Crystallography Times

Crystallography Newsletter
Volume 11, No. 02, February 2019

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PITTCON 2019
Philadelphia, PA, March 17 – 21, 2019

27th Annual Meeting of the German Crystallographic Society (DGK)
Leipzig, Germany, March 25 – 28, 2019

American Chemical Society National Meeting and Exposition (ACS Spring 2019)
Orlando, FL, March 31 – April 4, 2019

British Crystallographic Association Spring Meeting (BCA Spring Meeting 2019)
Nottingham, UK, April 15 – 18, 2019

Second Annual Industrial Biostructures America (IBA) Conference
La Jolla, California, May 19 – 21, 2019

102nd Canadian Chemistry Conference and Exhibition
Québec City, Canada, June 3 – 7, 2019

Join ROD on LinkedIn

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.

Crystallography in the News

February 5, 2019. Antibiotic resistance is the biggest challenge in modern medicine, Nobel laureate and renowned crystallographer Ada E. Yonath said during a public lecture organised by the Kerala State Higher Education Council (KSHEC) under its Erudite – Scholar in Residence programme at the Senate Chamber of the University of Kerala.

February 6, 2019. Researchers have made the first ever highly porous, mechanically flexible and stretchable inorganic nanomaterial that is both hydrophilic and hydrophobic at the same time. The material, which consists of interpenetrating hollow gallium nitride tetrapods, has similar properties to a biological cell membrane and it could find use in applications such as sensors, microfluidic devices and microrobotics.

February 6, 2019. Anna Ziegler's 2008 "Photograph 51" belongs to the growing body of literature helping women reclaim their rightful place in history in general and scientific history in particular. But the 90-minute play about Rosalind Franklin, the British chemist whose discovery of the DNA double helix in the early 1950s was long unappreciated, is no simple paean. Ziegler couples her portrait of a complicated woman in a world of sexist men with an examination of bigger "what if" questions.

February 7, 2019. The British-built Mars rover scheduled to be launched in 2020 has been named after scientist Rosalind Franklin. The ExoMars mission is designed to search for evidence of life on Mars. The name was revealed by astronaut Tim Peake and Science Minister Chris Skidmore after more than 36,000 people submitted ideas, which were narrowed down by a panel of experts.

February 11, 2019. Scientists from ASU's School of Molecular Sciences in collaboration with colleagues from Albert Einstein College of Medicine in New York City have captured snapshots of crystal structures of intermediates in the biochemical pathway that enables us to breathe. Published in the *Proceedings of the National Academy of Sciences*, their results provide key insights into the final step of aerobic respiration.

February 19, 2019. A natural quasicrystal is a solid whose atoms flout the laws of crystallography by having order that does not repeat. The first quasicrystal was in a rock that had been sequestered in a museum in Florence. In *The Second Kind of Impossible*, Steinhardt, a theoretical physicist, chronicles the detective work that led to his no-eureka-necessary moment — and sent him from Princeton University to the wilds of Siberia to find out how that rock had formed.

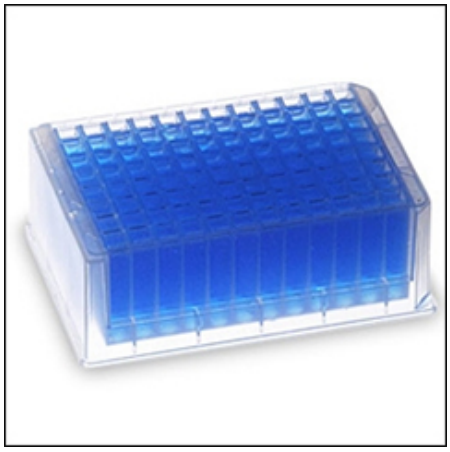
February 19, 2019. Researchers at Cardiff University have used X-ray crystallography and computer simulation to get a closer look at how viruses bind cells and cause infection. The new insight could help in the development of drugs and therapies for infections and further advance the exploitation of viruses for medical treatments.

February 20, 2019. A new antimicrobial-resistance gene, VCC-1, a ß-lactamase gene, has been discovered in benign close relatives of virulent *Vibrio cholerae*, which causes cholera. Using X-ray crystallography, a team of Canadian researchers has found a way to block the VCC-1 enzyme, which disables that resistance gene.

