Crystallography Times

Rigaku oxford diffraction

Crystallography Newsletter
Volume 11, No. 05, May 2019
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In this issue:

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ACS – Middle Atlantic Regional Meeting
Baltimore, Maryland, May 30 – June 1, 2019

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

ACS – Central Regional Meeting
Midland, Michigan, June 4 – 7, 2019

First Annual CSB Symposium
Montreal, Canada, June 17, 2019

ACS – Northwest Regional Meeting
Portland, Oregon, June 16 – 19, 2019

International Conference on the Chemistry of the Organic Solid State (ICCOSS XXIV)
New York, New York, June 16 – 21, 2019

ACS – Northeast Regional Meeting
Saratoga Springs, New York, June 22 – 27, 2019

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

Rigaku Reagents:
Lysozyme Crystallography Kit

Crystallography in the News

May 1, 2019. Microseeding is a method used in protein crystallography where small seed crystals can be used to induce the formation of larger crystals. Microseeding was first shown to generate untwinned crystals of a compound called LigM, an O-demethylase, using untwinned crystals as seeds.

May 1, 2019. Scientists from McGill, the University of Cambridge, the University of Copenhagen and Pontificia Universidad Católica de Chile uncovered an important property of the ionotropic glutamate receptor (iGluR) protein, which they believe will have important ramifications for biomedical research, as well as for future drug development.

May 2, 2019. Dr. Stephen Wallwork, who has died aged 93, was a chemist who made a significant contribution to the development of modern crystallography, and later became a historian of Beeston in Nottinghamshire. He published nearly 100 papers on his crystallographic research as well as a book for non-physical scientists in 1956, *Physical Chemistry for Students of Pharmacy and Biology*. He played a pivotal role in the founding of the British Crystallographic Association in 1982.

May 2, 2019. A study at The University of Texas MD Anderson Cancer Center identified a new therapeutic target in cancer cells and explains how new anti-cancer drugs called imipridones work by inducing cancer cell death in blood cancers, such as acute myeloid leukemia (AML) and mantle cell lymphoma. The study revealed a target in mitochondria, called caseinolytic protease P (ClpP), which, upon activation, breaks down proteins within mitochondria, a process known as mitochondrial proteolysis.

May 3, 2019. Scientists at the U.S. Department of Energy's Brookhaven National Laboratory and colleagues at Columbia University have developed a new approach for solving protein structures from tiny crystals using microdiffraction. To handle the tiny crystals, the team developed sample grids patterned with micro-sized wells. After pouring solvent containing the microcrystals over these well-mount grids, the scientists removed the solvent and froze the crystals that were trapped on the grids.

May 9, 2019. In a study led by Tony Holder's lab at the Crick and Ed Tate's satellite lab at the Crick and his lab at Imperial College London, scientists generated malaria parasites resistant to a promising new class of candidate antimalarial drugs. By analysing the structural changes behind the resistance, they identified novel compounds that were immune to this mechanism of resistance.

May 11, 2019. Researchers at Kolkata's the Indian Institute of Chemical Biology (CSIR-IICB) and the Indian Association for the Cultivation of Science (IACS) have designed and synthesised about 25 quinoline derivatives that show potent anticancer activity.

May 12, 2019. Have you ever taken a penicillin-based antibiotic? They're some of the most commonly prescribed, including amoxicillin, augmentin, and methicillin. Do you or someone you know have diabetes? If so, Dorothy Hodgkin is a name you should know — her scientific accomplishments made your healthcare possible.

May 14, 2019. Dr. Michael G. Rossmann, the Hanley Distinguished Professor of Biological Sciences at Purdue University, died in West Lafayette, Indiana. He was 88. He was a renowned scientist who gained worldwide attention in 1985 for discovering the structure of the common cold virus, using X-ray crystallography, and later the structure of the dengue virus.

May 20, 2019. A team of researchers from several institutions in Czech Republic has developed a way to determine the absolute stereochemistry of small, organic molecules. To overcome the problem of electron beams destroying nanocrystals before their stereochemistry could be recorded, the researchers simply used more beams — four of them. They fired them all at once at different parts of the nanocrystal and recorded information regarding the diffracting that occurred before the nanocrystal was destroyed.

