Crystallography Times
Rigaku

Crystallography Newsletter
Volume 11, No. 06, June 2019
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In this issue:

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ACA Annual Meeting
Covington, Kentucky, July 19 – 23, 2019

Denver X-ray Conference and International Congress on X-ray Optics and Microanalysis
Lombard, Illinois, August 5 – 9, 2019

European Crystallographic Meeting
Vienna, Austria, August 18 – 23, 2019

Rigaku Events at the ACA

Rigaku Users' Meeting
Saturday, July 20, 4 – 6 pm, location TBD

Rigaku Mixer
Sunday, July 21, 7 – 9:30 pm, Molly Malone's

Rigaku Booth Drawing
Tuesday, July 23, Afternoon Coffee Break

Rigaku Reagents:
Unipucks and Tools

Crystallography in the News

June 3, 2019. Amgen has discovered a drug to target a supposedly "undruggable" gene mutation, potentially paving the way for a new cancer treatment. The California-based biotech company presented very early data on its research into drugging the protein made by the KRAS gene — a mutation of which is found in many cancers including lung and colorectal.

June 4, 2019. Stephen Cusack and his research group at EMBL Grenoble have, for the first time, observed different functional states of the influenza virus polymerase as it is actively transcribing. It provides the first characterization of the movements of the polymerase during the so-called nucleotide addition cycle, whereby each successive nucleotide is added to the growing mRNA chain.

June 6, 2019. Rigaku and Merck KGaA, Darmstadt, Germany, have formed a partnership to develop lab consumables based on highly innovative crystalline sponge technology, which determines the absolute chemical structure of organic molecules and enables X-ray crystallography without crystallization of the analyte.

June 7, 2019. Groundbreaking research at the new long-wavelength macromolecular crystallography beamline (I23) at Diamond Light Source has for the first time demonstrated the location of potassium ions in bacterial ribosomes. Little was known of the sites of metal ions that are crucial for their structure and function.

June 10, 2019. Scientists at the Sloan Kettering Institute have combined biochemical and computational methods to visualize how an important cancer-related protein changes shape during a chemical reaction. The results will aid drug design.

June 10, 2019. New research reveals the molecular machinery behind the high-intensity sweetness of the stevia plant. The results could be used to engineer new non-caloric products without the aftertaste that many associate with sweetener marketed as Stevia.

June 11, 2019. Small molecule JH-RE-06 was developed by scientists at Duke University and tested in human cancer cell lines and a mouse model of human melanoma. JH-RE-06, which exploits a pair of half pockets that form a whole pocket when two TLS proteins combine, helps preserve the effectiveness of several forms of chemotherapy while also suppressing the ability of cultured cancer cells to mutate in the presence of DNA-damaging drugs.

June 17, 2019. In a scientific first, scientists in the Blavatnik Institute at Harvard Medical School have shown it is possible to determine the 3-D structures of a gene by assessing the effects of lab-made genetic mutations on protein functions. The team's findings represent a significant step toward linking sequence data with its function in cells. The tool is freely available at GitHub.

June 18, 2019. *C. trachomatis* pathogenicity relies on the creation of an intracellular parasitic niche called an "inclusion," which is made from the outer membrane of the host cell. When a human cell is infected with multiple *Chlamydia*, each bacterium will develop an individual inclusion, all of which will ultimately fuse together into one large inclusion. This unique fusion event depends on the chlamydial protein IncA. Microbiologist Fabienne Paumet teamed up with biochemist Gino Cingolani to determine an electron density map of the fusion protein.

June 19, 2019. Researchers have developed a technology to analyze the adsorption behavior of molecules in each individual pore of a metal organic framework (MOF). This system has large specific surface areas, allowing for the real-time observation of the adsorption process of an MOF.

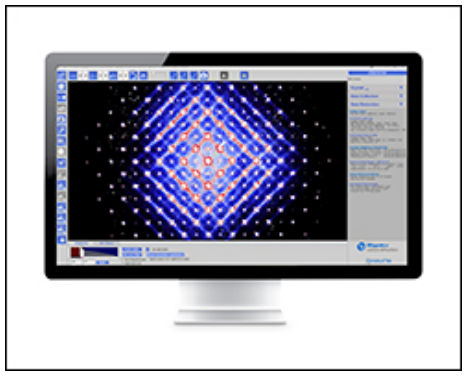
June 19, 2019. Using neutrons to collect structural information on RNA and DNA is no ordinary feat. Small biomolecular samples in dilute solutions often produce noisy scattering patterns, making the data difficult to analyze. Oak Ridge National Laboratory's Bio-SANS detector at the High Flux Isotope Reactor is one of few neutron instruments in the world with the capability to capture small and wide scattering angles simultaneously, combining both global- and local-scale details

