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Calendar of events

Rigaku will be attending the following conferences in the coming months:

- [Fragment-based Lead Discovery Conference](#), San Diego, CA, February 18-20
- [New York Structural Biology Group](#), Manhattan, NY, February 29
- [PITTCON 2008](#), New Orleans, LA, March 2-6
- [TMS 2008](#) (The Minerals, Metals & Materials Society), New Orleans, LA, March 9-13
- [APS](#) (American Physical Society), New Orleans, LA, March 10-14
- [ELRIG](#) (European Laboratory Robotics Interest Group), Cambridge, UK, April 1
- [ACS](#) (American Chemical Society) Spring National Meeting, New Orleans, LA, April 6-10
- [BCA](#) (British Crystallographic Association) Spring Meeting, York, UK, April 8-10
- [AAAS- SWARM](#) (The American Association for the Advancement of Science - Southwestern and Rocky Mountain Division), Albuquerque, NM, April 9-12
- [ICDD: Practical X-ray Fluorescence](#), Newtown Square, PA, April 28-

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A word from our president: Good to be back at work

What is it about the holiday period that makes one long to get back to work? While it is good to deviate from the daily routine and spend time with assorted family members, there is always a certain satisfaction in getting back to my desk. I turn to [Maslow's hierarchy of human needs](#) to try and understand this phenomenon.



Maslow's hierarchy is a way of describing the motivations that drive a human. At the bottom of the pyramid are the physiological needs. This need-class includes food, and let's face it; we all overfill this need during the holidays. Could the desire to go back to work be as simple as not wanting to move into a larger waist size?

The rest of the hierarchy categories are safety, love/belonging, self esteem, and finally self actualization. Self actualization is described as a basic human instinct to make the most of our abilities and do a good job. Our careers should satisfy that need but why do we jump over the love/belonging need which is left unfulfilled once we leave the family reunion and go back to work?

In reviewing the photographs taken during the visit by my in-laws I finally have the answer: the primal need for safety. The accompanying photograph is of one of my sister-in-law's sweet dogs performing one of its many "tricks" while visiting my wife and me over the holidays. Just looking at that image again raises the hair on the back of my neck. So at least for me, the satisfaction of getting back to work isn't about self-actualization, but simply about being in a place where I won't be bitten.

Paul N. Swepston

Max-Planck Institute of Biophysics chooses Rigaku X-ray crystallographic and crystallization equipment

Rigaku Americas Corporation is pleased to announce that the Max-Planck Institute of Biophysics (Frankfurt, Germany) has chosen to update their X-ray crystallography facility with the most advanced Rigaku protein crystallography and automated crystallization systems. The new equipment includes the world's brightest X-ray source, the Rigaku FR-E+ SuperBright™ equipped with Osmic™ VariMax™ HF optic, the recently introduced Rigaku Saturn 944+ CCD detector, and the advanced Rigaku CrystalMation™

March 2

Training Sessions

Rigaku is pleased to announce the following training sessions in 2008:

- Macromolecular
 - March 26-28
 - September 17-19
- XRD (MiniFlex II):
 - February 19-20
 - September 23-24
- XRD (Jade software):
 - February 20-21 (22)
 - May 20-21 (22)
 - November 4-5 (6)
- XRF:
 - February 5-7

All classes are held at Rigaku's applications laboratory in The Woodlands, TX.



PITTCON 2008

Visit Rigaku at Booth 5321 at [PITTCON 2008](#) to learn more about the world's most complete line of X-ray diffraction and fluorescence instruments, including: benchtop and laboratory powder diffractometers, high-resolution thin film diffractometers, X-ray reflectometers, diffraction and topography tools for the semiconductor industry, small angle scattering systems, rotating anode generators; sequential and simultaneous X-ray spectrometers, TXRF systems, and wafer analyzers.

Al Martin will be presenting a poster titled "A breakthrough in TXRF."

ACA preview

Angela Criswell will present poster W0327 at the upcoming [ACA meeting](#) in Knoxville. It is titled: [Automated Sample Handling, Data Collection and Structure Solution with ACTOR](#). Her co-authors are Amber Dowell, Robert Bolotovskiy and Jim Pflugrath.

Kris Tesh will present poster W0390 [New Optics for Macromolecular Crystallography](#). Co-authors are Angela Criswell, Licai Jiang, Bret Simpson, Boris Verman, Chang Yang, and Joseph Ferrara.

