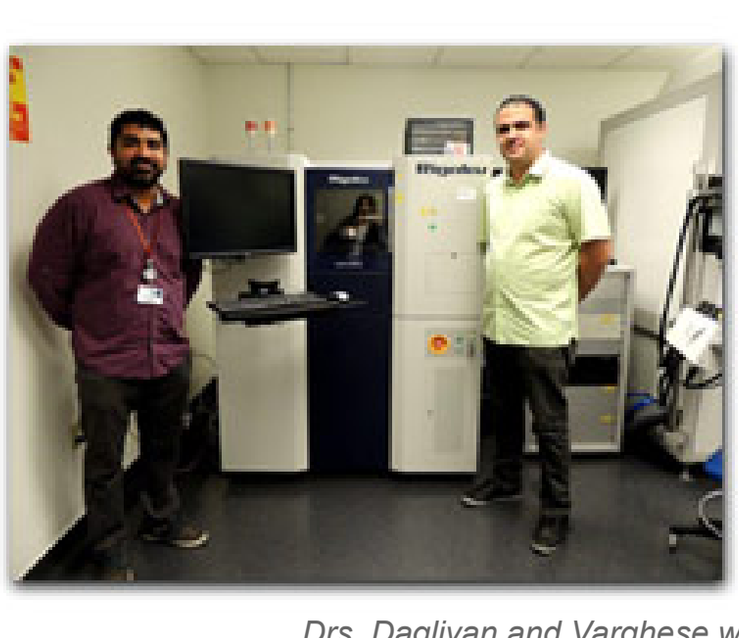
Welcome

We want to thank everyone who visited Rigaku at the 55th annual Eastern Analytical Symposium (EAS) in Somerset NJ during the middle of November. Attended by over 2,300 scientists, this conference featured 109 exhibitors and the usual plethora of oral sessions, workshops and posters. We wish to congratulate Purnendu Dasgupta, Professor in the Department of Physics at the University of Texas at Arlington, as winner of the 2016 EAS Award for Outstanding Achievements in the Fields of Analytical Chemistry.

Please come visit Rigaku in December at the following major events: AsCA (Hanoi, Vietnam), DLS-CCP4 Data Collection and Structure Solution Workshop (Oxford, UK), RSC Macrocyclic and Supramolecular Chemistry Meeting (Edinburgh, Scotland) and the Biological Structures Group Winter Meeting (London).




Drs. Dagliyan and Varghese with CTLab GX90 and nano3DX at the Molecular Imaging Center, The University of Southern California

This month's "Lab in the Spotlight" features the Molecular Imaging Center (MIC) at The University of Southern California (USC). The article below describes how the renovated facility included acquisition of two new computed tomography (CT) systems from Rigaku.

This month we feature two *Rigaku Journal* articles discussing the X-ray stress analysis technique and the fusion bead sample preparation method for XRF. Additional application papers include XRD, WDXRF, EDXRF and Raman technologies.

The video topic takes a break for November as we continue to celebrate Japanese Biologist Yoshinori Ohsumi, winner of the 2016 Nobel Prize for Medicine. The book review returns this month for a discussion of "the new physics." 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 XRD Rigaku Journal Article

X-ray stress analysis technique using the optimization of d_0 with error term Direct Refinement Solution (DRS) method

