Building the future of crystallography through active engagement

Suzanna Ward & Amy Sarjeant

ACA 2019 – Cincinnati, OH
Wednesday July 24th 2019
What we do

Charitable Objective:
Advancement of chemistry and crystallography for the public benefit

The CCDC is dedicated to the advancement of chemistry and crystallography for the public benefit through providing high quality information services and software. This is primarily achieved through compilation and dissemination of the Cambridge Structural Database (CSD). The CSD is an essential resource in the molecular sciences and is used extensively in medical research aimed at the drug design.
European Crystallographic Schools

- BCA School
- Zurich Crystallography School
- Erice
Engaging crystallographers

- Colombia Workshop
- Crystallography Schools – ACA, CCCW
- LACA Workshop – Merida, MX
- IUCr OpenLab - Uruguay
Engaging crystallographers – Asia / Oceania
Vietnam 2016

Cambridge Crystallographic Data Centre (CCDC)
6 December 2016

Today at Acadia 2016, CCDC’s Outreach and Education Manager, Amy Sarjeant is speaking about Using Metal-Organic Frameworks to Net Neon. She explains how MOFs have been used to elucidate the first ever crystal structures containing neon in an organic or metal-organic environment. http://www.ascada2016.org/programme.html

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From Dashi Umeda, third-year undergraduate student in the Department of Physical Chemistry, Tohoku University, Japan.

When I came for the first time to my current laboratory, I was particularly interested in one of the research topics within our laboratory, which is pharmaceutical crystals. However, since there is no crystallographer in our group, my professor (Professor Kohei Yonesaki) decided to make a collaboration from crystallography research group at Tokyo Institute of Technology (Professor Helmut Zelik).

During my experiments, one doctoral student from (Unica group) helps and supervises me in performing experiments. He also assists me to make a discussion about the project I am working on now. I am really interested working in the pharmaceutical crystal field because it can provide a better insight into understanding the physicochemical properties of drug materials. In my opinion, my experiences asked me to join the Acadia 2016 meeting which held in Hanoi, Vietnam. After discussing with my parents, I decided to attend this conference to get a new experience. I am the only student from my university to join this conference. However, one doctoral student from Tokyo Institute of Technology, Mr. Okf Dachinka Rasa, accompanied me during this trip.

Acadia 2016 was special conference as well as a special trip for me. It was the first international conference I attended and I was also my first journey abroad. Before arriving in Hanoi, I needed to transfer at Seoul. During my train ride in Japan, I used this time to enjoy Sushi and practice my presentation. As a third-year student, I was so nervous to speak in English because previously, English was not my native language. But I was determined to try my best to present my research. Finally, my presentation time was decided. I presented my poster on December 7th 2016. During my presentation, I met Sharlee Windle-Drick, Amy Foylan from CCDC, and we had a short discussion at the time. I also met some big professors in the field of crystallography, such as Professor Ohashi, Professor Oggse, and Professor Fronc, which many of the papers I have read before. Moreover, Professor Fronc from McGill University gave me a key chain from Crystal Growth and Design journal.

Since my goal was mostly to get experience, I did not expect that I would get an award at this conference. However, during the dinner, I was surprised that my name was mentioned by Professor Ian Williams from ICAG. It was such an honor for me to receive the poster prize award from CCDC. I am also deeply moved to be elected as one of the best poster among many interesting posters. My paper talked about the preparation, characterization, and physicochemical properties of pharmaceutical crystals. In the occasion, I used an antiplatelet inhibitor as a model compound. I also looked forward to getting our work to be published in the very near future.

Other than conference, I also tried to pack my schedule to explore Vietnam. Overall, I really like the autumn in Vietnam because it is warmer and more humid than Japan. In this trip, we can be considered as my full moon trip from cold winter in Japan. The food was also delicious, cheap, and spicy.

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From Archana K. M. Research Scholar at “The Functional Nanomaterials Group”, Material Science Division of Poomparvajee Institute of Scientific Research, Bangalore, India.

My research mostly focuses on Crystal structure analysis of functional oxide nanomaterials for photoluminescent and thermoelectric applications. I am in my second year PhD for which I synthesize nanomaterials and characterize them via various characterization techniques such as, XRD, Raman, FTIR, UV-DRIFT, SEM, TEM. Zero potential and more interesting, their bio-compatibility. Precise crystal structure analyses of these materials are carried out using Synchrotron and Neutron diffraction data to get more accurate crystallographic data such as bond angle and bond distances i.e., local environment of the luminescent ion. Since my area of research mostly focuses on luminescent materials and their crystal structure analysis, I do prefer to attend crystallography conferences. When I was searching for such conferences I came across Acadia 2016, I am very fortunate to present my work in Acadia 2016.

