Crystallography Times

Rigaku oxford diffraction

Crystallography Newsletter
Volume 10, No. 09, September 2018
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In this issue:

Come visit us at:

XVI International Small Molecule X-ray Crystallography Conference – SMCRA
Traverse City, Michigan, October 7 – 12, 2018

IACA III: Meeting of the Latin American Crystallographic Association
Valparaíso, Chile, October 10 – 12, 2018

74th Pittsburgh Diffraction Conference
Cleveland, Ohio, October 14–18, 2018

Rigaku Symposium at Yale University
New Haven, Connecticut, October 19, 2018

AsCA 2018/SCTA 32: Conference of the Asian Crystallographic Association (AsCA) and the Society of Crystallographers in Australia and New Zealand (SCANZ)
Auckland, New Zealand, December 2 – 5, 2018

Join RQO 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 Reagents:
JCSG Core Suite screens

JCSG Core Suite screens each contain 96 unique formulations delivered in a deep well block at 1.7 ml volumes. These screens were designed by analyzing over 500,000 high-throughput crystallization experiments performed at the JCSG. These screens have provided the highest hit ratios.

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Rigaku Oxford Diffraction Forum

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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 CrysAlisPro software for single crystal data processing.

We look forward to seeing you on there soon.

Survey of the Month

September 18 SCX Survey

The other day I came across a box of 4 mm tape cartridges from the early 80s. I have no means to read them, other than perhaps through some expensive archive retrieval service. Any results from them have been long published.

- Should I keep the tapes. just in case I might need them at some distant point in the future?
- Should I dispose of them properly?
- What are tapes?

Take the Survey

Last Month's Survey

The newsletter is currently distributed monthly. We are considering going to an extended format newsletter that will be distributed quarterly. Which would you prefer?

Videos of the Month

What is the significance of the sequence: 1,1,in,5,6,3,1 . I did not know until I came across this video at Numberphile. By the way, there is lots of other interesting information about numbers on this channel.

Watch the Video

Here is a video fresh from the Science website showing calcium signalling in a plant due to injury:

Watch the Video

Subscribe to Rigaku eNewsletters

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

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Crystallography in the News

September 1, 2018. Victoria Sheehan, a Scottish artist, collaborated with Dr. Linda Long, a biochemist at Uniwer Sheffield, to develop a method to generate music that represents the three-dimensional structure of proteins. Using the data from X-ray Crystallography, the computer assigns note sequences to specific features of the protein.

September 6, 2018. Andy Kerr, a graduate student at Uniwer Sheffield, discovered that a mutation of one gene in a mouse causes osteoporosis in mouse models. When scientists, led by Sahar Tamasi, Professor of Chemistry and the Princeton Faculty Fellow in the Science and Technology of Materials, at Princeton University compared the pattern of prime numbers among a length of genes in humans with the atomic patterns revealed when crystals are blasted with X-rays, they were surprised by the similarities.

September 6, 2018. One of the major known causes of amyotrophic lateral sclerosis (ALS) is a mutation in the gene encoding SOD1 that causes the protein to fold in the wrong way, and aggregated SOD1 has been found in the motor neurons of both familial and sporadic ALS patients. Scientists at the Gladstone Institute in Sweden have now discovered how the mouse protein can "transmit" its morbidity to other normal proteins.

September 6, 2018. Scientists at research groups in Bucharest and Iaşi Romania used X-ray crystallography to show how an antibiotic resistance enzyme (AadA) is able to recognise and inactivate two chemically different antibiotics (streptomycin and spectinomycin).

September 10, 2018. A research collaboration between Department of Molecular Biology and Genetics at Aarhus University and two American universities reveals that bacterial transcription elongation factors (EF-G1 and probably also factor 2)Phase – structure and function are far more complex than previously assumed. In Saren Tholp's group, X-ray crystallography revealed that a second EF-G (EF-G2) has shown that EF-G bound to a variant of GTP, GDPNP, can also occur in the "off" state, which is characterized by a more open structure.

September 12, 2018. Ten outstanding articles have been shortlisted for this year's Max Perutz Science Writing Award, which celebrates Perutz's annual writing competition. The award is named in honor of one of the UK's most outstanding scientists and communicators, Dr. Max Perutz, who, shortly after his death in 2002, was awarded the Nobel Prize in Chemistry for his work using X-ray crystallography to study the structures of globular proteins.

