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**Brent Nannenga wins the  
Margaret C. Etter Early Career Award**

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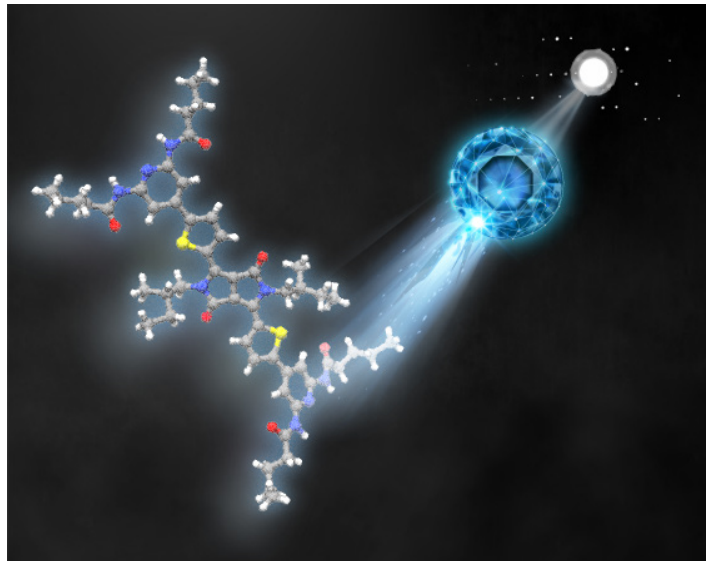
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### Table of Contents

Index of Advertisers.....	1
President's Column.....	2
2021 ACA Election Results.....	4
Call for Nominations.....	6
IUCr Workshop on raw diffraction data.....	7
Crystallographic Database Workshop.....	9
ACA 72nd Annual Meeting.....	10
Remembrance of Carroll Johnson (Chakoumakos) .....	15
Remembrance of Carroll Johnson (Brock/Scheidt).....	17
ACA Summer School 2022.....	18
BioXFEL Phase Retrieval Workshop.....	19
In Memoriam: L. Mario Amzel (Bianchet & Gabelli) .....	20
In Memoriam: L. Mario Amzel (Rose & Wolberger).....	22
In Memoriam: Nadrian "Ned" Seeman .....	24
In Memoriam: Farid R. Ahmed.....	25
In Memoriam: Donald E. Sands.....	27
In Memoriam: John Westbrook.....	28
Remembering Carlos A. Murillo.....	30
In Memoriam Jack D. Dunitz.....	34
2021 Award Donations.....	36
International SAXS Symposium 2022.....	38
ACA Living History Project - Update .....	40
Book Reviews.....	42
Spotlight on Stamps.....	46
Puzzle Corner.....	47
Corporate Sponsor News.....	49
Corporate Sponsor Members.....	52



### About the Cover:

Microcrystal electron diffraction, or MicroED, is a structure determination method that makes use of an electron microscope to collect high-resolution diffraction data from sub-micron crystals. Since its introduction in 2013, MicroED has been successfully applied to a variety of samples in structural biology, small molecule crystallography and pharmaceuticals, and materials science. The application and method development of MicroED is a major research focus for Brent Nannenga, Associate Professor of Chemical Engineering at Arizona State University and recipient of the 2022 Margaret C. Etter Early Career Award. Cover art was created by Vince Alrich.

### Index of Advertisers

Advertiser	Page
ThermoFisher	Inside Front
ATPS	3
Proto	3
Rigaku	13
Dectris	23
Bruker	53

Contributions to **ACA Reflexions** may be sent to *Editor*:

**Paul Swepston**.....[paulswepston@me.com](mailto:paulswepston@me.com)

Cover:	Paul Swepston	Book Reviews:	Joseph Ferrara
Historian:	Virginia Pett	Puzzle Corner:	Frank Fronczek
Photographer:	Richard Bromund	Spotlight on Stamps:	Daniel Rabinovich
Copy Editor:	Sue Byram		

Please address matters pertaining to advertisements, membership inquiries, or use of the ACA mailing list to:

Kristin Stevens, Executive Director of the ACA  
 American Crystallographic Association  
 P. O. Box 96, Ellicott Station  
 Buffalo, NY 14205  
 tel: 716-898-8692; fax: 716-898-8695  
[kstevens@hwi.buffalo.edu](mailto:kstevens@hwi.buffalo.edu)

**Deadlines for contributions to ACA Reflexions are: March 1 (Spring), June 1 (Summer), September 1 (Fall), and December 1 (Winter)**

**ACA Reflexions** (ISSN 1058-9945) Number 4, 2021. Published four times per year in the spring, summer, fall, and winter for the membership of the American Crystallographic Association, P. O. Box 96, Ellicott Station, Buffalo, NY 14205-0096.



**David Rose**  
**ACA President**

## **President's Column** **Winter 2021**

Everyone who has the honour to serve as ACA President has the opportunity to look back and reflect their term. I, personally, and I believe we as an organization have learned much and evolved significantly during the past year. The adage 'Everyone loves progress but hates change' has been put to the test over our past two annual meetings where, by necessity, we have had to make drastic changes to our format. While many of us are looking forward with crossed fingers to an in-person meeting in 2022, we have experienced some aspects of the virtual format that would be worth retaining, not least of which is the increased diversity of attendees (and members) in discipline, career stage, geography and employment/institution type. The precedent is set for a future that will include a mix of meetings throughout the year, virtual, in-person and hybrid. There is a strong argument that these changes made by necessity have led to progress in our vision of membership benefits and participation.

What has struck me most during the past year is the amazing level of commitment to the ACA by our members. Despite busy research, service and teaching schedules coupled with above-normal personal obligations, our members volunteer their time with enthusiasm to the many committees and tasks on behalf of the ACA. To me, this is a very healthy sign; we are all invested in the organization together. The ACA is what we, as members, want it to be.

Particularly gratifying to me is the 'baton-passing' to our early and mid-career colleagues. Almost

all our activities now include voices across the spectrum of experience and discipline; I am constantly amazed by how many early and mid-career members are stepping forward to chair committees and stand for elections. Those of us at the later stages of our careers feel energized in our interactions with the ACA; maybe change isn't so bad after all!

So now, we look forward with anticipation to our Portland meeting, as we come to grips with living with this endemic virus. Travel restrictions are starting to ease and borders gradually opening for international travel; many of our sister societies are already holding in-person conferences. Barring a major setback, we will soon be shaking hands, perhaps even a hug or two, and sharing Covid 'war stories' over coffee or a glass of wine.

With the upcoming meeting, while we escaped potential disaster from the past two years, thanks largely to Kristin, our staff and member volunteers, the ACA still is in a vulnerable position financially. I encourage everyone to make use of the ACA room block in Portland, even at the potential sacrifice of a few dollars per night. Meeting these obligations to the hotel permits us to obtain the best pricing on meeting room rentals, food and drink, and AV, thus easing the need to increase registration and membership fees. Plus, the hotel offers the security of not having to move around the city at night. As always, Council can consider requests for hardship, on a confidential basis.

To close, I must thank members of Council past and present. A special shout-out to members concluding terms on Council, who have devoted much valuable time to the ACA. Brian Toby has been a steady, thoughtful leader, and I have learned a lot by observing him. Ilia Guzei has done a remarkable job overseeing the all-important financial aspects of the organization, including the transition to a stable, transparent system. Our investments remain in a strong position due to his efforts. We wish Hanna Dabkowska the best in her new role as President of the IUCr. We will miss

her good humour and positive encouragement, but we know our parent organization is in excellent hands. Finally, a heartfelt thanks to all committee members and Chairs, SIG officers, all individuals who put their names forward for election, whether successful or not, meeting session organizers, Kristin Stevens, Kristina Vitale and their assistants, and, most important, you, the members of the ACA, who make the society what it is.

PS: The IUCr Congress to be held in Calgary in 2026 is searching for an International Program Chair. This is a busy but rewarding position that is critical to the success of the Congress. If you are interested in being considered, or if you know of someone who might be a strong candidate, please contact Kristin Stevens [kstevens@hwi.buffalo.edu](mailto:kstevens@hwi.buffalo.edu).

David Rose

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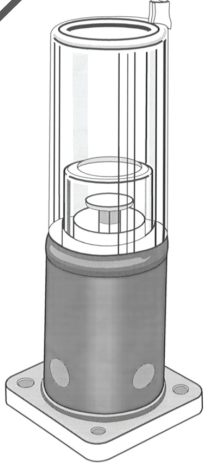
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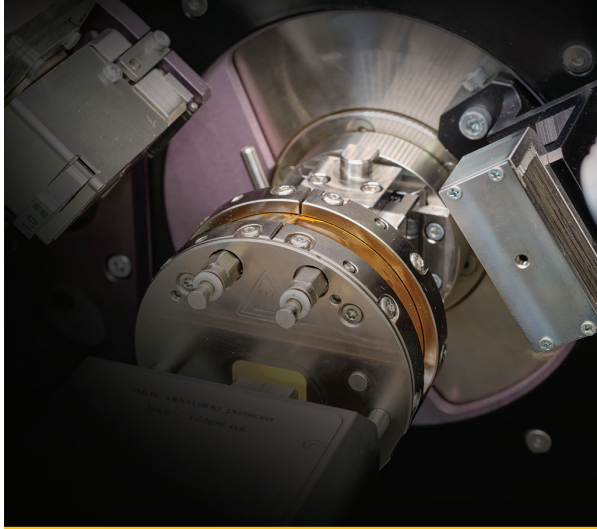
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# 2021 ACA Election Results

The results are in! Our appreciation goes out to all who participated in this year's election. All terms begin January 1, 2022 and the ACA website will be updated by January 1, 2022 to reflect all changes.

## *Council Officers*

---



Vice President 2022  
**Cora Lind-Kovacs**



Treasurer 22-23  
**Stephan Ginell**



USND President 22-23  
**Tamir Gonen**

## *Standing Committees*

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Education Committee  
**Veronica Carta**



Meeting Committee  
**Samantha Powell**



Communications  
Committee  
**Cassandra Eagle**

## SI&G Officers

 <p>BIOLOGICAL MACROMOLECULES Scientific Interest Group</p>	Chair Elect 2022 / Chair 2023: Krystle McLaughlin
 <p>BEST PRACTICES FOR DATA ANALYSIS &amp; ARCHIVING Scientific Interest Group</p>	Chair Elect 2022 / Chair 2023: Aaron Brewster Secretary/Treasurer 22-23: Charles Hespden
 <p>CANADIAN DIVISION Scientific Interest Group</p>	Chair Elect 2022 / Chair 2023: V. Nicholas Vukotic
 <p>CRYO EM Scientific Interest Group</p>	Chair Elect 2022 / Chair 2023: Yifan Cheng Secretary/Treasurer 22-23: Yirui Guo
 <p>GENERAL INTEREST Scientific Interest Group</p>	Chair Elect 2022 / Chair 2023: Lisa Katorcha Secretary/Treasurer 22-23: Mrittika Roy
 <p>INDUSTRIAL Scientific Interest Group</p>	Chair Elect 2022 / Chair 2023: Matthew Clifton Secretary/Treasurer 22-23: Elizabeth Sprague
 <p>LIGHT SOURCES Scientific Interest Group</p>	Chair Elect 2022 / Chair 2023: Denis Keane
 <p>MATERIALS Scientific Interest Group</p>	Chair Elect 2022 / Chair 2023: Jue Liu
 <p>NEUTRONS Scientific Interest Group</p>	Chair Elect 2022 / Chair 2023: Keith Taddei
 <p>POWDER Scientific Interest Group</p>	Chair Elect 2022 / Chair 2023: Wenqian Xu
 <p>SMALL ANGLE SCATTERING Scientific Interest Group</p>	Chair Elect 2022 / Chair 2023: Suzette Pabit Secretary/Treasurer 22-23: Thomas Fitzgibbons
 <p>SMALL MOLECULES Scientific Interest Group</p>	Chair Elect 2022 / Chair 2023: Brian Patrick
 <p>SERVICE Scientific Interest Group</p>	Chair Elect 2022 / Chair 2023: Dan Decato Secretary/Treasurer 22-23: Toby John Woods
 <p>YOUNG SCIENTIST Scientific Interest Group</p>	Chair Elect 2022 / Chair 2023: Alexander Erickson



## *Awards*

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The American Crystallographic Association is now accepting nominations for its 2023 awards. The ACA recognizes distinguished achievement in the field of crystallography through the presentation of various annual awards and prizes. The ACA relies on its experienced membership to recognize and bring attention to the accomplishments and contributions of their fellow members and colleagues.

