

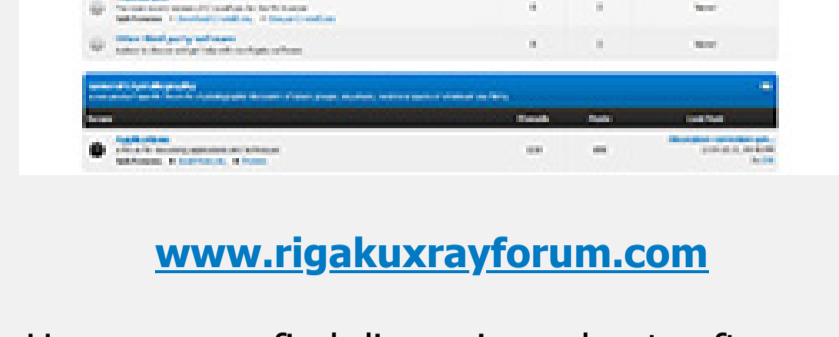
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Join ROD on LinkedIn

The 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 invites all users of Rigaku equipment to join us on our X-ray forum

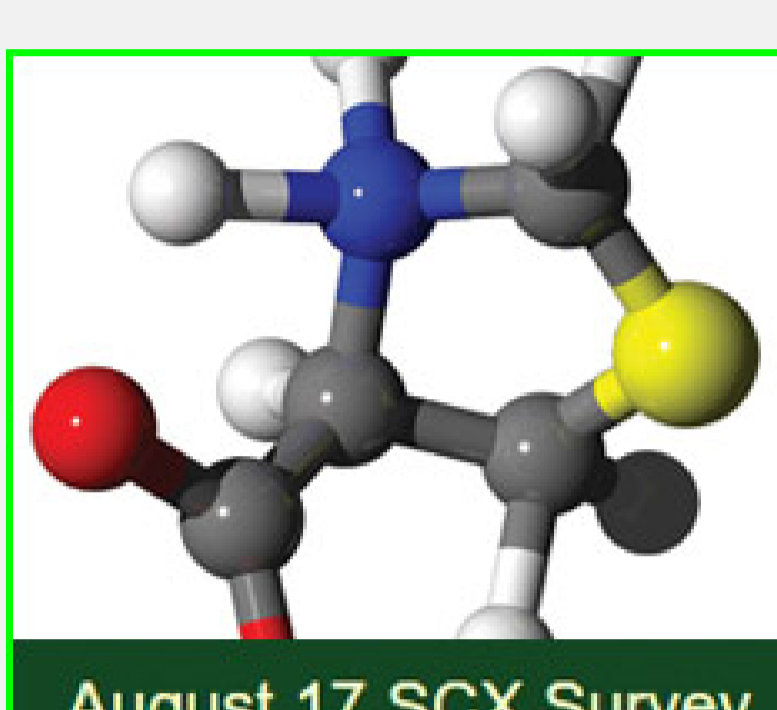


www.rigakuxrayforum.com

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



August 17 SCX Survey

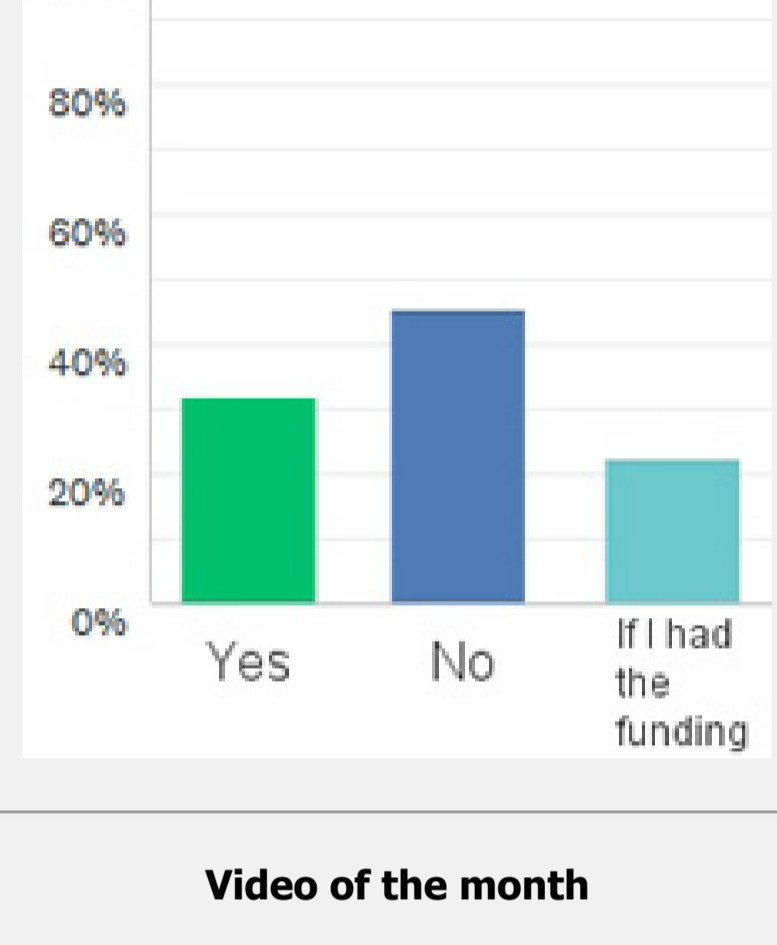
How many data sets does your departmental small molecule facility collect each month?

- <10
- 10-49
- 50-100
- >100
- I am a protein crystallographer

Take the Survey

Last month's survey

Will you be attending IUCr in Hyderabad?



Video of the month

Crystallography Innovator Dies



Here is a short news story on the passing of Phil Coppens. Interestingly, it appears the narrator is Siri.

Watch the Video

Upcoming events

Tomography for Scientific Advancement (ToScA)
Sept 6 – 8, 2017 in Portsmouth, UK

SPIE Photomask Technology
Sept 11 – 14, 2017 in Monterey, CA

SSRL Users Meeting
Sept 27 – 29, 2017 in Stanford, CA

[See full list >](#)

Greetings from IUCr in Hyderabad



A few notes on the conference ... IUCr attendees collected data on 37 single crystal samples at the Rigaku Oxford Diffraction LiveLab with 33 ready for publication. Sven Lidin of Sweden will be superseding Marv Hackert as president of the IUCr Executive Council. Finally, Melbourne has been selected as the venue for XXVII IUCr Congress and General Assembly in 2023.

Crystallography in the news