Rigaku Europe news

A collaborative team of scientists from Wake Forest University, Asahi Kasei Pharma, Oregon State University and Rigaku Europe have reported the first crystal structures of the enzyme α -glycerophosphate oxidase, a soluble bacterial homolog to the membrane-associated mitochondrial glycerol phosphate dehydrogenase which has been studied for over 70 years.

The GIpO structure reveals a multidomain flavoprotein with two domains similar in fold to those of flavoprotein amino acid oxidases and a novel fold in the C-terminal domain and may play a role in membrane association for the GIpD homologs.

T. Colussi, D. Parsonage, W. Boles, T. Matsuoka, T.C. Mallett, P.A. Karplus and A. Claiborne: (2008) *Biochemistry* **47**:965-977 [[abstract](#)]

Customer testimonials

"Since the Alchemist has arrived at Sareum Ltd the optimisation of initial hits

automated crystallization system.

Upgrading and expanding the X-ray crystallography facility at the Max-Planck Institute of Biophysics was part of an initiative by ESFRI-INSTRUCT (European Strategy Forum on Research Infrastructures - Integrated Structural Biology Infrastructure) to elevate the Max-Planck Institute of Biophysics to be one of the seven core European centers for structural biology. Prof. Hartmut Michel, winner of Nobel Prize for Chemistry in 1988, was chosen to lead the project. For the preparatory phase the BMBF (German Ministry of Education and Research) has funded the effort, with the majority of the funds being invested to improve the X-ray crystallographic equipment at the institute.

Commenting on the new acquisition, Dr. Juergen Koepke, Staff Scientist at the Max-Planck Institute of Biophysics, said "First, we decided to replace two 19 years old Rigaku RU200 X-ray sources with a new powerful, state of the art X-ray generator with optics and a CCD detector. Second, a fully automatic crystallization system was required that would be able to prepare 96 well crystallization plates with a pre-selected screen, store them at a chosen temperature, and image the wells on a regular basis."

Dr. Koepke continued, noting that "We chose a complete Rigaku system including an FR-E+ [SuperBright] X-ray generator with the latest VariMax-HF optic and a Saturn 944+ CCD detector to obtain the highest available brilliance and detector performance. The only worldwide available fully automatic crystallization system was the CrystalMation system from Rigaku. So we decided to start with a system that supports two Gallery 700 incubators, but with an Integration Module prepared to accept at least one additional Rigaku Minstrel HT/Gallery 700 combination. At the moment, we are investigating the possibility of adding a new room to the building, dedicated to the CrystalMation system, so as to be able to setup an Integration Module long enough to serve six incubators.

"It has turned out, that a high flexibility in temperature is required to optimize the crystallization conditions of protein complexes, especially for membrane proteins. Therefore the installed incubators will be set to such different temperatures, that high X-ray quality macromolecular crystals can be obtained with the new system. To avoid frequent trips to the synchrotron, the in-house X-ray power will be high enough, with the new Rigaku FR-E+ [SuperBright] and an already available Rigaku MicroMax-007 HF X-ray generator, to do both the screening and full data collection of crystals directly at our MPI facility. The preparation phase for the core center will be finished at the end of 2008 or in early 2009. After that initial phase the core center will provide the facilities also to European access groups."

FBLD 2008 Conference: X-ray crystallography teams up with complementary techniques to improve drug discovery timelines

Rigaku and ActiveSight® are organizing the first ever Fragment-based Lead Discovery Conference, FBLD 2008, taking place February 18-20th in San Diego. FBLD is a technique whereby smaller compounds and libraries are screened against drug targets, providing information that results in the development of efficiently binding lead compounds. The conference is a natural extension of the Fragment screening workshops ActiveSight has organized for the past several years, showcasing Rigaku's leading instrumentation for high-throughput X-ray crystallography. ActiveSight and Rigaku are actively involved in the FBLD/Drug Discovery community, bringing together FBLD thought leaders to participate at the conference and to give a perspective on its emerging role in creating high quality lead compounds efficiently. Sessions will include Success Stories, Chemical Biology in Drug Discovery, Methods & Emerging Technologies, and Lessons Learned. ActiveSight's Chief Scientific Officer, Vicki Nienaber, will give a presentation titled "Pulling it all together: Faster Better Lead Discovery through Integration of Technologies," covering one of ActiveSight's FBLD discovery programs. The closing plenary presentation will be given by Chris Lipinski, famous for creating the "Lipinski Rule of 5" for drug compounds, who will provide perspectives on current drug discovery paradigms.

obtained from 96 well factorial screens has been more accurate and comprehensive. This makes the process of obtaining good diffracting crystals more reproducible and quicker".