There are four award categories honoring individuals for distinction in the field of crystallography and structural science and this year we are accepting nominations for the following awards:

**David G. Rognlie Award:** To recognize an exceptional discovery or technical development of particularly high impact in any area of structural science, to be awarded at any stage of a scientist's career without prejudice based on age, gender, ethnicity, or race.

**A.L. Patterson Award:** To recognize and encourage outstanding research in the structure of matter by diffraction methods, including the methodology of structure determination and/or innovative application of diffraction methods and/or elucidation of biological, chemical, geological, or physical phenomena using new structural information.

**Elizabeth A. Wood Science Writing Award:** Persons who have written books or articles that bring science to the attention of a wider audience are eligible. Successful nominees need not be crystallographers or scientists and 'writing' could include artistic efforts, museum displays, etc. Nominations should include the titles of books, copies of articles, or other documentation (supporting letters, narrative and c.v. are not required).

**Margaret C. Etter Early Career Award:** This award was established to recognize outstanding achievement and exceptional potential in crystallographic research demonstrated by a scientist at an early stage of their independent career.

If you know a commendable individual, this is the opportunity to recognize their contributions by nominating them. Submit a nomination for one of the following awards by April 1, 2022. Please send your completed nomination packet to [kvitale@buffalo.edu](mailto:kvitale@buffalo.edu).

Awards will be presented at the 2023 ACA Annual Meeting in Baltimore, Maryland from July 7-11, 2023. For information and to submit a nomination, visit: <https://acas.memberclicks.net/awards>.

## *Fellows*

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The ACA Fellows program was established to recognize a high level of excellence in scientific research, teaching, and professional duties, but also service, leadership, and personal engagement in the ACA and the broader world of crystallography and science. Our Fellows program celebrates the excellence of our own members from within the ACA, and promotes their recognition worldwide to constituencies outside of the ACA, such as their employers, other scientific societies, and the government. See <https://www.amerocrystalassn.org/fellows> for information on the nomination procedure.

## *Questions?*

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Contact ACA HQ: [aca@hwi.buffalo.edu](mailto:aca@hwi.buffalo.edu)



## IUCr workshop on ‘When should small molecule crystallographers publish raw diffraction data?’

Simon Coles and Amy Sarjeant.

Nearly two years ago, we undertook a survey of the chemical crystallography community in order to better understand current practices and ideas around raw data management, archival and sharing. In early 2020 we presented a summary of the responses of nearly 200 survey participants in an IUCr Newsletter article (<https://www.iucr.org/news/newsletter/volume-28/number-1/raw-data-availability-the-small-molecule-crystallography-perspective>). To keep momentum building in the hopes of defining a set of community best practices, we began organising a workshop to run alongside the 2020 IUCr Congress in Prague. While our original workshop was delayed by a year due to the coronavirus pandemic, this additional time allowed us to engage more members of the chemical crystallography community, which ultimately resulted in a richly rewarding workshop for all involved. For those who could not attend, we present the following summary of the two-day virtual event.

Originally planned as an in-person, day-long workshop featuring invited presentations and a panel session from crystallographers at the leading edge of raw data usage and management practices, we adjusted both the schedule and platform to allow for as many international colleagues to attend as possible. The meeting was held via Zoom over two half-day sessions – we make a special thanks to our generous colleagues at Rigaku who provided this platform and helped with coordination. The workshop website (<https://www.iucr.org/resources/data/commdat/prague-workshop-cx>) shows the schedule and provides links to the presentations that were delivered.

Each day’s session began with a short summary of the survey results. On the first day, Amy Sarjeant presented an overview of survey

respondents’ demographics as well as their thoughts surrounding what uses a store of raw crystallographic data could have. This was followed by contributions from Michal Dusek, Kamil Dziubek, and Amber Thomson. Michal’s talk focused on the economic factors surrounding raw data archival, specifically in the field of modulated or incommensurate structures. He also gave a compelling case study of how a 1990’s dataset was revisited three different times over 20 years and drastically improved (R-factor going from 19% to 9%) along the way, thus becoming publishable, as new data processing and refinement software became available. Kamil highlighted efforts from the high pressure crystallography community to establish standards on metadata to accompany raw data archives. This is an activity that is well underway and we hope to see new CIF standards specifically supporting High Pressure crystallography emerging as a result. Amber shared several accounts underscoring the need for returning to original raw data files in order to solve complex structural problems and also raised the truly fundamental question – in the case of service crystallography, who really ‘owns’ the data?

After a coffee break, the session resumed with a presentation from Simon Grabowsky & Krzysztof Wozniak, highlighting the utility of raw data to validate assertions about electronic structure and properties in the field of quantum crystallography. This is an emergent aspect of crystallography that raises some major questions around what raw data actually is – if you are calculating a wavefunction based on a particular set of diffraction data, is that considered raw data? A further problem is where and how to store such a thing, as they are rather large for a CIF and there are no standard ways to describe them. Jim Britten provided a real-world application of raw diffraction data by demonstrating his 3D diffraction space visualizer, MAX3D. He showed so many beautiful examples that were a stark reminder that we don’t spend enough time looking at our raw diffraction data these days – and that if you do, you can often answer structural questions at some level or other despite how ‘bad’

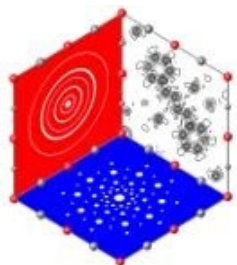
the data might appear! The session concluded with Joe Ferrara who provided a vendor perspective on what can be done to help the community adopt raw data management best practices and touched on the ideas of an archive of data processing software and conversion of formats.

The second day of the workshop focused more on community standards. Simon Coles started the session with an overview from the survey looking at current raw data management practices. Graeme Winter brought a massive amount of experience and insight from his work supporting raw data management across Diamond Light Source facilities, pulling out important points such as whether to use generic vs specific repositories and when, or 'who pays?' Loes Kroon Battenberg pointed out that most service crystallographers don't have any infrastructure to properly help them with raw data management. She also touched on the reusability of the raw data currently publicly available – just because you put it online doesn't mean that others can actually use it! Finally she touched on the importance of the concept of a 'CheckCIF for images', which would enable proper understanding and reusability of our raw data. Teodor Ivanoaica spoke about current data policies at the EU's Extreme Light Infrastructure. Their volumes and rates of data generation

are considerably greater than lab-based crystallography – however from about 150TB of data collected generally only 20TB is useful, which raises the question what to keep and what not to keep! The final speaker was Natalie Johnson from the CCDC who spoke about challenges in curating and maintaining a raw diffraction database, how it should be related to results data and how both of these interface to established ways of publishing. The workshop concluded with a group discussion of the various challenges highlighted throughout the previous talks, which was very vibrant and went on for three times the allocated slot – definitely a bonus of having such meetings online and not having to rush out to the next event at an in-person conference.

We left the workshop understanding several primary challenges facing widespread adoption of raw diffraction data. These mainly encompass the costs involved in maintaining an arguably huge data store, deciding which data should be archived if storing everything is cost-prohibitive, agreeing on what metadata to store and how best to record it, understanding what and how to 'publish', and finally, how to promote this within the community in order to effect widespread culture change. Though the challenges are many, the promise remains great.





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## The US National Committee for Crystallography

### 2<sup>nd</sup> Workshop Announcement

### Crystallographic Databases (March/April 2022)

The U.S. National Committee for Crystallography (USNC/Cr) is partnering with the National Institute of Standards and Technology (NIST) and the National Academy of Sciences (NAS) to provide an online short course for students and researchers on the use, development, and maintenance of crystallographic and structural databases. Encompassing macromolecular, small molecule, and powder diffraction information, the course will include training options for each of the following database resources:

**Crystallographic Open Database (COD)**

**Cambridge Structural Database (CSD)**

**Electron Microscopy Data Bank (EMDB)**

**International Center for Diffraction Data (ICDD)**

**Inorganic Crystal Structure Database (ICSD)**

**Integrated Resource for Reproducibility in Macromolecular  
Crystallography (IRRMIC)**

**RCSB Protein Data Bank (PDB)**

**SBGrid Data Bank**

Graduate students, postdoctoral fellows, faculty members and researchers in any of the crystallographic, diffraction, and imaging sciences affiliated with the International Union of Crystallography (IUCr) are encouraged to register and participate in the training options that interest them. Undergraduate students with appropriate research experience will be considered. More details on the registration process will be available in Winter 2021. For more information, please contact USNC/Cr member Joe Tanski, [jotanski@vassar.edu](mailto:jotanski@vassar.edu).

# 72nd ACA Annual Meeting

Portland, Oregon | July 29-August 2, 2022



## *Awards*

Bau Neutron Diffraction Awardee: **Arthur J. Schultz, Argonne National Laboratory**  
Fankuchen Memorial Awardee: **David S. Goodsell, Scripps Research Institute**  
Kenneth N. Trueblood Awardee: **Airlie McCoy, Cambridge University**  
Margaret C. Etter Early Career Awardee: **Brent L. Nannenga, Arizona State University**

## *Transactions Symposium*

**The Role of Structural Science in Tackling a Pandemic: COVID-19 as a Paradigm**

## *Workshops*

**WK1: Applications of Small Angle Scattering to Structural Biology: An Introduction**  
Organizer(s): Michal Hammel, Jesse Hopkins, Kushol Gupta, Richard Gillilan, Thomas Weiss  
& Steve Meisburger

**WK2: Crystallographic and CryoEM Structure Solution with Phenix**  
Organizer(s): Dorothee Liebschner

**WK3: Cryo-electron Tomography: State of The Art Methods**  
Organizer(s): JT Kaelber

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## *Workshops...cont.*

### **WK4: Hands-on single-particle cryo-EM data analysis with cryoEDU**

Organizer(s): Michael Cianfrocco, Mark Herzik,  
Elizabeth Kellogg & Melody Campbell

### **WK5: CryoEM Sample Preparation Training Using Center Merit Badges**

Organizer(s): Ed Eng, Craig Yoshioka, Claudia López, Michael Schmid, Peter Shen, Wen Jiang & Michael Cianfrocco