Shoichi Yasukawa, Rigaku Corporation

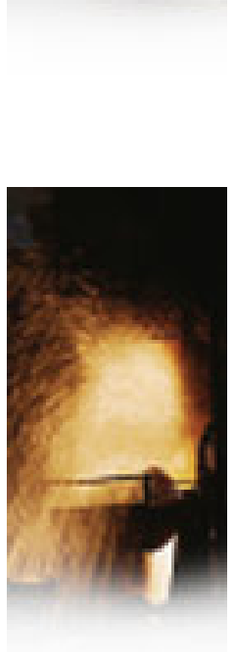
Stress analysis using X-ray diffraction is a well-known, effective technique for nondestructive evaluation of residual stresses in the surface of materials. Among X-ray stress analyses, the $\sin^2 \psi$ method is the most widely used and very common, especially in the industrial field. In this method, residual stress is calculated by assuming a plane stress condition as the stress state on the surface of materials. In detail, it is calculated by multiplying the X-ray stress constant specific to materials by the slope of a regression line between observed diffraction angle (2θ) and the $\sin^2 \psi$ function. As a result, it is not necessary to obtain the information on crystal lattice spacing (d-value) in the strain-free condition d_0, which is very difficult to know beforehand. This is why use of the $\sin^2 \psi$ method has become widespread as an effective analysis method. **For more >**

Featured XRF Rigaku Journal Article

Sample preparation for X-ray Fluorescence analysis V. Fusion bead method—part 2 practical applications

By Mitsuru Watanabe, Rigaku Corporation

The general preparation method of fusion bead, equipment, reagents and other important considerations were described in the previous article "Sample preparation for X-ray fluorescence analysis IV Fusion bead method—part 1 basic principles." In this article, the preparation methods of various applications such as ferroalloy, sulfide and carbide are described. **For full article >**



Lab in the Spotlight

Molecular Imaging Center, The University of Southern California

Reported by Yurika Takumi, Office of the President, Rigaku Corporation

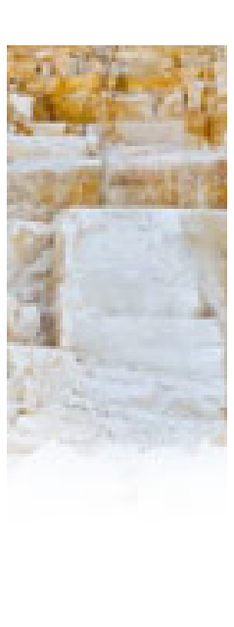
The Molecular Imaging Center (MIC) at The University of Southern California (USC) is one of the most important research facilities to provide a variety of imaging capabilities. Molecular imaging—that is, non-invasive visualization of the molecular processes of life in organisms of all levels of complexity—appears destined to become the primary mechanism by which new discoveries in molecular-based medicine are translated into clinical use and optimized for individual use. **For full report >**

XRD Application Note

MiniFlex300/600 Bulk sample measurement, Example 1 –Paper–

Rigaku Corporation

Powder X-ray diffractometers can readily measure bulk samples provided techniques are devised for sample preparation. In the case of samples in sheet form, such as paper or film, a diffraction pattern with no angular error can be obtained. **For more >**



WDXRF Application Note

Accurate Quantitative Analysis of Ferrosilicon by the Fusion Method Using ZSX Primus III+

Rigaku Corporation

Ferrosilicon is one of the most basic materials used in the steel making process. The iron alloys with the content of silicon between 15% and 90% are called "ferrosilicon", and are used in the reduction of the iron, removing oxygen and adding silicon when cast iron or steel alloys are produced. As part of controlling the steel making process, analyses of slag and raw materials such as quicklime are also required. X-ray fluorescence spectrometers are the most common analysis tools to analyze ferroalloy, slag, steel and added materials owing to the rapid analysis and the ability to measure both bulk metal and powders. This application note describes accurate ferrosilicon analysis using ZSX Primus III+, which is optimized for process control of steel making and ferrosilicon production. **For more >**

EDXRF Application Note

Measurement of $CaCO_3$, $MgCO_3$, Fe_2O_3, Al_2O_3 and SiO_2 in Dolomite

Applied Rigaku Technologies

Dolomite (calcium magnesium carbonate) is mainly used as an aggregate in concrete and asphalt for building roads. During mining and processing operations it is important to monitor and control the dolomite composition to ensure proper quality and characteristics desired for the various products. Rigaku meets this industry need with a high performance low cost benchtop EDXRF system. Rugged and reliable, the NEX QC+ is an ideal tool for measuring major carbonate and oxide components in dolomite, with simple and intuitive software designed for the non-technical at-line operator and for use in quality control labs. **For more >**

Raman Featured Article

Handheld Raman spectroscopy for the early detection of plant diseases: *Abutilon mosaic virus* infecting *Abutilon* sp.