September 12, 2018. A team of researchers at the University of Manchester has created the most tangled interlocked molecule ever. In their paper published in the journal Nature Chemistry, the researchers provide crystal structures that show that such knots will one day become useful.

September 13, 2018. Scientists at Monash University's Biomedicine Discovery Institute and the ARC Centre of Excellence in Advanced Molecular Imaging, working with the Australian Synchrotron, have presented a key question about how a dangerous bacterium, Clostridium perfringens, shares its genetic information.

September 16, 2018. Rutgers University leaders formally opened their new $115 million Science Building. The 180,000-square-foot Chemical Biology building was named after New Jersey's Building Our Future Bond Act. The four-story facility in Piscataway has everything students and researchers need to perform state-of-the-art research, school officials said. It has a humidity and temperature-controlled climate, a microscopy suite, and nuclear magnetic resonance spectroscopy and X-ray crystallography laboratories.

September 16, 2018. Sabrina Davies, a Ph.D. student at the University of Western Australia, was part of a team that used X-ray crystallography to identify a compound, kanchan, that causes clients to germinate. The work has implications for food security in the future.

September 17, 2018. Chemists from RUDN University (Moscow) carried out detailed analysis of the nature of intermolecular bonds between nitrogen and chlorine in the molecules of azo dyes and defined their photochromic properties. The scientists also clarified the importance of hydrogen and halogen intermolecular bonds in the stabilization of dyes structure. The research can be useful for all the types of azo dyes applications.

Product Spotlight

XtaLAB Synergy-S

If you want to remain under our minds, we have developed the XtaLAB Synergy-S X-ray diffractometer for single crystal X-ray diffraction. Using a combination of leading edge components and user-inspired software, put together through a highly pragmatic design architecture, the XtaLAB Synergy-S produces fast, precise data in an intelligent fashion.

The system is based around our PhotonJet-S series of microfocus X-ray sources that incorporate continuously variable divergence slits. These third-generation sources have been designed to maximize X-ray photons at the sample by using a combination of new optics, new, longer life, tubes and an improved alignment system. PhotonJets are available in Cu, Mo or Ag wavelengths either a single or dual source configuration.

The XtaLAB Synergy-S single crystal X-ray diffractometer comes with kappa goniometer that incorporates fast motor speeds and a unique telescopic two-theta arm to provide maximum flexibility for your diffraction experiment. The system is also equipped with your choice of HPC X-ray detector, including the HyPix-6000HE, PILATUS3 R 200K, PILATUS3 R 300K or EIGER 1M.

Benefits

- Extremely high performance due to bright source, noise-free X-ray detector and fast goniometer
- Continuously variable divergence slit option lets you resolve reflections from long unit cells.
- Minimal downtime with longer X-ray tube lifetime - supported by online diagnostics and predictive maintenance
- Compact design to fit in your laboratory

Features

- High source flux and increased goniometer speed to allow quicker, more agile experiments
- Unique telescopic two-theta arm to reach both longer and shorter crystal-to-detector distances
- Enhanced kappa goniometer design with symmetrical 2θ positioning
- Improved X-ray optic alignment mechanism for easy maintenance
- User-inspired cabinet design for improved workflow
- New electronically controlled brightness of cabinet and crystal lighting

School in the Spotlight

Zürich School of Crystallography 2018 in Tianjin, China

The highly regarded Zürich School of Crystallography (ZSC) this year took place in the School of Pharmaceutical Science and Technology (SPST) at Tianjin University from June 17 – 28. The school focuses on intensively training a small group of lucky participants. For this 8th school, 20 participants were handpicked from China, Hong Kong and Thailand. Regular lecturers Tony Linden, Oliver Blacque, Hans-Beat Bürgi, Lukas Palatinus, Michael Wörle, Bernd Schneider and Carolin Chapius were joined by Richard Cooper of Oxford, Ian Williams from HKUST and Junliang Sun from Peking University to train the participants. The ZSC endeavors to maintain a favorable student/tutor ratio of 2:1, ensuring each participant gets enough tutelage and leaves equipped with enough theory and practice to determine their own structures or recognize when to seek help.