I am very grateful to the Acadia 2016 committee for my abstract acceptance and for the travel support given to me to come across such a fruitful crystallography conference. In this context, Acadia 2016 covered diverse aspects of crystallographic research ranging from materials to life sciences utilizing several advanced techniques. It is more beneficial to my research by exposing me to those cutting-edge areas. I strongly believe that the discussion of my work with eminent speakers and researchers has given me more scientific direction to stretch my research towards these fields.

My special thanks to CCDC for recognizing my work. I attended few National and International conferences somewhere else also but as per my experiences Acadia 2016 is the best conference so far I attended. I convey my heartfelt thanks to all whose enriched my skills and strengthened my knowledge in the area of crystallography.

It’s immense pleasure to share our group experience and happiness with you. It was a pleasant stay at Hanoi, which is a lovely place and I was greatly inspired by their humble nature...
Courses in Kenya and Senegal - 2015

- Juliette Pradon (CCDC) and Lewis Whitehead (Novartis)

- Kenya – a series of lectures and workshops on crystallographic databases, and in-silico visualization and modelling applications in drug discovery.

- Senegal - first crystallography school and travelling laboratory. Over 50 participants from across francophone Africa

https://www.ccdc.cam.ac.uk/Community/blog/post-60/
Collaboration - CCDC & University of Kinshasa

• CCDC seminars and workshops at University of Kinshasa
  • Cambridge Structural Database for both research and teaching purposes
  • Electronic structure theory workshop
  • Drug discovery course

• Collaboration with Professor Zéphirin G. Yav (Chemistry Department, UNIKIN, D.R.C)
  • MSc and PhD student research support
Communicating research results

- International conferences
- Publications
- Manuscripts in preparation
2016 workshop in Ghana

Feedback:

• “I found that opportunity as a breakthrough in my research; especially how to assess the Cambridge crystallographic database.”

• “I believe it usage will add some touch of excellence to my research work.”

The Computational Chemistry Research Group of the Department of Chemistry hosted a five-day conference and workshop on Molecular/Materials Modelling, Catalysis and Crystallography on 1st - 5th August, 2016 on the theme "New Materials for a Sustainable Energy Future: Linking Computation with Experiment" as part of activities of the Royal Society – DFID-funded research and training project between the Department of Chemistry at KNUST, Cardiff University in Wales, the University of Namibia and the University of Botswana. The programme brought together scientists from Ghana, the UK, Botswana and Namibia who are engaged in fundamental research in the area of materials design for renewable energy applications to share the outcomes of their research and chart the course of future research in this area. Speakers and facilitators included Professor Nora H. de Leeuw, Professor of Computational Materials Science and Pro-Vice-Chancellor of Cardiff University; Professor Richard Catlow FRS, Professor of Catalytic and Computational Chemistry of Cardiff University; Professor Simon Coles, Professor of Structural Chemistry of the University of Southampton and Director of the UK National Crystallography Service; Professor Andrew Michael Beale, Professor of Inorganic Chemistry of University College London; Dr Sankar Meerakohsundaram of the Cardiff Catalysis Institute, Cardiff University; Dr. Jörg Saßmannshausen, University College London, UK; Dr. Suzanna C. Ward of the Cambridge Crystallographic Data Centre, Cambridge, UK; Dr. Alberto Reiland Martinz, Cardiff University, Wales; and Dr. Nelson Ozaide of Utrecht University, the Netherlands.
If you have much encouragement and more legislation that we signed up for the first ever Pan African Conference on Crystallography (PCCr) in Delft, Cape Town last October. For it was set to be a busy conference with talks, discussion sessions, a poster session, and an exhibition of new instruments related to the conference. But the opportunity to engage with the burgeoning community of crystallographers was too good to miss. What an experience if formed out to be on so many levels.

The key to the conference was that we wanted to experience it with a truly memorable experience. After a week’s sightseeing in Cape Town, a night in a hotel room in Oudtshoorn, and taking a scenic drive from Oudtshoorn to the Cape Winelands, we arrived back in Oudtshoorn for the conference. Along the way, we met many interesting people and engaged in discussions about the future of crystallography and its impact on society. We were also able to meet some of the latest research and developments in the field.

