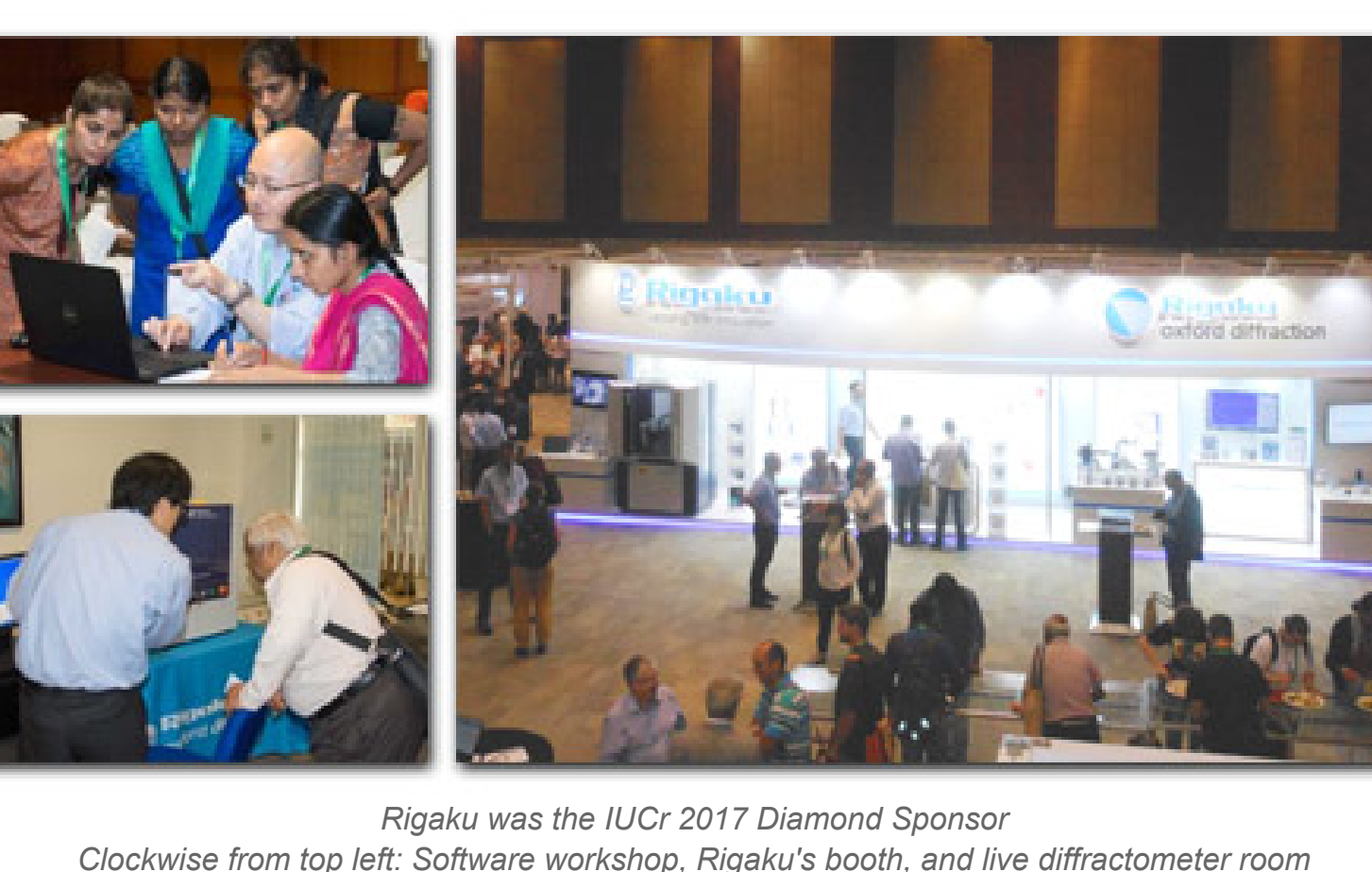
Rigaku
Leading With Innovation

X-ray Diffraction & Elemental Analysis

Welcome

Thanks again to everyone who came by our booths at DXC, PPXRD-15 and IUCr this month. It was great to see everyone and to have the chance to talk about our new and exciting products. Included in this issue is a review of the DXC in Big Sky, MT. In September, we invite members of the scientific, security and industrial communities to come see us at a variety of events listed below.