August 1, 2017. Two new discoveries from Edward Yu's Iowa State University laboratory are adding to the scientific understanding of how bacteria resist antibiotics. Yu and his research group have just described **two structures and mechanisms – efflux pumps and reinforced cell walls – that certain disease-causing bacteria use to keep antibiotics away.** That understanding could one day lead to new treatments that disable the structures and restore the effectiveness of drugs.

August 4, 2017. Researchers at Sanford Burnham Prebys Medical Discovery Institute (SBP) have published a study in *Nature Communications* shedding **new light on how K-80003 (TX803), an anti-cancer agent discovered at the Institute, prevents activation of the PI3K pathway,** resulting in inhibition of cancer cell growth.

August 9, 2017. The scientists, led by Fellow Emeritus in Trinity's School of Biochemistry and Immunology, Professor Martin Caffrey, used **next-gen X-ray crystallography techniques** to 'look under the bacterial bonnet' and produce a molecular blueprint that may be used to design drugs that minimize off-target effects and attack any structural weaknesses.

August 20, 2017. DGIST (Daegu Gyeongbuk Institute of Science and Technology) announced that the research team of Professor Ko Jae-won at the Department of Brain & Cognitive Sciences and the research team of Professor Kim Ho-min at KAIST (Korea Advanced Institute of Science and Technology) conducted a joint research and observed the three-dimensional **structure of proteins that regulate neuronal cell connections** for the first time in the world and have identified the control mechanisms of synapse formation.