The Universal V1-Puck (unipuck) is a sample pin storage and shipping container that is compatible with many automated sample mounting systems currently in use at synchrotrons and home laboratories worldwide. The unipuck was developed in collaboration between the ALS, APS, SBC-CAT and SSRL staff. The unipuck uses the standard AL tools for manipulation and has an outside form factor resembling the ALS pucks. There are many online resources for using unipucks, including the following manual from SSRL and helpful videos from Diamond Light Source.

The unipucks and tools are available to purchase individually or as kits. Each part of the V1-Puck has a unique serial number for identification. Custom serial numbers and puck coloring is available by request.

Contact ReagentOrders@Rigaku.com
For more information, visit the
Rigaku Reagents website.

CrysAlis^{Pro} v40 has been released on the Rigaku X-ray Forum



The major features of version 40 include:

- 32 and 64 bit versions
- Support of new AutoChem4.0 with an updated StructureExplorer
- Ewald3D live in the 64 bit version
- Extended support for multi-core use (in the 64 bit version, up to 32 cores)
- Significantly faster processing in dc profit
- Support of all new Synergy and ROD platforms
- Automated/manual version updating

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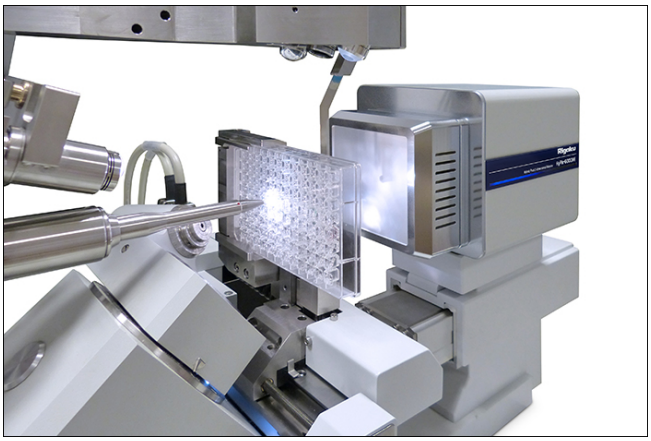
Rigaku Users' Meeting at the ACA Annual Meeting in Covington, KY

June 19, 2019. Memorial Sloan Kettering cancer biologist Michael Kharas's team reported that they have identified a molecule that appears to block the function of Musashi-2, a protein that plays a role in making cancer grow and spread. SKI computational chemist John Chodera, SKI structural biologist Dinshaw Patel, and Yehuda Goldgur, Head of MSK's X-Ray Crystallography Core Facility, helped determine the structure of the Musashi-2 protein and how Ro 08-2750 binds to it. SKI computational biologist Christina Leslie helped with the gene expression data generated from this research.

Product Spotlight



The XtalCheck System

The XtalCheck system is an automated tool for performing *in situ* crystallography experiments on your existing X-ray diffraction system. Protein crystallography often requires screening large numbers of crystals to identify samples that are suitable for X-ray diffraction experiments. Specifically, crystallographers usually loop and cryo-freeze samples for X-ray screening to identify whether the sample contains a protein or salt and to evaluate diffraction resolution, mosaicity and other crystal parameters. This iterative process of mounting and screening of many samples is time consuming and rarely automated. The XtalCheck system addresses this bottleneck by automating diffraction data collection for crystals directly from SBS format crystallization plates.

The XtalCheck system includes software that facilitates both visual and diffraction imaging of crystallization experiments. With the XtalCheck system, one can easily survey many crystallization experiments by eliminating the need to harvest and cryo-cool samples. Moreover, one can perform serial crystallography experiments, by collecting data from multiple crystals, to achieve complete data sets that can be used for structure solution.

Features:

- Quickly survey crystals prior to cryo-cooling
- Simple queuing of crystal objects for diffraction screening
- Data collection for sample queue progresses without user intervention
- Assign multiple crystal objects per drop

Lab in the Spotlight

The University of Alabama-Tuscaloosa

We are pleased to announce that following the success of this year's mini-user meeting at the 2019 BCA, we will be holding a short user meeting and discussion group at the 2019 ACA Annual Meeting. The meeting will start at 4 pm on Saturday July 20th and end at 6 pm just before the Celebration of Life for Michael Rossmann.