Rigaku Analytical Devices

Early detection of plant diseases is critical to the health of crops. Diseases can be spread very fast and can affect neighboring crops and large areas. A collaborative study by Escuela Politécnica Nacional, Central University of Venezuela, Oklahoma State University and Dr. Ciobotă, Application Scientist at Rigaku, was conducted using Rigaku's Progeny 1064 nm handheld Raman spectrometer for the identification of the *Abulation mosaic virus*. The results demonstrate that Raman can be used for fast and early detection of plant diseases.

Dr. Valerian Ciobotă is an Applications Scientist with Rigaku Analytical Devices. He received his Ph.D. from Friedrich Schiller University in Physical Chemistry. He has 5 years experience with optical technologies including Raman and Laser Induced Breakdown Spectroscopy or LIBS. Dr. Ciobotă has and continues to contribute to a variety of application studies using handheld Raman and handheld LIBS. **For more >**

Scientific Book Review

Fashion, Faith and Fantasy in the New Physics of the Universe

This book is the result of a series of lectures Roger Penrose gave at Princeton in the early 2000s. I heard about it on *Science Friday* so I bought a copy. Be forewarned: this is not light reading. This is not a text book, but the concepts might have been better related had this been presented as a textbook.

Read full review >

Material Analysis in the News

News for November 2016

November 1, 2016. Physicists at the University of Houston claim to have developed a method that forces a non-superconducting material into a superconductive state. Dr. Chu, coauthor of the paper, said the idea that superconductivity could be induced at the interface between two non-superconductive materials was first proposed in the 1970s, but hasn't been proved until now.

November 1, 2016. Professor Mohamed Eddaoudi, associate director of King Abdullah University of Science and Technology's Advanced Membranes and Porous Materials Research Center, led a team of researchers at KAUST who are developing porous solids called metal-organic frameworks (MOFs) for the selective removal of various gases from gas mixtures. Their latest breakthrough MOF can effectively take up carbon dioxide even when it is present at concentrations as low as 400 ppm and opens possibilities for capturing CO_2 as it is generated.

November 2, 2016. The mystery of the origin and diversity of the rings that surround Saturn, Uranus and Neptune has been solved by researchers from Japan's Tokyo Institute of Technology and Kobe University. The experts have suggested that the planetary rings formed four billion years ago when large celestial objects travelled very close to the planets and were destroyed.

November 3, 2016. Scientists at Lehigh University, in collaboration with Lawrence Berkeley National Laboratory, have demonstrated the fabrication of what they call a new class of crystalline solid by using a laser heating technique that induces atoms to organize into a rotating lattice without affecting the macroscopic shape of the solid.

November 4, 2016. Advanced simulations demonstrating the tetraneutron corroborate the first observational evidence of the tetraneutron in an experiment performed at the RIKEN Radioactive Ion Beam Factory (RIBF), in Saitama, Japan. The existence of the tetraneutron will add an interesting new entry and gap to the chart of nuclides.

November 8, 2016. A Japanese research project on silent tires has been recognized for its "highly accurate fluid analysis and data mining." The project, between Yokohama Rubber Co. and Japan's Institute of Space and Astronautical Science (ISAS), received the 'excellent achievement research project award' for general-use research themes using high performance computing infrastructure (HPCI).

November 8, 2016. Innovative technologies developed by researchers at the U.S. Department of Energy's (DOE's) Argonne National Laboratory and their partners earned three R&D 100 Awards. One of the awards was for Hard X-ray Scanning Microscope with Multilayer Laue Lens Nanofocusing Optics (X-ray Science Division, in partnership with Brookhaven National Laboratory).