August 21, 2017. The seven-day 24th Congress and General Assembly of the **International Union of Crystallography (IUCr) 2017** was inaugurated at Hyderabad International Convention Centre, India. Renowned scientists attended on the first day, including Professor Marvin Hackert, President, IUCr; Dr R Chidambaram, Principal Scientific Adviser to Govt of India; Prof Mike Glazer, Vice President, IUCr; Dr Rajiv Sharma, Principal Secretary, Department of Science and Technology; Dr Michael Heinz, Director Austrian Culture Forum and Prof. Gautam R Desiraju, Chair, Organising Committee.

August 24, 2017. High-resolution **crystal structure reveals a new pathway for RNA during a nontraditional form of transcription** – the process by which RNA is produced from a DNA template. The new crystal structure reveals RNA exiting the polymerase enzyme through an alternative channel to enable this unconventional mode of transcription.

Product spotlight: XtaLAB Synergy Custom

The XtaLAB Synergy Custom is the fully flexible system for laboratories requiring a bespoke solution for their unique crystallography applications. As its name suggests, you are able to customize to your own design, a system using a range of high quality components dedicated for single crystal X-ray diffraction.

The XtaLAB Synergy Custom is where you will find Rigaku's highest flux FR-X microfocus source delivering 2.5 times higher flux compared to the MicroMax-007 HF rotating anode generator. It may be configured to be dual port to accommodate a second diffractometer, perfect for high-throughput laboratories. It is possible to configure your system with any of Rigaku's X-ray sources, from microfocus sealed tubes to rotating anodes, to give the ultimate in flexibility.

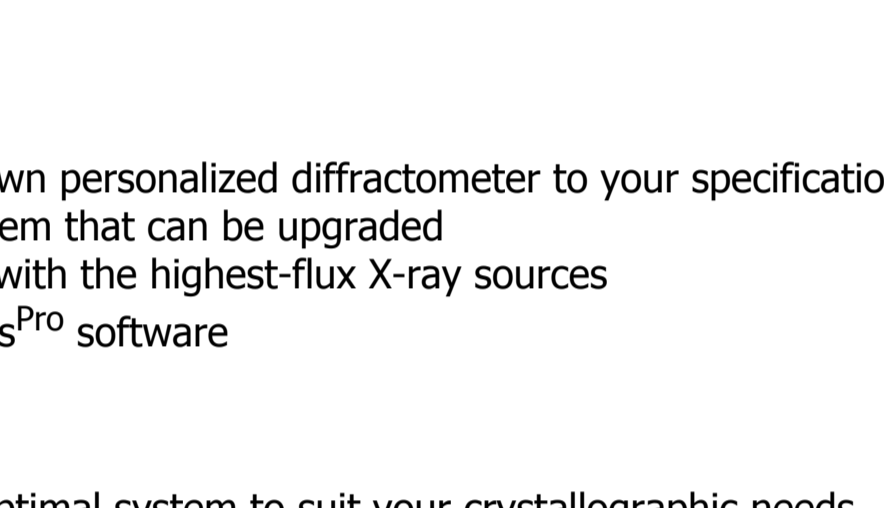
XtaLAB Synergy Custom systems can be configured with the popular and reliable four-circle kappa goniometer which is compatible with a wide range of detectors including the HyPix-6000HE and other Hybrid Photon Counting (HPC) detectors e.g. PILATUS and EIGER detectors.

HPC detectors are close to an ideal detector for a number of reasons:

- Photon counting detectors that directly detect X-ray photons without the need the intermediate step of converting X-ray photons to light with a phosphor
- High dynamic range and fast readout speed
- Extremely low noise
- An ideal point spread function of a single pixel

These combined features, along with shutterless data collection, means that you can collect more accurate data faster. As a result, the XtaLAB Synergy Custom system offers outstanding performance for single crystal diffraction experiments.

Select your accessories for the XtaLAB Synergy Custom, including the automated sample changing robot, the ACTOR or the XtalCheck for in-situ screening of macromolecules. The extra space around the goniometer enables tools such as a dewar or a microscope to be brought close into the goniometer for speedy mounting of samples.



