Crystallography Times

Rigaku oxford diffraction

Crystallography Newsletter
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Come visit with us at:

FASEB – Machines on Genes.
Snowmass, CO, June 24 – 29, 2018

NORM Northwest Regional Meeting – ACS.
Richland, WA, June 24 – 27, 2018

ACA Annual Meeting
Toronto, Canada, July 20 – July 24, 2018

ICCC 2018 – 3rd International Conference on Coordination Chemistry
Sendai, Japan, July 30 – August 4, 2018

Abstract Submission Deadlines

AxCA 2018
Due August 14, 2018

Join RQD on LinkedIn

Rigaku Oxford Diffraction LinkedIn group shares information and fosters discussion about X-ray crystallography and SAXS topics. Connect with other research groups and receive updates on how they use these techniques in their own laboratories. You can also catch up on the latest newsletter or Rigaku Journal issue. We also hope that you will share information about your own research and laboratory groups.

Rigaku Oxford Diffraction Forum

www.Rigakuxrayforum.com

Here you can find discussions about software, general crystallography issues and more. It's also the place to download the latest version of Rigaku Oxford Diffraction's CrysAlis^{Pro} software for single crystal data processing.

We look forward to seeing you on there soon.

Survey of the Month

Take the Survey

Last Month's Survey

The summer conference season will be upon us shortly. How many conferences will you attend?

Video of the Month

Here is a quick video from the American Red Cross on how to do hands-only CPR. You just might save a life with this little bit of knowledge.

Watch the Video

Upcoming Events

UK Synchrotron Radiation (UKSR50)
June 26 – 29, 2018 in Liverpool, UK

9th Conference on Aperiodic Crystals
July 8 – 13, 2018 in Ames, IA, USA

AFC French Crystallography Association 2018
July 10 – 13, 2018 in Lyon, France

See full list >

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Crystallography in the News

June 1, 2018. An international team of researchers, led by Marius Schmidt at University of Wisconsin-Milwaukee, has found a new way to investigate how TB bacteria inactivate an important family of antibiotics! They watched the process in action for the first time using an X-ray free-electron laser, or XFEL.

June 1, 2018. University of Saskatchewan researchers have found that chemicals commonly used to protect samples in synchrotron experiments actually help to damage those samples, potentially misleading scientists around the world. The findings apply to X-ray absorption spectroscopy and protein crystallography.

June 1, 2018. The antibiotic-resistant *Acinetobacter baumannii* bacterium is one of the most globally harmful bacteria that causes nosocomial infections. Researchers at the University of Turku, using X-ray crystallography, have discovered that the bacterium attaches to plastic medical devices using tiny finger-like structures.

June 4, 2018. Rice University scientists, led by George Phillips, used a rapidly pulsing X-ray laser to show how drug-resistant tuberculosis bacteria destroyed the antibiotic molecules intended to treat the deadly lung disease. The employed a technique called mix-and-inject serial crystallography.

June 5, 2018. Advances in detectors and X-ray microscopes at light sources such as Berkeley Lab's Advanced Light Source have made it possible to measure a ptychographic dataset in seconds. As a result, ptychography is used in a range of scientific domains, including condensed-matter physics, cell biology and electronics.

June 6, 2018. Paul Bover, who won the chemistry Nobel prize in 1997 for his work on the synthesis of the cellular energy source adenosine triphosphate (ATP), has died aged 99. In the 1970s Boyer put forward a theory of how the enzyme ATP synthase can turn adenosine diphosphate and inorganic phosphate into ATP, which is used to store and transport energy within biological cells.

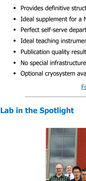
June 8, 2018. The Royal Society announced its 2018 Fellows who included protein crystallographer Harren Jhoti. A total of 50 scientists were announced as Fellows, as well as 10 new foreign members for their exceptional contributions to science, the Society said.

June 8, 2018. The Curiosity rover has been sampling on Mars for the past 5 years. Dr. Jennifer Eigenbrode and her colleagues used two instruments on the SAM (Sample Analysis at Mars) suite to catch traces of complex organics preserved in 3-billion-year-old sediments. Neither instrument uses an array of organics and relies instead on measurements of organic-rich sedimentary rock found on Earth.

June 12, 2018. Physicist Henry Moseley's early death was one of mankind's greatest losses. Moseley did a lot of fantastic and interesting work, mostly in the building field of X-Ray crystallography and spectrography, which had only just been formalized by the Braggs.

