Crystallography Times

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Crystallography Newsletter
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Final Thoughts for 2018

I would like thank Robert Tisdale, Bev Vincent and Dayva Beaudoin, who do most of the work in putting this newsletter together. This newsletter could not happen without them. I would also like to thank my daughter, Jeanette, who has been writing the books reviews for the last few months and will continue to do so during my year as President of the ACA.

Happy Holidays.

Joe

Crystallography in the News

November 22, 2018. Håkon Hope, who is considered the father of cryocrystallography, passed away after a short illness on November 22 at the age of 87.

December 3, 2018. DeepMind stunned the world as the UK's top AI team delivered their latest "wow moment" when their AI system AlphaFold topped the Critical Assessment of Structure Prediction (CASP) competition. CASP is a virtual protein-folding Olympics, where the aim is to predict the 3D structure of a protein based on its genetic sequence data.

December 4, 2018. Researchers from Charité – Universitätsmedizin Berlin, using X-ray crystallography, have demonstrated on a molecular level how a specific protein allows light signals to be converted into cellular information. When light hits a phytochrome, a complex process of transformation is triggered, which changes the 3D structure of the protein. Their findings have broadened the understanding of how plants and bacteria adapt to changes in light conditions that regulate essential processes such as photosynthesis.

December 5, 2018. Experiments in forest observation, protein crystal growth and in-space fuel transfer demonstration headed to the International Space Station following the launch of SpaceX's 16th mission for NASA under the agency's Commercial Resupply Services contract. Growth of large, perfect protein crystals for neutron crystallography (perfect crystals) crystallizes an antioxidant protein found inside the human body to analyze its shape. This research may shed light on how the protein helps protect the human body from ionizing radiation and oxidants created as a byproduct of metabolism.

December 6, 2018. Researchers from the UCLA Jonsson Comprehensive Cancer Center and the La Jolla Institute for Immunology have identified a new type of T cell called a phospholipid-reactive T cell that is able to recognize phospholipids, the molecules that help form cells' outer membranes.

December 12, 2018. Enzymes engineered to trap reaction intermediates: many enzymatic processes involve a mechanism in which reaction intermediates are covalently attached to the enzyme's active site. A strategy has been devised that enables mimics of these intermediates to be visualized.

December 13, 2018. Berkeley Lab researchers, in collaboration with scientists from SLAC National Accelerator Laboratory and the Max Planck Institute, have demonstrated that fluctuation X-ray scattering is capable of capturing the behavior of biological systems in unprecedented detail. Although this technique was first proposed more than four decades ago, its implementation was hindered by the lack of sufficiently powerful X-ray sources and associated detector technology, sample delivery methods, and the means to analyze the data.

December 14, 2018. The latest recipients of Germany's most prestigious research prize have been announced. The Joint Committee of the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) selected ten researchers, four women and six men, to receive the 2019 Gottfried Wilhelm Leibniz Prize.

December 17, 2018. A method called microcrystal electron diffraction can rapidly image

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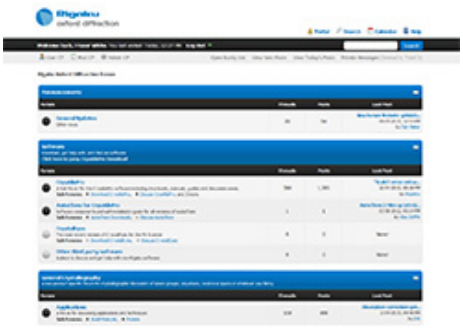

www.Rigakuxrayforum.com

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

the structures of small molecules, including those found in mixtures. Will it usurp X-ray crystallography for determining small-molecule structures?

Product Spotlight

XtaLAB Synergy-DW
One source with two high-flux wavelengths is the foundation of the revolutionary XtaLAB Synergy-DW single crystal X-ray diffractometer. It combines the increased flux of a rotating anode X-ray source with the flexibility of two different wavelengths, making it ideal for laboratories exploring a wide range of research interests.

The XtaLAB Synergy-DW diffractometer is based on the proven, low-maintenance MicroMax-007 HF microfocus rotating anode. The target is constructed with two different X-ray source materials (Cu and Mo) and is coupled with an auto-switching dual wavelength optic. Copper or molybdenum X-ray radiation is available at the click of a button. The XtaLAB Synergy-DW offers up to 12x higher flux compared to the standard sealed tube X-ray sources and, utilizing only one generator, means overall maintenance is reduced.

Rounding out the XtaLAB Synergy-DW configuration is the fast and efficient four-circle kappa goniometer which is compatible with a wide range of detectors including the HyPix-6000HE and other Hybrid Photon Counting (HPC) X-ray detectors e.g. PILATUS and EIGER detectors.