Features:

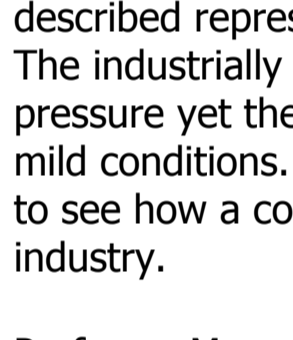
- Build your own personalized diffractometer to your specification
- Flexible system that can be upgraded
- Compatible with the highest-flux X-ray sources
- Uses CrysAlis^{Pro} software

Benefits:

- Design an optimal system to suit your crystallographic needs
- Expand your system as your research output increases or takes a new direction
- Reduce the need for synchrotron visits by using the brightest home-lab source
- Familiar software that is easy to use

[For more about XtaLAB Synergy Custom.](#)

Lab in the spotlight



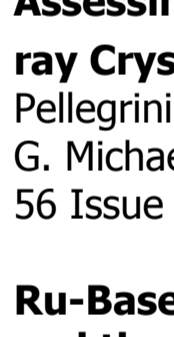
Prof. Marinella Mazzanti
Group of Coordination Chemistry GCC
Head of the Group

Marinella Mazzanti is from Vinci, Italy. She obtained her master's from the University of Pisa in 1985 and a PhD from the University of Lausanne in 1990 under the guidance of Carlo Floriani. Her career took her to the labs of W. Armstrong at UC Berkeley, Alan Balch at UC Davis and Jean Claude March at CEA Grenoble. In 1996 she began her independent research at CEA Grenoble. In September 2014 she joined the EPFL and founded the Group of Coordination Chemistry. She will continue to develop the chemistry of d and f block metals with particular focus on redox reactivity, supramolecular chemistry and small molecule activation.

Her most recent work appears in *Nature*, "Nitrogen reduction and functionalization by a multimetallic uranium nitride complex", doi:10.1038/nature23279. The chemistry described represents an exciting approach to the age-old problem of nitrogen fixation. The industrially important Haber-Bosch process requires relatively high temperature and pressure yet the multinuclear uranium complex described in the paper operates under mild conditions. Furthermore, it can add hydrogen or carbon to bound nitrogen. It is easy to see how a commercially viable version of this catalyst could change the chemical industry.

Professor Mazzanti is member of the Editorial Board of Dalton Transactions

Useful link: Stanford Engineering Everywhere



Here is a series of lectures by a very passionate instructor on the Fourier transform, starting with the basics and culminating in the use of the transform in crystallography and tomography (lectures 28 and 29).

Selected recent crystallographic papers

New developments in crystallography: exploring its technology, methods and scope in the molecular biosciences. Helliwell, John R. *Bioscience Reports*. Aug2017, Vol. 37 Issue 4, p1-13. 13p. DOI: 10.1042/BSR20170204.

Structures from poorly diffracting crystals: a new start for macromolecular crystallography? Hajdu, Janos. *Journal of Applied Crystallography*. Aug2017, Vol. 50 Issue 4, p982-984. 2p. DOI: 10.1107/S1600576717011293.

Assessing the Influence of Mutation on GTPase Transition States by Using X-ray Crystallography, ¹⁹F NMR, and DFT Approaches. Yi Jin; Molt Jr., Robert W.; Pellegrini, Erika; Cliff, Matthew J.; Bowler, Matthew W.; Richards, Nigel G. J.; Blackburn, G. Michael; Walther, Jonathan P. *Angewandte Chemie International Edition*. 8/7/2017, Vol. 56 Issue 33, p9732-9735. 4p. DOI: 10.1002/anie.201703074.

Ru-Based CO releasing molecules with azole ligands: interaction with proteins and the CO release mechanism disclosed by X-ray crystallography. Pontillo, Nicola; Ferraro, Giaria; Messori, Luigi; Tamasi, Gabriella; Merlino, Antonello. *Dalton Transactions: An International Journal of Inorganic Chemistry*. 8/7/2017, Vol. 46 Issue 29, p9621-9629. 9p. DOI: 10.1039/c7dt01991b.

