

**Crystallography Newsletter**  
Volume 11, No. 07, July 2019

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## In this issue:

- [Crystallography in the News](#)
- [Visit with Us](#)
- [Join ROD on LinkedIn](#)
- [Product Spotlight](#)
- [Custom Stock Solution Library](#)
- [Rigaku X-ray Forum](#)
- [Lab in the Spotlight](#)
- [Survey of the Month](#)
- [Last Month's Survey](#)
- [Useful Link](#)
- [Video of the Month](#)
- [Recent Crystallographic Papers](#)
- [Book Review](#)

## Visit with Us

[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

[ACS National Meeting & Expo](#)  
San Diego, CA, August 25 – 29, 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.

## Rigaku Reagents: Custom Stock Solution Library

## Crystallography in the News

**July 1, 2019.** In 2010 crystallographer [Dr. Julia Goodfellow](#) was appointed [Dame Commander](#) of the Order of the British Empire for her services to science. In 2018 Goodfellow became the third (current) president of the Royal Society of Biology.

**July 2, 2019.** A study published May 22 in the journal *Nature* notes the role of X-ray experiments at Berkeley Lab's Advanced Light Source (ALS) in detailing the [structure of a grouping of amino acids that are part of an important signaling protein](#). The protein, known as STING, plays an important role in activating the immune system.

**July 3, 2019.** Using biophysical techniques including x-ray crystallography and nuclear magnetic resonance, a University of Birmingham team were able to monitor the [movement of \(gram negative bacteria\) phospholipids from the inner membrane](#) towards the outer membrane directly through a series of proteins that form a pathway known as the Mla pathway.

**July 5, 2019.** Proteins are dynamic. Rearrangements of side chains, secondary structure, and entire domains gate functional transitions on time scales ranging from picoseconds to milliseconds. Weinert et al. used time-resolved serial [crystallography to study large conformational changes in the proton pump](#) bacteriorhodopsin that allow for redistribution of protons during the pumping cycle.

**July 10, 2019.** Happy 99th birthday to [Rosalind Franklin](#), July 25 1920 – April 16 1958. Her work with DNA and time at King's College London was critically important, however, her body of work expanded scientific knowledge throughout her robust yet short career. When we celebrate Franklin's work on DNA, we can also celebrate her as a person. There is no better day to celebrate her than July 25, her birthday. [The ExoMars rover](#) constructed by Roscosmos State Corporation for Space Activities of Russia in collaboration with the European Space Agency, which will likely land on Mars in February 2021, has been named for Franklin.

**July 11, 2019.** A German-Swiss team around Professor Oliver Daumke from the MDC has investigated how a [protein of the dynamin family deforms the inner mitochondrial membrane](#). The results, which also shed light on a hereditary disease of the optic nerve, have been published in *Nature*.

**July 11, 2019.** [A computational model](#) reveals the mechanism of the replication of prions. The study, from the Dulbecco Telethon Institute and the University of Trento in collaboration with the Italian National Institute of Nuclear Physics, will open up new research avenues to design drugs against incurable neurodegenerative disorders such as Mad Cow Disease.

**July 15, 2019.** Researchers have mapped the [crystal structure of a key protein that makes the metabolites responsible for the bitter taste](#) in *Brassica* vegetables like mustards, broccolis, and cabbages. The new study is the first snapshot of how the protein evolved and came to churn out such diverse byproducts in this agriculturally significant group of plants.

**July 19, 2019.** The American Crystallographic Association announced the Class of 2019 Fellows at its Annual Meeting in Covington, Kentucky. They are Craig Brown, National Institute of Standards and Testing; Susan Byram, Bruker Corp.; Charles Carter, Jr., University of North Carolina; Elspeth Garman, University of Oxford; and Xiaoping Wang, Oak Ridge National Laboratory.

**July 22, 2019.** Researchers from the Moscow Institute of Physics and Technology have published a [review on serial femtosecond crystallography](#), one of the most promising methods for analyzing the tertiary structure of proteins. This technique has rapidly evolved over the past decade, opening new prospects for the rational design of drugs targeting proteins previously inaccessible to structural analysis.