Please join us to discover the latest developments at Rigaku in single crystal diffraction and to chat about your research, experiences, and issues.

Register for this event.

Survey of the Month

June 2019 SCX Survey

Last year a Chinese scientist edited the CCR5 gene in human embryos, ultimately resulting in two infants that may or may not be HIV immune and may or may not have shortened life spans. Now a Russian scientist wants to make the same edits to human embryos. The scientific community should:

- Encourage this research
- Discourage this research
- Do everything to stop this research immediately

Take the Survey

The University of Alabama-Tuscaloosa recently took delivery of an XtaLAB Synergy-DW Cu/Mo, the first in the Western Hemisphere. Scientist Fengrui Qu says "The new instrument is much more powerful in every regard compared to our previous (aged) instrument. It cuts down the collection time dramatically, to roughly one fourth." Dr. Qu likes the "What Is This" (WIT) utility, which can provide a connectivity model in just a few minutes. While not good enough for publication, a WIT structure provides sufficient information to allow researchers to decide whether to collect a full data set if the material is interesting. Dr. Qu adds "This feature is very neat, esp. for some synthetic labs. We can use it as a walkup instrument (as NMR) in some cases." Furthermore, the instrument will also be used for diffuse scattering experiments on molecules and materials and for solving the structure of proteins and other large biomolecules. Beyond UA, it is a resource for regional colleges and universities and it will also be used heavily in teaching. Dr. Fengrui Qu (crystallographer), Dr. Elizabeth Papish (PI), Dr. Jared Allred (co-PI), Dr. Jack Dunkle (co-PI), Dr. Paul Rupar (co-PI), and Dr. Kevin Shaughnessy (co-PI) thank NSF CHE MRI 1828078 and UA for the purchase of the single crystal X-ray diffraction instrument.

Useful Link

AAAS Member Community

AAAS has a central website for all members and member communities (sections) with blogs, events, news and other useful information. You use your AAAS ID to sign in and you can participate in discussions with the greater AAAS membership, as well as the three sections to which you belong. You can also view activities in the 25 other sections. I have just begun to scratch the surface but this seems like a wealth of useful information.

Selected Recent Crystallographic Papers

Michael G. Rossmann (1930–2019), pioneer in macromolecular and virus crystallography: scientist, mentor and friend. Arnold, Eddy; Wu, Hao; Johnson, John E. *Acta Crystallographica: Section D, Structural Biology*. Jun2019, Vol. 75 Issue 6, p523-527. 5p. DOI: 10.1107/S2059798319008398.

HKLF5Tools: a program for processing diffraction data of non-merohedrally twinned crystals. Ivlev, Sergei I.; Conrad, Matthias; Kraus, Florian. *Zeitschrift für Kristallographie*. Crystalline Materials. Jun2019, Vol. 234 Issue 6, p415-418. 4p. DOI: 10.1515/zkri-2018-2147.

A new crystal structure and small-angle X-ray scattering analysis of the homodimer of human SFPQ. Hewage, Thushara Welwelwela; Caria, Sofia; Lee, Mihwa. Acta *Crystallographica: Section F, Structural Biology Communications*. Jun2019, Vol. 75 Issue 6, p439-449. 11p. DOI: 10.1107/S2053230X19006599.

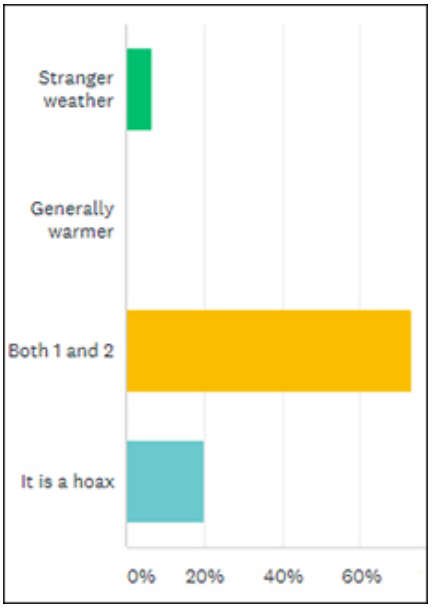
Structural Basis for YjbH Adaptor-Mediated Recognition of Transcription Factor Spx. Awad, Wael; Al-Eryani, Yusra; Ekström, Simon; Logan, Derek T.; von Wachenfeldt, Claes. *Structure*. Jun2019, Vol. 27 Issue 6, p923-923. 1p. DOI: 10.1016/j.str.2019.03.009.