—Marieke Lamers
Head of Protein Science
Sareum Ltd

"The SHINE optic works perfectly. I measured several 5 micron thin platelets which were impossible to run on the old monochromator. Routine measurements can often be done with one minute per frame. Really nice."

—Nils Trapp
Institut fuer Anorganische und Analytische Chemie
Universitaet Freiburg
Freiburg, Germany

What's new?

What's new at www.Rigaku.com:

- 01/28/2008 Job postings updated
- 01/23/2008 Introducing the Desktop Minstrel UV
- 01/21/2008 Max-Planck Institute of Biophysics chooses Rigaku X-ray crystallographic and crystallization equipment
- 01/11/2008 CrystalClear 1.4.0 now available
- 01/10/2008 Hear a customer talk about the SmartLab XRD system
- 01/03/2008 See the ACTOR SM in action
- 11/05/2007 XRF training session announced

Take our survey to express your opinion about the Rigaku web site

A pre-conference FBLD Methods & Implementation Workshop covering X-ray Crystallography, Surface Plasmon Resonance, NMR, Calorimetry, Chemistry, and Library Design/Maintenance will be covered. These technologies can all be used synergistically to screen fragment libraries and provide information about binding to the drug target. ActiveSight's John Badger will be discussing Library Design, and Robin Rosenfeld will present methods for Fragment screening using X-ray Crystallography. Separate registration is required for the FBLD 2008 Workshop. The Exhibit Hall will showcase new X-ray Crystallography and complementary technologies for FBLD with presentations and demonstrations from 12 companies. A list of FBLD 2008 exhibitors and their FBLD 2008 activities can be found [here](#). Rigaku will be demonstrating the ACTOR™ robotic system for automated crystal sample handling, along with the new MtGui software which bridges the gap between data collection and processing and includes full support for the new Rigaku RFID pins. In addition, researchers will learn about advances in CrystalMation, MIFit+, and the Ultimate HomeLab™.

The conference will take place at the [Paradise Point Resort in San Diego](#), and will attract Drug Discovery researchers from around the world.

Introducing the Desktop Minstrel™ UV

Rigaku introduced the Desktop Minstrel UV at the Advances in Protein Crystallography conference last week in San Diego. The Desktop Minstrel UV is the world's first fully automated UV imaging and protein crystal monitoring system that uses UV fluorescence microscopy. It allows experimenters to monitor crystal growth by distinguishing protein crystals from non-protein crystals, such as salt. The Desktop Minstrel UV uses Clean Light Technology™ and includes an ultraviolet microscope. Illumination is provided with the wavelength matching the absorption of fluorescing amino acids, such as tryptophan and the fluorescence is digitally recorded by a camera with a CCD sensor.



The Desktop Minstrel UV is built upon the platform of Rigaku's state-of-art imaging automation technology, the Desktop Minstrel, which makes the evaluation of a large number of crystallization experiments possible. The Desktop Minstrel UV enables researchers to accurately harvest protein crystals for data collection or design follow-up experiments.

Difficult analysis made easy with the ZSX Primus

Moving beyond standard quality control of manufactured sheet metals are a number of 'specialized' analysis that are needed and presently are difficult and awkward. One of these areas is wire analysis. Wires are manufactured in different sizes and many go on for brass or bronze coating.



Manufacturing failures due to inclusions in the wire are easily solved using

the Micro Analysis feature on the ZSX Primus series systems. With the built in CCD camera it is easy to 'snap' a picture of the failure/inclusion section then specify your analysis spot with the point and click feature of Micro Analysis. From there a Semi-quantitative analysis is preformed using spot sizes down to 0.5 mm on the failure area and a 'clean' area—do a comparison of the results and you have the answer of where along the production line your inclusion originated.

Coating analysis of wires is another area that is typically difficult to perform. This also is easily solved using the ZSX Primus series WDXRF systems. We have analyzed a number of these wires by forming a 'raft'—sections of wire cut to appropriate sizes and laid out side by side then joined by an adhesive backing. The rafts are inserted into the XRF system and analyzed for coating weight, elemental abundance (e.g. mg/gm, gm/kg, etc). This analysis typically was done via acid leaching of the coating followed by ICP analysis. XRF has shown itself to be an economical, efficient and safer successor to this older method.