With a structure of 2 hours of lectures followed by 2 hours of practical work, participants work through three sets of structures intended to familiarize them with structure determination and validation with the Olex² software package from OlexSys. While working through these problems, participant ability to solve structures improves to provide a challenging set of instructive problems to provide a large range of experience of crystallographic techniques and approaches.

The school made use of Rigaku equipment including a XtaLAB Synergy-S and a dual port XtaLAB Synergy-S Cryo. The XtaLAB Synergy-S was system at the SPST and was a hyper diffractometer at the School of Science. Through using these instruments, participants were able to gain hands-on experience with data collection procedures using their own samples on a range of instrumentation. Yan Zer from Rigaku Beijing China attended the school to assist with the hand-on sessions.

This was the first Zurich School in China and the very successful outcome of the final two-hour written exam showed how really hard everybody worked. Feedback from students was very positive, with comments such as "Excellent course" and "Very good organization".

If you are you interested in the next school, see
the Zürich School of Crystallography
University of Zürich, June 16 – 27, 2019
http://www.chem.uzh.ch/de/ezsc

Useful Link

DECOR

Amy Sarjeant, ACA Past President and GM at CCDC, pointed out this web site to me: https://decor.ccf.temple.edu/ which is a wiki-style repository of teaching tools for crystallography established by Mike Zdilla at Temple.

Selected Recent Crystallographic Papers

A high-performance protein crystallization platform pre-embedded with crosslinked protein microcrystals as seeds. Hou, Hao; Shi, Miao; Chen, Zhong-Hao; Ahmad, Rao; Liu, Hua; Yan, Fei; Kai; Luo, Chao; Li, Jing; Zhu, Cheng-Long; Dong, Ru-Dong; Yin, De-Chuan. CrystEngComm 2018, Vol. 20 Issue 33, p4713-4718. Ep: DOI: 10.1039/c8ce00819c

The impact of crystallosomic thermal contraction on proteins and protein crystals: volumes, conformation and order. Juers, Douglas H.; Farley, Christopher J.; Seeliger, Daniela; Weik, Martin; Zhang, Kaiqian; Jackson R. H.; Huberman Pearl, Ashley; Conor; Harrison, Kaitlin; Wu, Zhengqiu. Acta Crystallographica: Section D, Structural Biology 2018, Vol. 74 Issue 9, p922-936. 16p. DOI: 10.1107/S2059798318008750.

MBP-binding DARPins facilitate the crystallization of an MBP fusion protein. Gumpena, Rajesh; Lopez, Ana I.; Wasgo, Dylan E.; Kossiakoff, Anthony A. Acta Crystallo F, Structural Biology Communications. Sep2018, Vol. 74 Issue 9, p549-557. 8p. DOI: 10.1107/S2053230X18009991.

Crystallography and Its Impact on Carbonic Anhydrase Research. Lomelino, Carrie L.; Andring, Jacob T.; McKenna, Robert. International Journal of Medicinal Chemistry. 9/13/2018, p1-20. 20p. DOI: 10.1155/2018/1115921.

Identification of a novel tetrameric structure for human apolipoprotein-D. Kelkar, Chaula A.; Lee, Chen-Yu; Kanekar, Shreya; Vahidi, Siavash; Karuppiah, Tony; Oakley, Aaron J.; Whitten, Andrew E.; Gamer, Brett; Brown, Simon H.J. Journal of Structural Biology. Sep2018, Vol. 203 Issue 3, p205-218. 14p. DOI: 10.1016/j.jsb.2018.05.007.

Solubilisation behaviour of poorly water-soluble drugs during digestion of solid SMEDDS. Vinarov, Rauan; Gildey, Hawley; Adrian; Jannin, Vincent; Pouton, Colin; Bwo Ben J. European Journal of Pharmaceutics & Biopharmaceutics. Sep2018, Vol. 130, p236-246. 11p. DOI: 10.1016/j.ejpb.2018.06.024.