Features

- Access to two wavelengths in one compact system
- 12x higher flux than sealed tube X-ray sources
- Low maintenance, high performance system
- Uses CrysAlis^{Pro} software with both PX and SMX modes

Benefits

- Multi-functional diffractometer to cover you wherever your research takes you
- High flux performance means all your crystallography needs can be carried out 'in-house'
- Very little downtime and easy maintenance
- No need to purchase extra software for different applications

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Lab in the Spotlight

December 2018 SCX Survey

2018 is coming to a close. At the time of writing the US government is funding itself by continuing resolutions, Brexit is imminent, the yellow vests are rioting in France and Merkel is leaving office in Germany. Do you expect more funding for science in 2019?

- Yes
- No

Take the Survey

Videos of the Month

Here is a link to the 28th First Annual Ig Nobel awards. As always, science to make you laugh then think.

Watch the Video

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Rigaku Europe SE Application Laboratory

This past October we moved our application laboratory from Wrocław, Poland to the Rigaku Europe SE office in Neu-Isenberg, Germany, just ten minutes by car or bus from the Frankfurt airport. This move consolidates all of our European application labs in one easy-to-access location. The RESE facility also houses instruments for GP-XRD, SAXS and XRF. Now all of our European application scientists are in one location providing for cross-fertilization of ideas.

Normally, the XtaLAB Synergy-S, shown above, is configured with copper and molybdenum sources and a HyPix-6000HE detector. You may have noticed the snout on the detector in the picture seems a bit large. Right now we have the system configured with silver and molybdenum sources and a Dectris P300K CdTe detector. We will have this configuration running for the next few weeks. If you are interested in the advantages and capabilities of such a configuration for high pressure and/or charge density studies, please contact us to discuss the possibilities.

Useful Link

The Best Science Books Of 2018

Here is a link to the best science books of 2018 per Ira Flatow and a Science Friday panel. At the bottom of the page you'll find another list for young scientists.

Selected Recent Crystallographic Papers

Hydration Structures of the Human Protein Kinase CK2α Clarified by Joint Neutron and X-ray Crystallography. Shibazaki, Chie; Arai, Shigeki; Shimizu, Rumi; Saeki, Morihisa; Kinoshita, Takayoshi; Ostermann, Andreas; Schrader, Tobias E.; Kurosaki, Yuzuru; Sunami, Tomoko; Kuroki, Ryota; Adachi, Motoyasu. Journal of Molecular Biology. Dec2018, Vol. 430 Issue 24, p5094-5104. 11p. DOI: 10.1016/j.jmb.2018.09.018.

The first Fe(II) complex bearing end-to-end dicyanamide as a double bridging ligand: Crystallography study and Hirshfeld surface analysis; completed with a CSD survey. Setifi, Zouaoui; Geiger, David; Jelsch, Christian; Maris, Thierry; Glidewell, Christopher; Mirzaei, Masoud; Arefian, Mina; Setifi, Fatima. Journal of Molecular Structure. Dec2018, Vol. 1173, p697-706. 10p. DOI: 10.1016/j.molstruc.2018.07.049.

Crystallography, vibrational, electronic and optical analysis of 4-Bromo-2-(2,5-dichloro-phenylimino)-phenol. Soltani, Alireza; Javan, Masoud Bezi; Raz, Shima Ghafouri; Mashkoor, Reza; Khalaji, Aliakbar Dehno; Dusek, Michal; Fejfarova, Karla; Palatinus, Lukas; Rohlicek, Jan; Machek, Pavel. Journal of Molecular Structure. Dec2018, Vol. 1173, p521-530. 10p. DOI: 10.1016/j.molstruc.2018.01.009.

A combined X-ray crystallography and theoretical study of N—H…O*X* (*X* is =P and —C) hydrogen bonds in two new structures with a $(C—O)_2(N)P(=Y)$ (*Y* is O and S) skeleton. Vahdani Alviri, Banafsheh; Pourayoubi, Mehrdad; Farhadipour, Abolghasem; Necas, Marek; Bertolasi, Valerio. Acta Crystallographica: Section C, Structural Chemistry. Dec2018, Vol. 74 Issue 12, p1610-1621. 12p. DOI: 10.1107/S2053229618014006.