June 13, 2018. A group from Caltech, led by André Hoelz, used X-ray crystallography to give the first atomic-scale look at the specific components of human NPCs responsible for dropping mRNAs off in the cytoplasm. For an mRNA to be transported through an NPC (nuclear pore complex), it must be tagged with a nuclear export factor, a type of small protein.

Product Spotlight



Rigaku XtaLAB mini II

Single crystal X-ray diffraction on your benchtop
The XtaLAB mini™ II benchtop X-ray crystallography system is a compact single crystal X-ray diffractometer designed to produce publication-quality 3D structures. The perfect addition to any synthetic chemistry laboratory, the XtaLAB mini II will enhance research productivity by offering structure analysis capability without the necessity of relying on a shared departmental facility. By having a XtaLAB mini II in your lab, you no longer have to wait in line to determine your structure. Instead your research group can rapidly analyze new compounds as they are synthesized in the lab.

Teach single crystal X-ray diffraction through hands-on experience
At many universities, the departmental single crystal X-ray diffractometer is considered "off limits" to students because of the fear that the instrument might be damaged by inexperienced users. The XtaLAB mini II provides the opportunity for students to learn single crystal X-ray analysis by actually using a fully functional diffractometer. This is not a black box instrument. Rather, the important steps of mounting a crystal on the goniometer and physically centering the crystal in the position of the X-ray beam ensures that students learn the importance of mounting techniques and crystal selection. The simple, robust design of the XtaLAB mini II X-ray diffractometer makes it the ideal hands-on experimental device for students to learn crystallography.

Reduced size does not mean reduced data quality
The Rigaku XtaLAB mini II is a research grade chemical crystallography instrument that sits on the benchtop. No data quality compromises, no extended collection times. Results delivered are unambiguous and of publishable quality meeting *Acta Cryst* requirement.

Features

- Affordable design with low operating costs
- Requires minimal training and support
- Automatic structure solution software
- Provides definitive structural information
- Ideal supplement for a NMR spectrometer
- Perfect self-serve departmental lab instrument
- Ideal teaching instrument
- Publication quality results
- No special infrastructure required (110 VAC)
- Optional cryosystem available

For more about XtaLAB mini II

Lab in the Spotlight

The Matzger Group at the University of Michigan
Adam Matzger, Charles G. Overberger Collegiate Professor of Chemistry, College of LS&A; Professor of Macromolecular Science & Engineering, College of Engineering

The Matzger Group focuses on three principal areas: crystal polymorphism of pharmaceutical materials, porous materials and energetic materials

The Matzger Group's approach to the study of crystal polymorphism of pharmaceutical materials exploits polymers as phase directors. Combinatorial materials chemistry plays a vital role in these efforts, as do advanced analytical techniques including X-ray microdiffraction, thermal analysis, and Raman spectroscopy. Design of new polymeric systems for controlling pharmaceutical crystallization and elucidating mechanisms of form selection are topics of current interest, as well as developing novel pharmaceutical cocrystal materials.

Coordination polymers with high levels of porosity are being intensively investigated by the Matzger Group. New synthetic methods pioneered in the group are leading to materials with unprecedented structural properties. Both fundamental studies on processes such as gas adsorption, supramolecular isomerism, and host-guest chemistry are conducted alongside applications in gas (hydrogen, carbon dioxide, methane) storage and separations in liquids. Key techniques applied to characterize materials include X-ray diffraction, Raman spectroscopy, and adsorption analysis.

The Matzger Group is using cocrystallization, a method that combines existing compounds into a single crystal lattice to realize new and unique materials, as an alternative way to achieve significant improvements while avoiding the challenges and uncertainty associated with traditional methods. By cocrystallizing energetic compounds of complementary oxygen balance, stability, or density, novel and attractive energetic materials are created. Furthermore, energetic cocrystals have the potential to act as smart materials by offering solid state properties more complex than those of pure materials.

Useful Link

11 YouTube Channels Every Science Nerd Should Follow

Here is a useful link pointing to a number of great sites to connect science/nature videos for young and old, provided by the *Huffington Post*: *11 YouTube Channels Every Science Nerd Should Follow*

Selected Recent Crystallographic Papers

Quantum crystallography: A perspective. Massa, Lou; Matta, Chérif F. *Journal of Computational Chemistry*. 6/30/2018, Vol. 39 Issue 17, p1021-1028. Bp. DOI: 10.1002/jcc.25102.