Product Spotlight

This kit is designed to grow cryoprotected hen egg white lysozyme crystals that can be used for protein crystallography. The crystallographic space group is usually primitive tetragonal **$P4_32_12$** with until cell dimensions of **78 Å × 78 Å × 38 Å** and angles **90°, 90°, 90°**. The size of the crystals will vary from as large as 0.5 mm on an edge to shorter. The mosaicity of the crystals will vary depending on the handling, flash-cooling, and mounting techniques used.

Contact ReagentOrders@Rigaku.com
For more information, visit the
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CrysAlis^{Pro} 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

www.Rigakuxrayforum.com

Rigaku Oxford Diffraction Users' Meeting — July 20, 2019 Covington, KY

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

XtaLAB Synergy-S

With your success utmost in our minds, we have developed the XtaLAB Synergy-S X-ray diffractometer for single crystal X-ray diffraction. Using a combination of leading edge components and user-inspired software tied together through a highly parallelized architecture, the XtaLAB Synergy-S produces fast, precise data in an intelligent fashion.

The system is based around the PhotonJet-S series of microfocus X-ray sources that incorporate continuously variable divergence slits. These third generation sources have been designed to maximize X-ray photons at the sample by using a combination of new optics, new, longer life, tubes and an improved alignment system. PhotonJets are available in Cu, Mo or Ag wavelengths in either a single or dual source configuration.

The XtaLAB Synergy-S single crystal X-ray diffractometer comes with kappa goniometer that incorporates fast motor speeds and a unique telescopic 2θ arm to provide total flexibility for your diffraction experiment. The system is also equipped with your choice of HPC X-ray detector, including the HyPix-6000HE, PILATUS3 R 200K, PILATUS3 R 300K or EIGER 1M.

Benefits:

- Extremely high performance due to bright source, noise-free X-ray detector and fast goniometer speeds
- Continuously variable divergence slit option lets you resolve reflections from long unit cells
- Minimal downtime with longer X-ray tube lifetime – supported by online diagnostics and troubleshooting
- Compact design to fit in your laboratory

Features:

- High source flux and increased goniometer speed to allow quicker, more agile experiments
- Unique telescopic 2θ arm to reach both longer and shorter crystal-to-detector distances
- Enhanced kappa goniometer design with symmetrical 2θ positioning
- Improved X-ray optic alignment mechanism for easy maintenance
- User-inspired cabinet design for improved workflow
- New electronically controlled brightness of cabinet and crystal lighting

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Lab in the Spotlight

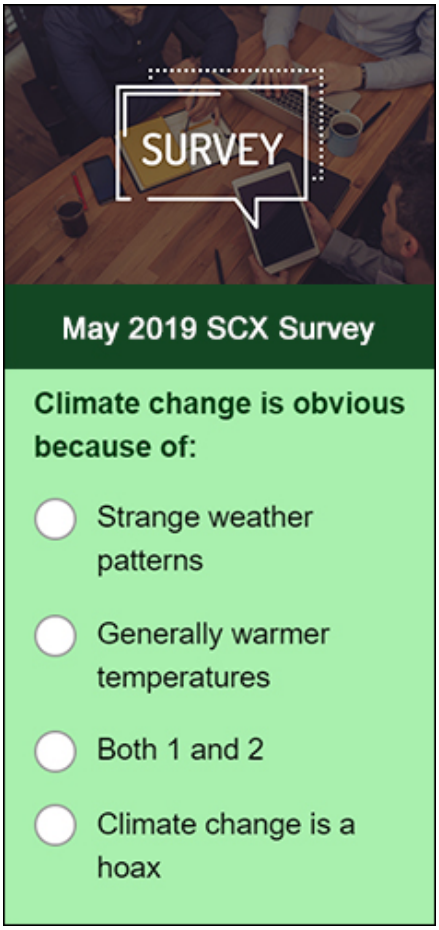
Oregon State University

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.