Atypical Lone Pair–π Interaction with Quinone Methides in a Series of Imido-Ferrociphenol Anticancer Drug Candidates. Wang, Yong; Pigeon, Pascal; Top, Siden; Sanz García, Juan; Troufflard, Claire; Ciofini, Ilaria; McGlinchey, Michael J.; Jaouen, Gérard. *Angewandte Chemie*. 6/17/2019, Vol. 131 Issue 25, p8509-8513. 5p. DOI: 10.1002/ange.201902456.

Laue diffraction and time-resolved crystallography: a personal history. Moffat,

Last Month's Survey

Climate change is obvious because of:



Video of the Month

Here is a TED talk by Pamela Meyers, author of *Liespotting*. Ms. Meyer provides some interesting insights into lying and lie detection. 18:50 minutes well spent.

Watch the Video

Join Us on LinkedIn

Our 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 X-ray Forum

Keith. *Philosophical Transactions of the Royal Society A: Mathematical, Physical & Engineering Sciences*. 6/17/2019, Vol. 377 Issue 2147, p1-10. 10p. DOI: 10.1098/rsta.2018.0243.

Light-Controlled Conformational Switch of an Aromatic Oligoamide Foldamer. Gole, Bappaditya; Kauffmann, Brice; Maurizot, Victor; Huc, Ivan; Ferrand, Yann. *Angewandte Chemie International Edition*. 6/11/2019, Vol. 58 Issue 24, p8063-8067. 5p. DOI: 10.1002/anie.201902378.

***P*-Aminophosphaalkenes with *C*-Isopropyldimethylsilyl Groups.** Bîrzoi, Roxana M.; Jones, Peter G.; Bartsch, Rainer; Mont, Wolf-W. *Zeitschrift für Anorganische und Allgemeine Chemie*. 6/3/2019, Vol. 645 Issue 10, p712-722. 11p. DOI: 10.1002/zaac.201900049.

Synthesis and crystal structures of chiral ferrocene and ruthenocene substituted aminomethylnaphthols obtained through Betti-condensation. Dikova, Krasimira; Kostova, Kalina; Simova, Svetlana; Linden, Anthony; Chimov, Angel; Dimitrov, Vladimir. *Polyhedron*. Jun2019, Vol. 165, p177-187. 11p. DOI: 10.1016/j.poly.2019.03.019.

Solid State Structure of cis-[$W(CO)_4(pip)(PPh_3)$]. Harkreader, Jennifer L.; Frost, Brian J. *Journal of Chemical Crystallography*. Jun2019, Vol. 49 Issue 2, p125-129. 5p. DOI: 10.1007/s10870-018-0743-1.

Koanolide A, antiproliferative germacrane-type sesquiterpene lactone from *Koanophyllon gibbosum*. Castillo, Quírico A.; Padrón, José M.; Wojtas, Lukasz; Keramane, Mehdi; Germosén, Evelyn A. *Tetrahedron Letters: International Organ for the Rapid Publication of Preliminary Communications in Organic Chemistry*. Jun2019, Vol. 60 Issue 25, p1640-1642. 3p. DOI: 10.1016/j.tetlet.2019.05.036.

Characteristics of twins in $Li(Ni_{0.67}Co_{0.33})O_2$ as a cathode material for lithium-ion batteries. Ai, YanLing; Zhang, M.Q.; Jiang, F.; Zhang, Ruizhi; Liu, Jun.; Wang, C.; Xiao, W.H. *Journal of Alloys & Compounds*. Jun2019, Vol. 791, p1167-1175. 9p. DOI: 10.1016/j.jallcom.2019.03.376.

Protein encapsulation in the hollow space of hemocyanin crystals containing a covalently conjugated ligand. Hashimoto, Tsubasa; Ye, Yuxin; Ui, Mihoko; Ogawa, Tomohisa; Matsui, Takashi; Tanaka, Yoshikazu. *Biochemical & Biophysical Research Communications*. Jun2019, Vol. 514 Issue 1, p31-36. 6p. DOI: 10.1016/j.bbrc.2019.04.062.

