Crystallography Times

Rigaku oxford diffraction

Crystallography Newsletter
Volume 10, No. 07, July 2018
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In this issue:

Come visit us at:

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

Denver X-ray Conference
Westminster, Colorado, August 6 – 10, 2018

31st European Crystallographic Meeting, ECM31
Oviedo, Spain, August 22 – 27, 2018

31st European Crystallographic Meeting, ECM31
Oviedo, Spain, August 22 – 27, 2018

XVII International Small Angle Scattering Conference – SAS2018
Traverse City, Michigan, October 7 – 12, 2018

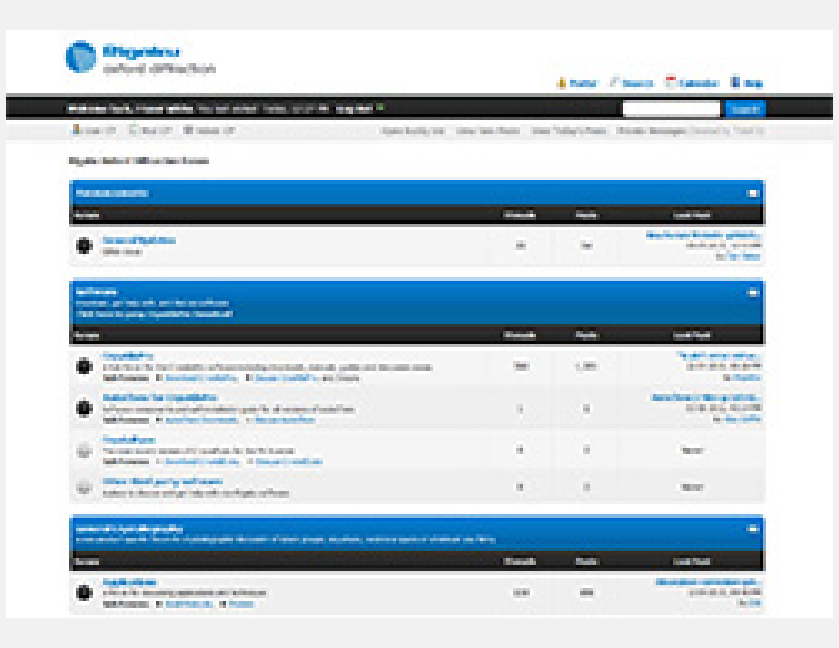
Abstract Submission Deadlines

AsCA 2018
Due August 14, 2018

Join ROD 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

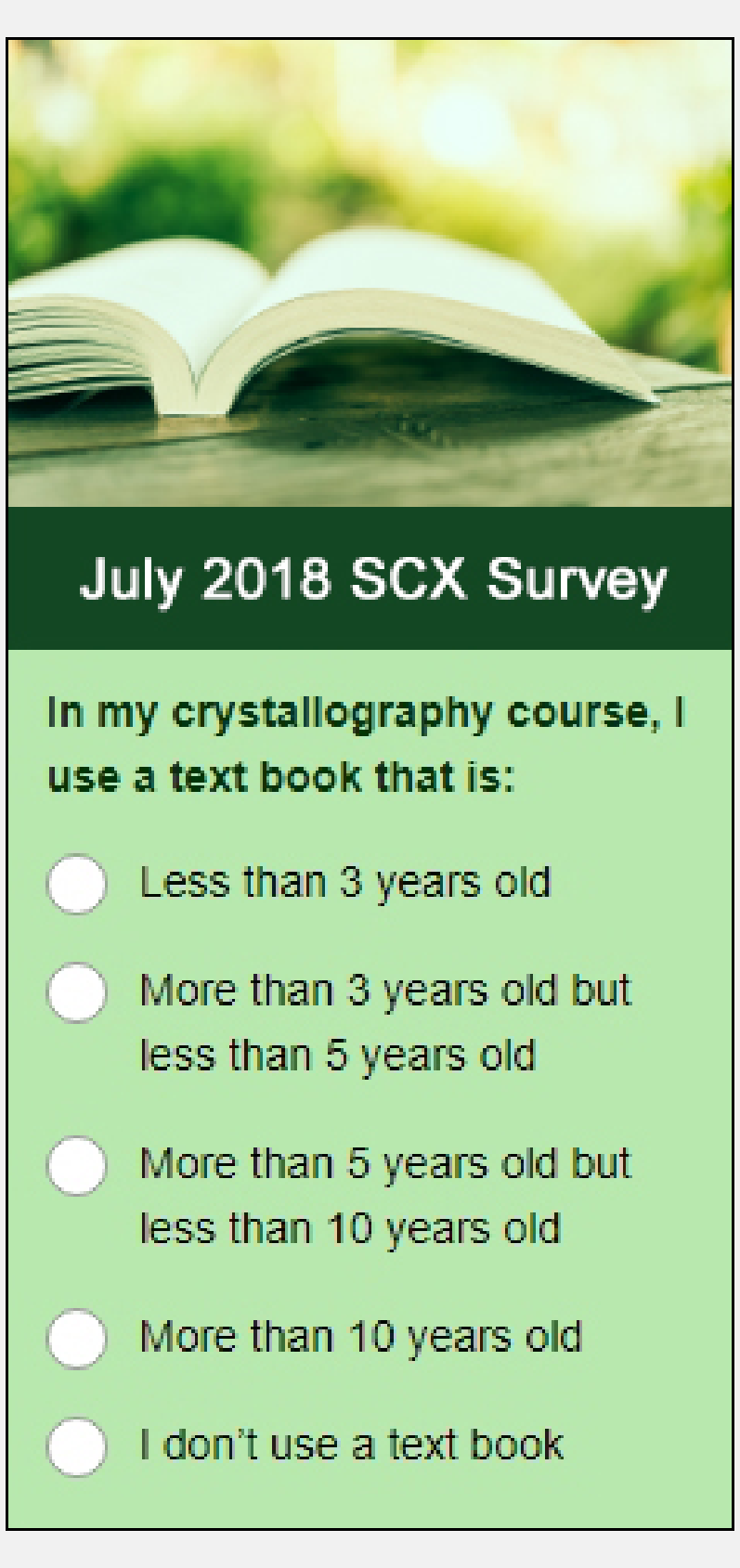


www.Rigakuxrayforum.com

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



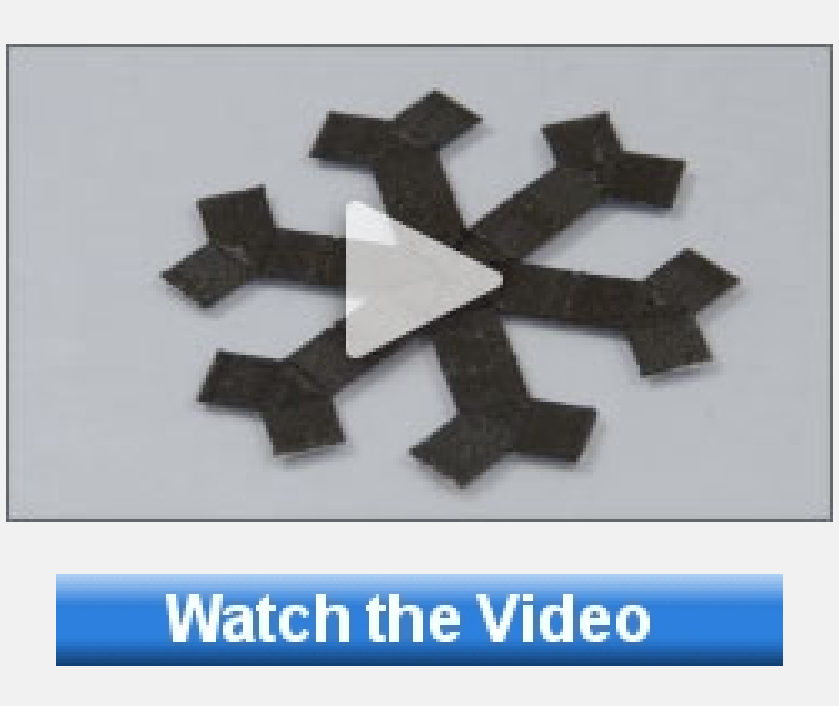
Take the Survey

Last Month's Survey

Big data has come to mean more than just the volumes of digital data being created today. It has also come to mean the analytics that extract useful information from the data itself.