Product Spotlight

XtaLAB mini II

Rigaku Reagents:
The Wizard pH Buffer Screen



The Wizard pH Buffer Screen is a set of 96 solutions containing 12 different buffer systems at 8 different pHs, ranging from ±1.4 pH units around the pKa. The screen covers the entire crystallization space with buffers ranging from pH 2.4 to pH 11.6. This set of buffers is designed to complement the use of any of our 96 formulation crystallization screens and can be employed to add another dimension to the search for optimal protein crystallization hits to simultaneously explore the effects of pH and buffer composition on crystal growth.

Wizard pH Buffer Screen
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List price: $240.00

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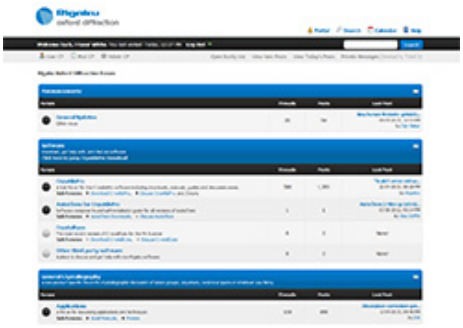
For more information, visit the
Rigaku Reagents website.

Rigaku Oxford Diffraction 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

Single crystal X-ray diffraction on your benchtop
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.

Teach single crystal X-ray diffraction through hands-on experience
In many universities, the departmental single crystal X-ray diffractometer is considered off limits to students because of fear that inexperienced users might damage the instrument. The XtaLAB mini II provides the opportunity for students to learn single crystal X-ray analysis by actually using a fully functional diffractometer. This is not a black box instrument. Rather, the important step of mounting a crystal on the goniometer and physically centering the crystal in the position of the X-ray beam ensures that students learn the importance of mounting techniques and crystal selection. The simple design of the XtaLAB mini II X-ray diffractometer minimizes the danger of students damaging the system.

Reduced size does not mean reduced data quality
The Rigaku XtaLAB mini II is a research grade chemical crystallography instrument that sits on the benchtop. No data quality compromises, no extended collection times. Results delivered are unambiguous. X-ray source tube lifetime is extended by running at 600 W. To compensate for running at lower power, a SHINE optic (specially curved mono-chromator) is utilized to produce usable X-ray flux comparable to a standard X-ray diffractometer.

Dedicated to producing publication quality single crystal X-ray structures
The chief design requirement when creating the XtaLAB mini II was that the structures produced would be publishable in the most demanding scientific journals. The HPC X-ray detector is positioned so that the maximum 2θ value is well outside of the *Acta Cryst.* requirements. The software provides all the tools you need to generate publication quality data that can be used to determine 3D structures from a variety of structure analysis packages.

Features

- Affordable design with low operating costs
- Requires minimal training and support
- Automatic structure solution software
- Provides definitive structural information
- Ideal supplement for a NMR spectrometer
- Perfect self-serve departmental lab instrument
- Ideal teaching instrument
- Publication quality results
- Air-cooled HPC detector
- No special infrastructure required
- Optional cryosystem available

We have a new price promotion for the XtaLAB mini II in the U.S. Please contact us for details.

Lab in the Spotlight

Department of Chemistry at the University of Rochester

February 2019 SCX Survey

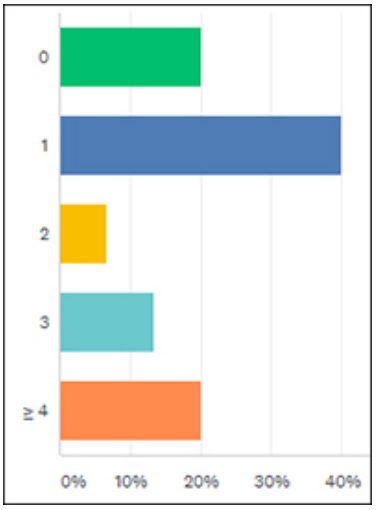
In the February 11 issue of *Nature*, C. K. Gunsalus, Marcia K. McNutt, Brian C. Martinson, Larry R. Faulkner & Robert M. Nerem call for a US advisory board on research integrity. Is it time for such a board "to ensure safety, efficiency, and integrity while facilitating scientific progress and the optimal use of researchers' time"?