The conference itself was well attended with about 300 participants from over 30 different countries, with the majority of these being from outside Africa. This is especially important in the light of the recent trends towards globalization and the need for international collaboration. Throughout the conference, there were plenary talks, poster sessions, and discussion panels. The plenary talks were held in the main conference hall, which was a spacious and comfortable environment.

The conference also featured a range of workshops and training sessions. These were held in smaller rooms and were designed to help participants learn new skills and techniques in crystallography. The training sessions were led by experts in the field and were aimed at both experienced researchers and those new to the field.

One of the highlights of the conference was the poster session, which was held in the exhibition hall. The posters were arranged in a circular format, with each poster containing a detailed explanation of the research being presented. The session was well attended, with many researchers stopping to discuss their work with each other.

The conference also featured a range of networking events, including a welcome reception and a conference dinner. These events were a great opportunity for participants to meet and discuss their work with others in the field.

In summary, the Pan African Conference on Crystallography was a successful event that brought together researchers from around the world to discuss the latest developments in the field. The conference was well-organized and provided a great opportunity for participants to learn new skills and techniques in crystallography.
Meeting new friends and familiar faces

Francoise Noa - one of the authors on the 750,000th CSD entry visiting our stand at ECM29 https://
Access to CSD-Enterprise in developing countries

- Frank Allen International Research and Education (FAIRE) Programme
  - Supports research & education in developing countries through use of the CSD
  - Three year award for researchers in developing countries who have a demonstrable hardship
    - Covers all of our data and software
    - Is a campus wide license
    - Requires users to mention FAIRE in acknowledgements

https://www.ccdc.cam.ac.uk/Community/FAIRE/
FAIRE in Africa

- 10 Universities
- >20 individual users
- 14 Publications made possible by the CSD

CSD-Enterprise has really revolutionized my approach to the teaching of coordination chemistry and inorganic chemistry.... I have been able to publish three articles in peer reviewed journals.

The authors thank the International Union of Crystallography (IUCr) and the Cambridge Crystallographic Data Center (CCDC) for their initiative to promote crystallography and structural studies in Africa and particularly in Cameroon.
PCCr2 – Meeting new friends and familiar faces
Educational resources and tutorials

Download a series of self-guided workshop materials for CCDC tools and features

Example 1. Generating Structure Views

In order to communicate science effectively, researchers must be able to provide clear images of their compounds for publication, meeting presentations, and presentations. The program Molecule contains many features which can assist in the production of high-quality, informative graphics of molecules. This example shows you how to build structure views such as packing diagrams, van der Waals, and intermolecular interactions, and how they can be output in graphics formats for use in various online environments. For these reasons, we will be using the Crystal Structure Viewer (CSV) to show how this is done. The CSV can be applied to any entry in the CCDC or any of your own structures. 

Generating a Simple Molecular View

In this section, you will learn how to manipulate molecule options in order to generate a simple molecular view:

1. Open Molecule by clicking the icon, or launching from the main menu.
2. In the Structure Viewer window, type the cif file name (CSD7000000) to bring up the structure of a complex diophane.
3. The whole molecule should be displayed in the viewer window. In this example, double-click on the two for hexagonal CSD and you will see half of the molecule disappear. Click the two to bring back the whole molecule. 
4. To generate the view in step 3 above, choose Publication from the Manager 3D viewer menu. Experiment by selecting other items from this menu.
5. To change the style of the atoms and bonds in the structure, but to keep the white background, use the Display option in the View window. Experiment with the by choosing other options. Select the “Ball and Stick” when you are done.

https://www.ccdc.cam.ac.uk/Community/educationalresources/workshop-materials/
New instructional videos

https://www.ccdc.cam.ac.uk/Community/educationalresources
Recorded workshop material
CSD Teaching Subset

- 750+ Structures for educational purposes
- Drug molecules
- Fundamental Chemistry
- Symmetry
- Metal-Orgaic Frameworks

https://www.ccdc.cam.ac.uk/Community/educationalresources
Engaging chemists

Metal-Organic Concepts
Click to download an introduction to Mercury using metal-organic complexes. This module was written by Anthony Fernandez - Associate Professor, Merrimack College.

Hydrogen-Bonding Concepts
Click to download a teaching module on hydrogen bonding. This module was written by Stefano Camossa - Università degli studi di Parma.