Video of the Month

Here is a video from *Nature* on the production and characterization of 11.4 nm silica dodecahedra. By the way, the link takes you to the *Nature* YouTube channel where you'll find lots of interesting videos.



Watch the Video

Subscribe to Rigaku eNewsletters

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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Crystallography in the News

July 1, 2018. New research by Prof. Timothy Hanusa at Vanderbilt University explains why some molecules have irregular forms. The new calculations show how dispersion and covalent effects can work together to change the structure of molecules.

July 2, 2018. A team from the University of Bristol has created new virtual reality (VR) cloud-based tools that could lead to new drug discoveries and boost the teaching of chemistry by combining real-time molecular simulations with VR technology.

July 3, 2018. Scientists have devised a new strategy for synthesizing notoriously difficult carbocyclic 5-8-5 fused ring systems, a molecular structure with broad therapeutic potential.

July 3, 2018. Researchers at Berkeley have produced the first detailed picture of the molecular structure of human telomerase, an enzyme that plays key roles in both the repair of aging cells and the endless cellular rejuvenation typical of cancers.

July 3, 2018. Atomic manipulation has been used to create the most complex molecule ever assembled using this technique. The structure is a molecular wire with a carbon backbone that was manipulated to have as many as eight triple bonds.

July 5, 2018. A new overview article on "X-ray Crystallography: Exploring Frontiers of Structural Biology" has been published on-line. The author, Dr. Alison Halliday, specializes in writing about research across the life sciences, medicine and health.

July 6, 2018. The Board on Higher Education and Workforce of the U.S. National Academies of Sciences, Engineering, and Medicine (NASEM) released a report recommending that humanities, arts, crafts, and design (HACD) practices be integrated with science, technology, engineering, mathematics, and medicine (STEMM) in college and post-graduate curricula.

July 6, 2018. A series of articles published by the Tye (HKUST)/Gao (Peking University) collaboration opens the door for deciphering the function of the DNA replication machinery at unprecedented resolutions. The third article now appears in *Nature*, detailing the atomic structure of the Origin Recognition Complex (ORC) that selects start sites genome-wide to initiate DNA replication.

July 6, 2018. Designing new molecules for pharmaceuticals is primarily a manual, time-consuming process that's prone to error. But researchers have now taken a step toward fully automating the design process, which could drastically speed things up – and produce better results.

July 6, 2018. Joachim Frank, a German-American Nobel Laureate in chemistry based at Columbia University, New York, traced the history of cryo-EM to the present day in his lecture at the 68th Lindau Nobel Laureate meeting in Germany.

July 7, 2018. Scientists from Lancaster University and the University of Leeds have discovered that a compound found in green tea, currently being studied for its ability to reduce amyloid plaques in the brain in Alzheimer's disease, also breaks up and dissolves potentially dangerous protein plaques found in the blood vessels.

July 9, 2018. Chemists at the University of Utah and the University of California San Diego used computer simulations of antifreeze proteins and water to understand what's going on at a molecular level. They found that the protein molecules just need to be parallel to ice crystal surfaces to bind to the ice – no need for the surrounding water molecules to organize into an ice-like structure before the proteins attached, like scientists previously supposed.

July 9, 2018. Deb Kelly, an associate professor at the Virginia Tech Carilion Research Institute, was awarded $2.1 million by the National Cancer Institute (NCI) to study the BRCA1 protein that gives rise to a hard-to-treat form of breast cancer. This is her third concurrent R01 grant, which funds a specific line of research for five years, from the NCI of the National Institutes of Health (NIH).

Product Spotlight

CrysAlis^{Pro}

CrysAlis^{Pro} v40

Now with full 64-bit compatibility!
Rigaku Oxford Diffraction single crystal X-ray diffractometers come complete with CrysAlis^{Pro}, our user-inspired data collection and data processing software for small molecule and protein crystallography. Designed around an easy-to-use graphical user interface, CrysAlis^{Pro} can be operated under fully automatic, semi-automatic or manual control.

The latest release, CrysAlis^{Pro} v.40, is now fully 64-bit compatible and ready for the future. As modern diffractometers increase in performance and speed, your experiments generate bigger and bigger images and datasets. Additionally, supporting large detectors with very high pixel counts, such as those commonly found at synchrotrons, requires large amounts of memory. Moving to 64-bit architecture gives applications access to more memory, enabling the handling of these very large image sizes and data sets more easily and speedily on any 64-bit computer.