Oxanion clusters with antileukotriene hydrogen bonding (AEHB) in tetrahydromonomer-bridged tripodalsalens. Ernesto; Marcetti; Sisquiera, Katarzyna Anna; Trzebiatowska, Monika; Nishinaradach, Naden; Kinzhybalo, Vasyl. CrystEngComm. 9/21/2018, Ed. ahead of print. 10p. DOI: 10.1039/c8ce00819c.

Revisit of Recentralized 30 nm chromatin fiber structures as Ensemble of Dynamic Structures. Zhou, Bing-Rui; Jiang, Jiansheng; Gharlanda, Rodolfo; Rorsuo, Davood; Sathish Yadav, Pamu; Feng, Hanqiao; Allahverdi, Yang; Zhang, Ping; Bowman, Victor Bis, Yawen. Journal of Molecular Biology. Sep2018 Part B, vol. 430 Issue 18, p3093-3110. 18p. DOI: 10.1016/j.jmb.2018.06.040.

Crystal structure of gluconate bound iron(III) complex: synthesis, characterization and electrochemical properties of the complex in aqueous solution Stewart, Christopher D.; Annan, Hadi; Benavides, Brenda; Muse, Ghezal T. New Journal of Chemistry. 9/21/2018, Ed. ahead of print. 4p. DOI: 10.1039/c8nj03189e. 9p. DOI: 10.1039/c8nj03189e.

Design and synthesis of a new class of 2,4-triazolidinedione based macrocycles suitable for Fe^{3+} sensing. Sepay, Nayim; Mallik, Sumitava; Saha, Pranab C.; Mallik, Asok K. New Journal of Chemistry. 9/21/2018, Vol. 42 Issue 18, p15729-15736. 7p. DOI: 10.1039/c8nj01536h.

Ferrocene-based anilides: synthesis, structural characterization and inhibition of butyrylcholinesterase. Arif, Ali; Hamayun, Muhammad; Lal, Bihari; Tahir, Muhammad Nawaz; Holder, Alvin A.; Badshah, Amin; Crans, Debbie C. Dalton Transactions: An International Journal of Inorganic Chemistry. 9/14/2018, Vol. 47 Issue 34, p11769-11781. 13p. DOI: 10.1039/c8dt03726c.

Structural characterization, hydrolytic stability and dynamics of cis-$Mo^{VI}O_2S^{VI}$-hydroxamato/phenolate complexes. Drouza, Chryssoula; Hadjithoma, Sofia; Nicolaou, Maria; Keramidas, Anastassia D. Polyhedron. Sep2018, Vol. 152, p22-30. 9p. DOI: 10.1016/j.poly.2018.06.046.

Mixed μ-azido-Schiff-base cyclometallated Pd (II) complexes as a template for novel palladacycles bearing bridging carbodithioate, tetrazolate and 1,2,3-betaxole-thiolate linkers. Jang, Yuchun; Li, Manxia; Liu, Dailiang; Song, Xi-Ming; Chang, Xiaohong. Journal of Organometallic Chemistry. Sep2018, Vol. 871, p103-110. 8p. DOI: 10.1016/j.joma.2018.06.009.

Structure and function of I-threonine-3-dehydrogenase from the parasitic protozoan Trypanosoma brucei revealed by X-ray crystallography and geometric simulations. Adjogatse, Evans; Erskine, Peter; Wells, Stephen A.; Kelly, Jamie M.; Coker, Alun R.; Wood, Steve P.; Cooper, Jeremy B. Acta Crystallo D, Biological Crystallography. Sep2018, Vol. 74 Issue 9, p861-876. 15p. DOI: 10.1107/S2059798318005508.

New insights into ionic ligands: Synthesis and characterization of 1D chains by the use of pyridine-2-sulfonate and polycarboxylates. Mylonas-Margaritis, Ioannis; Weirbach, Hegner; Efthymiou, Constantinos G.; Lazarides, Theodore; Mondal, Patrick; Papatriantafyllopoulou, Constantina. Polyhedron. Sep2018, Vol. 151, p360-368. 9p. DOI: 10.1016/j.poly.2018.05.027.

Metallo-macrocycles from the use of flexible linkers: 1D cobalt(II) coordination polymers and a supramolecular pipe. Manna, Paulami; Ramalhosaemo, Mukesh; Sanyal, Suresh; Sen, Sankar K. Polyhedron. Sep2018, Vol. 151, p394-400. 7p. DOI: 10.1016/j.poly.2018.05.047.