- Yes
- No
- It doesn't matter, the world is just too FUBAR.

Take the Survey

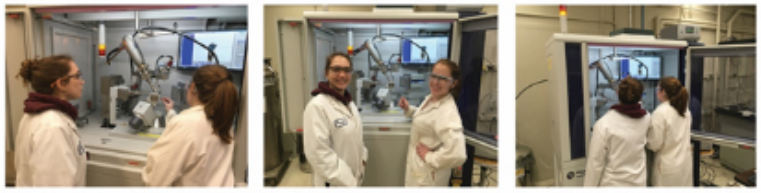
Last Month's Survey

How many scientific conferences do you plan to attend in 2019?



After careful consideration, the Department of Chemistry at the University of Rochester chose a Rigaku XtaLAB Synergy-S diffraction system, equipped with dual Cu and Mo microfocus X-ray sources, a HyPix-6000HE HPC detector, and a Cryostream 800 temperature controller to supplement their existing diffractometer. The XtaLAB Synergy-S is housed in the X-ray Crystallographic Facility in B04 Hutchison Hall and has been operational for one year now. The XtaLAB Synergy-S supports the research efforts of Professors William Jones, Rich Eisenberg, Ellen Matson, Michael Neidig, Daniel Weix and Kathryn Knowles, and crystallographer Dr. William Brennessel. The XtaLAB Synergy-S is capable of collecting complete data for publication in as little 10–20 minutes, although most small molecule experiments take 1–4 hours and two to three data collections per day are not unusual. Identification of substances can occur within minutes. In addition to the fast turnaround, the new instrument can produce high-quality data on small powder samples and efficiently collect data on small macromolecules or preliminary data for larger proteins. Perhaps the most amazing capability is its ability to yield high-quality structures from extremely tiny crystals, samples that were unable to be examined on the old diffractometer.

Obtaining funding for the new instrument is only half of the success story. The usage statistics tell the rest. The number of publishable crystal structures has increased by 180% from the calendar year 2017 (old diffractometer) to 2018 (new diffractometer), and that for structures of strictly organic molecules has gone up by 750%. The huge increase of the latter is due in large part to the ability to work with smaller crystals.



Graduate students Theresa Boddle and Stephanie Carpenter mount and center a crystal in preparation for data collection.

Students and researchers are fully trained on the diffractometer by taking a graduate level course, X-ray Crystallography. Additionally, undergraduate students are introduced to the instrument during a laboratory session in Advanced Laboratory Techniques. As part of the outreach program, researchers at local colleges and universities can submit samples for *pro bono* analysis.

Useful Link

CXRO X-ray Data Booklet

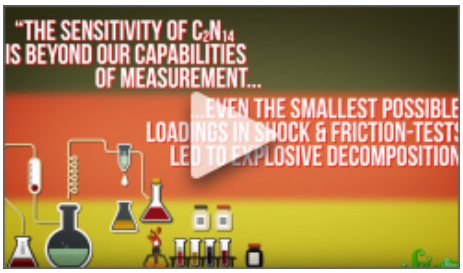
I recently introduced a colleague to the CXRO X-ray Data Booklet produced by Al Thompson and others. This booklet has been around for over 30 years and was most recently updated in 2009. I have found this reference work invaluable and use it so often I have a hot-key for the pdf: ctrl-alt-x. You can access it via HTML or download the pdf.

UCSD JANA Workshop Summary

Nearly thirty crystallographers from academia, industry and government labs recently gathered for the 2018 Jana Modulation Workshop organized and hosted by Drs. Milan

Videos of the Month

Here is a link to a YouTube channel called SciShow. I enjoyed "5 of the World's Most Dangerous Chemicals". Some minor technical details were not quite right, for example calling thioacetone a thiol, but very interesting.



Watch the Video

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Gembicky and Curtis Moore of the University of California, San Diego. The workshop was led by Profs. Václav Petříček and Michal Dušek of the Czech Academy of Sciences, two of the co-authors of the Jana2006 software. The participants came from a wide variety of backgrounds, including chemistry, geology and materials science, and their experience level ranged from graduate students to emeriti faculty. More than half a dozen US states, two Canadian provinces and three other foreign countries were represented.