**July 24, 2019.** Crystallographer and Professor Emeritus [Dr. Gary D. Anderson of Marshall University's Department of Chemistry](#) was named a [Fellow with the American Chemical Society](#) and will be recognized at the society's fall national meeting in San Diego in

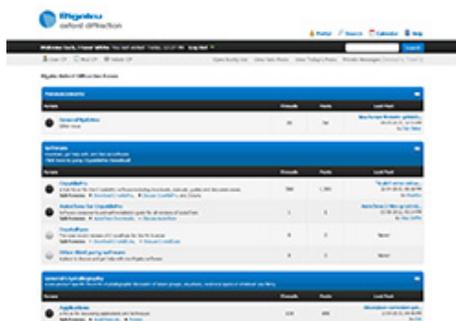


Rigaku Reagents can help you build your own customized solution library so that you never run out of a stock solution. These stock solutions are ideal for systematic grid-screening of initial crystallization hits. Select the stock solutions you use from our buffers, salts, polymers and precipitants, or let Rigaku Reagents know what type of solution, container, volume or label you need and we'll prepare it for you.

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### Rigaku Oxford Diffraction Forum



[www.Rigakuxrayforum.com](http://www.Rigakuxrayforum.com)

CrysAlisPro V40 has been released on the Rigaku Oxford Diffraction 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

August. The ACS Fellows program honors members for outstanding achievements in and contributions to science, the profession and the society.

**July 24, 2019.** As technology and science continue to play an even greater role in everyday lives, training and developing the next wave of scientists needs to evolve. Noncognitive factors and new strategies to more fully engage each student and promote an inclusive classroom are being considered for [improved learning experiences in STEM courses](#).

**July 25, 2019.** The ACA announced the winners of the 2020 A. L. Patterson Award, 2020 David G. Rognlie Award and the 2020 Margaret C. Etter Early Career Award. They are Václav Petříček, The Institute of Physics of the Czech Academy of Sciences; James Holton, Lawrence Berkeley National Laboratory; and Nozomi Ando, Cornell University, respectively.

**July 25, 2019.** Rigaku Oxford Diffraction (ROD) is pleased to announce its attendance at the 69th [Annual Meeting of the American Crystallographic Association](#) (ACA), Saturday, July 20, through Wednesday, July 24, 2019 at the Northern Kentucky Convention Center in Covington, Kentucky. Rigaku Oxford Diffraction, a Ruby Sponsor of the event, is presenting their macromolecular and small molecule crystallography instrumentation at booths 206 and 208.

## Product Spotlight

### [XtaLAB Synergy Custom](#)



The XtaLAB Synergy Custom is the fully flexible single crystal X-ray diffractometer for laboratories requiring a bespoke solution for their unique crystallography applications. As its name suggests, you are able to customize to your own design, a system using a range of high quality components dedicated for single crystal X-ray diffraction.

### Configuration

The XtaLAB Synergy Custom is where you will find Rigaku's highest flux [FR-X](#) microfocus source delivering 2.5 times higher flux compared to the [MicroMax-007 HF](#) rotating anode X-ray generator. It may be configured to be dual port to accommodate a second X-ray diffractometer, perfect for high-throughput laboratories. It is possible to configure your system with any of Rigaku's X-ray sources, from microfocus sealed tubes to rotating anodes, to give the ultimate in flexibility.

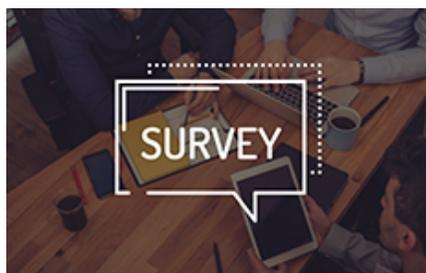
XtaLAB Synergy Custom systems can be configured with the popular and reliable four-circle kappa goniometer which is compatible with a wide range of detectors including the [HyPix-6000HE](#) and other Hybrid Photon Counting (HPC) X-ray detectors e.g. PILATUS and EIGER detectors.

HPC X-ray detectors are close to an ideal detector for a number of reasons:

- Photon counting detectors that directly detect X-ray photons without the need the intermediate step of converting X-ray photons to light with a phosphor
- High dynamic range and fast readout speed
- Extremely low noise
- An ideal point spread function of a single pixel

These combined features, along with shutterless data collection, means that you can collect more accurate data faster. As a result, the XtaLAB Synergy Custom single crystal x-

## Survey of the Month



### July 19 SCX Survey

What is the best way for scientists to reduce their carbon footprint?

- Stop driving
- Stop flying
- Stop eating beef
- What's a carbon footprint?