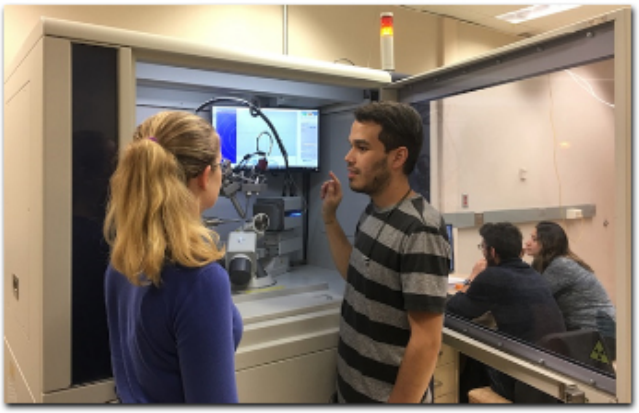
Survey of the Month



Take the Survey

Last Month's Survey

I have dialed up all the privacy settings on my social media apps:



Oregon State University recently took delivery of a dual source XtaLAB Synergy-S diffractometer. The new diffractometer was funded through the generosity of the Murdock Charitable Trust, which supports scientific and engineering research in the Pacific Northwest, and matched by private funds from the College of Science Renaissance Fund and other donor-supported funds from the colleges of Agricultural Sciences, Engineering and Pharmacy. The new diffractometer is located in the Agricultural Life Science Building.

Within the first week after installation, the new diffractometer produced enough data for eight new structures, all fit for publication in peer-reviewed science journals. It is not only fast — "What used to take two hours now takes eight minutes!" exclaims chemist May Nyman — it is capable of analyzing smaller crystals, has fewer runtime errors, and has two X-rays to pick from to optimize imaging for different crystals.

Students are trained in all of the steps of diffraction data gathering and interpretation. They gain a valuable skill set that not only yields rapid knowledge to advance research, but also can translate to marketable skills in a wide range of careers in chemistry research from academia to government to industry.

The new diffractometer's ability to analyze smaller crystals than any other diffractometer in Oregon has already attracted scientists from the University of Oregon and interest from other regional universities and industries who would like to take advantage of this fantastic capability. And anyone who grows single crystals on campus will use the diffractometer, including students, postdocs and faculty. The new diffractometer is expected to open up new avenues of research on campus and across Oregon.

Useful Link

Imagine a crystal's inner life

Here is a freebie (albeit 5 years old) on the history of crystallography from *Nature*. Remember Bragg's Law came before the Laue equations!

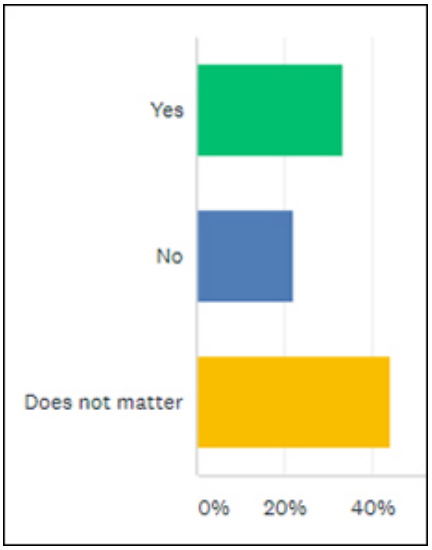
Selected Recent Crystallographic Papers

Optical control, selection and analysis of population dynamics in ultrafast protein X-ray crystallography. Hutchison, Christopher D. M.; van Thor, Jasper J. *Philosophical Transactions of the Royal Society A: Mathematical, Physical & Engineering Sciences*. 5/20/2019, Vol. 377 Issue 2145, p1-18. 18p. DOI: 10.1098/rsta.2017.0474.

The CSD Drug Subset: The Changing Chemistry and Crystallography of Small Molecule Pharmaceuticals. Bryant, Mathew J.; Black, Simon N.; Blade, Helen; Docherty, Robert; Maloney, Andrew G.P.; Taylor, Stefan C. *Journal of Pharmaceutical Sciences*. May2019, Vol. 108 Issue 5, p1655-1662. 8p. DOI: 10.1016/j.xphs.2018.12.011.

Findable Accessible Interoperable Re-usable (FAIR) diffraction data are coming to protein crystallography. Helliwell, John R.; Minor, Wladek; Weiss, Manfred S.; Garman, Elspeth F.; Read, Randy J.; Newman, Janet; van Raaij, Mark J.; Hajdu, Janos; Baker, Edward N. *Acta Crystallographica: Section D, Structural Biology*. May2019, Vol. 75 Issue 5, p455-457. 3p. DOI: 10.1107/S2059798319004844.