Workshop participants were introduced to the Jana2006 software and to the concept of modulation through a combination of lectures and step-by-step activities that they worked through on their own computers individually or in pairs. To familiarize themselves with Jana2006, the attendees first learned how to solve and refine non-modulated structures from both single-crystal and powder data. As they gained confidence and experience, more advanced concepts were introduced to the exercises. By the end of the four-day workshop, which ran from December 10–13, 2018, participants were modeling twins and various modulation functions, and visualizing the results in Diamond and Vesta. Everyone was sent back to their universities or companies with several more datasets to keep practicing on.

In order to make sure that participants had all the necessary tools to generate and process their own datasets in the future, several other software packages were also demonstrated and distributed during the workshop. Dr. Jim Britten of McMaster University gave a lecture on Max3D, a powerful program for visualizing reciprocal space in three dimensions. Because Jana2006 can handle data from virtually any diffractometer, Dr. Bruce Noll of Bruker AXS and Dr. Eric Reinheimer of Rigaku Americas each gave lectures to demonstrate best practices for collecting and processing crystallographic data using the APEX3 and CrysAlis^{Pro} software suites, respectively. Dr. Milan Gembicky of University of California, San Diego reinforced the message of their lectures – the importance of proper collection and processing strategies – by leading everyone through a hands-on integration and scaling of modulated single-crystal data. All of these lecturers made themselves available for one-on-one interactions with the workshop participants throughout the meeting.

The formal instruction periods of the workshop were supplemented with a number of social activities to promote networking among the participants. Each day started with a continental breakfast in the lecture hall, where everyone could mingle and discuss science with the other attendees. These discussions continued during the coffee breaks, as well as the three lunches and two dinners that were provided to the attendees. The UCSD crystallography lab, known as *Diffractopia*, was open before, during and after the workshop, and several people brought challenging crystals from their home labs to run on one of the nine state-of-the art, custom-built diffractometers in the UCSD facility. Tours of other famous UCSD landmarks, including the Geisel Library and the Fallen Star House, were offered, as was a sunset hike through the Scripps Coastal Reserve near campus. No matter what their research interests and experience level was, everyone who came to this workshop learned something new and left a better scientist than when they arrived.

Selected Recent Crystallographic Papers

Using Mathematica as a platform for crystallographic computing. Ramsnes, Stian; Larsen, Helge Bøvik; Thorkildsen, Gunnar. *Journal of Applied Crystallography*. Feb2019, Vol. 52 Issue 1, p214-218. 5p. DOI: 10.1107/S1600576718018071.

Design, 3D printing and validation of a novel low-cost high-capacity sitting-drop bridge for protein crystallization. Talapatra, Sandeep K.; Penny, Matthew R.; Hilton, Stephen T.; Kozielski, Frank. *Journal of Applied Crystallography*. Feb2019, Vol. 52 Issue 1, p171-174. 4p. DOI: 10.1107/S1600576718017545.

Implementation of software for data processing of X-ray optical measurements for the analysis of structural parameters. Petrakov, Dmitry S.; Smirnov, Dmitry I.; Gerasimenko, Nikolay N.; Medetov, Nurlan A.; Jikeev, Azamat A. *Journal of Applied Crystallography*. Feb2019, Vol. 52 Issue 1, p186-192. 7p. DOI: 10.1107/S1600576718016837.

Total chemical synthesis and racemic protein crystallography of toxin proteins. Gao, Shuai; Qu, Qian; Tan, XiaoDan; Liu, Lei. *Toxicon*. 2019 Supplement 1, Vol. 158, pS76-S77. 2p. DOI: 10.1016/j.toxicon.2018.10.262.

Druggability Simulations and X-Ray Crystallography Reveal a Ligand-Binding Site in the GluA3 AMPA Receptor N-Terminal Domain. Lee, Ji Young; Krieger, James; Herguedas, Beatriz; García-Nafría, Javier; Dutta, Anindita; Shaikh, Saher A.; Greger, Ingo H.; Bahar, Ivet. *Structure*. Feb2019, Vol. 27 Issue 2, p241-241. 1p. DOI: 10.1016/j.str.2018.10.017.

