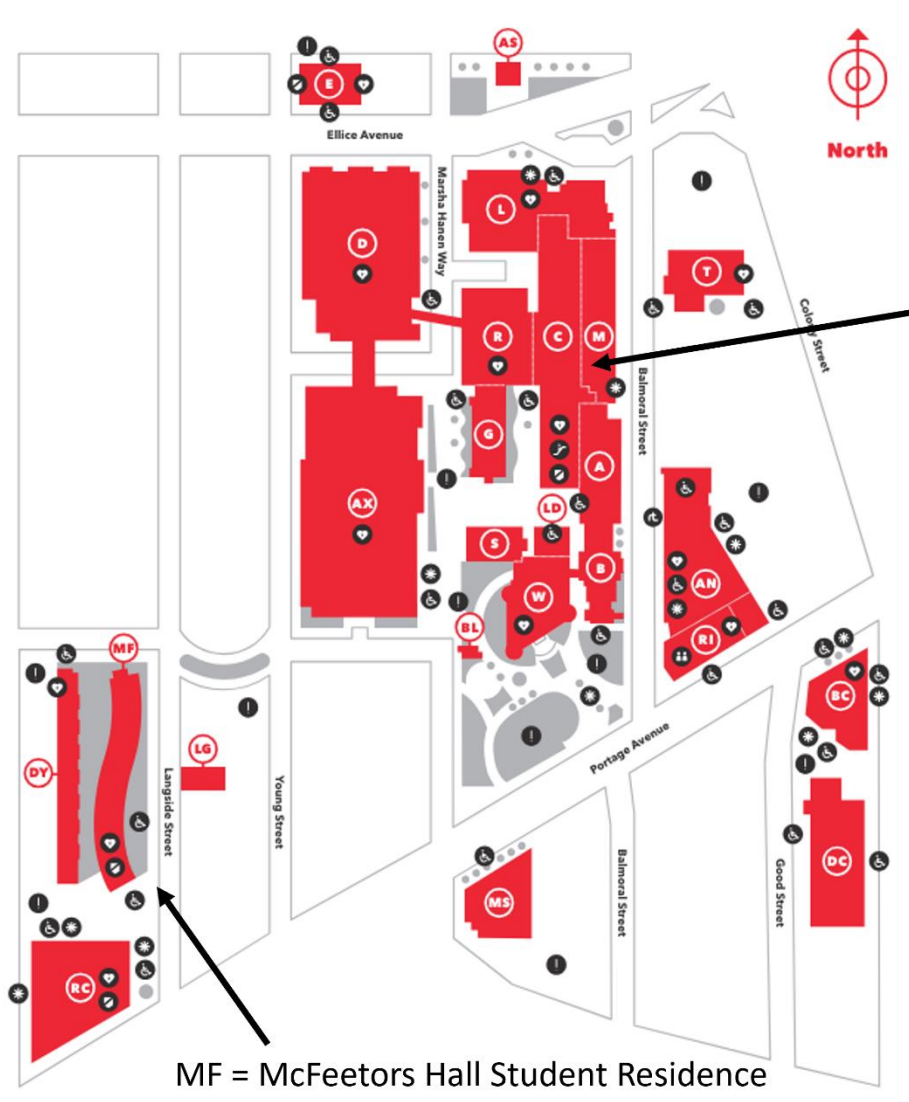
Campus Map



M = Manitoba Hall (workshop location)
C = Centennial Hall (Saturday entry to workshop location)

There are two main ways to get from the hostel (MF residence) to Centennial Hall. Each is about a 5-7 minute walk:

A) Go north on Langside St, turn right and go across the green corridor and cross Young St. Then walk past the RecPlex sports facility. Once past it, turn left and keep going until you see the bike racks on the right. Turn right, and the entrance to Centennial Hall will be ahead on the left.

Or

B) Go south on Langside St, then turn left and follow the sidewalk on Portage Ave until you get past Spence Street. Just past the bus stop turn left onto the pathway and walk around the front lawn (there is currently a peaceful encampment on the lawn). When the path branches go left to walk between Wesley Hall (the castle-looking building) and Bryce Hall. Keep going straight and you will reach the entrance to Centennial Hall.

Once inside Centennial Hall, take the stairs (or escalator or elevator) up one level, then turn right, following the sign for Manitoba Hall. Once through the doorway turn left. The workshop room, 2M70, will be on the right.

Practical Considerations

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

2. Location: We will be in the Manitoba Hall Boardroom - 2M70. The building location is denoted as "M" on this map. On the final day, we will need to enter via Centennial Hall, and will need to show ID to security. Centennial Hall is "C" on the linked map.

3. Wifi: For academic participants, Eduroam is available. For those affiliated with institutions that do not support Eduroam, a visitor network will be available. Instructions on access to this network were sent by email.

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

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 Wednesday, May 29 at Local Public Eatery (274 Garry St; about an 18 minute walk or five minute car ride from Centennial Hall). Buffet-style appetizers and one drink ticket per person will be available. Attendees can purchase additional food and beverages at their own expense.

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

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. 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.

8. 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 1. 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.)