Crystallographic elucidations of indium(III) porphyrin conformations, morphology and aggregation behaviour: Comparative optical study of free base porphyrins and their indium(III) derivatives at varying pH. Dechan, Padma; Bajju, Gauri Devi; Sood, Puneet; Dar, Umar Ali. *Journal of Molecular Structure*. May2019, Vol. 1183, p87-99. 13p. DOI: 10.1016/j.molstruc.2019.01.064.



Videos of the Month

This video, which provides the starting point for the book selected for this month's book review, should make you realize that we are not the only animals on the planet capable of emotion.

Watch the Video

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.

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Diffractive–refractive optics: X-ray focusing splitter. Hrdý, Jaromír. *Nuclear Instruments & Methods in Physics Research Section A*. May2019, Vol. 925, p106-108. 3p. DOI: 10.1016/j.nima.2019.02.008.

A unique copper coordination structure with both mono- and bi-dentate ethylenediamine ligands. Sharma, Jai; Jiang, Zhelong; Bhutani, Ankita; Behera, Piush; Shoemaker, Daniel P. *CrystEngComm*. 5/7/2019, Vol. 21 Issue 17, p2718-2726. 9p. DOI: 10.1039/c8ce02188k.

Dioxygen reacts with metal–carbon bonds in thorium dialkyls to produce bis(alkoxides). Settineri, Nicholas S.; Shiau, Angela A.; Arnold, John. *Dalton Transactions: An International Journal of Inorganic Chemistry*. 5/7/2019, Vol. 48 Issue 17, p5569-5573. 5p. DOI: 10.1039/c9dt00811j.

Group 6 metal carbonyl complexes of cyclo-(P_5Ph_5). Yufanyi, Divine Mbom; Grell, Toni; Sárosi, Menyhárt-Botond; Lönnecke, Peter; Hey-Hawkins, Evamarie. *Pure & Applied Chemistry*. May2019, Vol. 91 Issue 5, p785-796. 12p. 4 Diagrams, 3 Charts, 1 Graph. DOI: 10.1515/pac-2018-0905.

Investigation of crystallographic structure, *in vitro* cytotoxicity and DNA interaction of two La(III) and Ce(IV) complexes containing dipicolinic acid and 4-dimethylaminopyridine. Adibi, Hadi; Abdolmaleki, Sara; Shahabadi, Nahid; Golabi, Aynaz; Mahdavi, Mohammad; Zendehcheshm, Saba; Ghadermazi, Mohammad; Ansari, Mohabbat; Amiri Rudbari, Hadi; Bruno, Giuseppe; Nemati, Andya. *Polyhedron*. May2019, Vol. 163, p20-32. 13p. DOI: 10.1016/j.poly.2019.02.009.

Synthesis, crystal structure, experimental and theoretical studies of tetradentate N_2O_2 Schiff base ligand and its Ni(II) and Pd(II) complexes. Kargar, Hadi; Torabi, Vajiheh; Akbari, Alireza; Behjatmanesh-Ardakani, Reza; Tahir, Muhammad Nawaz. *Journal of the Iranian Chemical Society*. May2019, Vol. 16 Issue 5, p1081-1090. 10p. DOI: 10.1007/s13738-018-01583-1.

A space for lattice representation and clustering. Andrews, Lawrence C.; Bernstein, Herbert J.; Sauter, Nicholas K. *Acta Crystallographica. Section A, Foundations & Advances*. May2019, Vol. 75 Issue 3, p593-599. 7p. DOI: 10.1107/S2053273319002729.

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Piano-stool Ru (II) arene complexes that contain ethylenediamine and application in alpha-alkylation reaction of ketones with alcohols. Kavukcu, Serdar Batikan; Günnaz, Salih; Sahin, Onur; Türkmen, Hayati. *Applied Organometallic Chemistry*. May2019, Vol. 33 Issue 5, pN.PAG-N.PAG. 1p. DOI: 10.1002/aoc.4888.