Specificity of *Escherichia coli* Heat-Labile Enterotoxin Investigated by Single-Site Mutagenesis and Crystallography. Heggelund, Julie Elisabeth; Heim, Joel Benjamin; Bajc, Gregor; Hodnik, Vesna; Anderluh, Gregor; Krengel, Ute. International

Journal of Molecular Sciences. Feb2019, Vol. 20 Issue 3, p703. 1p. DOI: 10.3390/ijms20030703.

Synthesis, X-ray crystallography, computational studies and catecholase activity of new zwitterionic Schiff base derivatives. Boulemche, Hakima; Anak, Barkahem; Djedouani, Amel; Touzani, Rachid; François, Michel; Fleutot, Solenne; Rabilloud, Franck. *Journal of Molecular Structure*. Feb2019, Vol. 1178, p606-616. 11p. DOI: 10.1016/j.molstruc.2018.10.078.

Syntheses of and structural studies on some square planar dithiophosphonato Ni(II) complexes, octahedral pyridine derivatives thereof and X-ray crystallography, DFT and molecular docking studies of the latter. Saglam, Ertugrul Gazi; Bulat, Elif; Zeyrek, Celal Tugrul; Dal, Hakan; Hökelek, Tuncer. *Journal of Molecular Structure*. Feb2019, Vol. 1178, p112-125. 14p. DOI: 10.1016/j.molstruc.2018.09.084.

A new polymorph of the common coformer isonicotinamide. Vicatos, Alexios I.; Caira, Mino R. *CrystEngComm*. 2/7/2019, Vol. 21 Issue 5, p843-849. 7p. DOI: 10.1039/c8ce01588k.

Organic molecular tessellations and intertwined double helices assembled by halogen bonding. Ng, Chun-Fai; Chow, Hak-Fun; Mak, Thomas C. W. *CrystEngComm*. 2/21/2019, Vol. 21 Issue 7, p1130-1136. 7p. DOI: 10.1039/c8ce02133c.

Crystallographic Analysis of the Catalytic Mechanism of Phosphopantothenoylcysteine Synthetase from *Saccharomyces cerevisiae*. Zheng, Peiyi; Zhang, Mengying; Khan, Muhammad Hidayatullah; Liu, Hejun; Jin, Yuping; Yue, Jian; Gao, Yongxiang; Teng, Maikun; Zhu, Zhongliang; Niu, Liwen. *Journal of Molecular Biology*. Feb2019, Vol. 431 Issue 4, p764-776. 13p. DOI: 10.1016/j.jmb.2019.01.012.

Phase transformation in the C form of myristic-acid crystals and DFT calculations. Miranda, J.R.S.; de Castro, A.J.R.; da Silva Filho, J.G.; Freire, P.T.C.; Pinheiro, G.S.; Moreira, S.G.C.; Saraiva, G.D.; de Sousa, F.F. *Spectrochimica Acta Part A: Molecular & Biomolecular Spectroscopy*. Feb2019, Vol. 208, p97-108. 12p. DOI: 10.1016/j.saa.2018.09.065.

Crystallographic and computational studies of a new organoarsenate compound: o-anisidinium dihydroarsenate. Harchani, Ali; Trzybinski, Damian; Pawledzio, Sylwia; Wozniak, Krzysztof; Haddad, Amor. *Acta Crystallographica: Section C, Structural Chemistry*. Feb2019, Vol. 75 Issue 2, p128-134. 7p. DOI: 10.1107/S2053229619000172.

Encapsulation of biomacromolecules by soaking and co-crystallization into porous protein crystals of hemocyanin. Hashimoto, Tsubasa; Ye, Yuxin; Matsuno, Asuka; Ohnishi, Yuki; Kitamura, Akira; Kinjo, Masataka; Abe, Satoshi; Ueno, Takafumi; Yao, Min; Ogawa, Tomohisa; Matsui, Takashi; Tanaka, Yoshikazu. *Biochemical & Biophysical Research Communications*. Feb2019, Vol. 509 Issue 2, p577-584. 8p. DOI: 10.1016/j.bbrc.2018.12.096.