Structure, Hirshfeld surface and theoretical study of a new inorganic organic arsenate compound $NaH_2AsO_4{\cdot}(C_{12}H_8N_2){\cdot}1.5H_2O$. Harchani, Ali; Kaminsky, Werner; Haddad, Amor. *Journal of Molecular Structure*. Jun2019, Vol. 1186, p60-67. 8p. DOI: 10.1016/j.molstruc.2019.03.018.

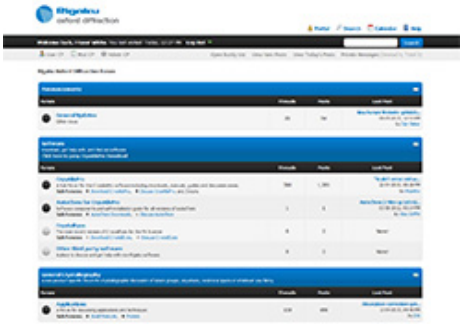
Half-sandwich Ni(II) complexes [Ni(Cp)(X)(NHC)]: From an underestimated discovery to a new chapter in organonickel chemistry. Banach, L.; Gunka, P.A.; Zachara, J.; Buchowicz, W. *Coordination Chemistry Reviews*. Jun2019, Vol. 389, p19-58. 40p. DOI: 10.1016/j.ccr.2019.03.006.

A Microporous Metal-Organic Framework Supramolecularly Assembled from a Cu^{II} Dodecaborate Cluster Complex for Selective Gas Separation. Zhang, Yuanbin; Yang, Lifeng; Wang, Lingyao; Duttwyler, Simon; Xing, Huabin. *Angewandte Chemie International Edition*. 6/11/2019, Vol. 58 Issue 24, p8145-8150. 6p. DOI: 10.1002/anie.201903600.

Accurate and efficient representation of intramolecular energy in *ab initio* generation of crystal structures. II. Smoothed intramolecular potentials. Sugden, Isaac J.; Adjiman, Claire S.; Pantelides, Constantinos C. *Acta Crystallographica: Section B, Structural Science, Crystal Engineering & Materials*. Jun2019, Vol. 75 Issue 3, p423-433. 11p. DOI: 10.1107/S2052520619005778.

Effect of water of crystallization on aggregation-induced emission in structurally similar crystals. Hayashi, Naoto; Okamoto, Naoki; Onoue, Masaya; Yamamoto, Kensuke; Yoshino, Junro. *Tetrahedron Letters: International Organ for the Rapid Publication of Preliminary Communications in Organic Chemistry*. Jun2019, Vol. 60 Issue 25, p1663-1666. 4p. DOI: 10.1016/j.tetlet.2019.05.040.

Structural basis for efonidipine block of a voltage-gated Ca^{2+} channel. Xu, Fuyan; Xiong, Weixi; Huang, Yiman; Shen, Jianghua; Zhou, Dong; Tang, Lin. *Biochemical & Biophysical Research Communications*. Jun2019, Vol. 513 Issue 3, p631-634. 4p. DOI: 10.1016/j.bbrc.2019.03.176.



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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 CrysAlis^{Pro} software for single crystal data processing.

We look forward to seeing you on there soon.

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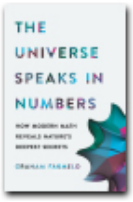
Zinc-oxaprozin compounds: Synthesis, structure and biological activity. Lazou, Marialena; Hatzidimitriou, Antonios G.; Papadopoulos, Athanasios N.; Psomas, George. *Journal of Inorganic Biochemistry*. Jun2019, Vol. 195, p101-110. 10p. DOI: 10.1016/j.jinorgbio.2019.03.016.

Probing the antibacterial and anticancer potential of tryptamine based mixed ligand Schiff base Ruthenium(III) complexes. Malik, Manzoor Ahmad; Raza, Md Kausar; Dar, Ovas Ahmad; Amadudin; Abid, Mohammad; Wani, Mohmmad Younus; Al-Bogami, Abdullah Saad; Hashmi, Athar Adil. *Bioorganic Chemistry*. Jun2019, Vol. 87, p773-782. 10p. DOI: 10.1016/j.bioorg.2019.03.080.

Pyrazolyl-phosphinoyl nickel (II) complexes: synthesis, characterization and ethylene dimerization studies. Junges, C.H.; Dresch, L.C.; Costa, M.T.; Tirloni, B.; Casagrande, O.L.; Stieler, R. *Applied Organometallic Chemistry*. Jun2019, Vol. 33 Issue 6, pN.PAG-N.PAG. 1p. DOI: 10.1002/aoc.4887.