[Take the Survey](#)

### Last Month's 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:

ray diffractometer offers outstanding performance for your diffraction experiments.

Select your accessories for the XtaLAB Synergy Custom diffractometer, including the automated sample changing robot, the [ACTOR](#) or the [XtalCheck](#) for *in-situ* screening of macromolecules. The extra space around the goniometer enables tools such as a dewar or a microscope to be brought close into the goniometer for speedy mounting of samples.

#### Features

- Build your own bespoke diffractometer to your specification
- Flexible system that can be upgraded
- Compatible with the highest-flux X-ray sources
- Uses CrysAlis<sup>Pro</sup> software

#### Benefits

- Design an optimal system to suit your crystallographic needs
- Expand your system as your research output increases or takes a new direction
- Reduce the need for synchrotron visits by using the brightest home-lab source
- Familiar software that is easy to use

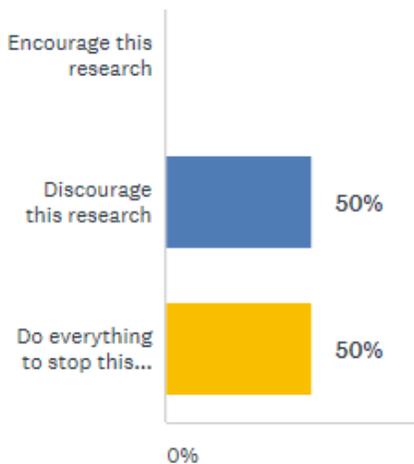
### Lab in the Spotlight

#### [The University of Reading, United Kingdom](#)

In March this year, the Chemical Analysis Facility in the University of Reading took delivery of a Rigaku XtaLAB Synergy-S diffraction System (dual micro-focus source) single-crystal diffractometer with a HyPix 6000HE single-photon counting detector. The system was funded by a special allocation from the Research Endowment Trust Fund of the University, on the advice of the Environment and Health Sciences research divisions. It supports both research and teaching across the University, and is free at the point of use for Reading users. Commercial work is also possible by [contacting Nick Spencer](#) (pictured). The [first published work](#) from the instrument was carried out by our newly promoted full Professor Kenneth Shankland, making use of the high sensitivity for measuring small and weakly diffracting crystals.

Dr James Hall (pictured) is using the new instrument for studies of DNA crystals and their damage processes along with Megan Lambert (pictured). Two attachments are playing important roles in this work - a humidity controller (Arinax) for controlled dehydration studies, and a plate screening attachment (XtalCheck-S) for the rapid assessment of macromolecular crystal quality within crystallisation plates. The newly promoted Professor Ann Chippindale, who is also the laboratory head, is using the instrument for variable temperature studies of metal cyanides and related materials, particularly those displaying negative thermal expansion properties. She also collaborates with a range of colleagues to solve challenging small molecule structures.

Professor Christine Cardin has published extensively on the binding modes of [ruthenium polypyridyl complexes to DNA](#). She, together with colleagues and students, will use this instrument in future studies in this area, greatly enhancing the speed and sensitivity compared with the previous Oxford Diffraction instrument, purchased with EPSRC funding as long ago as 2005. The new instrument is based on similarly reliable hardware, but enormously expanded range.



### Videos of the Month

Here is a short video of the lunar excursion module landing on the moon.



[Watch the Video](#)

### Subscribe to Rigaku eNewsletters



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

[www.Rigaku.com/en/subscribe](http://www.Rigaku.com/en/subscribe)

**ROD European Users' Meeting**  
**26th-27th September 2019**  
**Rigaku Europe, Neu Isenburg, Germany**



Left to right: Megan Lambert (PhD student), Nick Spencer (Senior technician in charge), Drs James Hall and Elena Kabova (Lecturers in Pharmaceutical Chemistry).

### Useful Link



Fifty years ago we landed on the moon and took our first steps on a celestial body other than Earth. Here is a link to the mission history at the NASA website.

[https://www.nasa.gov/mission\\_pages/apollo/missions/apollo11.html](https://www.nasa.gov/mission_pages/apollo/missions/apollo11.html)

And here is a collection of articles from Nature on the same topic:

<https://www.nature.com/collections/bfhghadfcc>

BTW, if you haven't signed up for Spot the Station, here you go:

<https://spotthestation.nasa.gov/> Spot-the-station gatherings are a great way to endear science to your neighbors.