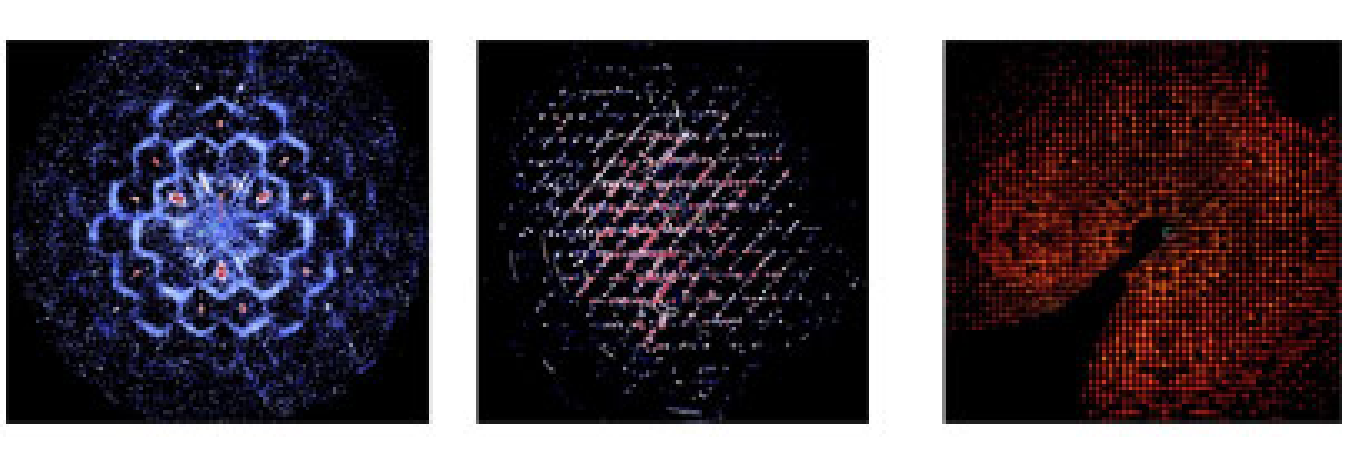
Also, in this release, is further expanded support for older Rigaku instrumentation. New third party hardware support is also increased.

CrysAlis^{Pro}: Seamless from start to finish
CrysAlis^{Pro} combines automated crystal screening, the fastest and most accurate strategy available, concurrent data reduction and automatic small molecule structure solution. Visual feedback is provided for each step with clear, color-coded guidance so that both novices and experts can collect high-quality data in the shortest time possible.

We also understand that not everyone likes automation. CrysAlis^{Pro} is built on a command line interface and the GUI retains full manual control options for those that want them. It is your choice how to analyse your data. Processing data is, of course, very important too. CrysAlis^{Pro} incorporates many sophisticated algorithms to provide the highest quality data. Our software team is always adding new approaches for data analysis and processing.

Processing of challenging and non-standard data collections
CrysAlis^{Pro} contains a comprehensive and highly effective range of tools for dealing with a full range of samples from easy to challenging, and non-standard crystal samples. EwaldExplorer and Ewald3D (NEW!) are the tools that have been developed to easily identify effects, problems or artifacts in difficult or problematic datasets.

Ewald3D allows visualization of measured reciprocal space in 3 dimensions and in an undistorted way. Identifying diffuse scatter, modulation, subtle twinning, or incorrect instrument models is quick and easy with this new feature.