D+: software for high-resolution hierarchical modeling of solution X-ray scattering from complex structures. Ginsburg, Avi; Ben-Nun, Tal; Asor, Roi; Shemesh, Asaf; Fink, Lea; Tekoah, Roee; Levartovsky, Yehonatan; Khaykelson, Daniel; Dharan, Raviv; Fellig, Amos; Raviv, Uri. *Journal of Applied Crystallography*. Feb2019, Vol. 52 Issue 1, p219-242. 24p. DOI: 10.1107/S1600576718018046.

Analysis of styrene maleic acid alternating copolymer supramolecular assemblies in solution by small angle X-ray scattering. Brady, Nathan G.; Qian, Shuo; Bruce, Barry D. *European Polymer Journal*. Feb2019, Vol. 111, p178-184. 7p. DOI: 10.1016/j.eurpolymj.2018.11.034.

Sodium ascorbate (SA) and l-ascorbic acid (AA) as modifiers of burn affected skin –A comparative analysis. Pielesz, Anna; Slusarczyk, Czeslaw; Binias, Dorota; Bobinski, Rafal. *Spectrochimica Acta Part A: Molecular & Biomolecular Spectroscopy*. Feb2019, Vol. 209, p55-61. 7p. DOI: 10.1016/j.saa.2018.10.021.

Book Review

Broken Ballots: Will Your Vote Count?
By Douglas W. Jones and Barbara Simons
ISBN 978-1-57586-637-6

Broken Ballots: Will Your Vote Count? is the product of a collaboration between Douglas W. Jones, a computer science professor at the University of Iowa, and Barbara Simons, a

former IBM Research employee. *Broken Ballots* takes a deep, methodical dive into the popular vote tradition in American electoral history and the automation of the voting process, making certain repeating patterns of election controversy quite clear.

Jones and Simons begin with a brilliant opening line: "This book should never have been written." It's a bold opening statement that's immediately followed up with a detailed explanation: "In 1934, the Brookings Institution published a great book by Joseph Harris, entitled *Election Administration in the United States*. Had people followed Harris' advice, there would be no need for our book." However, to state the obvious, people—namely the government officials making election-related decisions for the past eighty years—did not follow Harris' advice. It's startling to consider that election tampering and voter fraud was enough of a concern 80 years ago for someone to write a book about it. And these election-related cracks in American democracy were not new then—they'd been slowly spreading since the birth of the nation. How far we simply haven't come becomes quite apparent the further the reader gets into *Broken Ballots*.

Given the extensive government inquiry following the 2016 presidential election and the level of turmoil regarding the validity of each American's vote, one might suspect that *Broken Ballots* was published in the aftermath of that election. They would be incorrect.

Broken Ballots was published in 2012—and the tumultuous election to which the authors make the most reference is that of 2000. For those readers who need a refresher on what made the outcome of that election so contentious, Al Gore lost the electoral college vote to George W. Bush thanks to Florida even though he won the popular vote. After a recount and a Supreme Court decision, Bush was declared the winner. But many suspected that certain discrepancies in the voting process could be attributed to flaws in the Votomatic machines that many Floridians used to cast their vote.

Swap out Bush for Trump, Gore for Clinton, and the Florida debacle with Russian election tampering, and the overall outcome of the 2016 election parallels that of the 2000 election quite eerily. Even though Simons' and Jones' book is almost 7 years old at this point, the content is hardly dated. If anything, it should be required reading for high school students taking AP Government. Jones and Simons address the dangers of online voting and the ease with which voting machines can be tampered and internet voting can be hacked by a third party. More than four years before the 2016 election, they were basically telling their readers how it would end.

It's not clearly marked which chapters or sections were authored by Jones or Simons. The writing is clear and seamless—no one section seems more or less well written than any other. Anytime either author appears as a character in the narrative, so to speak, they are referred to in the third person. The rather interesting narrative decision has the effect of conveying to the reader both that Jones and Simons themselves have nothing to hide and emphasizes their importance in the perhaps rather small sphere of academically inclined experts in electronic voting.

Simons and Jones have the unique talent of taking a rather pedantic subject and making it more than palatably interesting. I recommend reading *Broken Ballots* before the next time you cast a vote.

Review by Jeanette S. Ferrara, MA

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