Sonication-assisted synthesis of a new cationic zinc nitrate complex with a tetradentate Schiff base ligand: Crystal structure, Hirshfeld surface analysis and investigation of different parameters influence on morphological properties. Mousavi, M.; Montazerozohour, M.; Mahmoy, Lakshan; A.; Rahmaudi, G.; White, J.M. Ultrasonics Sonochemistry. Sep2018, Vol. 46, p28-35. 10p. DOI: 10.1016/j.ultsonch.2018.03.004.

Metal- and Multicharge-Assisted Supramolecular Self-Assembly in Metal-Organic Framework-Ion Hybrid Materials. Huang, Zhong; Zhang, Qian; Li, Yuan; Shanshan; Li, Bo; Duan, Wenxin. Journal of Chemical Crystallography. Sep2018, Vol. 48 Issue 3, p125-130. 6p. DOI: 10.1007/s10870-018-0713-1.

Co-crystallization of a Versatile Building Block Benzoquanamine with Two Flexible Cyclohexanedicarboxylic Acids. Zheng, Ling Ling; Zhou, Ai Ju; Ma, Zheng. Journal of Chemical Crystallography. Sep2018, Vol. 48 Issue 3, p117-124. 8p. DOI: 10.1007/s10870-018-0718-3.

Crystal structure, optical properties, DFT analysis of new morphotropic based Schiff base ligands and their copper(II) complexes: DNA, protein docking analyses, antibacterial and antifungal activities. Gopalakrishnan, Dhanagopal; Karuthamoorthi; Kesavan, Mookkandi Palaniyappan; Gujuluva Gangatharan Vinoth, Kumar; Rajesh, Jegathapallavathan; Rajan, Lakesh; Rajagopal, Subramanian. Materials Science & Engineering: C. Sep2018, Vol. 90, p119-130. 12p. DOI: 10.1016/j.msec.2018.04.027.

Mosquito-larvicidal binary toxin receptor protein (Cpm1): crystallization and X-ray crystallographic analysis. Mathew, Mathew; Lakshmi, Ashwitha; Gupta, Gopal D.; Kumar, Vinay. Acta Crystallographica Section F, Structural Biology Communications. Sep2018, Vol. 74 Issue 9, p571-577. 6p. DOI: 10.1107/S2053230X18010673.

Book Review

***Biological Small Angle Scattering: Theory and Practice*, Eaton E. Lattman, Sean E. Grant and Edward P. Gillis, Oxford University Press, Oxford, 2018, 288 pages, ISBN: 978-019967087-1.**

Biology is a complex subject and most one often does use small angle scattering (SAS), this volume really addresses the current theory and practice with sufficient detail to be a skilled practitioner but accessible to people a study in biological small angle scattering. The book is divided into five parts.

Part 1, the introduction, conveys the basic reasons you might perform a SAS experiment and interpreting the results. The second half of Part 1 considers various aspects of instrumentation both at home and at the beamline, special experimental setups, and neutron scattering.

Part 4 looks at some interesting examples of the application of SAS to biological problems. Here, the authors provide initial findings from XFELs and describe an interesting concept that many well recognize as an upcoming one for Shake-and-Bake approaches to SAS problems. The authors conclude with a short epilogue listing a number of references for operating various software packages.

Part 5 contains an appendix, a list of acronyms, a glossary, a list defining major variables, references, and an index.

Review by Joseph Ferrara
Deputy Director, X-ray Research Laboratory, Rigaku

* I should disclose I have known two of the authors for many years, there is a picture of a Rigaku system on page 139 and I have no financial interest.

Rigaku Corporation
e-mail: info@rigaku.com
Tel: +(81) 3-3479-9681
Fax: +(81) 3-3479-6094

Rigaku Americas
e-mail: info@rigaku.com
Tel: (281) 362-2300
Fax: (281) 364-3628

Rigaku Europe
e-mail: info@rigaku.com
Tel: +(44) 1732 763 367
FAX: +(44) 1732 763 757

Rigaku China
e-mail: info@rigaku.com.cn
Tel: +(86) 010-88575768
FAX: +(86) 010-88575768