Introduction to Crystallography for General Chemistry Students
Click to download an introduction to crystallography using Mercury. Click to download an introduction to crystallography using the Teaching Subset. These modules were written by Tim Roweppa - Professor, University of West Florida.

Introduction to Mercury
The Cambridge Crystallographic Data Centre (CCDC) distributes Mercury, which is a program that can be used to view and analyze crystal structure data. We will be using it over the course of the semester and this exercise will provide an introduction to the software package.

First, the program must be obtained from the CCDC using the link provided below. http://www.ccdc.cam.ac.uk/Solutions/CSDSystem/Pages/Mercury.aspx
This program is a freely available and there are versions for Mac, Windows, and Linux operating systems.

Once the program is installed and you open the program, you will see the following screen.

VIPER
VIRTUAL INORGANIC PEDAGOGICAL ELECTRONIC RESOURCE: A COMMUNITY FOR TEACHING STUDENTS OF INORGANIC CHEMISTRY

Home > Isomerism in Coordination Complexes
Submit by Anthony L. Fernandez, Merrimack College

My Notes
Add to Favorites (2 favorites)
I Have Adopted This (1 adopted)

Categories
Prequisitese:
General Chemistry
Co-requirese:
No Co-requisites
Course Level:
Second year
Upper Division

Description:
Students are confronted with a number of new types of isomerism as they move from organic chemistry into inorganic chemistry. This can be confusing and students often struggle. The program uses active visualizations to help students learn and understand isomerism.

Topics Covered:
Coordination Chemistry
Molecular Structure and Bonding

Getting Started:
1. To use the CCD "Access Structures" function you will require a computer or laptop with access to the internet.
2. You will then need to find CCD "Access Structures" page using one of these methods:
   1. Type in the web address https://www.ccdc.cam.ac.uk/structures
   2. Type in the search engine such as google "inorganic structure" and click on the "Get it!" button for the "Access Structures" page.

Basics:
To view a particular structure, you need to click to access the structures provided on the CCD website. The purpose of the file is to help students study the crystal structure of caffeine.

The "inorganic" tab on the VIPER website can be used to change the view.

The "latest step" button can be used to view different steps in the molecule.

Folding systems can be used to look at large crystal structures, e.g. the unit cell and the unit cell of the whole crystal.

You will notice that caffeine also has an "inorganic" representation in the crystal structure which appears to have no normal inorganic name. If it's any consolation, caffeine is not a normal inorganic crystal.
Engaging chemists

Learning point-group symmetry through 3D printed models

Click to download the worksheet for use in the classroom
Click to download the answer key
This module was developed by Anton Savchenkov and uses 3D printed models from the Shapeways site.
International Year of The Periodic Table in Crystals

• Community project
• Linked from educational materials
• Shows elements in the CSD
• #IYPTcrystals
• #IYPT2019

https://www.ccdc.cam.ac.uk/Community/educationalresources/PeriodicTable/
The wonders of crystals and the periodic table

• Next steps
  • Creation of educational activities based on resource
  • Targeting:
    • Uniform group badges
    • Science festival activity packs
    • STEM ambassador events
Cambridge Botanic Gardens

Campanum annuum (chilli pepper)

Capsaicin

Capsaicin is the chemical compound that accounts for the heat in chilli peppers. The burning sensation is caused by stimulation of heat sensors, but does not actually increase body temperature.

Capsaicin is the principal ingredient in pepper spray, used for riot control and personal protection. Tarantula venom activates the same pain pathway as capsaicin.

Medically, it can be applied topically in ointments and creams to treat pain. This effect is believed to result from nerves being overwhelmed by the burning sensation and temporarily unable to "report" pain.

The hotness of different varieties of chilli is measured using the Scoville Scale, named after Wilbur Scoville who developed the test in 1912. As originally devised, a solution of the pepper extract is diluted in sugar water until the 'heat' is no longer detectable to a panel of tasters; the degree of dilution gives its measure on the Scoville scale.
Engaging a new generation
Science festival activities
Engaging activities
Engaging the future

Classroom Teaching Module: Structure Exploration
Click to download the packet for use in the classroom
This module was developed for use in the classroom based on hands-on exercises used at the Cambridge Science Festival (Wilfrid Laurier University) for assistance with curriculum benchmarking.