Evaluation of a crystallographic surrogate for kallikrein 5 in the discovery of novel inhibitors for Netherton syndrome. Thorpe, James H.; Edgar, Emma V.; Smith, Kathrine J.; Lewell, Xiao Q.; Rella, Monika; White, Gemma V.; Polyakova, Oxana; Nassau, Pamela; Walker, Ann L.; Holmes, Duncan S.; Pearce, Andrew C.; Wang, Yichen; Liddle, John; Hovnanian, Alain. *Acta Crystallographica: Section F, Structural Biology Communications*. May2019, Vol. 75 Issue 5, p385-391. 7p. DOI: 10.1107/S2053230X19003169.

Characterisation of an n-type segmented BEGe detector. Abt, I.; Caldwell, A.; Donmez, B.; Etrillard, C.; Gooch, C.; Hauertmann, L.; Lampert, M.O.; Liao, H.; Liu, X.; Ma, H.; Majorovits, B.; Schulz, O.; Schuster, M. *Nuclear Instruments & Methods in Physics Research Section A*. May2019, Vol. 925, p172-183. 12p. DOI: 10.1016/j.nima.2019.02.005.

Construction of a new double phenoxo bridged asymmetric manganese(III) Schiff base complex: Observation of ferromagnetic interaction within the dimer and antiferromagnetic interaction between dimers. Sarkar, Nandita; Ghosh, Kousik; González-Prieto, Rodrigo; Herrero, Santiago; Chattopadhyay, Shouvik. *Polyhedron*. May2019, Vol. 164, p138-145. 8p. DOI: 10.1016/j.poly.2019.01.061.

Synthesis, structure and palladium coordination of ambiphilic, pyridine- and phosphine-tethered N-boryl imine ligands. Lorenzini, Fabio; Lagueux-Tremblay, Pierre-Louis; Kayser, Laure V.; Anderson, Ethan; Arndtsen, Bruce A. *Dalton Transactions: An International Journal of Inorganic Chemistry*. 5/7/2019, Vol. 48 Issue 17, p5766-5772. 7p. DOI: 10.1039/c8dt05100c.

Structural analysis of a replication protein encoded by a plasmid isolated from a multiple sclerosis patient. Kilic, Turgay; Popov, Alexander N.; Burk-Körner, Amelie;

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

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Koromyslova, Anna; zur Hausen, Harald; Bund, Timo; Hansman, Grant S. *Acta Crystallographica: Section D, Structural Biology*. May2019, Vol. 75 Issue 5, p498-504. 7p. DOI: 10.1107/S2059798319003991.

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Transmetallation of bis(6-diphenylphosphinoxy-acenapth-5-yl)mercury with tin tetrachloride, antimony trichloride and bismuth trichloride. Olaru, Marian; Krupke, Sandra; Lork, Enno; Mebs, Stefan; Beckmann, Jens. *Dalton Transactions: An International Journal of Inorganic Chemistry*. 5/7/2019, Vol. 48 Issue 17, p5585-5594. 10p. DOI: 10.1039/c9dt00827f.

Synthesis, characterization, and biological evaluation of a novel Zn(II)-Naproxen complex. Chu, Yi-Chun; Wang, Tian-Tian; Wang, Lin-Jian; Luo, Qing-Yang; Jia, Ru; Hong, Tao-Cheng; Wang, Xiao-Ming; Zhu, Hai-Liang. *Polyhedron*. May2019, Vol. 163, p71-76. 6p. DOI: 10.1016/j.poly.2019.01.040.

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Synthesis, characterization and antitumor activity of (E)-2-methyl-3-ferrocenyl-N-acrylamide derivatives. Liu, Yan-Wei; Cheng, Hui-Jie; Ruan, Ban-Feng; Hu, Qiao. *Journal of Organometallic Chemistry*. May2019, Vol. 887, p71-79. 9p. DOI: 10.1016/j.jorganchem.2019.02.021.

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Synthesis and X-ray Crystal Structures of $Ru_3(CO)_9(\mu\text{-arphos})(L)$ [L = $AsPh_3$, $As(m\text{-}C_6H_4Me)_3$, $As(p\text{-}C_6H_4Me)_3$]. Syaida Sirat, Siti; Shawkataly, Omar Bin. *Zeitschrift für Anorganische und Allgemeine Chemie*. 5/15/2019, Vol. 645 Issue 9, p683-687. 5p. DOI: 10.1002/zaac.201900013.