Structural studies of *Neurospora crassa* LPM09D and redox partner CDHIIA using neutron crystallography and small-angle scattering. Bodenheimer, Annette M.; O'Dell, William B.; Stanley, Christopher B.; Meilleur, Flora. *Carbohydrate Research*. Aug2017, Vol. 448, p200-204. 5p. DOI: 10.1016/j.carres.2017.03.001.

The first C(O)NHP(O)-based phosphoric triamide structure with an N-H...N hydrogen bonding: A combination of X-ray crystallography and theoretical study to evaluate the strength of hydrogen bonds. Taherzadeh, Maryam; Pourayoubi, Mehrdad; Afzali, Raheleh; Necas, Marek. *Phosphorus, Sulfur & Silicon & the Related Elements*. 2017, Vol. 192 Issue 8, p936-944. 9p. DOI: 10.1080/10426507.2017.1295960.

Understanding pre-mRNA splicing through crystallography. Espinosa, Sara; Zhang, Lingdi; Li, Xueni; Zhao, Rui. *Methods*. Aug2017, Vol. 125, p55-62. 8p. DOI: 10.1016/j.ymeth.2017.04.023.

Protein-ligand complex structure from serial femtosecond crystallography using soaked thermolysin microcrystals and comparison with structures from synchrotron radiation. Naitow, Hisashi; Matsura, Yoshinori; Tono, Kensuke; Joti, Yasumasa; Kameshima, Takashi; Hatsui, Takaki; Yabashi, Makina; Tanaka, Rie; Tanaka, Tomoyuki; Sugahara, Michihiro; Kobayashi, Jun; Nango, Eriko; Iwata, So; Kunitshima, Naoki. *Acta Crystallographica Section D: Structural Biology*. Aug2017, Vol. 73 Issue 8, p702-709. 7p. DOI: 10.1107/S2059979817008919.

Combining NMR and small angle X-ray diffraction and the study of biomolecular structure and dynamics. Mertens, Haydn D.T.; Svergun, Dmitri I. *Archives of Biochemistry & Biophysics*. Aug2017, Vol. 628, p33-41. 9p. DOI: 10.1016/j.abb.2017.05.005.

Solution structure of human steroidogenic acute regulatory protein STARD1 studied by small-angle X-ray scattering. Sluchanko, Nikolai N.; Tugaeva, Kristina V.; Maksimov, Eugene G. *Biochemical & Biophysical Research Communications*. Aug2017, Vol. 489 Issue 4, p445-450. 6p. DOI: 10.1016/j.bbrc.2017.05.167.

Probing the internal and external micelle structures of differently sized casein micelles from individual cows milk by dynamic light and small-angle X-ray scattering. Day, L.; Raynes, J.K.; Leis, A.; Liu, L.H.; Williams, R.P.W. *Food Hydrocolloids*. Aug2017, Vol. 69, p150-163. 14p. DOI: 10.1016/j.foodhyd.2017.01.007.

Halogen bonded cocrystal polymorphs of 1,4-di(4'-pyridyl)-1,3-diacetylene. Zhang, Pan; Bolla, Geetha; Qiu, Gege; Shu, Zhibin; Yan, Qingqing; Li, Qingyuan; Ding, Shang; Ni, Zhenjie; Zhu, Weigang; Dong, Huanli; Zhen, Yonggang; Hu, Wenping. *CrystEngComm*. 8/21/2017, Vol. 19 Issue 31, p4505-4509. 5p. DOI: 10.1039/c7ce00892a.

Interaction between aromatic rings as organizing tools and semi-coordination in Cu(II) compounds. Martínez-Vargas, Sergio; Dorazco-González, Alejandro; Hernández-Ortega, Simón; Toscano, Rubén A.; Barquera-Lozada, José Enrique; Valdés-Martínez, Jesús. *CrystEngComm*. 8/21/2017, Vol. 19 Issue 31, p4595-4604. 10p. DOI: 10.1039/c7ce00871f.