A few notes on the IUCr conference: attendees collected data on 37 single crystal samples at the Rigaku Oxford Diffraction LiveLab, with 33 being 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 XXVI IUCr Congress and General Assembly in 2023.



Rigaku was the IUCr 2017 Diamond Sponsor
Clockwise from top left: Software workshop, Rigaku's booth, and live diffractometer room

This month's issue contains a new Rigaku Journal article describing crystal structure analysis from powder X-ray diffraction data using the high-temperature attachment for capillaries on the Rigaku SmartLab. On the theme of SmartLab, a press release on the installation of one at the University of Manchester is included.

Application papers are also included for TXRF, WDXRF and EDXRF techniques, with the WDXRF AppNote highlighting "Sulfur Analysis in Petroleum Products by Benchtop WDXRF According to ASTM D2622-10." The book review this month covers Protein Crystallography: Methods and Protocols. Finally, this month's video link is from the University of Southampton and covers single crystal X-ray diffraction familiarisation featuring the Rigaku XtaLAB mini. Check out the news and papers sections at the bottom of the page for the latest developments in materials science.

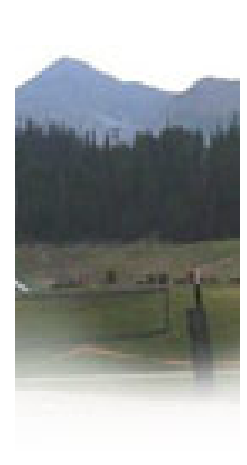
Enjoy the newsletter.

R.C. Tisdale, Ph.D. – Editor

Featured Rigaku Journal Article

Crystal structure analysis from powder X-ray diffraction data using high-temperature attachment for capillaries
By Hisashi Konaka and Akito Sasaki, Rigaku Corporation

The physical and chemical properties of a crystalline solid depend heavily on the conformations of the molecules and the arrangement of atoms and molecules, that is, the "crystal structure", as well as on the composing elements and molecular structures. The single crystal structure analysis technique is used in many fields as a good tool to precisely clarify the crystal structures required to understand the mechanisms of developing physical properties of crystalline materials.
Full article >



Conference report

The 66th Annual Denver X-ray Conference
By Kousuke Kawakyu

Big Sky Resort, a basecamp to Yellowstone National Park, is located 2200 meters above sea level in the grandeurs of the Rocky Mountains. Almost 300 researchers and students from five continents congregated here to present and learn about the latest in X-ray science and technology over the course of five days. **For more >**

TXRF Application Note

Benchtop TXRF spectrometer NANOHUNTER II
Ultra-trace Analysis of Aqueous Liquids by Internal Standard Method
Rigaku Corporation

An incident X-ray beam impinges upon the sample at a shallow angle resulting in virtually complete reflection of the excitation beam away from the silicon drift detector. This affords dramatically reduced background contributions in the measured energy dispersive X-ray fluorescence spectra. Ultra-trace elemental analysis of the liquid sample becomes possible using the NANOHUNTER II and "Drop and Dry" sample preparation technique. **For more >**

WDXRF Application Note

Sulfur Analysis in Petroleum Products by Benchtop WDXRF According to ASTM D2622-10
Rigaku Corporation

Crude oil contains sulfur in concentration from 0.5 mass% to 5.0 mass% typically, and sulfur is one of critical elements in refinery processes and final products. Sulfur in petroleum-based fuels contributes to atmospheric pollution; therefore, sulfur content in fuels, especially in automobile fuels, is strictly controlled. Sulfur also causes damage to process components such as catalysts in refinery processes. Therefore, control of sulfur content is very important in the petroleum industry from the standpoints of both environmental and production costs. **For more >**

EDXRF Application Note

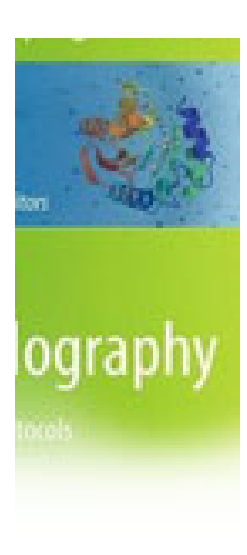
Co, Br, Mn IN TPA AND PTA
Applied Rigaku Technologies