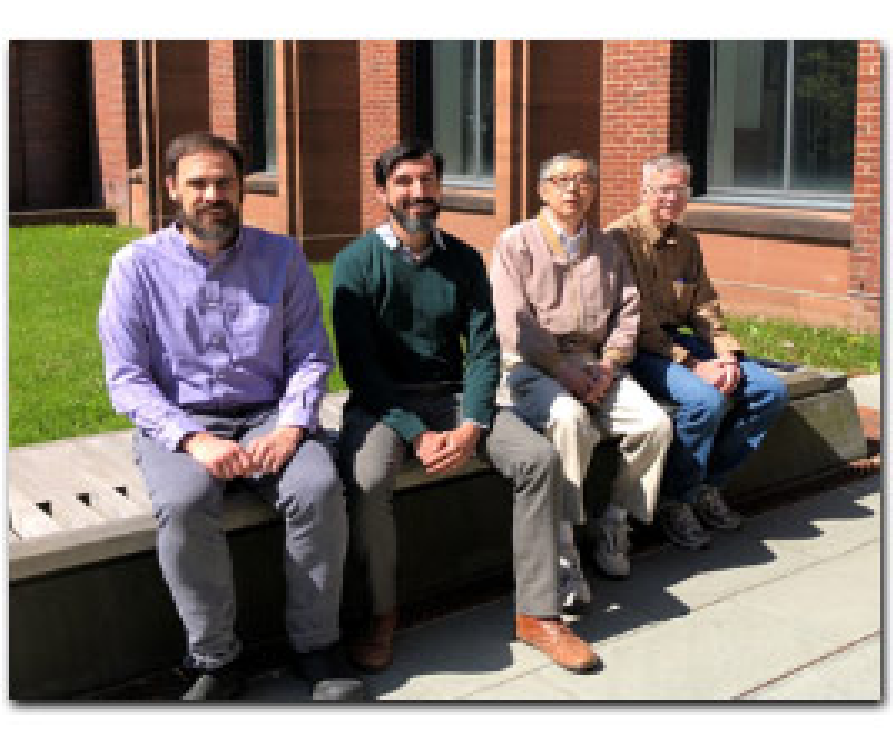
From left to right: An example of diffuse scattering, multiple crystals and a protein.

Supporting a range of crystallographic setups and applications
In addition to standard data collection routines, CrysAlis^{Pro} contains tools for working with non-standard experimental setups and sample types, including:

- High pressure data collections
- Variable temperature and multi-wavelength experiments
- Powder experiments (data collection and processing)
- Automatic screening or full data collections of several *in situ* protein crystals
- Highly absorbing samples
- Up to 8-fold twinned samples
- Charge density measurements
- Absolute structure determination

How to get CrysAlis^{Pro}
CrysAlis^{Pro} is freely available for users of Rigaku Oxford Diffraction single crystal X-ray instruments and can be downloaded from our forum. Please register at https://www.rigakuxrayforum.com. Any queries related to the software may be answered on the forum.

Lab in the Spotlight



From left to right, Eric Paulson, Ph.D., Director of CBIC and NMR spectroscopist, Brandon Mercado, Ph.D. Crystallographer, Xiaoling Wu, Ph.D., NMR spectroscopist, David Keller, research support.

The **Chemical and Biophysical Instrumentation Center (CBIC)** X-Ray facility in the Department of Chemistry at Yale University conducts characterizations by a number of X-ray techniques. The majority of data collected in the CBIC X-ray lab are diffraction images of macromolecular, small-molecule organic or inorganic single crystals. The lab is also equipped with X-ray sources that can be used for powder diffraction, small angle X-ray scattering, and microCT scanning. The majority of samples are submitted by members of research groups in the chemistry department. As an extension service, the facility also accepts sample submissions from other departments at Yale, as well as local, national, and international collaborators in academia and industry. The CBIC also hosts a comprehensive instrument suite that includes a vast array of medium and high frequency NMR spectrometers; GC/LC/MALDI-TOF mass spectrometers; UV/vis/NIR/fluorescence/Raman spectrometers; polarimeter; CD; DLS; ITC; AU. The facility is operated by full-time staff who can provide detailed analyses for submitted samples. Students interested in learning the practical application and theory of X-ray diffraction are encouraged to take CHEM553, Small Molecule Crystallography, taught by Dr. Brandon Mercado. The Departmental X-ray Crystallography Facility houses six diffractometers that are available to the research community. The lab has roughly 1200 sq ft. of contiguous space and currently houses:

- R-AXIS RAPID with a SPIDER imaging plate, copper sealed tube with SHINE optics, Oxford 700 cryostream
- SCXmini with a Mercury275R CCD, molybdenum sealed tube with SHINE optics, Oxford 700 cryogenic system for cooling crystals
- MicroMax-007 HF+ copper rotating anode with two active ports
  - Right port: AFC11/Saturn 994 HG CCD, X-stream cryogenic system
  - Left port: AFC11/Saturn 994+, Oxford 700 cryogenic system
- MicroMax-007 ArcSecVHF+ molybdenum rotating anode and AFC kappa/PILATUS 200K detector
- MiniFlex 600 powder diffractometer