### **WK6: Advanced Software Tools for Single Crystal Diffraction**

Organizer(s): Xiaoping Wang, Zachary Morgan,  
Christina Hoffmann & Feng Ye

### **WK7: Visualizing Structure**

Organizer(s): Nichole Valdez

### **WK8: MicroED of Small and Macromolecules**

Tamir Gonen, Jessica Bruhn & Brandon Mercado

## *Meeting Committee*



Nozomi Ando



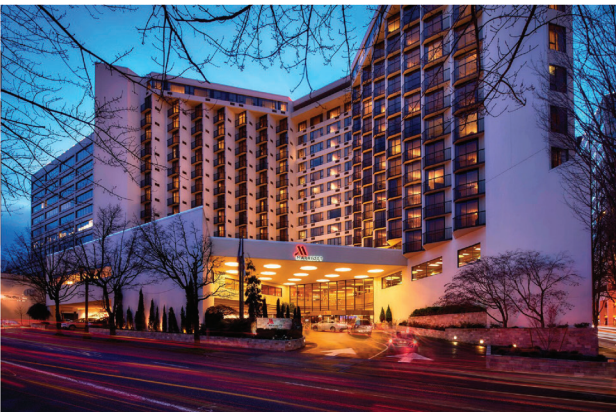
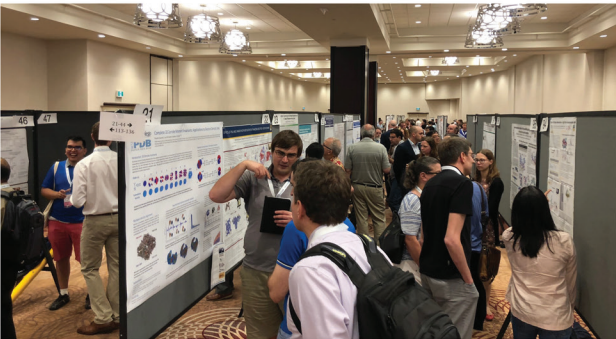
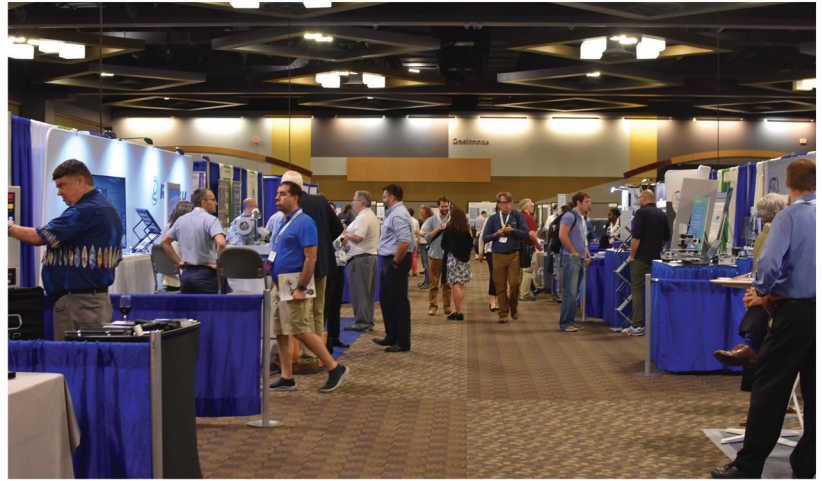
Anna Gardberg  
(21-24)



Brandon Mercado  
(20-23)



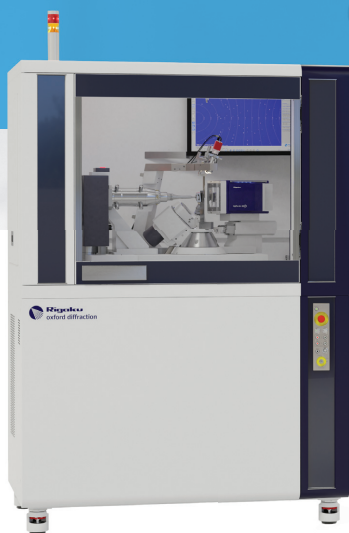
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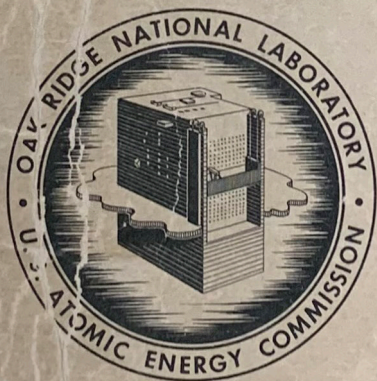
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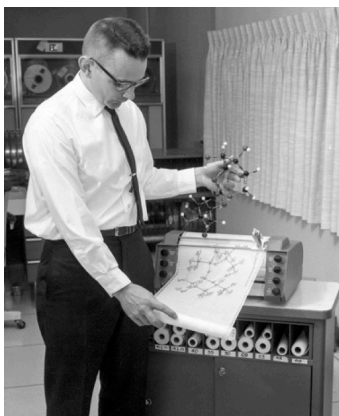
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## Carroll K. Johnson, 1929 – 2021

Carroll Johnson's professional career adhered to the postulate that one should change directions every five years to avoid stagnation. His career-profile in approximately five-year segments as he described himself starting in 1955 was as follows:



(1) graduate school (MIT-PhD): biophysics & fiber diffraction theory, (2) postdoc positions: X-ray crystallography (Institute for Cancer Research, Philadelphia) & neutron diffraction (Oak Ridge National Laboratory), (3) staff member ORNL until retirement in 1996:

thermal motion & computer graphics, (4) crystal physics, (5) artificial intelligence concepts, (6) artificial intelligence applications, (7) machine vision engineering & project management, and (8) crystallographic topology & neutron diffraction. Carroll remained very active in retirement. His post retirement activities involved "crystallographic topology, personal computing and enjoying life." He personally noted selected professional activities in his career: 1975-76 sabbatical, studying artificial intelligence at the Computer Science Department, Stanford University, 1977 President of the American Crystallographic Association (ACA), 1981 studying more artificial intelligence at the Naval Research Laboratory, 1996 Chairing the ACA General Interest Group, and 1997 receiving the ACA Buerger Award.

He was a native of Colorado and started a pre-med program in 1947 at the University of Colorado, which was put on hold by four years in the United States Marine Corps, which included a year in the Korean war. Afterwards, he completed a B.S. degree in Animal Nutrition and Physiology (1955) from the Colorado State University. He went on to complete a Ph.D. degree in Biophysics (1959) at M.I.T., doing his thesis on polypeptide packing

studied by X-ray diffraction. After that, he did a post-doc (1959-1962) at the Institute for Cancer Research (now the Fox Chase Cancer Center), Philadelphia with Lindo Patterson, whose group at that time included Jenny Glusker, Dick van der Helm, Max Taylor, Eric Gabe, and Jean Minkin. It was during his post-doc in Philadelphia that he began working on the computer program for plotting atomic thermal ellipsoids, which he later finished at ORNL.

Carroll started at ORNL in 1962 beginning as a post-doc working on neutron diffraction in Henri Levy's group. After converting to a staff scientist, he spent his entire professional career in the Chemistry Division at ORNL, retiring in 1996. Over the years at ORNL his immediate colleagues and his group's mission changed a lot. In the early days he worked with Henri Levy, Bill Busing, and George Brown. Later he worked with Michael Burnett on many programming applications. He was an independent thinker, mathematically inclined, and pursued projects always at the forefront and often beyond current thinking. Carroll Johnson's scientific success grew markedly with the publication of his most celebrated computer program, *ORTEP* (Oak Ridge Thermal-Ellipsoid Plot Program), which rapidly became a favorite of crystallographers and protein crystallographers to make illustrations of crystal structures for conference presentations and publications. *ORTEP* was first released in an ORNL Technical Report in 1965; see historical note <https://www.umass.edu/molvis/francoeur/ortep/ortepnews.html>. A key strength of *ORTEP* was its capacity to generate stereoscopic images automatically. *ORTEP 2* was released in 1976 and *ORTEP 3* in 1996. The latter is still available from the official *ORTEP* website, <https://ornl-ndav.github.io/ortep/ortep.html>. *ORTEP* is one of the most cited and miscited publications in crystallography with over 30,000 citations. *ORTEP* even is commonly used as a word for a crystal structure drawing with atomic displacement ellipsoids, whether it was made with *ORTEP* or not. A Google search on "ORTEP" returns 798,000 hits. Atomic displacement ellipsoid

drawing options are now standard in all the major crystal and molecular structure drawing programs. Carroll was an expert on thermal motion analysis as studied by diffraction and sought better and new ways to use this aspect of crystal structure analysis.

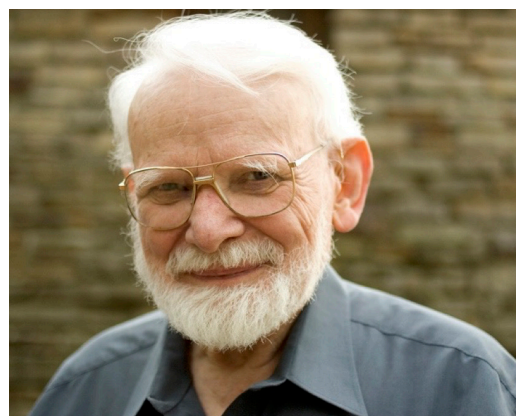
Bill Busing, Henri Levy, Hal Smith, and Pete Peterson had built and were operating a three-circle neutron diffractometer at the Oak Ridge Research Reactor for several years doing chemical crystallography prior to Carroll Johnson's arrival at ORNL. Data collection by that diffractometer was controlled by a computer program run on the ORACLE (an early main-frame computer at ORNL) which prepared a paper punch control tape which conveyed the angle settings to the motors. The intensities were also recorded on paper punch tape. When minicomputers became available in 1965, Busing and Levy programmed the PDP-5 computer to control a four-circle Picker diffractometer, first as an X-ray instrument and then for a neutron instrument at ORNL's High Flux Isotope Reactor (HFIR), which had just started operating. Seminal crystal structural studies of hydrogen containing compounds were done with the HFIR diffractometer, but the science it could do was limited because no low temperature sample cooling device was available on the instrument. The HFIR four-circle diffractometer was operated only intermittently through the 1980's. After a 3+ year safety review shutdown of HFIR ending in 1990, Carroll Johnson and Michael Burnett upgraded the neutron diffractometer at HFIR, with a new Huber goniometer, a low temperature sample stage (5K-300K) and a new 7-pixel array detector. I was responsible for the powder diffractometer at HFIR at that time but was interested in doing structural studies with single-crystals as well, so I got with Carroll to learn as much as I could about the operation of his single-crystal diffractometer. The interest in single-crystal neutron diffraction studies by the Chemistry Division kept dwindling with each retirement and passing of Levy's old group members. Carroll had been the youngster in that group when he started, but now he was

ready for a change, retirement was next, and it was at that time that he transferred the HFIR four-circle diffractometer to me in the neutron scattering group. Since then, we have upgraded that instrument multiple times, and it has grown with the help of a new younger generation of scientists hired in the ORNL Neutron Scattering Division to be extremely productive doing research in materials physics and chemistry. I thank Carroll for setting us on that course.

The American Crystallographic Association was his professional society home. He began attending ACA meetings in 1964 and with few exceptions attended all their meetings until he retired, and some after that. The ACA was an extended family for him, and he often planned family vacations around the annual meetings, bringing along Carol, his wife, and his children, which numbered five in the end. He gave back to the ACA in presenting many talks and posters, serving on the Crystallographic Computing Committee in 1965-1967, serving as President-elect in 1976, President in 1977, and Past-President in 1978, and Chairing the General Interest Special Interest Group 1994-1996.

Carroll Johnson was married to Carol for 69 years and had five children, ten grandchildren and seven great grandchildren. His family especially enjoyed how his curiosity and inquisitiveness were not limited to his work and touched all aspects of his life.