### Selected Recent Crystallographic Papers

**The potential benefits of using higher X-ray energies for macromolecular crystallography.** Dickerson, Joshua L.; Garman, Elspeth F. *Journal of Synchrotron Radiation*. Jul2019, Vol. 26 Issue 4, p922-930. 9p. DOI: [10.1107/S160057751900612X](https://doi.org/10.1107/S160057751900612X).

**Comprehensive model for X-ray-induced damage in protein crystallography.** Close, David M.; Bernhard, William A. *Journal of Synchrotron Radiation*. Jul2019, Vol. 26 Issue 4, p945-957. 13p. DOI: [10.1107/S1600577519005083](https://doi.org/10.1107/S1600577519005083).

**(F)uridylylated Peptides Linked to VPg1 of Foot-and- Mouth Disease Virus (FMDV): Design, Synthesis and X-Ray Crystallography of the Complexes with FMDV RNA-Dependent RNA Polymerase.** de Castro, Sonia; Ferrer-Orta, Cristina; Mills, Alberto; Fernández-Cureses, Gloria; Gago, Federico; Verdaguer, Nuria; Camarasa, María-José; Seley-Radtke, Katherine L.; Dayie, Theodore K. *Molecules*. 7/1/2019, Vol. 24 Issue 13, p2360. DOI: [10.3390/molecules24132360](https://doi.org/10.3390/molecules24132360).

**DeepCentering: fully automated crystal centering using deep learning for macromolecular crystallography.** Ito, Sho; Ueno, Go; Yamamoto, Masaki. *Journal of Synchrotron Radiation*. Jul2019, Vol. 26 Issue 4, p1361-1366. 6p. DOI: [10.1107/S160057751900434X](https://doi.org/10.1107/S160057751900434X).

**Stepwise construction and destruction of nickel thiolate Ni<sub>3</sub> cluster revealed by mass spectrometry and crystallography.** Tu, Min; Wang, Jie; Liu, Bin; Zeng, Ming-Hua. *Inorganic Chemistry Communications*. Jul2019, Vol. 105, p208-211. 4p. DOI: [10.1016/j.inoche.2019.05.014](https://doi.org/10.1016/j.inoche.2019.05.014).

**Computational Modeling of Designed Ankyrin Repeat Protein Complexes with Their Targets.** Radom, Filip; Paci, Emanuele; Plückthun, Andreas. *Journal of Molecular Biology*. Jul2019, Vol. 431 Issue 15, p2852-2868. 17p. DOI: [10.1016/j.jmb.2019.05.005](https://doi.org/10.1016/j.jmb.2019.05.005).

**Isolation of a Relatively Air-Stable, Bulky Silyl-Substituted, Neutral Silicon-**



We are pleased to announce that we will be holding a two day user meeting and discussion group at the Rigaku Europe HQ in Neu Isenburg near Frankfurt Airport. The meeting will start at 10am on Thursday 26th September running until the afternoon of Friday 27th September. This year's meeting will be jointly held between the single-crystal and powder diffraction groups.

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

[Register](#)

**Centered Radical.** Holzner, Richard; Kaushansky, Alexander; Tumanskii, Boris; Frisch, Philipp; Linsenmann, Fabian; Inoue, Shigeyoshi. *European Journal of Inorganic Chemistry*. 7/7/2019, Vol. 2019 Issue 25, p2977-2981. 5p. DOI: [10.1002/ejic.201900522](https://doi.org/10.1002/ejic.201900522).

**Partial functionalisation of C<sub>4</sub>-symmetric tetramethoxyresorcinarenes.** Tan, Daniel A.; Massera, Chiara; Mocerino, Mauro. *Supramolecular Chemistry*. Jul2019, Vol. 31 Issue 7, p442-450. 9p. DOI: [10.1080/10610278.2019.1620949](https://doi.org/10.1080/10610278.2019.1620949).

**Direct measurement of X-ray-induced heating of microcrystals.** Warren, Anna J.; Axford, Danny; Owen, Robin L. *Journal of Synchrotron Radiation*. Jul2019, Vol. 26 Issue 4, p991-997. 7p. DOI: [10.1107/S1600577519003849](https://doi.org/10.1107/S1600577519003849).