November 9, 2016. India and Japan have signed a memorandum of understanding (MoU) for the advancement of academic research in the field of earth sciences for the benefit of the peace and human welfare. The union cabinet on Tuesday approved the MoU signed between Japan Agency for Marine-Earth Science and Technology (JAMSTEC) and the ministry of earth sciences, Government of India.

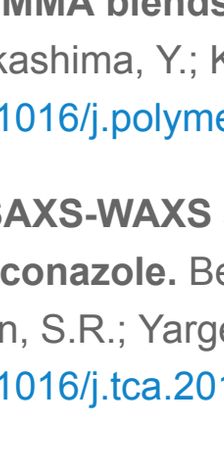
November 11, 2016. A startup founded by maverick Japanese entrepreneur Takafumi Horie is poised to launch a test rocket as early as January. If the trial succeeds, it will be Japan's first private rocket to reach an altitude of 100 km. Interstellar Technologies, based in Hokkaido, plans to use the data from the test flight to make technical improvements.

November 14, 2016. A multi-institutional collaboration driven by a group of London Centre for Nanotechnology (LCN) researchers has just published their results on the interaction of water with a metal oxide, TiO_2. Scanning tunnelling microscopy results from UCL and surface X-ray diffraction measurements taken at the European Synchrotron Radiation Facility (ESRF) in Grenoble were used to elucidate the structure of this model photocatalytic interface at a quantitative level, which has terminal hydroxyls in the contact layer.

November 21, 2016. After ramping up their respective 16nm/14 nm finFET processes, chipmakers are moving towards 10 nm and/or 7 nm, with 5 nm in R&D. But as they move down the process roadmap, they will face a new set of fab challenges. In addition to lithography and interconnects, there is metrology.

November 22, 2016. New technology could revolutionize printed electronics by enabling high quality semiconducting molecular crystals to be directly spray-deposited on any surface. University of Surrey and National Physical Laboratory's research allows to convert organic semiconducting inks into isolated crystals through a scalable process, suitable for a wide range of molecules.

November 22, 2016. Researchers at MIT, the German Synchrotron, and the University of Hamburg in Germany describe a new technique for generating ultrashort electron bursts, which could be the basis of a shoebox-sized device that consumes only a fraction as much power as its predecessor. The researchers' approach has the potential to lower their duration to a single femtosecond. An electron burst of a single femtosecond could generate attosecond X-ray pulses, which would enable real-time imaging of cellular machinery in action.



Recent Scientific Papers of Interest

Papers for November 2016

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

Assessing silicon deposits in Zilfi province, Saudi Arabia, using XRF and XRD techniques. Attaelmanan, Atta G.; Suleman, Nawal M.; El Agib, Ibrahim A.; Al-Sewaidan, Hamed A. *XRS: X-ray Spectrometry*. Nov/Dec2016, Vol. 45 Issue 6, p325-329. 5p. DOI: 10.1002/xrs.2708.

***In-situ* XRD investigation of re-crystallization and selenization of CZTS nanoparticles.** Sayed, Mohamed H.; Brandl, Marco; Chory, Christine; Hammer-Riedel, Ingo; Parisi, Jürgen; Gütay, Levent; Hock, Rainer. *Journal of Alloys & Compounds*. Nov2016, Vol. 686, p24-29. 6p. DOI: 10.1016/j.jallcom.2016.05.313.

Effect of miscible PMMA chain length on disordered morphologies in epoxy/PMMA-*b*-PnBA-*b*-PMMA blends by *in situ* simultaneous SAXS/DSC. Asada, M.; Oshita, S.; Morishita, Y.; Nakashima, Y.; Kunimitsu, Y.; Kishi, H. *Polymer*. Nov2016, Vol. 105, p172-179. 8p. DOI: 10.1016/j.polymer.2016.10.025.

A SAXS-WAXS study of the endothermic transitions in amorphous or supercooled liquid itraconazole. Benmore, C.J.; Mou, Q.; Benmore, K.J.; Robinson, D.S.; Neuefeind, J.; Ilavsky, J.; Byrn, S.R.; Yarger, J.L. *Thermochimica Acta*. Nov2016, Vol. 644, p1-5. 5p. DOI: 10.1016/j.tca.2016.10.004.