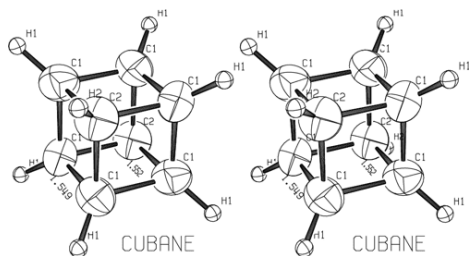
*Bryan Chakoumakos, October 6, 2021*



## In Praise of Carroll Johnson

Carroll Johnson was a visionary. He was so far out ahead of his colleagues that he did not always get the credit he deserved.

Carroll once confirmed as true the story I had heard about how he came to be a crystallographer: As a senior majoring in Animal Nutrition and Physiology at Colorado State University he needed one more elective course to graduate, and the textbook for the crystallography course was cheaper than the textbook for the other possibility.



At ORNL, where he had his first and only permanent position, Carroll became interested in thermal motion in solids because the neutron diffraction studies being done there gave reliable displacement parameters for the H atoms as well as for the “heavy” atoms. This interest led to his writing the Oak Ridge Thermal Ellipsoid Plotting Program (ORTEP), which was hugely influential. Bill Busing once told me that he had had to protect Carroll from their superiors at ORNL, who thought Carroll was wasting his time.

In the mid 1970s Carroll worked on a structure (TTF7I5) that turned out to be incommensurate because the dimensions of the TTF and iodide substructures don't quite match. His 1976 paper on the structure with postdoc C. R. Watson, Jr. in the *Journal of Chemical Physics* was one of the first detailed reports of an aperiodic structure. The 16-pg. paper also describes the methodology developed to refine the structure. This project led Carroll to organize a workshop on modulated structures that was held on the Big Island the week before the 1979 ACA meeting in Honolulu.

Later Carroll became interested in artificial intelligence and in crystallographic topology. The terms critical net, groupoid, and orbifold started appearing in his abstracts and writings in the 1990s, well before the topic became popular.

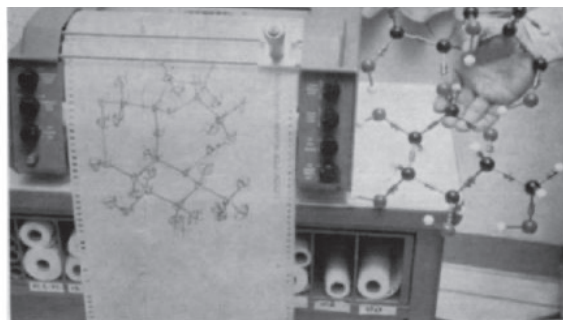
How lucky it was for the crystallographic community that financial considerations led such a gifted mathematician and thinker into our field.

*Carol Brock*

## Thank you Carroll Johnson!

My most vivid recollection of Carroll Johnson was meeting him at the 1970 meeting at Ames, Iowa (Iowa State University), I sat at a table (this must have been at the Student Union) with Carroll Johnson (CJ) at breakfast. I was a starting assistant professor and somewhat in awe of everyone at the meeting. I told CJ that I had been the first person to prepare publication quality ORTEP plots at the University of Michigan and I subsequently used the plotting program during my postdoc at Cornell. I was effusive in my praise for the quality and usefulness of ORTEP. But CJ was having none of that, “The program has many shortcomings especially since it does not solve the hidden line problem and additional manual labor is needed to have a quality illustration.” Of course the hidden line problem was solved in a subsequent version. The importance of ORTEP plots (originally produced on CALCOMP plotters) in solid state science publications cannot be overstated.

*Bob Scheidt*





## ACA Summer Course in Chemical Crystallography

June 12<sup>th</sup> – June 18<sup>th</sup>, 2022

Purdue University, West Lafayette, IN

The ACA Summer Course in Chemical Crystallography is a week long program that is now well into its third decade of instruction here in the United States. The course is directed towards Single-Crystal Chemical Crystallography and Powder Diffraction techniques, as applicable to small molecule studies and is designed to instruct attendees in the theory and practice of these two aspects of crystallography. Mornings feature lectures on the theory of the experiment and afternoons and early evenings are covering hands-on workshops.

**Applications will be accepted starting January, 2022**

[www.acasummercourse.net](http://www.acasummercourse.net)

Sponsored by:

The American Crystallographic Association, The US National Committee for Crystallography, Triclinic Labs, Inc., Improved Pharma, Rigaku Americas, Bruker AXS, Oxford Cryosystems, MiTeGen, The International Centre for Diffraction Data, The Cambridge Crystallographic Data Centre, The Pittsburgh Diffraction Society, Anton Paar, Huber Diffraction and Positioning Equipment, and STOE



**PURDUE**  
UNIVERSITY

Northwestern  
University



[BioXFEL](#) sponsored a remote Phase Retrieval Workshop Monday, October 18 through Tuesday, October 19 2021. The workshop featured a mix of lectures and virtual demonstrations delivered by BioXFEL staff, scholars, and collaborators.

This two-day online event was delivered to an international audience of over 60 people. On the first day we held a teaching session where we covered the basic math, physics, algorithms, and biological applications of phase retrieval methods. Day 2 was focused on research talks presented by invited speakers discussing their current research pertaining to phase retrieval methods. The talks were recorded and posted to [YouTube](#).

**Invited Speakers and Lecturers:**

Joe Chen (ASU) Organizer  
Jeffrey Donatelli (LBNL) Organizer  
Kanupriya Pande (LBNL) Organizer  
Zixi Hu (LBNL)  
Rainier Mobley (ASU)  
Rick Kirian (ASU)  
Tom Grant (UB)  
Elijah Gonzalez (Rice University)  
George Phillips (Rice University)  
Sabine Botha (ASU)  
Dorothee Liebschner (LBNL)  
Iris Chang (SLAC)

## Phase Retrieval Workshop 2021 Agenda

### Day 1 Teaching Talks

- Welcome and Introduction
- Physics and Fourier optics
- Coherent Diffractive Imaging and Phase Retrieval Algorithms
- Basic phasing with Python Hands-on tutorial
- Basic introduction to crystallography for those who need it.
- Crystallographic phasing (MAD/SAD)
- Crystallographic phasing (MR/Direct method)
- The discrete Fourier transform and the phase problem for 2D and 1D crystals
- Trivia/Quiz

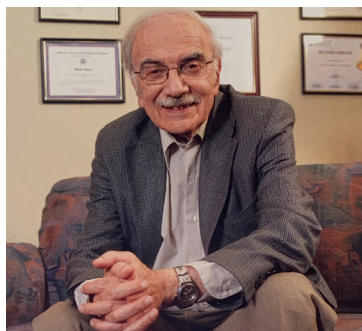
Joe Chen  
Rick Kirian  
Jeff Donatelli  
Joe Chen  
Joe Chen  
Sabine Botha  
George Phillips  
Rick Millane  
Joe Chen

### Day 2 Research Talk Speakers

- Multi-tiered iterative phasing for solving complex inverse problems
- A mathematical algorithm for estimating rotational diffusion coefficient from X-ray photon correlation spectroscopy data
- Scaling and accelerating algorithms for single-particle imaging
- The Monte Carlo expand-maximize-compress algorithm
- Phase retrieval for 1D solution scattering profiles
- Ab initio structure determination from fluctuation x-ray scattering
- Ab initio phasing of high solvent content crystals using a hybrid input-output algorithm
- Phase determination in Macromolecular crystallography with Phenix

Jeff Donatelli, LBNL  
  
Zixi Hu, LBNL  
Iris Chang, Stanford  
Benjamin Mobely, ASU  
Tom Grant, Univ. at Buffalo  
Kanupriya Pande, LBNL  
  
Elijah Gonzalez, Rice Univ.  
Dorothee Liebschner, LBNL

### In Memoriam: L. Mario Amzel



As the first Latino chair of a department at the Johns Hopkins School of Medicine he was a role model for many and specially for the under-represented minorities in our community. He led the transformation

of what we know today as the Biophysics and Biophysical Chemistry Department. Under his leadership, the department hired eight faculty, sponsored five faculty promotions, expanded the central techniques of the department, as well as opened multiple core facilities to benefit the whole JHU community.

Mario was born in Buenos Aires, Argentina and was educated in the public school system. Convinced of the power of education as a force of social transformation he graduated with an emphasis in elementary school education and then applied to the Facultad de Ciencias Exactas y Naturales (FCEN), Universidad de Buenos Aires (UBA). He graduated in chemistry as a “Licenciado”. He then obtained his PhD in physical chemistry at the Universidad de Buenos Aires where his studies focused on structural thermodynamics of plastic crystals under the mentorship of Dr. Leo Becka. During this time, and given his strong support of graduate education, it is not a surprise that Mario was an active representative of the graduate student association at the Universidad de Buenos Aires. During the disruption of the Argentinian academic environment resulting from the politically motivated repression that become known as the ‘night of the long batons’, Mario left Argentina. He joined the lab of Dr. Roberto Poljak at JHU as a postdoctoral fellow and was later invited to join the faculty of the Biophysics and Biophysics Chemistry Department at Johns Hopkins University where he spent his entire academic career.

Mario’s scientific journey in molecular structure

determination veered from plastic crystals to macromolecular crystallography that led to the determination of the first antibody structure. Mario’s contribution synergized thermodynamics and structural biology to establish the specificity determinants of lectins and antibodies. He was part of the team that determined the first structure of antibodies and as part of his own studies, he established the structural basis of angiotensin II recognition by an anti-idiotypic antibody. His body of work provided insights into the mechanism of enzymes that catalyze the synthesis of signal molecules. These include lipoxygenase, peptidylglycine alpha-hydroxylating monooxygenase, (PHM) and phosphatidylinositol 3 kinase (PI3K). In addition to these studies, Mario made significant contributions to our understanding of membrane proteins including the mitochondrial FoF1-ATPase, the cytoplasmic domain of the voltage gated sodium channels and the Na<sup>+</sup>/I<sup>-</sup> symporter, NIS. These structural studies not only contributed to our fundamental understanding of these proteins, but they also led to clinically important insights. For example, these studies were important for mapping mutations in cardiac patients with arrhythmia and established models to overcome their deleterious effect.

Mario was an excellent teacher and collaborator. As the department Director, his office had two physical entrances; one gated by his secretary



L. Mario Amzel, S. Gabelli, M. Bianchet and M. Nadella at the X-ray Laboratory at JHU, 2006

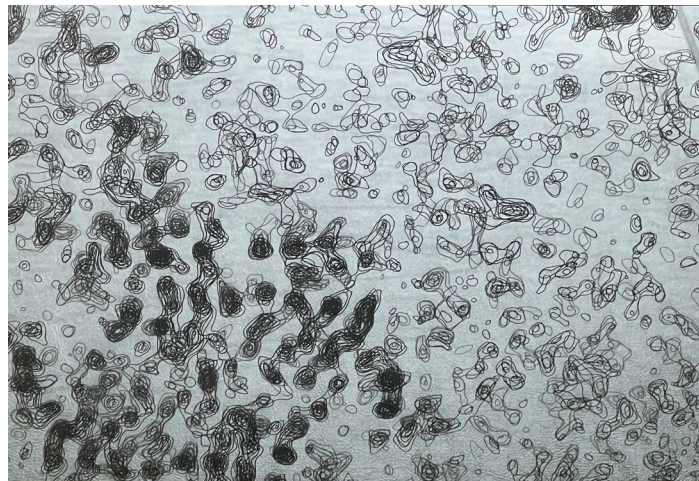
and administrative staff, while the other ungated, always open “for science”. When discussing science, he readily grabbed the chalk or the pencil to describe the scientific basis of a particular

phenomenon, present hypothesis for recent data, and suggest new experiments to test the hypothesis. He had an amazing ability to calm the stress of students and postdocs struggling with their data. We often heard him in the x-ray lab, where someone would be struggling to process their data, and say, “don’t worry, if the program can’t do it, it can be done by hand” and then sat with the trainee to figure it out, or give them the confidence to solve it for themselves. Mario was also great with ‘hands on’ teaching even to those that, as he would say, “had never pulled apart a bike and put it back”. He inspired in them to tackle both intellectual and instrumentation challenges in a warm and supportive manner.