**The role of gelsolin domain 3 in familial amyloidosis (Finnish type).** Zorgati, Habiba; Larsson, Mårten; Ren, Weitong; Sim, Adelene Y. L.; Gettemans, Jan; Grimes, Jonathan M.; Wenfei Li; Robinson, Robert C. *Proceedings of the National Academy of Sciences of the United States of America*. 7/9/2019, Vol. 116 Issue 28, p13958-13963. 6p. DOI: [10.1073/pnas.1902189116](https://doi.org/10.1073/pnas.1902189116).

**Structure and catalytic mechanistic insight into *Enterobacter aerogenes* acetolactate decarboxylase.** Ji, Fangling; Feng, Yanbin; Li, Mingyang; Long, Feida; Yang, Yongliang; Wang, Tianqi; Wang, Jingyun; Bao, Yongming; Xue, Song. *Enzyme & Microbial Technology*. Jul2019, Vol. 126, p9-17. 9p. DOI: [10.1016/j.enzmictec.2019.03.005](https://doi.org/10.1016/j.enzmictec.2019.03.005).

**Dicationic ditelluride salts stabilized by N-heterocyclic carbene.** Nakata, Norio; Kawauchi, Fumihiko; Takahashi, Shintaro; Ishii, Akihiko. *New Journal of Chemistry*. 7/21/2019, Vol. 43 Issue 27, p10894-10898. 5p. DOI: [10.1039/c9nj02138h](https://doi.org/10.1039/c9nj02138h).

**Catalytic ring-closing reactions of gold compounds containing bis(phosphino)ferrocene ligands.** Michaels, Toni A.; Pritchard, Olivia F.; Dell, Justine S.; Bezpalko, Mark W.; Kassel, W. Scott; Nataro, Chip. *Journal of Organometallic Chemistry*. Jul2019, Vol. 889, p1-8. 8p. DOI: [10.1016/j.jorganchem.2019.03.006](https://doi.org/10.1016/j.jorganchem.2019.03.006).

**An unexpected mixed valence tetranuclear copper(I/II) complex: Synthesis, structural characterization, DNA/protein binding, antioxidant and anticancer properties.** Anu, D.; Naveen, P.; VijayaPandiyan, B.; Frampton, Christopher S.; Kaveri, M.V. *Polyhedron*. Jul2019, Vol. 167, p137-150. 14p. DOI: [10.1016/j.poly.2019.04.021](https://doi.org/10.1016/j.poly.2019.04.021).

**Benzene Triimides: Facile Synthesis and Self-Assembly Study.** Tuo, De-Hui; He, Qing; Wang, Qi-Qiang; Ao, Yu-Fei; Wang, De-Xian. *Chinese Journal of Chemistry*. Jul2019, Vol. 37 Issue 7, p684-688. 5p. DOI: [10.1002/cjoc.201900146](https://doi.org/10.1002/cjoc.201900146).

**Combining random microseed matrix screening and the magic triangle for the efficient structure solution of a potential lysin from bacteriophage P68.** Truong, Jia Quyen; Panjekar, Santosh; Shearwin-Whyatt, Linda; Bruning, John B.; Shearwin, Keith E. *Acta Crystallographica: Section D, Structural Biology*. Jul2019, Vol. 75 Issue 7, p670-681. 12p. DOI: [10.1107/S2059798319009008](https://doi.org/10.1107/S2059798319009008).

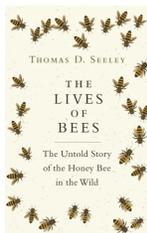
**Synthesis of two new symmetrical macroacyclic Schiff base ligands containing homopiperazine moiety and their mononuclear complexes: Spectral characterization, X-ray crystal structural, antibacterial activities, antioxidant effects and theoretical studies.** Aidi, Maryam; Keypour, Hassan; Shooshtari, Amir; Mahmoudabadi, Masoumeh; Bayat, Mehdi; Ahmadvand, Zeinab; Karamian, Roya; Asadbegy, Mostafa; Tavatli, Sarah; Gable, Robert William. *Polyhedron*. Jul2019, Vol. 167, p93-102. 10p. DOI: [10.1016/j.poly.2019.02.030](https://doi.org/10.1016/j.poly.2019.02.030).

**Productive reorientation of a bound oxime reactivator revealed in room temperature X-ray structures of native and VX-inhibited human acetylcholinesterase.** Gerlits, Oksana; Xiaotian Kong; Xiaolin Cheng; Wymore, Troy; Blumenthal, Donald K.; Taylor, Palmer; Radic, Zoran; Kovalevsky, Andrey. *Journal of Biological Chemistry*. 7/5/2019, Vol. 294 Issue 27, p10607-10618. 12p. DOI: [10.1074/jbc.RA119.008725](https://doi.org/10.1074/jbc.RA119.008725).