Terephthalic acid (TPA) and purified terephthalic acid (PTA) are precursors in the making of polyester PET for polyester films, PET bottle resin, textile fabrics, and specialty chemicals. During production and use of TPA and PTA the catalysts Co, Br and Mn must be closely monitored to ensure optimum product quality. Since TPA and PTA are aggressive solutions, an on-line measurement is ideal. Continuous monitoring minimizes lab testing requirements, allows for process optimization, and is a critical step in insuring the end product meets specifications. The Rigaku NEX OL offers a simple and low maintenance on-line analytical technique for trending your process streams. **For more >**

Press Release

New Rigaku SmartLab XRD system installed at the Henry Royce Institute at The University of Manchester
Rigaku Corporation

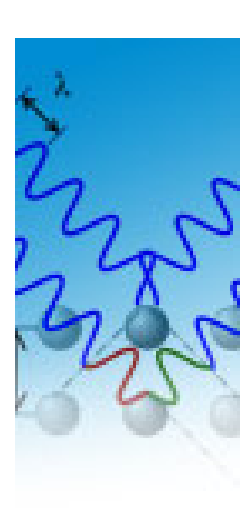
Rigaku and Scientific and Medical Products (SciMed) are proud to announce the installation of a new Rigaku SmartLab system within the National Graphene Institute at The University of Manchester (UoM) as part of the leading advanced materials work being carried out on campus. Research in this area will become part of the activity to support the Henry Royce Institute, which will have its hub based in Manchester. The Institute will lead the accelerated discovery and development of new materials systems for the economic and social benefit of the UK. The key theme within the Institute will be the application of 2D Materials, in collaboration with the National Graphene Institute, an area pioneered in the UK, and one where the UK has a lead in the terms of the fundamental physics of such materials.
For more >



Book Review

Protein Crystallography: Methods and Protocols: Alexander Wlodawer, Zbigniew Dauter and Mariusz Jaskolski, Eds., Springer Science+Business Media, New York, 2017, 672 pp., ISBN-13: 978-1-4939-6998-2
Reviewed by Joseph D. Ferrara, Ph.D., Deputy Director, X-ray Research Laboratory, Rigaku

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. **Full review >**



Material Analysis in the News

News for August 2017

August 1, 2017. A new, lightweight multilayer, hexagonal boron-nitride nanocrystal composite material for energy storage in flexible electronics, electric vehicles, and aerospace applications has been experimentally shown to store energy at operating temperatures well above current commercial polymers, according to a team of Penn State scientists. This polymer-based, ultrathin material can be produced using techniques already used in industry.

August 2, 2017. Researchers at Kyoto University's Institute for Integrated Cell-Material Sciences (iCeMS) and the University of Tokyo have developed a light-responsive crystalline material that is flexible and amenable to repeated use. The flexible material changes its ability to absorb carbon dioxide when exposed to light.

August 3, 2017. Physicists have spotted elusive subatomic particles called neutrinos pinging off atomic nuclei in a way predicted more than 40 years ago, but never before observed. Even more remarkably, they spotted the scattering effect with a device the size of a milk jug. The advance could open the way to portable neutrino detectors that could monitor nuclear facilities.

August 7, 2017. Physicists were able to perform the first extreme ultraviolet radiation (XUV) coherence tomography experiment at laboratory scale. This radiation has a wavelength of between 20 and 40 nanometers – from which it is just a small step to the X-ray range.

August 8, 2017. A senior scientist at the Air Force Research Laboratory's Materials and Manufacturing Directorate, Dr. Sheldon "Lee" Semiatin, will receive the prestigious 2018 ASM International Albert Sauvuer Achievement Award in the fall of 2018. He will be recognized for significant contributions to materials research and development that have led to the establishment of the discipline of Processing Science, impacting the worldwide research endeavor.

August 9, 2017. Osaka University researchers used X-ray crystallography and electron microscopy to resolve the assembly of the export gate apparatus in *Salmonella*. The new details of this nanomachine are expected to clarify how bacteria infect eukaryotic cells and present new molecular targets for drug discovery.