Mario was a highly respected scientist. His body of work garnered more than 19000 citations from more than 240 peer-reviewed publications. In addition to his numerous invitations to present his work at national and international conferences he served as a reviewer for multiple scientific journals as well as national and international grant review panels. Mario received a Doctor Honoris causa from the University of Buenos Aires (Argentina), as well as the prestigious “Raices” award as an accomplished Argentinian scientist who had continued to support Argentinian research development. He was also a fellow of the Biophysical Society and the American Association for the Advancement of Science. He was a constant and fervent promoter of integration, and not of assimilation to reach the shared goal of a diverse faculty and student population in academic medicine. Mario’s influence went well beyond his mentorship within JHU. Besides the PhDs and postdoctoral fellows that trained in his lab from a variety of Hopkins programs, his wisdom shaped collaborations and careers throughout most of South America, that included Argentina, Colombia, Venezuela, Brazil, and Mexico. Impressively, the power of his imprint generated graduate programs in regions where there had been none.

Beyond science, and on a personal note, we bonded over our many discussions that ranged

from politics to science, and from wine to charcuterie. As Mario’s mentees, we learned the



*Map of the first antibody in glass*

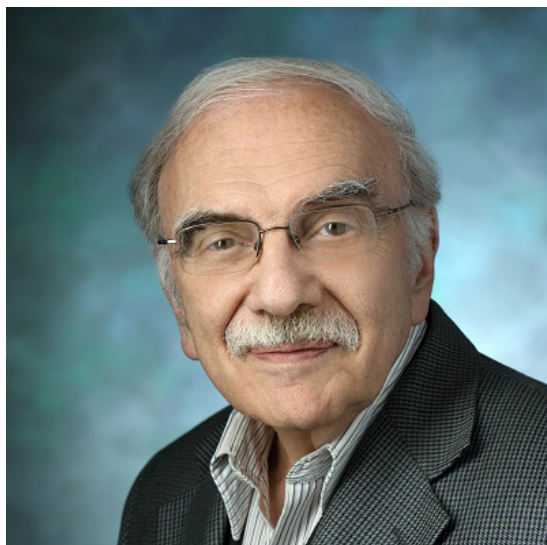
benefits of reaching out to colleagues, of listening to dissenting opinions, and of giving space for all growth. He opened generously his house to visiting colleagues, particularly at ‘end-of-the-year’ parties overlooking the fireworks on the Baltimore inner harbor as well as to lab parties and picnics, where he would personally grill for us a never-ending plethora of meats no matter the weather. These discussions and events were examples of his scientific generosity and enormous humanity. He will be greatly missed.

*Mario A. Bianchet and Sandra B. Gabelli*



*Lab picnic Summer 2019*

## In Memoriam: L. Mario Amzel



By George D. Rose<sup>1</sup> and Cynthia Wolberger<sup>2</sup>

<sup>1</sup>*Department of Biophysics, The Johns Hopkins University*

<sup>2</sup>*Department of Biophysics and Biophysical Chemistry, The Johns Hopkins University School of Medicine*

This past August we lost L. Mario Amzel, crystallographer and polymath. He made seminal contributions to structural studies of antibodies and a variety of enzymes of central importance to human health. He also trained students and fellows who went on to become leaders in the field. As chair of the Department of Biophysics and Biophysical Chemistry at the Johns Hopkins School of Medicine for 15 years, he hired most of the current faculty. Throughout his career, he was actively involved with science in Latin America, giving lectures, participating in scientific affairs, and bringing Latin American students to Hopkins. He was a founding member of the Latino American Biophysical Society and also served a term as its president. He is deeply missed.

Mario was born and educated in Buenos Aires, Argentina, receiving his Ph.D. in physical chemistry from the University of Buenos Aires in

1968. One year later, he arrived at Johns Hopkins, where he joined the laboratory of Roberto Poljak to work on determining the first structure of an antibody. Mario's work on antibody structure, which continued after he established his own group in the Hopkins Biophysics department, ushered in today's therapeutic strategies to harness the immune response.

Mario Amzel's predominant focus was on the relationship between biological structure and thermodynamics, including statistical thermodynamics. His work on mitochondrial ATPases spanned a quarter of a century and provided ground-breaking insight into both the structure of F1-ATPase and the detailed understanding of the mechanism of ATP synthesis. The list of additional structure-based contributions includes numerous proteins of physiological interest: alcohol dehydrogenase, lipoygenase, cystolic quinone reductases, odorant binding proteins, lectins, monooxygenases, ADP-ribose pyrophosphatase, the sodium/iodide symporter and Na<sup>+</sup>-driven transporters, and aspects of the HIV1 protease.

For Mario, the quest to uncover underlying physical-chemical principles in biology guided his research throughout. In addition to specific systems, his publications range over broad topics that include energetics and kinetics in biological systems, enzyme mechanisms, allostery, methodology, and data analysis. He was ever curious about the workings of things - all things: societies, government, geography, the internet, lab instruments ... with passions that spanned literature, poetry, opera and wine, especially fine Argentinean wines. When asked whether he planned to retire, he responded, "I have many interests as an amateur but only one thing as a professional, so why would I want to give that up?"

Mario was a gifted and generous teacher and mentor, who trained 33 students and 15 postdoctoral fellows. He was always willing to put aside other matters for them and for the steady



stream of faculty colleagues, who routinely sought him out as a tutor, to brainstorm a problem, or at times just for wise advice. As an administrator, he could see around corners, with an uncanny ability to foresee and avert potential problems.

Self-promotion was not Mario's long suit. His overriding goal was to understand biological phenomena at a root level, not to seek honors, although honors came anyway. He was elected Fellow of the Biophysical Society and the American Association for the Advancement of Science and was both an honorary professor and an honorary doctorate recipient from the University of Buenos Aires, his Alma Mater. His teaching awards were well-deserved and especially meaningful. It's a long list.

Mario was our cherished colleague and friend. "He was our scientist's scientist – one of our deepest and broadest thinkers – and a thoughtful, warm and caring colleague, who always put people –

especially students –above all else," said Bertrand Garcia-Moreno, professor and former chair of the Department of Biophysics at the Krieger School of Arts and Sciences, and vice dean for natural sciences at Johns Hopkins. Speaking for all of us, Mario's long-time friend and colleague, Professor Eaton Lattman, put it succinctly: "it's hard to imagine our world without him."

*George D. Rose and Cynthia Wolberger*



**Macromolecular  
crystallography**  
with guest speakers from  
DLS, ORNL & SPring-8

**High energy  
experiments**  
with guest speakers  
from ESRF, STOE & APS

**WATCH HERE!**

## In Memoriam: Nadrian "Ned" Seeman



Professor Nadrian Seeman, New York University, NY, USA, passed away on November 16, 2021. He founded and developed the field of DNA nanotechnology. DNA nanotechnology involves the design and construction of

nanostructures from nucleic acids, i.e., DNA is used as a "building material" for nanostructures. The method relies on base pairing: The DNA used is designed in such a way that complementary base sequences bind together in specific places and connect DNA strands. Thus, the DNA selectively assembles to form the target nanostructures.

Seeman built, for example, nanocubes, nanotubes, polyhedra, two- and three-dimensional lattices, and other structures using DNA strands. The approach has also been used to build nanorobots and other machines, as well as knotted DNA molecules, and has applications in DNA computing.

Nadrian Charles "Ned" Seeman was born in Chicago, IL, USA, on December 16, 1945. He studied biochemistry at the University of Chicago and received his Ph.D. in biochemistry and X-ray crystallography from the University of Pittsburgh, PA, USA, in 1970. He was a Postdoctoral Fellow at Columbia University, New York, NY, USA, and the Massachusetts Institute of Technology (MIT), Cambridge, MA, USA. Seeman then joined the faculty at the State University of New York at Albany, USA, and in 1988, he became Professor of Chemistry at New York University.

Nadrian Seeman has received numerous awards, including the 1995 Feynman Prize in Nanotechnology, the 2010 Kavli Prize in Nanoscience, and the 2016 Benjamin Franklin Medal from the Franklin Institute. In 2017, he

was elected to the American Academy of Arts and Sciences. He also was a Fellow of the Royal Society of Chemistry and the American Association for the Advancement of Science and a Member of the Norwegian Academy of Science and Letters.

[ChemistryViews](#)

ACA History Website

### The Crystallographic Roots of DNA Nanotechnology

Nadrian C. Seeman  
2014

I was born in Chicago at the end of 1945 as an only child in a middle-class Jewish family. My father sold fur garments in Chicago (from 1953 in his own store), but after my birth my mother did not return to teaching until my grandmother died in 1963. In 1951, we moved to the suburb of Highland Park, where we remained until I went to college in 1962. I was a quiet child who preferred reading over sports, a characteristic that has persisted. Sputnik was launched in October, 1957; a year later, I became a "Sputnik Kid" who was brought daily to the high school in the early morning, where I took a special algebra class, before spending the rest of the day at my middle school. As a nocturnal person, I didn't do all that well, but I was set on a path of advanced math and science courses from then until the end of high school. A year earlier, my father had begun a campaign to convince me that I wanted to be a physician. The math and science that I liked were not incompatible with my father's goal, so he gave me no flack about them. At about the time I got to high school, I lost whatever faith I might have had, and I've been an atheist ever since.

[Read the full history>](#)

**In Memoriam: Farid R. Ahmed  
(1924-2021)**



After graduating in 1950 with a BSc Honours in mathematics from the University of Leeds, I wanted to continue my study for a PhD in mathematics. However, the Mathematics Dept. told me to see E. G. Cox, head of the Inorganic and Physical Chemistry

Dept. Cox introduced me to Durward W. J. Cruickshank. They explained that they would be interested in having me pursue a PhD degree in crystallography. Durward would be my supervisor, and the title of my thesis would be Development of Mathematical Methods for the Determination of Molecular Structures by X-ray Analysis. I agreed to give it a try.

The first year was spent learning about crystallography and Hollerith equipment (business punch-card machines in the UK) and their use for crystallographic calculations as described by Cox, Gross & Jeffrey (1949). Our use of the Ferranti Mark II electronic digital computer at the University of Manchester started soon after its installation in the summer of 1951. The article by Ahmed & Cruickshank (1953) gives some details of the computer and the crystallographic programs that we devised in that period. They were for the calculation of structure factors, differential syntheses with correction for finite summations as described by Booth, and for the estimation of errors according to Cruickshank. For maximum efficiency, those initial programs were space-group specific. However, sections of the programs could be altered easily to adapt them for other space groups.

The photograph of Durwood and me was taken in 1953 after the farewell party that the Chemistry Department held before my return to Egypt. For the next two years, I taught mathematics to



*Farid R. Ahmed, and Durward William John Cruickshank, U. of Leeds, UK, 1953*

engineering students at the University of Alexandria.