**Water-stable Zeolitic Tetrazolate-Imidazolate Frameworks (ZTIFs) with GIS topology.** Li, Min-Yu; Wang, Fei; Zhang, Jian. *Inorganic Chemistry Communications*. Jul2019, Vol. 105, p59-62. 4p. DOI: [10.1016/j.inoche.2019.05.002](https://doi.org/10.1016/j.inoche.2019.05.002).

**Multipole electron densities and atomic displacement parameters in urea from accurate powder X-ray diffraction.** Svane, Bjarke; Tolborg, Kasper; Jørgensen, Lasse Rabøl; Roelsgaard, Martin; Jørgensen, Mads Ry Vogel; Brummerstedt Iversen, Bo. *Acta Crystallographica. Section A, Foundations & Advances*. Jul2019, Vol. 75 Issue 4, p600-609. 10p. DOI: [10.1107/S205327331900799X](https://doi.org/10.1107/S205327331900799X).

[Book Review](#)



***The Lives of Bees: The Untold Story of the Honey Bee in the Wild***

**By Thomas D. Seeley**  
**ISBN 9780691166766**

Thomas D. Seeley's *The Lives of Bees* is the culmination of over four decades of formal research and nearly a lifetime's worth of personal interest in honeybees. Indeed, *The Lives of Bees* feels more like an incredibly thoughtful, well-written, and meticulously researched doctoral dissertation than a work of popular science—but not in a bad way. What distinguishes *The Lives of Bees* from other works in the genre—as Seeley himself declares early on—is that it concerns itself not with domesticated honeybees but with wild ones.

Honeybee populations around the world are declining rapidly—both wild and cultivated. Seeley takes a deep, detailed dive into the behaviors and patterns of wild honey bees to hopefully better inform human beekeeping practices, which he describes in the final chapter, "Darwinian Beekeeping." Fair warning—this final chapter is not for the faint of heart. Human-assisted natural selection plays a heady role.

But that's getting ahead. Seeley starts his book with the singular event that sparked his fascination with honey bees, specifically wild honey bees. As an almost 11-year-old boy, he witnessed a honey bee colony swarm a hole in a black walnut tree in the woods near his home. The desire to know what caused that swarm to choose that tree on that particular day has fueled his academic pursuits ever since. Only someone truly captivated by honey bee behavior could have conducted the decades' worth of research that went into this book.

From his brief personal preface, Seeley moves into an overview of the wild honey bee populations he studies. They predominantly live in the Arnot Forest of upstate New York, near Cornell University, where Seeley works as a professor of neurobiology and behavior. After introducing his wild honey bee population, Seeley offers his readers a brief history of the human relationship with honey bees and their honey, as well as the process of domesticating these wild animals. Seeley presents the argument that although humans may claim to have successfully domesticated honey bees, they are largely deluding themselves. He rests his case on the evidence presented in subsequent chapters, that the lack of distinction between the behavior of honey bees living in the wild and those living in man-made apiaries suggests that they might not be so very different after all.

He starts with the nest—where the worker bees build their combs, the queen bee lays her eggs, and, most importantly to humans and to bears, where the honey is made. Perhaps one of the most interesting tidbits this chapter has to offer has very little to do with honeybees themselves, but rather the nature of the scientific research process. Seeley admits that he originally believed most honey bee nests to be close to the ground, based on earlier surveys of the forest. However, further research revealed the opposite to be true. Many honey bee swarms seem to purposefully choose nest locations higher up in trees, making them less susceptible to attack by a hungry black bear seeking a sweet treat. After describing the living conditions of the wild honey bee, Seeley moves into their annual life cycle, colony reproductive processes, methods of food collection, temperature control techniques utilized in cold winter months, and colony defense mechanisms, before finally addressing his recommendations for Darwinian beekeeping.

*The Lives of Bees* is very technical, but Seeley does an excellent job illustrating his subject matter, both with his careful and descriptive diction and his numerous figures and diagrams, all printed in full color on thick, glossy paper. I wouldn't recommend this book unless you have a healthy interest in bees, beekeeping, or even insects in general. But if you do, you'll definitely enjoy it.

Review by Jeanette S. Ferrara, MA



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