Early days of quantum crystallography: A personal account. Tsirelson, Vladimir. *Journal of Computational Chemistry*. 6/30/2018, Vol. 39 Issue 17, p1029-1037. 10p. DOI: 10.1002/jcc.24893.

Design, synthesis and X-ray crystallography of selenides bearing benzenesulfonamide moiety with neuroprotific pain modulating effects. Angeli, Andrea; di Cesare Mannelli, Lorenzo; Lucarini, Elena; Pinat, Thomas S.; Ghelardini, Carla; Supuran, Claudiu T. *European Journal of Medicinal Chemistry*. Jun2018, Vol. 154, p210-219. 10p. DOI: 10.1016/j.ejmech.2018.05.026.

A novel water-soluble tetranuclear copper (II) Schiff base cluster bridged by 2, 6-bis-{(2-hydroxyethylimino)methyl}-4-methylphenol in interaction with BSA: Synthesis, X-ray crystallography, docking and cytotoxicity studies. Asadi, Zahra; Sedehi, Maryam; Eigner, Vaclav; Dusek, Michal; Amirghofran, Zahra. *Journal of Photochemistry & Photobiology A: Chemistry*. Jun2018, Vol. 361, p93-104. 12p. DOI: 10.1016/j.jphotochem.2018.05.010.

Experimental and theoretical studies of the neutron diffractometer at J-PARC for protein crystallography covering crystals with large unit cell volume. Kurihara, Kazuo; Hirano, Yu; Oikawa, Kenichi; Harada, Masahide; Nakamura, Tatsuya; Tamada, Taro. *Journal of Applied Crystallography*. Jun2018, Vol. 51 Issue 3, p596-605. 9p. DOI: 10.1107/S1600576718006723.

Real-space refinement in *PHENIX* for cryo-EM and crystallography. Afonine, Pavel V.; Poon, Billy K.; Read, Randy J.; Sobolev, Oleg V.; Terwilliger, Thomas C.; Urzhumtsev, Alexandre; Adams, Paul D. *Acta Crystallographica Section D, Structural Biology*. Jun2018, Vol. 74 Issue 6, p531-544. 13p. DOI: 10.1107/S2059798318006551.

Quantum crystallography: From the intersection to the union of crystallography and quantum mechanics. Matta, Chérif F. *Journal of Computational Chemistry*. 6/30/2018, Vol. 39 Issue 17, p1019-1020. 2p. DOI: 10.1002/jcc.25352.

Crystallography on Mars: Curiosity's Bragging right. Velbel, Michael A. *American Mineralogist*. Jun2018, Vol. 103 Issue 6, p837-838. 2p. DOI: 10.2138/am-2018-6468CCBYNCND.

Synthesis and single crystal X-ray diffraction analysis of five isostructural 2D MOCs. Singh, Sandeep K.; Srivastava, Krishna; Banerjee, Rahul; Prasad, Jagdish. *Polyhedron*. Jun2018, Vol. 147, p49-54. 6p. DOI: 10.1016/j.poly.2018.02.031.

Crystal structure analysis of a star-shaped triazine compound: a combination of single-crystal three-dimensional electron diffraction and powder X-ray diffraction. Goenka, Tatiana E.; van de Streek, Jacco; Meier, Herbert; Andernach, Lars; Opatz, Till. *Acta Crystallographica: Section B, Structural Science, Crystal Engineering & Materials*. Jun2018, Vol. 74 Issue 3, p284-29. 7p. DOI: 10.1107/S2052520618006686.

Structural Investigation, UV-Vis Analysis and Crystal Packing of Spiro[chromeno[4,3-*b*]quinoline-6,1′-cycloalkan]-7-amine: Novel Tacrine Hybrids by Single Crystal X-Ray Diffraction. Bonacorso, Hélio G.; Campos, Patrick T.; Silva, Letícia B.; Iglesias, Bernardo A.; Zanatta, Nilo; Hörner, Manfredo. *Journal of Chemical Crystallography*. Jun2018, Vol. 48 Issue 1/2, p19-31. 13p. DOI: 10.1007/s10870-018-0706-6.