Before 1955, the University of Toronto installed a Ferranti Mark II computer just like the one we had used at Manchester. The X-ray diffraction group at the National Research Council of Canada (NRC) decided to use that computer for their crystallographic calculations. W. H. Barnes and David C. Phillips met

in Ottawa with Peter J. Wheatley, who was a crystallographer at the University of Leeds. They decided that crystallographic computing in Ottawa would benefit by bringing in someone with my experience and I received an offer to join the NRC as a postdoctorate fellow for one year. I accepted gladly because of my love for crystallography and computers. My wife Jean and I then immigrated to Canada in 1955.



*A Ferranti Model No. 1 computer of the 1950s installed at the U. of Manchester, UK*

The NRC crystallographers got permission to use the Ferranti computer at the U. of T. (FERUT) as much as they needed. At that time, crystallography in Canada was already well established at a few universities and government laboratories. They did powder diffraction and single-crystal analyses of organic and inorganic compounds as well as minerals and metal complexes. Their crystals had varied space groups. It was therefore essential to devise generalized crystallographic programs, which could handle all space groups, and economize on the calculations by taking full advantage of the space group symmetries, and the corresponding structure factor and electron-

density expressions, given in the International Tables for X-ray Crystallography (1952). To achieve that, the appropriate equations for the space groups were represented by a simple pseudo code, which directed a short interpretive routine to make the necessary changes to the main program. The article by Ahmed & Barnes (1958) gives some details of the NRC generalized crystallographic programs.



Co-authors of the NRC FORTRAN package of programs: (top left) William Howard Barnes, second Head of crystallography at the NRC (circa 1966); (top right) Sydney R. Hall (circa early 1970s); (bottom left) Carol P. Huber (photo taken in April 1997) and (bottom right) Margaret E. Pippy (photo taken July 29, 1988).

After FERUT was retired we used computers in Ottawa, starting with the IBM 650 then the IBM 1620, and in each case we used the symbolic codes of those computers. Finally in 1965 the NRC Computation Center installed an IBM 360. This time all our crystallographic programs were written in FORTRAN IV, by F. R. Ahmed, S. R. Hall, C. P. Huber & M. E. Pippy. That was the last rewrite of the NRC generalized crystallographic programs. These programs served us till about 1986. By that time our crystallography group became part of the NRC Institute of Biological Sciences, under the new name of Protein Crystallography Group. Our main research was now directed to the study of macromolecular structures. Computer programs for these studies were imported from other

laboratories. The program FRODO for computer graphics was in daily use by our group.

The programs that we wrote in machine or symbolic language lasted for an average of 3.3 years, while the FORTRAN programs lasted for 20 years. The FORTRAN package was also more versatile for distribution to other laboratories in Canada and abroad. The technical advances of the last half century including powerful X-ray beams, automatic data collection with diffractometers/area detectors, and computers with phenomenal speeds, have benefited most areas of crystallography. I consider myself lucky to have witnessed these interesting developments.

I am grateful to Lachlan M. D. Cranswick for inviting me to write this article, and for his help with the Figures.

*Farid R. Ahmed*

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This article appeared in a Crystallography in Canada edition of the [IUCr Newsletter, 2009, Volume 17, Number 4.](#)

### In Memoriam: Donald E. Sands



Donald E. Sands, chemistry professor at the University of Kentucky for 37 years, died on September 22, 2021 at the age of 92. During his final months he amused himself, as he had all his life, by solving difficult puzzles of all types. Upon

waking up in the morning he converted the time to a digital number and mentally factored it into its primes.

Don was born in Leominster, MA, did his undergraduate work at nearby Worcester Polytechnic Institute, and completed a Ph.D. at Cornell in 1955 under the direction of J. Lynn Hoard. One of Don's papers with Hoard, "The Structure of Tetragonal Boron", became a classic; a few months later Linus Pauling [wrote to Hoard](#) saying: I have just been reading, for the second time, your paper on tetragonal boron and I am writing primarily to tell you my opinion of it. I think that it is one of the best crystal-structure determinations that has ever been made. Also, I am pleased with the excellent writing in this paper. Too often scientific papers are written in a discouragingly dull way.

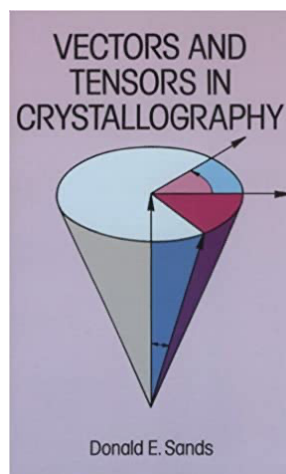
Don's first professional position was as a Senior Chemist at Lawrence Livermore. After having worked on the structures of boron allotropes in graduate school he studied inorganic borides and beryllides at the California lab. While his work was primarily scientific and led to 20 publications, the Lawrence lab at that time had strong interests in nuclear-weapons research. Expectations that Don participate eventually led him to look for a position elsewhere.

Don joined the University of Kentucky as an Assistant Professor in 1962; he was a full professor by 1968. In Lexington he did not at first have

access to good equipment but eventually there was a working lab with students and publications. One of his early papers, on the structure of the disordered monoclinic polymorph of sulfur (1965), is well known still because the solid-state orthorhombic-monoclinic phase transition of sulfur is so often discussed in undergraduate physical chemistry courses. Also noteworthy is his 1965 paper with undergraduate Victor Day on one of the low-temperature phases of cyclooctane.

Among his colleagues in the Chemistry Department Don became known as the guru of Physical Chemistry. He worked the problems in textbooks for relaxation and could (unlike the rest of us) solve them all – and make doing so look simple. His students admired him for his orderly lectures and fair exams, his dry wit, and his concern for their welfare. Don's interest in teaching led to a very successful book, *Introduction to Crystallography*, (1969; 1993; Spanish edition in 1974).

Don also enjoyed, and was very good at, more formal mathematics. His first paper in that area, "Transformations of Variance-Covariance Tensors" was published in 1966; eventually there was a book (*The Vectors and Tensors of Crystallography*, 1982) that became a classic. Reprinted in 1995, it is now available as a free pdf download. Don also wrote an article ("Distances, Angles, and their Standard Uncertainties") for *The International Tables for Crystallography* (1993 through the current 2010 edition).



Being smart, thoughtful, witty, and good with both numbers and words, Don's eventual move into university administration was a near certainty. Over the years he served as Department Chair, Associate Dean, Acting Dean (on three separate occasions), and Vice Chancellor

for Academic Affairs. He spent two years at the National Science Foundation as Section Head of the Division of Teacher Preparation and Enhancement.

*International Tables for Crystallography* (2010). Vol. B, Section 3.1.1, p. 404.

### 3.1. Distances, angles, and their standard uncertainties

By D. E. SANDS

Don retired formally in 1999 and so had more time to play chess, to enjoy museums and the arts, and to spend time with his granddaughters, but he also remained active in a variety of projects. One of those was teaching physical chemistry to a young inmate of the federal prison in Lexington. That student later graduated from UK, earned a Ph.D. elsewhere, and is now employed as a chemist. Don also took on more formal roles, such as Acting Director of the University of Kentucky Art Museum in 2001, and Board Member and then Chair (1999) of the Central Kentucky Civil Liberties Union (ACLU – KY). The latter group honored Don with its Thomas L. Hogan Award in November 2015. Back in the years when various forms of discrimination were acceptable to many they were never acceptable to Don.

Don was a central, if quiet, presence at the University of Kentucky and around Lexington for nearly sixty years. His influence has been perhaps mostly strongly felt in how things are done, or at least how we think they ought to be done. He could take strong, principled positions (as Dean he was known to ask professors who had canceled class when they were going to make up the time students had paid for) but he always listened, always considered all the circumstances, and often leavened his opinions with humor.

Don was a wonderful mentor for many, including the greenhorn assistant professor that I was.

Carolyn P. Brock

## In Memoriam: John Westbrook



John D. Westbrook Jr. (1957-2021), Research Professor at Rutgers University and Data & Software Architect Lead for the RCSB PDB, passed away on October 18, 2021.

He was incredibly beloved and respected by his colleagues at Rutgers and throughout the world, known for his dry wit and endless enthusiasm for thinking about all aspects of data and data management.

John had a long and highly successful career developing ontologies, tools, and infrastructure in data acquisition, validation, standardization, and mining in the structural biology and life science domains. His work established the PDBx/mmCIF data dictionary and format as the foundation of the modern Protein Data Bank (PDB) archive ([wwPDB.org](http://wwPDB.org)).

More than twenty-five years ago, while still a graduate student, John recognized the importance of a well-defined data model for ensuring delivery of high quality and reliable structural information to data users. He was the principal architect of the mmCIF data representation for biological macromolecular data. Based on a simple, context-free grammar (without column width constraints), data are presented in either key-value or tabular form. All relationships between common data items (e.g., atom and residue identifiers) are explicitly documented within the PDBx Exchange Dictionary ([mmcif.wwpdb.org](http://mmcif.wwpdb.org)). Use of the PDBx/mmCIF format enables software applications to evaluate and validate referential integrity within any PDB entry. A key strength of the mmCIF technology is the extensibility afforded by its rich collection of software-accessible metadata.

The current PDBx/mmCIF dictionary contains more than 6,200 definitions relating to experiments involved in macromolecular structure determination and descriptions of the structures themselves. The first implementation of this schema was used for the Nucleic Acid Database, a data resource of nucleic acid-containing X-ray crystallographic structures. Today, this dictionary underpins all data management of the PDB. Since 2014, it has served as the Master Format for the PDB archive. It also forms the basis of the Chemical Component Dictionary ([wwpdb.org/data/ccd](http://wwpdb.org/data/ccd)), which is used to maintain and distribute small molecule chemical reference data in the PDB.

In 2011, the Worldwide Protein Data Bank (wwPDB) PDBx/mmCIF Working Group was established to enable direct use of PDBx/mmCIF format files within major macromolecular crystallography software tools and to provide recommendations on format extensions required for deposition of larger macromolecule structures to the PDB. This was a key step in the evolution of the PDB archive, which enabled studies of macromolecular machines, such as the ribosome, as single PDB structures (instead of split entries with atomic coordinates distributed among different entry files). In 2019, mandatory submission of PDBx/mmCIF format files for deposition was announced (Adams et al. *Acta Crystallographica* D75, 451-454).



To ensure the success of the PDBx/mmCIF dictionary and format, John worked with a wide range of community experts to extend the framework to encompass descriptions of macromolecular X-ray crystallographic experiments, 3D cryo-electron microscopy experiments, NMR spectroscopy

experiments, protein and nucleic acid structural features, diffraction image data, and protein production and crystallization protocols. Most recently, these efforts have been focused on developing compatible data representations for X-ray free electron (XFEL) methods, and for integrative or hybrid methods (I/HM). I/HM structures, currently stored in the prototype PDB-Dev archive ([pdb-dev.wwpdb.org](http://pdb-dev.wwpdb.org)), presented new challenges for data exchange among rapidly evolving and heterogeneous experimental repositories. Proper management of I/HM structures in PDB-Dev also required extension of the PDBx/mmCIF data dictionary to include coarse-grained or multiscale models, which will be essential for studying macromolecular structures in situ using cryo-electron tomography and other bioimaging methods.

John contributed broadly to community data standards enabling interoperability and data integration within the biology and structural biology domains. His efforts have included (i) describing the increasing molecular complexity of macromolecular structure data, (ii) representing new experimental methodologies, including I/M techniques, and (iii) expanding the biological context required to facilitate broader integration with a spectrum of biomedical resources. John's work has been central to connecting crystallographic and related structural data for biological macromolecules to key resources across scientific disciplines. His efforts have been described in more than 120 peer-reviewed publications, one of which has been cited more than 21,000 times according to the Web of Science (Berman et al. *Nucleic Acids Research* 28, 235-242). Eight of his most influential published papers have appeared in the *International Tables of Crystallography*.