Synthesis and characterization of nanocrystaline hexagonal boron nitride powders: XRD and luminescence properties. Matović, Branko; Luković, Jelena; Nikolić, Marko; Babić, Biljana; Stanković, Nadežda; Jokić, Bojan; Jelenković, Branislav. *Ceramics International*. Nov2016, Vol. 42 Issue 15, p16655-16658. 4p. DOI: 10.1016/j.ceramint.2016.07.096.

Study of the Decomposition and Phase Transition of Uranium Nitride under UHV Conditions via TDS, XRD, SEM, and XPS. Xiaofang Wang; Zhong Long; Ren Bin; Ruilong Yang; Qifa Pan; Fangfang Li; Lizhu Luo; Yin Hu; Kezhao Liu. *Inorganic Chemistry*. 11/7/2016, Vol. 55 Issue 21, p10835-10838. 4p. DOI: 10.1021/acs.inorgchem.6b01260.

Measurement of *d*-spacing of crystalline samples with SAXS. Wei, Yanru; Li, Zhihong. *Measurement* (02632241). Nov2016, Vol. 93, p473-479. 7p. DOI: 10.1016/j.measurement.2016.07.051.

Influence of dopant metal ions on the formation of cordierite using combined SAXS/WAXS and EXAFS/WAXS techniques. Sankar, Gopinathan; Dent, Andrew. J.; Dobson, Barry; Bras, Wim. *Journal of Non-Crystalline Solids*. Nov2016, Vol. 451, p16-22. 7p. DOI: 10.1016/j.jnoncrysol.2016.07.030.

Occurrence characteristics of free iron oxides in soil microstructure: evidence from XRD, SEM and EDS. Zhang, X.; Kong, L.; Cui, X.; Yin, S. *Bulletin of Engineering Geology & the Environment*. Nov2016, Vol. 75 Issue 4, p1493-1503. 11p. DOI: 10.1007/s10064-015-0781-2.

Thermodynamic and XRD analysis of reaction behaviors of gangue minerals in roasting mixture of scheelite and calcium carbonate for Ca_3WO_6 preparation. Li, Xiaobin; Xu, Xiangming; Zhou, Qiusheng; Qi, Tiangui; Liu, Guihua; Peng, Zhihong; Cui, Yuanfa; Li, Jianpu. *International Journal of Refractory Metals & Hard Materials*. Nov2016, Vol. 60, p82-91. 10p. DOI: 10.1016/j.ijrmhm.2016.07.007.

Orthorhombic boron oxide under pressure: *In situ* study by X-ray diffraction and Raman scattering. Cherednichenko, Kirill A.; Godec, Yann Le; Kalinko, Aleksandr; Mezouar, Mohamed; Solozhenko, Vladimir L. *Journal of Applied Physics*. 2016, Vol. 120 Issue 17, p1-8. 8p. 1 Diagram, 4 Charts, 7 Graphs. DOI: 10.1063/1.4966658.

Characterization of the effective atomic number for first row transition elements by the ratio of coherent to compton scattering intensities obtained by wavelength dispersive X-ray fluorescence. Boydaş, Elif; Yılmaz, Demet; Cömert, Esra. *Instrumentation Science & Technology*. 2016, Vol. 44 Issue 6, p642-650. 9p. DOI: 10.1080/10739149.2016.1176928.

Determination of Zn in Dry Feeds for Cats and Dogs by Energy-Dispersive X-Ray Fluorescence Spectrometry. Ávila, Dayara Virgínia L.; Souza, Sidnei O.; Costa, Silvânio Silvério L.; Araujo, Rennan Geovanny O.; Garcia, Carlos Alexandre B.; Alves, José Do Patrocínio H.; Passos, Elisangela A. *Journal of AOAC International*. 2016, Vol. 99 Issue 6, p1572-1575. 4p. 5 Charts. DOI: 10.5740/jaoacint.16-0105.