A new high-spin iron(III) bis(aqua) complex with the meso-tetra(para-chlorophenyl)porphyrin: X-ray crystallography, Hirshfeld surface analysis, magnetic, EPR and electrochemical properties. Dhifaoui, S.; Hajji, M.; Nasri, S.; Guerfel, T.; Daran, J. C.; Nasri, H. Research on Chemical Intermediates. Dec2018, Vol. 44 Issue 12, p7259-7276. 18p. DOI: 10.1007/s11164-018-3555-1.

Each month, Rigaku distributes two eNewsletters: *The Bridge*, which focuses on Materials Analysis, and *Crystallography Times*, which concentrates on X-ray crystallography.

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New phosphorus ylide palladacyclic: Synthesis, characterization, X-Ray crystal structure, biomolecular interaction studies, molecular docking and *in vitro* cytotoxicity evaluations. Karami, Kazem; Rahimi, Mahzad; Zakariazadeh, Mostafa; Buyukgungor, Orhan; Amirghofran, Zahra. Journal of Organometallic Chemistry. Dec2018, Vol. 878, p60-76. 17p. DOI: 10.1016/j.jorganchem.2018.09.018.

21st century developments in the understanding and control of molecular solids. Steed, Jonathan W. Chemical Communications. 12/7/2018, Vol. 54 Issue 94, p13175-13182. 8p. DOI: 10.1039/c8cc08277d.

Crystal polymorphs and *ab initio* calculation of 2,3,4,5,6-pentachlorobenzoic acid. Ozaki, Koji; Okuno, Tsunehisa. Journal of Molecular Structure. Dec2018, Vol. 1173, p959-963. 5p. DOI: 10.1016/j.molstruc.2018.07.067.

Crystallographic and spectroscopic studies as well as DFT quantum chemical calculations of hydrazo-bond conformation in 4,4'-dimethyl-3,3',5,5'-tetranitro-2,2-hydrazobipyridine. Kucharska, E.; Bryndal, I.; Lis, T.; Hermanowicz, K.; Hanuza, J. Journal of Molecular Structure. Dec2018, Vol. 1173, p750-762. 13p. DOI: 10.1016/j.molstruc.2018.07.040.

Crystallographic, dynamic and Hirshfeld surface studies of charge transfer complex of imidazole as a donor with 3,5-dinitrobenzoic acid as an acceptor: Determination of various physical parameters. Alam, Kehkashan; Khan, Ishaat M. Organic Electronics. Dec2018, Vol. 63, p7-22. 16p. DOI: 10.1016/j.orgel.2018.08.037.

The Structural and Functional Organization of Ribosomal Compartment in the Cell: A Mystery or a Reality? Karpova, Elizaveta A.; Gillet, Reynald. Trends in Biochemical Sciences. Dec2018, Vol. 43 Issue 12, p938-950. 13p. DOI: 10.1016/j.tibs.2018.09.017.

Two 3D Co(II) coordination polymers modulated by rigid tris(imidazolyl) ligands: Syntheses, structural diversity and photo-degradation properties. Fan, Chuanbin; Bi, Caifeng; Zong, Ziao; Zhu, Zheng; Xu, Cungang; Meng, Xiangmin; Zhang, Xia; Fan, Yuhua. Polyhedron. Dec2018, Vol. 156, p123-130. 8p. DOI: 10.1016/j.poly.2018.09.032.

Crystallographic and Computational Studies of Non-Covalent Interactions of Molecular Clips with a Series of Small Solvent Molecules. Alaparthi, Madhubabu; Vogel, Dayton Jonathan; Sykes, Andrew G. Journal of Chemical Crystallography. Dec2018, Vol. 48 Issue 4, p131-137. 7p. DOI: 10.1007/s10870-018-0720-8.

Design, synthesis and crystal structure of six macrocyclic complexes as efficient and effective nitric oxide scavengers. Cheng, Qingrong; Wan, Yuqi; Wang, Liwen; Liao, Guiying; Pan, Zhiquan. Polyhedron. Dec2018, Vol. 156, p249-256. 8p. DOI: 10.1016/j.poly.2018.08.061.

4'-(2H-tetrazol-5-yl)-[1,1'-biphenyl]-4-carboxylic acid: Synthetic approaches, single crystal X-ray structures and antimicrobial activity of intermediates. Ardeleanu, Rodinel; Dascalu, Andrei; Shova, Sergiu; Nicolescu, Alina; Rosca, Irina; Bratanovici, Bogdan-Ionel; Lozan, Vasile; Roman, Gheorghe. Journal of Molecular Structure. Dec2018, Vol. 1173, p63-71. 9p. DOI: 10.1016/j.molstruc.2018.06.086.