August 11, 2017. Researchers at the U.S. Department of Energy's (DOE) Brookhaven National Laboratory have developed a less expensive and more efficient way of controlling X-ray beams. The new beam-shaping devices, invented by Brookhaven mechanical engineer Sushil Sharma, can be made from a single piece of copper, which dramatically reduces the time and complexity of their construction – and their cost.

August 11, 2017. Investigators have developed a new sensor array-based instrument, a SQUID-based detector that offers ultra-low noise detection of small amounts of energy for applications in fields as diverse as nuclear materials accounting, astrophysics and X-ray spectrometry.

August 18, 2017. Known as a metal-organic framework (MOF), the new porous, or cage-filled, superstructure called NU-1301 is quite large, with the largest unit cell of any non-biological material. In addition, it is the lowest density MOF reported to date. The low density means the MOF is a highly porous material, like a super sponge, which is great for storage applications including, but not limited to, storage of nuclear waste.

August 21, 2107. Researchers at Nagoya University have demonstrated how the TMTTF (tetramethyltetrathiafulvalene) salt shows a charge disproportionation transition at 67 Kelvin but no relevant changes in its crystal structure. This transition is a long-standing mystery known as a 'structure-less' transition. Using the X-ray source at SPring8, in Hyogo Japan, the team were able to precisely determine the crystal structure at each stage. The structure-less transition involves the formation of a two-dimensional Wigner crystal, based on a change in the distribution pattern of electrons in the structure.

August 24, 2017. A team of scientists, including scholars from the University of Chicago, appear to have found the first X-rays coming from type Ia supernovae. Astronomers are fond of type Ia supernovas, created when a white dwarf star in a two-star system undergoes a thermonuclear explosion, because they burn at a specific brightness. This allows scientists to calculate how far away they are from Earth, and thus to map distances in the universe.

Recent Scientific Papers of Interest

Papers for August 2017

Recent Scientific Papers of Interest is a monthly compilation of material analysis papers appearing in recently released journals and publications. *See below*

Stoichiometry Calculation in $Ba_xSr_{1-x}TiO_3$ Solid Solution Thin Films, Prepared by RF Cosputtering, Using X-Ray Diffraction Peak Positions and Boltzmann Sigmoidal Modelling. Reséndiz-Muñoz, J.; Fernández-Muñoz, J. L.; Corona-Rivera, M. A.; Zapata-Torres, M.; Márquez-Herrera, A.; Meléndez-Lira, M.; Caballero-Briones, F.; Chale-Lara, F.; Zelaya-Ángel, O. Journal of Nanomaterials. 8/9/2017, p1-8. 8p. DOI: 10.1155/2017/4308294.

Analysis of InGaN nanodots grown by droplet heteroepitaxy using grazing incidence small-angle X-ray scattering and electron microscopy. Woodward, J. M.; Nikiforov, A. Yu.; Ludwig Jr., K. F.; Moustakas, T. D. Journal of Applied Physics. 2017, Vol. 122 Issue 6, p065305-1-065305-16. 16p. 6 Color Photographs, 4 Black and White Photographs, 2 Charts, 6 Graphs. DOI: 10.1063/1.4986272.

Low-energy shelf response in thin energy-dispersive X-ray detectors from Compton scattering of hard X-rays. Michel-Hart, N.; Elam, W.T. Nuclear Instruments & Methods in Physics Research Section A. Aug2017, Vol. 863, p1-6. 6p. DOI: 10.1016/j.nima.2017.04.039.

Soot with 10^{13} cm^{-3} high concentration and 25 Å radius of gyration as detected by small-angle X-ray scattering in a premixed ethylene-air flame at sooting threshold. di Stasio, Stefano. Journal of Aerosol Science. Aug2017, Vol. 110, p11-24. 14p. DOI: 10.1016/j.jaerosci.2017.05.003.

Hydrodemetallation and Hydrodesulfurization Spent Catalysts Elemental Analysis: Comparison of Wavelength Dispersive X-ray Fluorescence and Atomic Emission Spectrometries. Garoux, Laetitia; Gourhand, Sébastien; Hébrant, Marc; Schneider, Michel; Diliberto, Sébastien; Meux, Eric. Applied Spectroscopy. Aug2017, Vol. 71 Issue 8, p1884-1893. 10p. DOI: 10.1177/0003702817694382.