Grazing incidence resonant soft X-ray scattering for analysis of multi-component polymer-fullerene blend thin films. Schaffer, Christoph J.; Wang, Cheng; Hexemer, Alexander; Müller-Buschbaum, Peter. *Polymer*. Nov2016, Vol. 105, p357-367. 11p. DOI: 10.1016/j.polymer.2016.05.056.

Distribution of sulfur in styrene-butadiene rubber studied with anomalous small-angle X-ray scattering at sulfur *K*-edge. Shinohara, Yuya; Seike, Haruka; Kishimoto, Hiroyuki; Tamenori, Yusuke; Amemiya, Yoshiyuki. *Polymer*. Nov2016, Vol. 105, p368-377. 10p. DOI: 10.1016/j.polymer.2016.06.016.

Local structure of Ca^{2+} induced hydrogels of alginate–oligoguluronate blends determined by small-angle-X-ray scattering. Yuguchi, Yoshiaki; Hasegawa, Ami; Padol, Anna Maria; Draget, Kurt Ingar; Stokke, Bjørn Torger. *Carbohydrate Polymers*. Nov2016, Vol. 152, p532-540. 9p. DOI: 10.1016/j.carbpol.2016.07.020.

Miniaturized X-ray powder diffraction assay (MixRay) for quantitative kinetic analysis of solvent-mediated phase transformations in pharmaceutics. Kirchmeyer, Wiebke; Grassmann, Olaf; Wyttenbach, Nicole; Alsenz, Jochem; Kuentz, Martin. *Journal of Pharmaceutical & Biomedical Analysis*. Nov2016, Vol. 131, p195-201. 7p. DOI: 10.1016/j.jpba.2016.08.028.

Effect of the concentrations of nucleating agents ZrO_2 and TiO_2 on the crystallization of $Li_2O–Al_2O_3–SiO_2$ glass: an X-ray diffraction and TEM investigation. Kleebusch, Enrico; Patzig, Christian; Höche, Thomas; Rüssel, Christian. *Journal of Materials Science*. Nov2016, Vol. 51 Issue 22, p10127-10138. 12p. DOI: 10.1007/s10853-016-0241-9.

Solid acetone structure dependence on pressure: a new fibre textured thin film crystallographic structure studied by grazing-incidence X-ray diffraction. Ferrer, P.; da Silva, I.; Puente-Orench, I. *CrystEngComm*. 11/14/2016, Vol. 18 Issue 42, p8220-8228. 9p. DOI: 10.1039/c6ce01333c.

Observing structural reorientations at solvent–nanoparticle interfaces by X-ray diffraction - putting water in the spotlight. Zobel, Mirijam. *Acta Crystallographica.* *Section A, Foundations & Advances*. Nov2016, Vol. 72 Issue 6, p1-11. 11p. DOI: 10.1107/S2053273316013516.

User Influence on Two Complementary Residual Stress Determination Methods: Contour Method and Incremental X-Ray Diffraction. Levieil, B.; Bridier, F.; Doudard, C.; Thevenet, D.; Calloch, S. *Experimental Mechanics*. Nov2016, Vol. 56 Issue 9, p1641-1652. 12p. DOI: 10.1007/s11340-016-0189-3.

Non-Destructive or Noninvasive? The Potential Effect of X-Ray Fluorescence Spectrometers on Luminescence Age Estimates of Archaeological Samples. Huntley, Jillian; Westaway, Kira E.; Gore, Damian B.; Aubert, Maxime; Ross, June; Morwood, Michael J. *Geoarchaeology*. Nov/Dec2016, Vol. 31 Issue 6, p592-602. 11p. DOI: 10.1002/gea.21574.

Analytical approaches for determination of bromine in sediment core samples by X-ray fluorescence spectrometry. Pashkova, Galina V.; Aisueva, Tatyana S.; Finkelshtein, Alexander L.; Ivanov, Egor V.; Shchetnikov, Alexander A. *Talanta*. Nov2016, Vol. 160, p375-380. 6p. DOI: 10.1016/j.talanta.2016.07.059.