Rigaku welcomes Stan Cameron

Rigaku Americas is proud to host [T. Stanley Cameron of Dalhousie University](#) for his fifth sabbatical at RAC (formerly Rigaku/MSC and MSC). Stan started life in New Jersey, moved to England during WWII, received a D. Phil from Oxford in 1968 and began his teaching career in Northern Ireland. In 1976, he joined the faculty at Dalhousie. Among Stan's many honors is his role as science ambassador to India for Canada. Stan is also a renowned teacher and was the recipient of the Alumni Award for Teaching Excellence from Dal in 2001.



During his last sabbatical in 2004 he collected several charge density sets which were used to probe hydrogen bonding in non-conventional motifs. The results of that work have been published in three articles cited below. Stan takes advantage of the time away from teaching to work on the really difficult crystallographic problems that come through his lab. Thus far Stan has already tackled and solved some interesting problems and is looking forward to several months of extensive data collection at our application lab in the The Woodlands. The warm weather (0-15°C) versus -20°C in Halifax is a also a big draw for Stan.

We look forward to an enjoyable five months with Stan and his wife Liz.

1. David Wolstenholme, Manuel A.S. Aquino, T. Stanley Cameron, Joseph D. Ferrara, and Katherine N. Robertson (2006) A topological analysis of the interior interactions of tetraphenylphosphonium squarate. *Can. J. Chem.* **84**, 804-811.

2. Deepak Chopra, T. S. Cameron, Joseph D. Ferrara, Tayur N. Guru Row (2006) Pointers Toward the Occurrence of C-F F-C Interaction: Experimental Charge Density Analysis of 1-(4-Fluorophenyl)-3,6,6-trimethyl-2-phenyl-1,5,6,7-tetrahydro-4H-indo 1-4-one and 1-4-(4-Fluorophenyl)-6-methoxy-2-2-phenyl-1,2,3,4-tetrahydroisoquinoline. *J. Phys. Chem. A*, **110**, 10465-10477.

3. Parthapratim Munshi, Elinor Cameron, Tayur N. Guru Row, Joseph D. Ferrara, and T. Stanley Cameron (2007) Investigation of Inter-Ion Interactions in N,N,N',N'-Tetramethylethylenediammonium Dithiocyanate via Experimental and Theoretical Charge Density Studies. *J. Phys. Chem. A*, **111**, 7888-7897.

2007 Customer satisfaction survey

Beginning in November, Rigaku Americas Corporation customers were asked to participate in our semi-annual Customer Satisfaction Survey. Delivered by both e-mail and "snail mail", the response was almost 30% of our installed base worldwide. We wish to thank all of those who took the time to help us help you.

Vastly different from a marketing or installation survey, or other "nut and bolts" questionnaires, this survey was designed to measure perceptions of Rigaku products and

- CIF output and other structure results are placed in a sample subdirectory.
- Setup and optimized have been simplified for the SCXmini X-ray source, goniometer, and Mercury 2 detector hardware.
- Support for the new d*TREK[®] 9.7 processing package.
 - Dramatically increased speed (up to 3X) for d*TREK processing server using optimized MSCSServProceDTREK.exe.
 - Improved CrystalClear server interface to Director with support for the multiple-scan strategy features now provided by d*TREK 9.7.
 - Crystal ranking has been improved for use both with ACTOR and manual use.
 - Improvements in indexing, scaling, and space group determination.
- Support for the latest enhancements in the FS_Process package.
- Support for the upgraded TwinSolve 1.67 processing package for twinned crystals which now includes support for the Rigaku Kappa goniometer.
- Support for the Rigaku Kappa goniometer and new Saturn 724, 724+, 944, 944+, and Mercury 2 CCD detectors.
- Updated Instrument Servers (CCD, R-AXIS, and RAPID/SPIDER) with support for new hardware options.
- Expanded support for the separate JXG X-ray generator control, including a new pre-collection JXG script running mechanism.
- Incorporation of XML database file generation allowing ASCII text editing/viewing of program default parameter databases.
- Updates to the image viewer including new circle masking and middle mouse button support for dragging operations.
- Still image collection capability.
- Updated/improved collision detection XML files for various instruments.
- Updated site defaults for all instruments.
- Expanded configuration file control for various CrystalClear operations.
- Improved support for Japanese character display when using Japanese Windows[®] OS.
- FS_ABSCOR absorption correction algorithm as an optional alternative to the Jacobson REQAB algorithm.
- Improved CIF file generation and versioning.
- Numerous fixes and minor enhancements.
- Improved installation and setup.

This release is available to all customers who are under warranty or under a current software support contract. If you are not currently under software support you can gain access to the new version by buying a one year software support contract.



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