CCCW2024 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. Highly recommended: ORCA 5.0.4 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 CCCW24 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 CCCW24 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 2024-05-02)

All times are Winnipeg local time

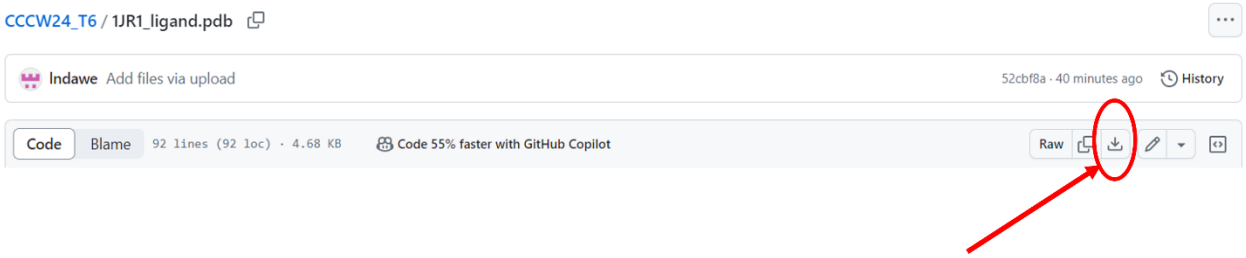
	Tuesday, May 28	Wednesday, May 29	Thursday, May 30	Friday, May 31	Saturday, June 1
9 – 10 am	Last minute technical check-in and Welcome **(Decken/Dawe)**	L3. Point Symmetry **(P. Boyle)**	L7. Data collection and reduction **(B. Patrick)**	T5. NoSphereA2 **(R. Boeré)**	L11. High Pressure: Crystallography and Synchrotrons **(C. Beavers)**
10 – 11 am	L1. Introduction to Crystals, Crystallography, and Crystal Growth **(Ritch/Dawe)**	L4. Space Groups **(A. Decken)**	L8. Absolute structure / absolute configuration determination **(C. Beavers)**		T8. Modeling disorder: Solvent masks **(L. Dawe)**
11 – 11:15 am	Short Break	Short Break	Short Break	Short Break	Short Break
11:15 am – 12:15 pm	L2. Bragg's Law and Miller Indices **(B. Patrick)**	L5. Reciprocal Space and Precession Images **(A. Schmidt)**	T4. Modeling disorder: Fixed positions and fragment libraries Extended time for extra practice and OLEX2 Q&A **(L. Dawe + Other Instructors)**	L10. Twinning **(J. Britten)**	L12. Crystallographic Information Framework and Validation: The cif file and checkCIF **(B. Patrick)**
12:15 – 1:15 pm	T1. Introduction to OLEX2 **(L. Dawe)**	T3. Introduction to the CSD **(Y. Olatunji-Ojo)**		T6. Data analysis using the CSD **(Y. Olatunji-Ojo)**	Break
1:15 – 2:30 pm	Break	Break	Break	Break	Participant Presentations
2:30 – 4pm	Group work and one-on-one discussions using home or supplied data	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	T2. Data collection and reduction demonstration 1 **(A. Schmidt)**	L6. Structure Factors **(P. Boyle)**		T7. Data collection and reduction demonstration 2 (Twinning) **(C. Beavers)**	Formal End of Workshop
5:30	Formal End of Day	**Networking Night sponsored by Bruker (Start time ~6 pm)**		Formal End of Day	

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 – 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)
Pre-Workshop Activities		*Please refer to page 7 of this program book.*
L1. Introduction to Crystals, Crystallography, and Crystal Growth	Jamie Ritch and Louise Dawe	2024 Crystal Growing Slides 2022 Slides Crystal Growing Guides
L2. Bragg's Law and Miller Indices	Brian Patrick	2024 Slides Interactive Miller Planes Viewer
L3. Point Symmetry	Paul Boyle	2024 Slides
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	Ashley Schmidt	2022 Lecture Slides Additional Notes
L6. Structure Factors	Paul Boyle	2024 Slides
L7. Data collection and reduction	Brian Patrick	2022 Slides

L8. Absolute structure / absolute configuration determination	Christine Beavers	2023 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	2024 Lecture Slides 2024 Twinning Data Twin_introduction_Regine_Herbst-Irmer Twinpseudomero_Regine_Herbst-Irmer Ton Spek's Presentation on TwinRotMat
L11. High Pressure: Crystallography and Synchrotrons	Christine Beavers	A night at the beamline | Careers | Chemistry World Dropbox link to talk slides
L12. Crystallographic Information Framework and Validation: The CIF file and checkCIF	Brian Patrick	2023 Lecture Slides IUCr Crystallographic Information Framework Ton Spek's Powerpoint presentations
T1. Introduction to OLEX2	Louise Dawe	2024 Tutorial Slides 2024 Tutorial Data Notes on OLEX2 by Ilia A. Guzei

		Crystallographic problems
T2. Data collection and reduction demonstration 1	Ashley Schmidt	
T3. Introduction to the CSD	Yinka Olatunji-Ojo	2024 worksheets were sent by email. Other resources: CCDC Introduction Videos Playlist Free teaching tutorials for WebCSD
T4. Modeling disorder: Fixed positions and fragment libraries	Louise Dawe	2024 Tutorial Slides 2024 Tutorial Data Notes on OLEX2 by Ilia A. Guzei Crystallographic problems
T5. NoSphereA2	René Boeré	2024 Slides 2024 Tutorial Data
T6. Data analysis using the CSD	Yinka Olatunji-Ojo	2024 worksheets were sent by email. 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)

T7. Data collection and reduction demonstration 2 (Twinning)	Christine Beavers	2023 Slides
T8. Modeling disorder: Solvent masks	Louise Dawe	2024 Tutorial Slides 2024 Tutorial Data Using smtbx.mask in OLEX2 OLEX2 disorder across symmetry elements and a Solvent Mask PLATON SQUEEZE by Ton Spek
T9 Max3D (Not formally part of the schedule, but we will fit this in!)	Jim Britten	Max3D Slides (PDF; for PPTX, please contact Jim Britten) Max3D software for academic users
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.

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 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.

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.

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.

Ashley Schmidt, Bruker AXS

Dr. Ashley (Weiland) 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.