Other resources include:

- 4 microscopes, one with a CRT monitor for teaching, another with an X-stream cryogenic cooling system to screen temperature/air/moisture sensitive samples
- Sample preparation and wet-lab areas
- Mosquito nanoliter drop setter for crystallization tray preparation
- Nikon XT H 225 microCT imaging system
- 8 computer terminals running Windows 10 with access to CrysAlisPro, Cambridge Structural Database, SHELX and OLEX2 software packages for small molecule refinement
- A LINUX-based workstation with SBgrid and HKL2000 software packages for macromolecular refinement
- A Windows 10 terminal with PDXL2 and FullProf software packages for powder phase ID and Rietveld refinement

Useful Link

About IUCr

Here is a useful link to a poster describing the IUCr in a nutshell: International Union of Crystallography

Selected Recent Crystallographic Papers

Towards the synthesis of prenylated phloroglucinol derivatives: An X-ray crystallographic and DFT study of unexpected reaction products. Akerman, Matthew P.; van Heerden, Fanie R.; Mkhize, Zimbili. *Journal of Molecular Structure*. Jul2018, Vol. 1164, p438-446. 9p. DOI: 10.1016/j.molstruc.2018.03.097.

Cinnamamide pharmacophore for anticonvulsant activity: evidence from crystallographic studies. Zeslawska, Ewa; Nitek, Wojciech; Marona, Henryk; Gunia-Krzyzak, Agnieszka. *Acta Crystallographica: Section C, Structural Chemistry*. Jul2018, Vol. 74 Issue 7, p782-788. 6p. DOI: 10.1107/S2053229618007660.

Evaluation of N—H...S and N—H...p interactions in *O,O'*-diethyl *N*-(2,4,6-trimethylphenyl)thiophosphate: a combination of X-ray crystallographic and theoretical studies. Torabi Farkhani, Elham; Pourayoubi, Mehrdad; Izadyar, Mohammad; Andreev, Pavel V.; Shchegravina, Ekaterina S. *Acta Crystallographica: Section C, Structural Chemistry*. Jul2018, Vol. 74 Issue 7, p847-855. 8p. DOI: 10.1107/S2053229618007933.

Electron diffraction and three-dimensional crystallography for structural biology. Clabbers, Max T. B.; Abrahams, Jan Pieter. *Crystallography Reviews*. Jul2018, Vol. 24 Issue 3, p176-204. 29p. DOI: 10.1080/0889311X.2018.1446427.

***Cinder*: keeping crystallographers app-y.** Rosa, Nicholas; Ristic, Marko; Marshall, Bevan; Newman, Janet. Acta Crystallographica: Section F, *Structural Biology Communications*. Jul2018, Vol. 74 Issue 7, p410-418. 8p. DOI: 10.1107/S2053230X18008038.

Exploiting the full quantum crystallography. Massa, Lou; Matta, Chérif F. *Canadian Journal of Chemistry*. 2018, Vol. 96 Issue 7, p599-605. 7p. DOI: 10.1139/cjc-2017-0667.

What is behind a successful academic carrier? Editorial for Crystallography Reviews, Issue 3 of 2018. Bombicz, Petra. *Crystallography Reviews*. Jul2018, Vol. 24 Issue 3, p147-148. 2p. DOI: 10.1080/0889311X.2018.1478639.

Nucleic acid crystallography: methods and protocols. Soler-Lopez, Montserrat; Leonard, Gordon. *Crystallography Reviews*. Jul2018, Vol. 24 Issue 3, p211-214. 4p. DOI: 10.1080/0889311X.2018.1437724.

ClusPro FMFT-SAXS: Ultra-fast Filtering Using Small-Angle X-ray Scattering Data in Protein Docking. Ignatov, Mikhail; Kazennov, Andrey; Kozakov, Dima. *Journal of Molecular Biology*. Jul2018, Vol. 430 Issue 15, p2249-2255. 7p. DOI: 10.1016/j.jmb.2018.03.010.