Crystal structure of a hydrogen sulfide sorption complex of anhydrous Mn^{2+}-exchanged zeolite Y (FAU, Si/Al = 1.56). Moon, Dae Jun; Lim, Woo Taik; Seff, Karl. *Microporous & Mesoporous Materials*. May2019, Vol. 279, p432-438. 7p. DOI: 10.1016/j.micromeso.2019.01.027.

Crystal structure and electrical conduction of the organic–inorganic compound $(C_6H_9N_2)_2ZnI_4$. Mao, Wenhui; Wang, Jilin; Liao, Hejie; Zhou, Bing; Zheng, Guoyuan; Mo, Shuyi; Long, Fei; Zou, Zhengguang. *Polyhedron*. May2019, Vol. 164, p48-54. 7p. DOI: 10.1016/j.poly.2019.02.029.

Book Review

Mama's Last Hug: Animal Emotions and What They Tell Us about Ourselves
By Frans de Waal, ISBN: 9780393635065

Frans de Waal's latest book, *Mama's Last Hug*, derives its name from a singular event. In 2016, an elderly professor named Jan van Hoof visited a dying female chimpanzee named Mama at the Burgers' Zoo in the Netherlands. Van Hoof had known Mama for over forty years, having spent many of them studying her behavior and the behavior of her fellow chimpanzees in the zoo's colony.

Van Hoof entered her evening enclosure, known as a night cage, and as soon as Mama recognized him her face burst into a wide grin and she started to make vocalizations indicating she was happy to see him. When van Hoof got close enough, she wrapped her arms around him in a warm embrace.

Even though van Hoof had known Mama for over four decades, he had never interacted with her without being safely behind bars. Any grooming sessions or conversations had taken place with a physical barrier between them. Despite any cute or cuddly appearances, an adult chimpanzee can and will kill a human without hesitation. However, Mama's deteriorating condition facilitated extenuating circumstances, and van Hoof was able to enter her enclosure—still only with her permission. The event was unprecedented—and the video footage went viral.

Despite choosing *Mama's Last Hug* as the title of his book, de Waal only covers the titular event in-depth in the first chapter. The aging Mama's final hug serves as an entry point and, later, a touchstone for a larger narrative regarding expressions of animal emotions, not only of primates but other mammals as well—including humans. The following six chapters cover a broad variety of topics, from anthropomorphism to bartering to alpha male bullying. De Waal occasionally relates the current topic of discussion back to Mama and her role in the Burgers' Zoo chimpanzee colony.

One interesting social behavior de Waal covers—which directly pertains to the title of the book—is the alpha female. Mama was a matriarchal figure in her colony. If Mama liked you, you were going to be just fine, and if Mama did not like you, you were not. Even in patriarchal societies, alpha females can and do wield a tremendous amount of social-emotional power.

De Waal illustrates the concept of the alpha female by directly referencing a passage from Bruce Springsteen's 2016 autobiography *Born to Run*. When Springsteen was an up-and-coming musician, he used to play at a club in New Jersey. The success of the band's performance was determined by one young woman in the audience—Kathy. If Kathy liked the music, she would get up to dance and everyone else would follow suit. If Kathy didn't like the music, the night was a bust. But even so, they didn't want Kathy to like them too much—that would cause tension and foster a detrimental rivalry with the alpha males who hung around the club vying for Kathy's attention.

After describing Springsteen's youthful experience with alpha female control, de Waal brings the narrative back to Mama and the Burgers' Zoo chimpanzee colony, likening Mama's control over the colony's social hierarchy to Kathy's control over the success of a band's evening performance at a hole-in-the-wall club.

Passages like this one in *Mama's Last Hug* serve to provide helpful context for the reader regarding the social and behavioral phenomena de Waal describes. They also underscore several of de Waal's key points about animal emotions, human emotions, and humans as social animals with emotions. De Waal has a unique gift for condensing decades of his own scientific research into a concise, digestible format that flows naturally and is easy to read with little to no background in behavioral studies.

Review by Jeanette S. Ferrara, MA

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