Crystal structure, quantum mechanical investigation, IR and NMR spectroscopy of two new organic perchlorates: $(C_8H_{18})_2(CH_3)_4N_2O$ (I) and $(C_8H_{18})_2N_2)\cdot ClO_4(II)$. Bayar, I.; Khedhiri, L.; Soudani, S.; Lefebvre, F.; Ferretti, V.; Ben Nasr, C. *Journal of Molecular Structure*. Jun2018, Vol. 1161, p486-496. 11p. DOI: 10.1016/j.molstruc.2018.02.038.

Synthesis of highly fluorescent dibiphenyl dibenzo chrysene. Dhanunjayarao, Kunchala; Mukundam, Vanga; Ranga Naidu Chinta, Ramu V.; Venkatasubbaiah, Krishnan. *Journal of Organometallic Chemistry*. Jun2018, Vol. 865, p234-238. 5p. DOI: 10.1016/j.jorganchem.2018.04.026.

Structure Determination and Characterization of a Family of Primary Alcohol Solvates. Vasudevan, Kalyan V.; Peterson, Matthew L. *Journal of Pharmaceutical Sciences*. Jun2018, Vol. 107 Issue 6, p1489-1497. 9p. DOI: 10.1016/j.xphs.2018.01.020.

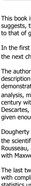
Aureochaeglobosins A–C, Three [4 + 2] Adducts of Chaetoglobosin and Azaanthracene Derivatives from *Chaetomium globosum*. Ming-Hua Yang; Mei-Ling Gu; Chao Han; Xiao-Jiang Guo; Guo-Ping Yin; Pei Yu; Ling-Yi Kong. *Organic Letters*. 6/1/2018, Vol. 20 Issue 11, p3345-3348. 4p. DOI: 10.1021/acs.orglett.8b01243.

Structural properties of barium stannate. Phelan, D.; Lopez-Bezanilla, A.; Rong, Y.; Zhang, Junjie; Zheng, H.; Krogstad, M.J.; Han, F.; Yang, Wenge; Gim, Y.; Cooper, S.L.; Parshall, D.; Feygenson, M.; Chen, Yu-Sheng. *Journal of Solid State Chemistry*. Jun2018, Vol. 262, p142-146. 7p. DOI: 10.1016/j.jssc.2018.03.016.

Confusion over the description of the quartz structure yet again. Glazer, A. M. *Journal of Applied Crystallography*. Jun2018, Vol. 51 Issue 3, p915-918. 3p. DOI: 10.1107/S1600576718004546.

Protonation of inorganic 5-Fluorocytosine salts. Souza, Matheus S.; Da Silva, Cecília C.p.; Almeida, Leonardo R.; Diniz, Luan F.; Andrade, Marcelo B.; Ellena, Javier. *Journal of Molecular Structure*. Jun2018, Vol. 1161, p412-423. 12p. DOI: 10.1016/j.molstruc.2018.02.071.

Book Review



***The Evolution of Scientific Knowledge: From Certainty to Uncertainty* by Edward O. Dougherty, SPIE Press, Bellingham, 2016, ISBN: 9781510607354.**

I came across this title at the book shop at a conference for the International Society for Optics and photonics (SPIE). The author is on the faculty of Texas A&M in the department of Electrical Engineering and Computer Science, as well as an SPIE fellow.

This book is about scientific epistemology—the theory of scientific knowledge. As the title suggests, the book covers how scientific knowledge has evolved from the time of Aristotle to that of genomics.

In the first two chapters the author takes us through an introduction to epistemology. In the next chapter he explains pre-17th century science.

The author posits the revolution in science occurs with the transition from the Copernican description of planetary motion to Kepler's three laws of planetary motion. Kepler's laws demonstrate the four basic components of a theory for the first time: observation, analysis, modeling and prediction of future events. This revolution culminates in the 17th century with Bacon, Galileo and Newton. The next step is determinism, in which Descartes, Laplace and Pascal all contribute greatly. Determinism is the paradigm that, given enough information, the future can be predicted.

Dougherty then spends a chapter looking at the philosophical changes brought about by the scientific revolution of the 17th century through the writings of Locke, Hume, Kant and Rousseau, as well as some later philosophers. The age of uncertainty in science begins with Maxwell and continues into the quantum era with the particle/wave duality crisis.

The last two chapters focus on the problem of big data and the modeling of large systems with complicated interdependencies. The author provides a brief description of Bayesian statistics using a simple mathematical model as an example.

The book is short—only 136 pages—but demanding, especially the chapter on philosophy.

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