Adsorption of lysozyme on pH-responsive PnBA-b-PAA polymeric nanoparticles: studies by stopped-flow SAXS and ITC. Filippov, Sergey K.; Papagiannopoulos, Aristeidis; Riabtseva, Anna; Pispas, Stergios. *Colloid & Polymer Science*. Jul2018, Vol. 296 Issue 7, p1183-1191. 9p. DOI: 10.1007/s00396-018-4329-4.

Effects of a lysophosphatidylcholine and a phosphatidylcholine on the morphology of taurocholic acid-based mixed micelles as determined by small-angle X-ray scattering. Aizawa, Hideki; Ichikawa, Sosaku; Kotake-Nara, Eiichi; Nagao, Akihiko. *Journal of Dispersion Science & Technology*. 2018, Vol. 39 Issue 7, p1003-1009. 7p. 1 Chart, 3 Graphs. DOI: 10.1080/01932691.2017.1380529.

New topology of levyne B under quasi-equilibrium conditions: A temperature-dependent *in situ* single crystal X-ray diffraction study. Cametti, G. *Microporous & Mesoporous Materials*. Jul2018, Vol. 265, p162-171. 10p. DOI: 10.1016/j.micromeso.2018.02.002.

Single-crystal x-ray diffraction structures of covalent organic frameworks. Ma, Tianqiong; Kapustin, Eugene A.; Yin, Shawn X.; Liang, Lin; Zhou, Zhengyang; Niu, Jing; Li, Li-Hua; Wang, Yingying; Su, Jie; Li, Jian; Wang, Xiaoge; David Wang, Wei; Wang, Wei; Sun, Junliang; Yaghi, Omar M. *Science*. 7/6/2018, Vol. 361 Issue 6397, p48-52. 5p. 4 Diagrams. DOI: 10.1126/science.aat7679.

First copper(II)-cyclophosphato complex with macrocyclic N-donor ligand: Single crystal structure elucidation with Hirshfeld surface analysis, optical, electrochemical and antioxidant properties. Hemissi, Hanène; Fezai, Ramzi; Mezni, Ali; Besbes-Hentati, Salma; Rzaigui, Mohamed. *Journal of Solid State Chemistry*. Jul2018, Vol. 263, p1-10. 10p. DOI: 10.1016/j.jssc.2018.04.004.

Influence of rare earth gadolinium nitrate addition on structural, dielectric, linear and nonlinear optical properties of glycine single crystals. Vijayalakshmi, V.; Dhanasekaran, P.; Ganesan, N.M. *Journal of Crystal Growth*. Jul2018, Vol. 493, p30-33. 4p. DOI: 10.1016/j.jcrysgro.2018.04.021.

Synthesis, characterization, single crystal structure and theoretical studies of trans-Ni(II)-complex with dithiophosphonate ligand. Karakus, Mehmet; Kara, Izzet; Çelik, Ömer; Orujalipoor, Ilghar; Ide, Semra; Yilmaz, Hamza. *Journal of Molecular Structure*. Jul2018, Vol. 1163, p128-136. 9p. DOI: 10.1016/j.molstruc.2018.02.110.

New complexes constructed based on (1*H*-tetrazol-5-yl)phenol: Synthesis, structures and properties. Xie, Fei; Du, Ceng-Ceng; Dong, Jun-Liang; Du, Jia-Qiang; Han, Ying-Zhi; Wang, Duo-Zhi. *Polyhedron*. Jul2018, Vol. 149, p17-24. 8p. DOI: 10.1016/j.poly.2018.04.016.

MoF_5 revisited. A comprehensive study of MoF_5. Stene, Riane E.; Scheibe, Benjamin; Pietzonka, Clemens; Karttunen, Antti J.; Petry, Winfried; Kraus, Florian. *Journal of Fluorine Chemistry*. Jul2018, Vol. 211, p171-179. 9p. DOI: 10.1016/j.jfluchem.2018.05.002.

Perfluoroalcohols: The Preparation and Crystal Structures of Heptafluorocyclobutanol and Hexafluorocyclobutane-1,1-diol. Baxter, Amanda F.; Schaab, Jonas; Christe, Karl O.; Haiges, Ralf. *Angewandte Chemie*. 7/2/2018, Vol. 130 Issue 27, p8306-8309. 4p. DOI: 10.1002/ange.201804101.