A beam path-based method for attenuation correction of confocal micro-X-ray fluorescence imaging data. Liu, Peng; Ptacek, Carol J.; Blowes, David W.; Finfrock, Y. Zou. JAAS (Journal of Analytical Atomic Spectrometry). Aug2017, Vol. 32 Issue 8, p1582-1589. 8p. DOI: 10.1039/c7ja00148g.

X-ray fluorescence – a non-destructive tool in investigation of Czech fine and applied art objects. Trojek, T.; Musílek, L. Radiation Physics & Chemistry. Aug2017, Vol. 137, p230-233. 4p. DOI: 10.1016/j.radphyschem.2017.01.007.

X-ray diffraction, dielectric and Raman studies of the $Ba_{1-x}Na_xTi_{1-x}(Nb_{1-y}Sb_y)_xO_3$ ceramics. Chihaoui, Sonia; Chaker, Hanèn; Chaker, Chiheb; Khemakhem, Hamadi. Ceramics International. Aug2017, Vol. 43 Issue 12, p8938-8943. 6p. DOI: 10.1016/j.ceramint.2017.04.032.

***In operando* X-ray diffraction of lithium–oxygen batteries using an ionic liquid as an electrolyte co-solvent.** Knipping, E.; Aucher, C.; Guirado, G.; Fauth, F.; Aubouy, L. New Journal of Chemistry. 8/7/2017, Vol. 41 Issue 15, p7267-7272. 6p. DOI: 10.1039/c7nj01027c.

Validation of missed space-group symmetry in X-ray powder diffraction structures with dispersion-corrected density functional theory. Hempler, Daniela; Schmidt, Martin U.; van de Streek, Jacco. Acta Crystallographica: Section B, Structural Science, Crystal Engineering & Materials. Aug2017, Vol. 73 Issue 4, p756-766. 10p. DOI: 10.1107/S2052520617005935.

Solvent exchange in a metal–organic framework single crystal monitored by dynamic *in situ* X-ray diffraction. Cox, Jordan M.; Walton, Ian M.; Bateman, Gage; Benson, Cassidy A.; Mitchell, Travis; Sylvester, Eric; Chen, Yu-Sheng; Benedict, Jason B. Acta Crystallographica: Section B, Structural Science, Crystal Engineering & Materials. Aug2017, Vol. 73 Issue 4, p669-674. 5p. DOI: 10.1107/S2052520617008447.

Sourcing and processing of ochre during the late upper Palaeolithic at Tagliente rock-shelter (NE Italy) based on conventional X-ray powder diffraction analysis. Cavallo, Giovanni; Fontana, Federica; Gonzato, Federica; Guerreschi, Antonio; Riccardi, Maria; Sardelli, Giorgia; Zorzin, Roberto. Archaeological & Anthropological Sciences. Aug2017, Vol. 9 Issue 5, p763-775. 13p. DOI: 10.1007/s12520-015-0299-3.

The pair distribution function of liquid water: Truncation problem in light of recent X-ray diffraction data. Naberukhin, Yu. I. Journal of Molecular Liquids. Aug2017, Vol. 239, p45-48. 4p. DOI: 10.1016/j.molliq.2016.12.053.

Solar Technologies go Hybrid: Structure of Organometal Halide Perovskite Films as Determined with Grazing-Incidence X-Ray Scattering Methods. Schlipf, Johannes; Müller-Buschbaum, Peter. Advanced Energy Materials. 8/23/2017, Vol. 7 Issue 16. 1p. DOI: 10.1002/aenm.201770084.

CHARMed PyMca, Part I: A Protocol for Improved Inter-laboratory Reproducibility in the Quantitative ED-XRF Analysis of Copper Alloys. Heginbotham, A.; Solé, V. A. Archaeometry. Aug2017, Vol. 59 Issue 4, p714-730. 17p. DOI: 10.1111/arcm.12282.