John has also done yeoman service to the crystallographic community over many years and was recognized with the inaugural Biocuration Career Award from the International Society for Biocuration in 2016.

For the International Union of Crystallography, John served on the Commission for Maintenance of CIF Standard (COMCIFS), the Working Group on Data Diffraction Deposition (DDDWG), and the Committee on Data (CommDat). He also served as an Associate Editor for *Acta Crystallographica* Section F.

John was a long-standing member of the American Crystallographic Association, and served on the Data, Standards & Computing Committee. He also served on the Metadata Interest Group for the Research Data Alliance.

John is survived by his wife, Bonnie J. Wagner-Westbrook, Ed.D. and his devoted Mother-in-Law, Joan N. Wagner of Clinton Twp., NJ; many cousins including Chandler Turner (of Portsmouth, VA), Ann (Turner) Heyes (of Tasmania, Australia) and Louise (Turner) Brown (of Oakland CA).

Memorials can be made to Capicats (<http://www.capiccats.com/>) or an organization of choice in his honor.



*John Westbrook at the 2017 Congress and General Assembly of the International Union of Crystallography in Hyderabad, India*

## REMEMBERING CARLOS A. MURILLO



*Carlos A. Murillo*

*Larry Falvello, Lee M. Daniels, Xiaoping Wang, Bruce Foxman, Joseph Reibenspies*

*December, 2021*

### Larry Falvello

We present here remembrances of Carlos Murillo, who died on November 6, 2021.

The youngest of nine siblings, Carlos was born near San José, Costa Rica. With a deep-rooted scientific curiosity, he studied chemistry at the University of Costa Rica as an undergraduate (“Bachiller,” 1973) and at Texas A&M as a graduate student, obtaining his Ph.D. in 1976 under the direction of Al Cotton. Following a post-doctoral stay with Malcolm Chisholm at Princeton (1976-1977), he joined the chemistry faculty at the University of Costa Rica, rising to Professor by 1986. At UCR Carlos was also Associate Dean for Postgraduate Studies.

Through the 1980’s Carlos maintained a collaborative link with Al Cotton’s group (by then formally known as the Laboratory for Molecular Structure and Bonding, LMSB), visiting often for short or long stays. Carlos possessed uncanny skill as a hands-on synthetic chemist, which made him a go-to person for difficult syntheses.

In the 1990’s Carlos moved to Texas A&M on a long-term basis. He took on teaching duties and also assumed more of a leadership role at LMSB, becoming Executive Director. During these years he also participated as co-author -- with Cotton, Geoffrey Wilkinson and Manfred Bochmann -- of



the Sixth Edition of Advanced Inorganic Chemistry.

From the beginning of his research career as a student in the 1970's, Carlos was closely familiar with crystal structure analysis, which was often the first line of characterization for the products of his synthetic wizardry.

With the untimely death of Al Cotton in 2007, the LMSB was wound down and Carlos moved to the National Science Foundation. There he would become Director of the Chemistry Research Instrumentation and Facilities Program. That role brought Carlos more contact with members of the crystallographic community.

Carlos possessed a rare combination of strong will and respectful mild manners. He was devoted to family, steadfast in his friendships, and meticulous and exacting at work. In his varied professional roles -- hands-on bench chemist, professor, teacher & research leader, textbook author, and science administrator, he earned the respect of those who worked with him and of those whose work or studies brought them into contact with him. It is hoped that the following remembrances by people who knew Carlos will convey more details of his exceptional professional and personal character.

### **Bruce Foxman**

I received my Ph. D. under the supervision of Professor F. Albert Cotton at MIT during the 1960's. I knew most of the group who got their degrees before me, and carefully kept track of the research done by Al's group - and as many of the students as I could - after Al moved to Texas A&M. One day over 30 years ago, I received a phone call from Al, who asked me if I knew his excellent colleague, Carlos Murillo. I explained that of course I knew his work well, but we had never met. "Well," Al said, "... he'll be at a meeting in Boston in two weeks, and will arrive the weekend before: you should arrange to pick him up and show him around ... you'll become the best of friends ... I HAVE NO DOUBT!" I agreed

to host his visit, and Al was of course correct. Our weekend together was the beginning of a glorious and close friendship. I have been tickled pink to think of it as an "arranged friendship" that never faltered, and grew stronger every day.

After the initial meeting Carlos and I kept in close contact in person, and by phone & email. He immediately referred to me as El Zorro (The Fox), and I always signed our correspondence as "Z". When he became the MRI Program Director at NSF, I was regularly invited to be a panel member, and was always impressed with the manner in which the panels were run, with the highest senses of integrity, fairness, and clarity. Junior investigators at a number of institutions remarked to me that Carlos provided advice that was extremely beneficial, and led to a successful outcome for their proposals. I smile when I think of one dinner we had after a panel, where I had a dizzy spell after the meal. Carlos helped me get back to the hotel, and later always referred to this event as "I had to wheel Zorro back to his hotel in a grocery cart." This "shopping experience" usually came up in our phone calls every few months thereafter!

After Al was brutally attacked in 2006, Carlos' wonderful wife Debbie led a team that included Carlos, Larry Falvello and myself; we served as co-editors and helped to complete Al's autobiography [1], which had remained unfinished owing to his untimely passing. I found that project to be an uplifting experience, and was very grateful to Debbie, Carlos and Larry for including me. Carlos, Larry and I also wrote a paper on the 50th anniversary of the quadruple bond that served as a remembrance of the great work that Al and his co-workers carried out [2]. I fondly remember and miss Carlos' scientific brilliance, integrity, warmth, sense of humor and good judgement. He was a great pal, and a unique, lovable individual.

### **Lee M. Daniels**

I met Carlos when I was a grad student at Texas

A&M, but didn't really get to know him until several years later when I returned to A&M to support the crystallographic work in Al Cotton's research group (empire?). Shortly after the start of my 11-year stay there, Carlos arrived. His presence immediately influenced the quality and quantity of work produced by the group.

Carlos was the master of organometallic synthesis. (From which I was a drop-out!) So I trusted him with the wet lab work, and he trusted me with the crystallography. While I could only marvel at his synthetic skills, his crystallographic intuition kept my enthusiasm in check when an interesting new structure was in question. I have records of over 200 papers on which we were both authors (and all but a handful of those with F. A. Cotton). Nearly every one of those involved Carlos providing a selection of beautiful crystals, then following each step of the process with intense curiosity. In those days, the process could take 2 or 3 weeks.

While I supported the crystallographic work of a decade of grad students moving through the Cotton labs, Carlos not only mentored them in synthetic methods but committed himself to ensuring that each of them upheld the high standards of scientific rigor, proof, and documentation expected in that stimulating environment. Each of these former students are part of Carlos' legacy. When Al passed away unexpectedly, Carlos gathered the PhD candidates and ensured that they completed their work and received their degrees.



Carlos was instrumental in the creation of the [F.A. Cotton Medal](#), an annual ACS honor awarded to recognize excellence in chemical research. He alone was responsible for the design of the actual

medal and coordinated the establishment of the award along with the ACS Texas A&M University Section.

Even after leaving the lab for his NSF position, Carlos continued to collaborate and publish. One of my favorites is his 2015 paper "The  $\delta$  Bond and Trigonal Paddlewheels before the Dawn of the Quintuple Bond" - *Comments on Inorganic Chemistry*, 35: 1–20, 2015 (DOI: 10.1080/02603594.2014.1002033).

Despite his declining health, Carlos agreed to present at the 2021 ACA meeting last August. His talk at the "Economics of Crystallography" session, titled "Diffraction in the Context of the National Science Foundation," provided us the latest information on what's important to do (and to avoid!) when seeking funding. Many of us benefited from his assistance when seeking support from the NSF, and we'll continue to feel his influence.

While Carlos was direct and demanding in his work, he did not let that overshadow his love of people and his sense of humor. He was open and honest with his colleagues, always willing to provide support and counsel when asked, and to ask for help when needed. I cherish the memories of making discoveries with him, but more so the laughs and experiences.

### Xiaoping Wang

Carlos was a wonderful mentor, colleague, and friend. I first met Carlos when I was a graduate student in 1993. Since the discovery of the first metal-metal multiple bonds by F. A. Cotton in 1964, progress in the related chemistry for the early 3d transition metals has been slow. Carlos made a breakthrough in 1992, soon after his return to Texas A&M as the director of LMSB. He synthesized the first dinuclear vanadium(II) paddlewheel compound  $V_2\{(p\text{-tol})NC(H)N(p\text{-tol})\}_4$ , with the divanadium unit held together by a  $\sigma^2\pi^4$  triple bond between the two vanadium atoms. Al once told me that 'Carlos has magic hands. You can learn from him how to make new compounds no others could'. As the director of the Laboratory for Molecular Structure and Bonding at A&M, Carlos had trained many graduate students and

postdocs in the Cotton group. He was always available to help whenever I had questions developing strategies for sample preparations or growing single crystals.

Carlos was a strong advocate for crystallography throughout his career. He had witnessed the development of X-ray crystallography since the seventies when diffractometers were slow and scarce, and crystallographic studies were far from being routine. Nowadays, a crystal structure can be determined in only a few hours or even seconds. However, in his eyes, the importance of crystallography to the advance of scientific knowledge had never diminished. As a program manager at NSF, he was very supportive in developing new techniques and capabilities for research and providing help to underrepresented universities and colleges in their grant applications for research instrumentation.

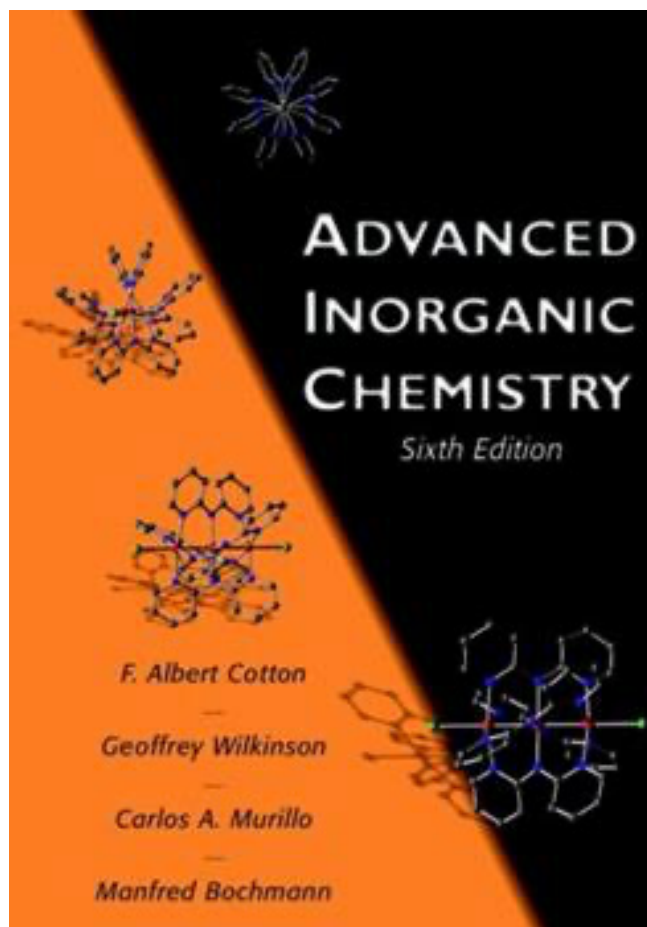
I saw Carlos the last time at his talk in the 2021 ACA virtual meeting in August (See picture below). His charming smile will be sorely missed by all of us.