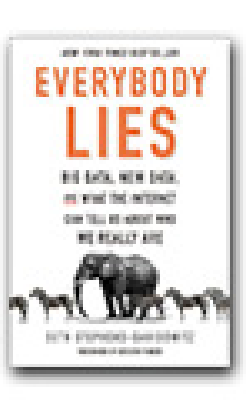
Syntheses, crystal structures and photoluminescence properties of five Cd/Zn–organic frameworks. Xue, Dong-Xu; Zhang, Yu-Feng; Zhang, Zong-Hui; Gao, Ziwei; Li, Qing. *Journal of Molecular Structure*. Jul2018, Vol. 1164, p123-128. 6p. DOI: 10.1016/j.molstruc.2018.03.048.

Crystal structure, vibrational studies and optical properties of a new molybdo-tellurate $Na_6(TeMo_6O_{24})(H_2SO_4)_2\cdot 12H2O$. Bouallegui, Thamer; Chebbi, Hamouda; Haddad, Amor; Ayed, Brahim. *Journal of the Iranian Chemical Society*. Jul2018, Vol. 15 Issue 7, p1505-1511. 7p. DOI: 10.1007/s13738-018-1348-5.

A New Metal–Organic Framework with Pentanuclear Zinc Clusters as Secondary Building Units. Xue, Xiaofei; Liu, Yuqi; Liu, Qiang; Wang, Xinying; Li, Wei; Peng, Jinhui. *Journal of Cluster Science*. Jul2018, Vol. 29 Issue 4, p625-632. 8p. DOI: 10.1007/s10876-018-1377-3.

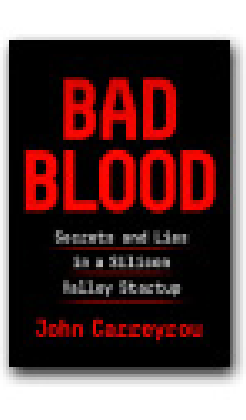
Molecular structures of some bivalent metal complexes of 1-(4-acetylphenyl)imidazole and co-ligands. Behera, Nibedita; Manivannan, Vadivelu. *Polyhedron*. Jul2018, Vol. 149, p84-94. 11p. DOI: 10.1016/j.poly.2018.04.023.

Book Reviews



***Everybody Lies: Big Data, New Data, and What the Internet Can Tell Us About Who We Really Are* by Seth Stephens-Davidowitz, HarperCollins, New York, 2017, 352 pages, ISBN-13: 978-0062390851.**

Seth Stephens-Davidowitz is a former Google data scientist and currently a lecturer at the Wharton School. He hypothesizes that surveys and Facebook do not reflect our true inner selves. The answers we provide in surveys and what we put on Facebook reflect what we want other people to think, not what we actually think. On the other hand, the anonymity of the Google search, and the ability to slice and dice the resultant data, allows one skilled in the art of analytics to extract a true view of what we are thinking and feeling in near real-time. Stephens-Davidowitz provides many examples including tracking the flu, unemployment and racial slurs and how the results compare to Centers for Disease Control, Bureau of Labor Statistic and election results. He also demonstrates the ease with which hypotheses can be tested on the general population through big data in ways that would not pass ethics reviews otherwise. Warning: there is a lot of explicit language in this book – it is not for youngsters.



***Bad Blood: Secrets and Lies in a Silicon Valley Startup* by John Carreyou, Penguin Random House, New York, 2018, 352 pages, ISBN-13: 978-1524731656.**

I hate to use a cliché, but this book is a page-turner, even though I already knew that the principals of Theranos, Elizabeth Holmes and Ramesh "Sunny" Balwani, had been indicted on multiple charges of wire fraud and conspiracy to commit wire fraud. Carreyou does a superb job of narrative setup before he comes on the scene as a reporter for *The Wall Street Journal*, then outlining the details of how he and the *WSJ* brought the facts to light, and kept going in spite of all manner of legal threats.

Theranos proposed using modern biochemistry and microfluidics to analyze a drop of blood using a small benchtop analyzer. It's a great idea, but Theranos could not execute it, failed to deliver on promises, and began to lie. The lies took many forms, but the most egregious was the production of false results on the very blood tests that made them famous. Patients were being misdiagnosed. Imagine learning your potassium level is so high you could have a heart attack at any moment, when you previously thought you were not at risk? Here is an example of vaporware with the possibility of tragic consequences.

Review by Joseph Ferrara
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