Classroom Teaching Module: Crystallization
Click to download the packet for use in the classroom
This module was developed for use in the classroom based on hands-on exercises used at the Cambridge Science Festival (Wilfrid Laurier University) for assistance with curriculum benchmarking and Prof. Robert Pike at The College of William and Mary resources.
Engaging the future

Understanding molecules by exploring crystal structures

Chemistry, Physics
Target age group: High school/A-Level/University students (16+ y.o.)

Description: This learning module exposes students to the structures of molecules by allowing them to explore common chemicals through crystal structures contained in the Cambridge Structural Database (CSD). Students will be able to visualize 3D chemical structures as a way to understand concepts of bonding, chirality and isomerism. These activities can be run in series as part of a science learning day event or can be incorporated into classroom activities.

Expected Outcomes
• Familiarity with the Cambridge Structural Database (CSD)
• Ability to relate 2D chemical diagram to 3D molecular structure
• Understanding the nature of chirality (right- and left-handed molecules)
• Understanding the nature of isomerism (same chemical formula, different connectivity)
• Understanding the nature of common chemicals found in everyday objects
• Understanding differences between model kits and experimental data

Materials
Required
• Printed hand-outs
• Examples of everyday objects
  o Lemon, sugar, chocolate, mothballs, aspirin
• Computer with internet access
• Molecular model kit

Optional

Using this activity in the classroom:

This activity was originally designed as part of The Cambridge University Science Festival. If you are interested in using this as part of your course curriculum, please see below for some places where this might fit into your classroom.

Guide to Science Curriculum from Ontario, Canada:

Areas where this activity might fit in your courses:
Grade 11 (University Prep Course) - Overall Expectations
By the end of this course, students will:
B1. analyse the properties of commonly used chemical substances and their effects on human health and the environment, and propose ways to lessen their impact; (pg 94)
B2. investigate physical and chemical properties of elements and compounds, and use various methods to visually represent them; (pg 94)
B2.6 build molecular models, and write structural formulae, for molecular compounds containing single and multiple bonds (e.g., CO2, H2O, C2H4), and for ionic crystalline structures (e.g., NaCl) (pg. 96)

Grade 12 (University Prep Course) - Overall Expectations
By the end of this course, students will:
B2. investigate organic compounds and organic chemical reactions, and use various methods to represent the compounds; (pg 108)
B3. demonstrate an understanding of the structure, properties, and chemical behaviour of compounds within each class of organic compounds. (pg 108)
B3.3 build molecular models for a variety of simple organic compounds (pg 108)
C3. demonstrate an understanding of atomic structure and chemical bonding, and how they relate to the physical properties of ionic, molecular, covalent network, and metallic substances. (pg 110)
C3.5 describe a Canadian contribution to the field of atomic and molecular theory (e.g., the work of...
Building a collection of resources

Building a collection of:
• CCDC educational material
• Community driven educational material

Let us know if:
• You have material based on the CSD that you would like us to host or link to
• You have ideas or requests for future CCDC educational material
• You would like us to provide specific material for a workshop or event you are involved with

https://www.ccdc.cam.ac.uk/Community/educationalresources/
Event support

Sponsorship Guidelines

If you are interested in receiving sponsorship or support for an event or an award, please note the following.

Events or awards will be considered if they:

1. Focus on an area related to the mission of the CCDC
   1. Crystallography
   2. Structural chemistry / biology
   3. Pharmaceutical research / methodology
   4. Computational chemistry
   5. Database resources / data management
2. Promote participation of students and young scientists in these fields
3. Provide educational opportunities related to CCDC’s core mission
4. Allow for participation of CCDC staff for educational purposes and/or include CSD as part of the educational experience

Requests will be reviewed on a regular basis must be received at least 6 months in advance of the event in line with the schedule below:

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<tr>
<th>Proposed Event Date</th>
<th>Due Date</th>
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<td>June 1st – Sep 30th</td>
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<td>Oct 1st – Jan 31st</td>
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https://www.ccdc.cam.ac.uk/Community/awardsandsponsorship/
Thank You

Thank you and...
Colleagues at the CCDC
The IYPT in Crystals team
The many contributors to the CSD
The many educators who use the CSD
Those who have contributed educational materials
Susan Bourne, Simon Coles, Caroline Davies,
Louise Dawe, Graciela Diaz, Anthony Fernandez, Greg Ferrence, Delia Haynes,
Peter Hoare, Dean Johnston, Patrice Kerfoot, Tim Power, Dmitriy Soldatov,
Samuel Tetteh, Michele Zema

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