A rapid total reflection X-ray fluorescence protocol for micro analyses of ion profiles in *Arabidopsis thaliana*. Höhner, Ricarda; Tabatabaei, Samaneh; Kunz, Hans-Henning; Fittschen, Ursula. *Spectrochimica Acta Part B*. Nov2016, Vol. 125, p159-167. 9p. DOI: 10.1016/j.sab.2016.09.013.

Forensic Application of X-ray Fluorescence Spectroscopy for the Discrimination of Authentic and Counterfeit Revenue Stamps. Melendez-Perez, Jose Javier; Nascimento Correa, Deleon; Veri Hernandes, Vinicius; de Morais, Damila Rodrigues; de Oliveira, Rodrigo Borges; de Souza, Wanderley; Machado Santos, Jandyson; Nogueira Eberlin, Marcos. *Applied Spectroscopy*. Nov2016, Vol. 70 Issue 11, p1910-1915. 6p. DOI: 10.1177/0003702816645352.

Video of the Month

The Nobel Prize for Medicine 2016

Japanese Biologist Yoshinori Ohsumi has won the first Nobel Prize of the season for Medicine. His research into Autophagy in cells gained him the prestigious prize. **Watch video >**

Conferences and Workshops

Join Rigaku at future meetings

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

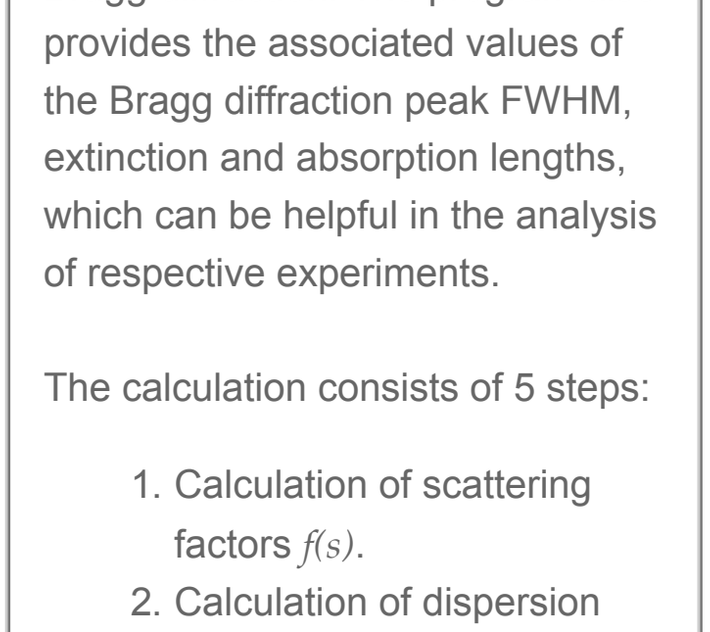
International Metal Technology 2016
Kaohsiung, Taiwan
December 6 & 8, 2016

BRSG Christmas Meeting 2016
London, UK
December 14, 2016

RSC Macrocyclic and Supramolecular Chemistry Meeting (2016)
Edinburgh, Scotland
December 15 – 16, 2016

See the complete list >

Useful link of the Month



X0h – Sergey Stepanov's X-ray Server

This useful link is an interface to program *X0h* for calculating crystal susceptibilities X_0, X_h (*chi-zero, chi-h*) for X-ray scattering and Bragg diffraction. The program also provides the associated values of the Bragg diffraction peak FWHM, extinction and absorption lengths, which can be helpful in the analysis of respective experiments.

The calculation consists of 5 steps:

1. Calculation of scattering factors $f(s)$.
2. Calculation of dispersion corrections df' and df''.
3. Calculation of dipole and quadrupole absorption cross sections.
4. Calculation of Debye-Waller temperature factors.
5. Finally, calculation of X_0 and X_h by summation of atomic scattering over crystal unit cell.

For more >