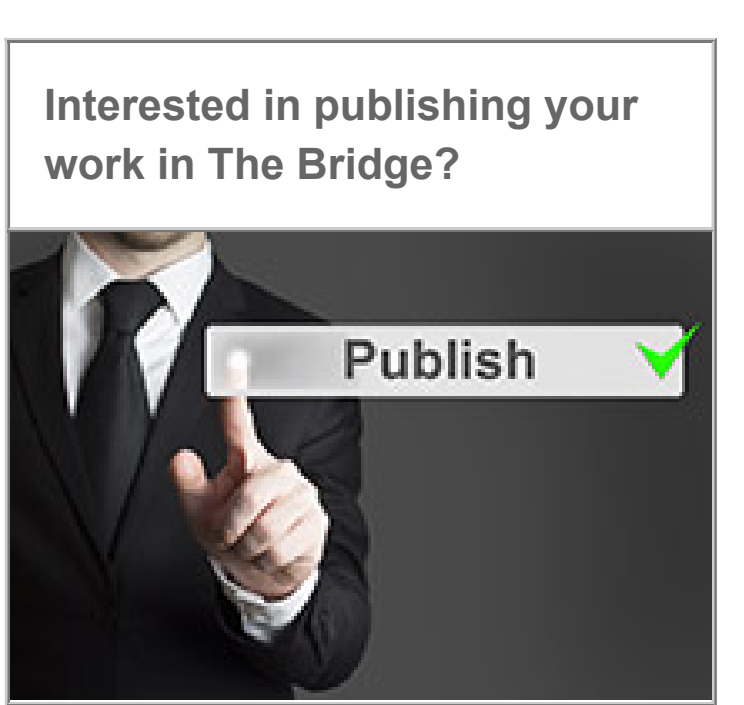
***In-situ* XRD investigation of selenization of CZTS nanoparticles.** Brandl, Marco; Sayed, Mohamed H.; Chory, Christine; Hammer-Riedel, Ingo; Parisi, Jürgen; Hock, Rainer; Gütay, Levent. Journal of Alloys & Compounds. Aug2017, Vol. 714, p35-38. 4p. DOI: 10.1016/j.jallcom.2017.04.199.

Elemental analysis of solids, liquids, powders, alloys and thin films

Supermini200

As the world's only high-power benchtop sequential wavelength dispersive X-ray fluorescence (WDXRF) spectrometer for elemental analysis of oxygen (O) through uranium (U) of almost any material, the Rigaku Supermini200 uniquely delivers low cost-of-ownership (COO) with high resolution and lower limits-of-detection (LLD). **For more >**

Interested in publishing your work in The Bridge?



Publish Your Work Here

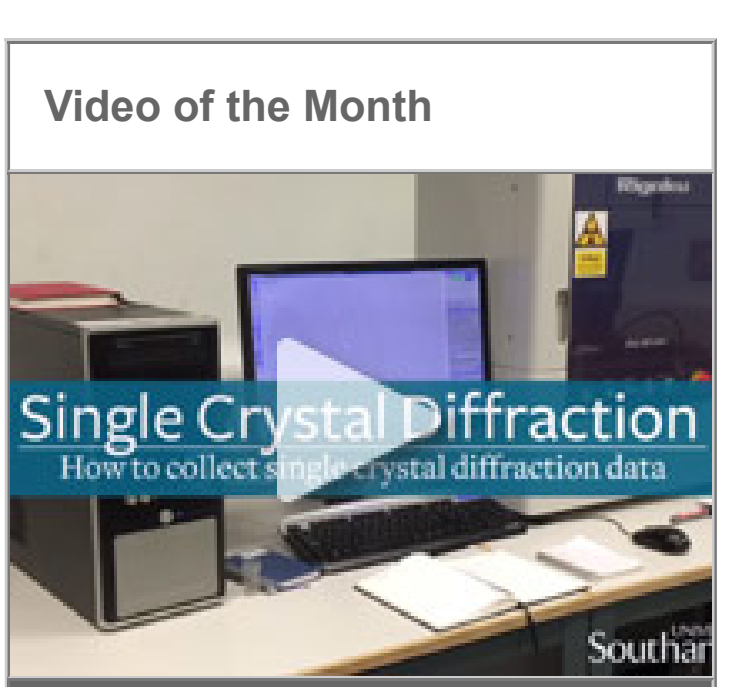
The Bridge now welcomes manuscripts, communications, and papers that describe techniques and applications of all forms of X-ray fluorescence (XRF) and X-ray diffraction (XRD, including SAXS) that are of interest to fellow scientists in industry, academia, and government. Manuscripts, in PDF format, are only accepted with the understanding that they are not commercial in nature. Authors are responsible for all statements made in their work. If illustrations or other material in a manuscript have been published previously, the author is responsible for obtaining permission to republish. Please send copy to the editor at Rigaku.newsletter@Rigaku.com