Protein topology determines substrate-binding mechanism in homologous enzymes. Herrera-Morande, Alejandra; Castro-Fernández, Victor; Merino, Felipe; Ramírez-Sarmiento, Cesar A.; Fernández, Francisco J.; Vega, M. Cristina; Guixé, Victoria. BBA - General Subjects. Dec2018, Vol. 1862 Issue 12, p2869-2878. 10p. DOI: 10.1016/j.bbagen.2018.09.007.

Copper(II) complexes of bidentate mixed ligands as artificial nucleases: Synthesis, crystal structure, characterization and evaluation of biological properties. Jayamani, Arumugam; Bellam, Rajesh; Gopu, Gopalakrishnan; Ojwach, Stephen O.; Sengottuvelan, Nallathambi. Polyhedron. Dec2018, Vol. 156, p138-149. 12p. DOI: 10.1016/j.poly.2018.09.011.

A new potassium-based coordination polymer with hydrogen bonding and zigzag metallophilic interactions. Moghadam, Zarin; Akhbari, Kamran; White, Jonathan; Phuruangrat, Anukorn. Applied Organometallic Chemistry. Dec2018, Vol. 32 Issue 12, pN.PAG-N.PAG. 1p. DOI: 10.1002/aoc.4613.

Synthesis, X-ray structure, in silico calculation, and carbonic anhydrase inhibitory properties of benzylimidazole metal complexes. Bouchouit, Mehdi; Bouacida, Sofiane; Zouchoune, Bachir; Merazig, Hocine; Bua, Silvia; Bouaziz, Zouhair; Le Borgne, Marc; Supuran, Claudiu T.; Bouraiou, Abdelmalek. Journal of Enzyme Inhibition & Medicinal Chemistry. Dec2018, Vol. 33 Issue 1, p1150-1159. 10p. DOI: 10.1080/14756366.2018.1481404.

Book Review

The Tangled Tree: A Radical New History of Life
By David Quammen

David Quammen's *The Tangled Tree* is an absolute delight. In many ways, it feels like a biography of Carl Woese, the microbiologist who defined the domain of Archaea in 1977. Despite over 40 years having passed since then, Woese's definition challenged our fundamental understanding of evolutionary biology.

However, *The Tangled Tree* is more than just a biography—calling it that does an insult to the work and the writer—it's more like a biographical history of evolutionary biology. Quammen declares in his introduction "this book is about a new method of telling that story [of life], a new method of deducing it, and certain unexpected insights that have flowed from the new method. The method has a name: molecular phylogenetics." The line that follows illustrates the engaging tone Quammen takes throughout the book (and the wordiness): "Wrinkle your nose at that fancy phrase, if you will, and I'll wrinkle with you, but, in fact, what it means is fairly simple: reading the deep history of life and the patterns of relatedness from the sequence of constituent units in certain long molecules, as those molecules exist today within living creatures."

In other words, "molecular phylogenetics" means using patterns in DNA, RNA, and certain proteins to determine how life evolved on Earth. This shouldn't come as a surprise. The Human Genome project largely concluded in 2003, and researchers have been charting the genome of various species for quite some time now. Scientists have long known that the key to evolution lies in DNA—perhaps not only ours, but that of other organisms, namely single-celled nucleus-less ones, i.e. Archaea.

The heart of Quammen's book isn't just science—it is scientists. He introduces Woese early on, along with numerous other key players in this history of the history of life, including Lynn Margulis (also known as the first wife of famed astrophysicist Carl Sagan) and Ford Doolittle, a biologist who published an essay called "Uprooting the Tree of Life"—that sought to do just that.

Quammen starts the book, post-introduction, where you might suspect he would: with Charles Darwin. He gives a brief introduction to Darwin, his studies and his *Origin of Species*, but only enough to give quality context to the chapters ahead. Darwin occupies Part I of VII—only eight short chapters in a book of eighty-four. His work laid the foundation for modern evolutionary biology, and so it must be taken into consideration.

From Darwin, Quammen moves quickly to Crick and others, before settling on Woese in Chapter 11, where he stays for quite some time, straying to others in the field like Margulis and Doolittle, but ultimately always tying the story back in to Woese. You'll have to read the book to find out how—and I highly recommend it.

Quammen's prose is artistic and informative. His presentation and attention to detail flows naturally—it is easy to forget you are reading a work of nonfiction, because the characters and the story are so captivating. His chapters, though numerous, have a fairly short average length—a good metaphor for his storytelling style. Quammen has a lot to tell, and tells it well and concisely. Each chapter ties into the narrative neatly, pushing the reader further on. As a reader, you have the context and explanation you need to keep the story and the science moving forward. Should you want more, there is an extensive index at the end.

Review by Jeanette S. Ferrara, MA

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