Book Review



The Universe Speaks in Numbers: How Modern Math Reveals Nature's Deepest Secrets
By Graham Farmelo, ISBN: 978-0-465-05665-1

In *The Universe Speaks in Numbers*, Graham Farmelo presents a concise version of the history of the relationship between mathematics and physics. As Farmelo explains in his book, the relationship, though perhaps a natural one, has not always been an easy one. He even goes so far as to describe it as one that has gone through a long divorce and subsequent reconciliation.

Farmelo begins by describing Einstein's philosophy, that a purely mathematical and theoretical approach to the study of physics could wield meaningful insights into the natural world, as opposed to a purely experimental one. Even though Einstein's genius was celebrated in his own time as it is now, such an approach was considered laughable by many of his peers and fellow physicists. A young Robert Oppenheimer once described Einstein as "completely cuckoo," Farmelo explains. And Oppenheimer wasn't the only one.

But, as with many great minds, Einstein was simply ahead of his time. A significant amount of scientific research up to that point was observation- and experiment-based. Now, the use of mathematics to study and describe physics on a theoretical level is widely practiced—string theory comes to mind as perhaps the most famous example of theoretical physics in the forefront of the zeitgeist.

After beginning with Einstein, Farmelo goes back to the basics—classical physics. It's a field that Isaac Newton—a mathematician by practice and title—helped describe. Newton, despite being well-known in high school and college physics courses today for his Laws of Motion, would not have considered himself a physicist in his own time. Newton described his use of mathematics to explain what he saw in nature in his *Principia*—now considered a foundational text of calculus. Today, calculus and physics are essentially married subjects—but, in Newton's time, the idea of wedding mathematical calculations with experimental insights to support theoretical observations was revolutionary, to say the least. His work catalyzed the integrated study of mathematics and science in an unprecedented way that would culminate in the invention of modern physics in the twentieth century.

Farmelo makes sure to pay his respects to some of Newton's "giant" predecessors, upon whose shoulders Newton stood to see further. These include Aristotle and Galileo, amongst others. But the main focus of Farmelo's first chapter is Newton. After Newton, he details James Clerk Maxwell's mathematical investigations into electromagnetism—the culmination of which is a series of equations that bear his name. From there, Farmelo moves on to the two revolutionary discoveries that define modern physics: basic relativity and quantum mechanics.

Then, Farmelo comes to the aforementioned long divorce. In the mid-twentieth century, many physicists, Freeman Dyson among them, felt physics stood alone from mathematics. Experimentation and observation were the foundations of the field. Dyson and his fellow physicists viewed the mathematical foundations of theoretical physics with skepticism. Now 92, Dyson—along with others in the field—have changed their tune. It's intriguing to read *The Universe Speaks in Numbers* not long after reading Dyson's memoir *Maker of Patterns: An Autobiography through Letters*. He's gone from being the narrator to the narrated, so to speak—from the director of the show to an actor in it, and it's an interesting transition. If you want more on Dyson after reading *The Universe Speaks in Numbers*, or even if you want a scientist's immediate perspective on the events Farmelo describes in his own book, I recommend checking out Dyson's memoir. [A review of Maker of Patterns will appear here next month – JDF]

It's humbling to note, as Farmelo does, that it took three centuries to get from Newton to the Standard Model of particle physics, and only four decades to get from the Standard Model to where we are today. The last four decades occupy the second half of *The Universe Speaks in Numbers* and, as you might expect, more modern characters like Stephen Hawking make an appearance, while Dyson continues to pop up as the fields of theoretical physics and mathematics begin to repair their relationship and reconcile. If you want to learn how, you'll have to read it for yourself.

Farmelo is both a professor of physics and a skilled science writer—and it shows. He demonstrates a firm command of the subject matter, which coupled with his accessible language and writing style makes *The Universe Speaks in Numbers* a delightful and insightful read.

Review by Jeanette S. Ferrara, MA

Rigaku Corporation
e-mail: info@Rigaku.com
Tel: +[81] 3-3479-0618
FAX: +[81] 3-3479-6112

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

Rigaku China
e-mail: info@Rigaku.com.cn
Tel: +[86] 010-88575768
FAX: +[86] 010-88575748

Rigaku Europe
e-mail: info@Rigaku.com
Tel: +[49] 6102 77999 51
FAX: +[49] 6102 77999 99