Benchtop chemical crystallography system for 3D small molecule structure determination

XtaLAB mini II

The Rigaku XtaLAB mini II benchtop X-ray crystallography system is a compact single crystal X-ray diffractometer designed to produce publication-quality 3D structures. The perfect addition to any synthetic chemistry laboratory, the XtaLAB mini II will enhance research productivity by offering affordable structure analysis capability without the necessity of relying on a departmental facility. With the XtaLAB mini II, you no longer have to wait in line to determine your structures. Instead your research group can rapidly analyze new compounds as they are synthesized in the lab.
For more >

Video of the Month



Single Crystal X Ray Diffraction familiarisation video – Southampton Diffraction Centre

University of Southampton Single Crystal X Ray Diffraction familiarisation video features the Rigaku XtaLAB mini.
Watch video >

Conferences and Workshops

Join Rigaku at future meetings

Rigaku will be sponsoring, attending or exhibiting at the following conferences and trade shows:

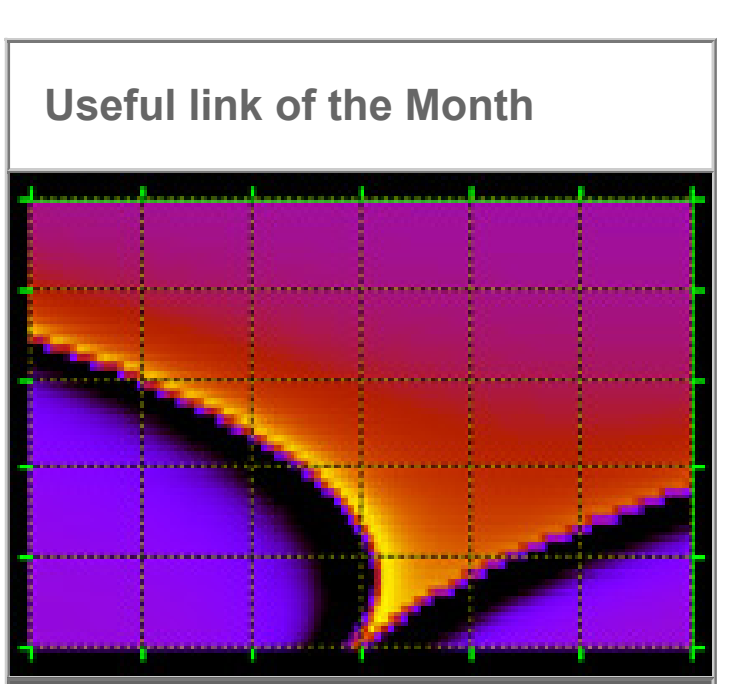
The Continuing Challenge
Sacramento, CA, USA
September 5 – 8, 2017

Canadian Mineral Analysis (CMA 2017)
Kamloops, BC, Canada
September 11 – 14, 2017

Massachusetts Hazmat Conference
Plymouth, MA, USA
September 20 & 21, 2017

See the complete list >

Useful link of the Month



X-Ray Server: BRL, GID_sl, TER_sl, TRDS_sl, MAG_sl, and X0h

X-ray Server was launched in 1997 with the goal to provide a wide scientific community with access to personal research results and for refining X-ray scattering models and scientific software via WWW technologies. The Server delivers a number of programs implementing the author's models in the fields of X-ray diffraction and scattering. Since computations are provided via a Web interface, there is no need to download, compile or install code. **For more >**

Planning to Submit a Grant?

Rigaku is happy to assist

If you are planning on submitting an instrument grant proposal, Rigaku will be happy to assist you. We can help you determine the correct instrument and configuration best suited for your analytical needs. **Start the process >**

Rigaku's Materials Analysis eNewsletter, The Bridge

Join us

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

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