Structural Biology and the Design of New Therapeutics: From HIV and Cancer to Mycobacterial Infections: A Paper Dedicated to John Kendrew. Thomas, Sherine E.; Mendes, Vitor; Kim, So Yeon; Malhotra, Sony; Ochoa-Montaño, Bernardo; Bernasconi, Michal; Blundell, Tom L. *Journal of Molecular Biology*. Aug2017, Vol. 429 Issue 17, p2677-2693. 17p. DOI: 10.1016/j.jmb.2017.06.014.

Reversible Protonated Resting State of the Nitrogenase Active Site. Morrison, Christine N.; Spatzal, Thomas; Rees, Douglas C. *Journal of the American Chemical Society*. 8/9/2017, Vol. 139 Issue 31, p10856-10862. 7p. DOI: 10.1021/jacs.7b05695.

3D-NuS: A Web Server for Automated Modeling and Visualization of Non-canonical 3-Dimensional Nucleic Acid Structures. Patro, L. Poonoo Prasad; Kumar, Abhishek; Kolimi, Narendar; Rathinavelan, Thennalarchelvi. *Journal of Molecular Biology*. Aug2017, Vol. 429 Issue 16, p2438-2448. 11p. DOI: 10.1016/j.jmb.2017.06.013.

Metal-Organic Frameworks: Examples, Counterexamples, and an Actionable Definition. Seth, Saona; Matzger, Adam J. *Cryst Growth & Design*. Aug2017, Vol. 17 Issue 8, p4043-4048. 6p. DOI: 10.1021/acs.cgd.7b00808.

Pitfalls in metal-organic framework crystallography: towards more accurate crystal structures. Øien-Ødegaard, S.; Shearer, G. C.; Wragg, D. S.; Lillerud, K. P. *Chemical Society Reviews*. 8/21/2017, Vol. 46 Issue 16, p4867-4876. 10p. DOI: 10.1039/c6cs00533k.

Dispersion and Halogen-Bonding Interactions: Binding of the Axial Conformers of Monohalo- and (±)-trans-1,2-Dihalo-cyclohexanes in Enantiopure Allenone-Acetylenic Cages. Cropp, T. Husch, N. Trapp, M. Reher, F. Diederich. *J. Am. Chem. Soc.* August 15, 2017. DOI: 10.1021/jacs.7b05461.

Book review

Zbigniew Crystallography: Methods and Protocols, Alexander Wlodawer, Business Review Group and Mariusz Jaskolski, Eds., Springer Science+Business Media, New York, 2017, 672 pp., ISBN-13: 978-1-4939-6998-2

This book is a compilation of 27 reviews by 50 contributors on current methods in protein crystallography. The contributors are all recognized as leaders in their area of specialization, adding gravitas to each review.

The book starts with a chapter (1) on preparation and purification, followed by a chapter (2) on traditional crystallization. The micrographs in this chapter of growth steps are beautiful and instructive. Three more chapters (3-5) cover state-of-the-art processes in crystallizing problem proteins. Another chapter (6) on finding crystals for the diffraction experiment illustrates the problems of selecting an object from the background when there is little contrast.

Once crystals are grown, the next step is data collection. The next five chapters (7-11) cover conventional data collection, microbeam data collection, serial synchrotron data collection and time-resolved data collection. Chapter 12 covers structure determination with X-ray free-electron laser data while Chapter 13 reviews the problems of data processing from XFELs.

Chapters 14-19 cover experimental solutions to phasing without derivatization, anomalous diffraction and long-wavelength data collection, and computational methods via Patterson and direct methods and molecular replacement. Chapter 20 covers the issues of radiation damage and even loops back to experimental phasing using radiation damage.

With an initial model, the book flows through five chapters (21-25) on modeling, refinement and validation. The book closes with two chapters (26 and 27) on databases in crystallography.

What is missing from this tome are reviews on cryo-techniques and conventional data processing. Nevertheless, I believe this modern volume will replace the venerable Volumes 276 and 277 of *Methods in Enzymology* on many shelves.

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