### Joseph Reibenspies

Carlos was a great friend to Crystallography and the Structural Sciences. His work has enhanced all of our lives. He has given us the garden to make our scientific seeds bloom. The gardens that Carlos left us are thriving, and now others must take his work and keep them alive, healthy and flourishing. We all must continue to do the hard work to feed, water and hoe the gardens so that we may someday, walk the forest, fields and flowers and find a place where we too can rest. Rest in peace my friend and know your work is good.

1. Cotton, F. A. *My Life in Chemistry : More Fun Than Fun*; Falvello, L. R.; Foxman, B. M., Murillo, C. A.; Murillo, D., Assoc. Eds.; Elsevier, Waltham, MA, 2014.
2. Falvello, L. R.; Foxman, B. M.; Murillo, C. A. *Inorg. Chem.* 2014, 53, 9441–9456.



## In Memoriam: Jack D. Dunitz



*In the group coffee room during the spring of 1981.*

A few weeks ago I needed to reread one of Jack Dunitz's major articles from the 1980s and was struck all over again by his greatness. He was gifted at mathematics, a master with words, and interested in anything new or intriguing. He had a nearly perfect memory. He knew a great deal about literature, art, music, *etc.* and would come up with appropriate quotes in their original languages. Still, he did not take himself too seriously, and he was kind and generous, especially with his time. He treated all with respect and was especially good with students presenting their work in talks or poster sessions. He always asked good questions.

Writing about such a giant is daunting; any piece is guaranteed to be incomplete. Since others have attempted to summarize his scientific impact I will only describe what it was like to work in his lab. In 1979, after difficult journeys to tenure, my husband and I were planning sabbaticals. In the end we decided on a year apart; during 1980-81 he was in Oxford and I was in Jack's lab at the ETH.

It was a wonderful year. The lab had good equipment and two expert assistants – Paul Seiler for data collection and Bernd Schweizer for computing. The diffractometer and cameras

were in the basement but the offices and labs were five and six floors above ground. Jack's office on H and the group coffee room on I were at the SW corner of the building, which was on a hill overlooking the city. Those rooms featured glass windows all along two sides that gave spectacular views of central Zurich, the lake, the hills, and, on good days, the mountains.

The lab ran on the American model – it started later in the morning than the Hauswirtin of my apartment building thought proper. There was lots of freedom; the emphasis was on originality and results rather than on time spent. Ski outings in the middle of the week were fine as long as they were only occasional.

The atmosphere could be intense, if only because we were in the presence of such an exceptional mind. After departmental seminars, at which attendance was expected, Jack would ask, because he really wanted to know, what we thought and what we had learned. At the informal group coffee after lunch the subject could be chemistry, computers, philosophy of science, linguistics, current events, or whatever. On Mondays we visitors were often asked what interesting things we had done over the weekend because Jack was curious and because he wanted us to enjoy Switzerland. He particularly liked its well-marked walking paths and hiking trails.

Working on a paper with Jack was a major undertaking because he wanted to get it just right and because word processors hadn't yet been invented. Having come from a department that valued "efficiency" I once asked him how he could justify spending so much time on a manuscript. He replied simply that he did it to please himself.

Jack could be sage and pithy; his advice that all bad experiences should be assessed for their story potential has proved particularly useful. He could also be quite funny, especially when annoyed. In 1980 *JACS* rejected his submission, with Doyle Britton, of a paper on an application of the structure-

correlation method that Jack had developed with Hans-Beat Bürgi. The stated reason for rejection was the absence of new data; Jack replied with a "review" of Mendeleev's supposed report of the periodic table (see Figure). *JACS* reconsidered; the paper with Doyle was published in 1981. Just recently a Google search for "Jack Dunitz Mendeleev" revealed that chemist and historian Jeffrey Seeman had found the "review" in Roald Hoffmann's files and had written an essay about it that appeared in the 2019 volume of *Helvetica Chimica Acta*.

It is impossible to think about Jack without also thinking of his wife Barbara, who was concerned about us all and who produced memorable dinner parties.

It was my great good fortune to collaborate with Jack for another dozen or so years and to be in contact with him for four decades. In later years

he often talked about how lucky he had been to be a professor during a time in which he could pursue ideas that interested him without having to think much about their potential economic or social benefits (see his 2013 essay in *Helvetica* titled *La Primavera*). He also talked about the history of crystallography and how as a graduate student, and maybe later too, he knew the details of every structure that had ever been published.

Jack influenced science and scientists for ca. 70 years. Even at 98 he was well and interesting (see the 2021 YouTube interview with the *JACS* Editor-in-Chief Erick Carreira). It is wonderful that Jack was with us for so long and that he left us while still on top of his game.

Carol Brock

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COMMENTS OF REFEREE \_\_\_\_\_ I \_\_\_\_\_

AUTHOR: MENDELEEV

TITLE: Periodic System ...

Would the article be suitable for publication:

1. without change? no 2. after minor revision? no 3. after major revision? maybe

Is *JACS* the best medium for publishing this article? no If not, what other Journal would you suggest? Analyt. Chem. Please be as specific as possible if revision by the author is recommended. Indicate specifically whether descriptions of method, tables of data, etc. should be reduced or eliminated with the understanding that they would be available to the specialist in the form of microfilm or in some other way. Does the nomenclature used conform with accepted practice as exemplified by Chemical Abstracts and the recommendations of the Committee on Nomenclature, Punctuation and Spelling of the Society? Are hazardous procedures clearly identified as such?

COMMENTS:

The paper by Mendeleev examines atomic weights to suggest possible speculations about missing elements. While the paper presents an interesting review of existing data, I see little definitiveness in the conclusions. Essentially the paper is a review and the main result is a cataloging of atomic weights with a few inferences about missing elements. Correlations among chemical properties of elements are proposed but not backed up by statistical significance tests, so it is not clear to what extent the correlations are due to chance and to what extent to selection of data. The assertion that the atomic weight of tellurium must lie between 123 and 126 has no basis.

While the paper is interesting to atomic weight specialists and warrants publication I feel *JACS* is not the proper medium. I see little significance to the conclusions. I suggest eliminating the Table, which is merely a rearrangement of already known data.

The "review" of Mendeleev's "report" of the periodic table as scanned from a copy given by JDD to CPB. In that copy the right edge of the text was truncated slightly.

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# ACA HISTORY

AMERICAN CRYSTALLOGRAPHIC ASSOCIATION



## ACA:SSS History Project Update



Virginia Pett

### 2021 ACA Annual Meeting

Two excellent lectures from the Annual Meeting are now online at ACA History.



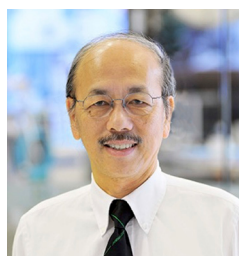
Jacqueline M. Cole

[Jacqueline M. Cole](#), Head of the Molecular Engineering group in the Cavendish Laboratory at the University of Cambridge, is the recipient of the 2021 B. E. Warren Diffraction Physics Award. This award “recognize[s] an important recent contribution

to the physics of solids or liquids using X-ray, neutron or electron diffraction techniques.”

In her lecture, “[Molecular Engineering of Single-Crystal Optical Actuators](#)” Cole described her experimental work with a solid-state light-induced molecular switch that she engineered to have optical tunability. She investigated the photolysis of ruthenium complexes with an SO<sub>2</sub> ligand. She was able to match the observed the metal-to-ligand charge transfer spectrum over time with the changes in structure to deduce the mechanism of conversion. An amazing piece of work.

[Wah Chiu](#), the Wallenberg-Bienenstock Professor at Stanford University and SLAC National Accelerator Laboratory, is the recipient of the 2021 M. J. Buerger Award which “recognize[s] mature scientists who have made contributions of exceptional distinction in areas of interest to the ACA.”



Wah Chiu

Chiu’s lecture, “[CryoEM Structures of Macromolecules](#)” provided a fascinating overview of the tremendous advances in electron microscopy; many of these advances were powered by his own work. There

are now more than 4,000 structures between 1-4 Å now deposited. In 2020 more structures of molecular complexes were determined by electron microscopy than by X-ray diffraction, a significant turnabout just since 2014. Advanced data processing can even be used to distinguish structural variations in membrane ion channels and RNA. Applications of cryoEM range from single particles to entire cells!

### PDB50



The Protein Data Bank celebrated its 50th anniversary in 2021 with more than 170,000 molecular structures available online. Here is a [video](#) for general audiences describing the history

of the PDB as well as the scientific techniques (X-ray crystallography, NMR, 3D electron microscopy) that enable us to visualize proteins and DNA in three dimensions. This video is a good introduction for students and non-scientists who want to understand why this database is such a valuable resource for structural biology — the PDB makes available crucial information for therapeutics and vaccines.

See also [journal collections and articles](#) celebrating the 50th anniversary with highlights from the past and a preview of the future in structural biology. Scroll down on [this page](#) to see other available materials with a structural theme like playing cards designed by David Goodsell. You can download the intriguing PDB50 game created by Brian Hudson or play the game online with friends.



Stephen K. Burley

The 2021 Transactions sessions, “Function Follows Form: Celebrating the 50th Anniversary of the Protein Data Bank” were outstanding, as you know if you attended the meeting (virtually). One of the speakers, Stephen K. Burley, Director of the RCSB PDB, published an article “[Impact of structural biologists and the Protein Data Bank on small-molecule drug discovery and development.](#)” He presented three examples showing how PDB structures were crucial in development of antineoplastic drugs.

Volume 296 of Journal of Biological Chemistry, where Burley’s article appeared, was a special issue with many other great articles celebrating the PDB. See “[How the Protein Data Bank](#)

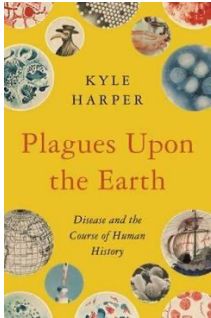
[changed biology](#): An introduction to the JBC Reviews thematic series, part 1” by Helen M. Berman and Lila M. Gierasch for a description of the other articles. To give just one example, there is an article by Peter B. Moore, “[The PDB and the Ribosome.](#)” The full text articles are freely available and could be very useful in teaching; simply click on the footnote reference number to read each contribution.

See other recent articles describing the [Impact of Structural Science](#) on science in general and upon society on the Impact page of ACA History online.

If you have suggestions for other articles to be featured on the Impact page, contact [Virginia Pett](#).



## Book Review: *Plagues Upon the Earth: Disease and the Course of Human History*



**By Kyle Harper**  
**ISBN: 9780691192123**

Kyle Harper's *Plagues Upon the Earth: Disease and the Course of Human History*

is longer than your average read these days, clocking in at 509 pages not including the nearly 200 pages of appendices and indexes. But it's not as long as you might expect, given the title and the subject matter--in fact, it might almost seem rather short. Despite the book's length and density--both literal and figurative--*Plagues Upon the Earth* is a solid read for anyone looking to take a dive into the history of humanity and its diseases.

Harper assumes a rather daunting task as he sets out to document and describe the dual histories of humanity and the infectious diseases humans are susceptible to. It is a tricky duality to balance between "microorganisms" and "macrohistory," but Harper does an excellent job, never veering too deeply into the historical context or the microbiological sciences. He interweaves the two narratives quite seamlessly, making it evident that as impactful as plagues have been on human history, the course of human history has in many ways dictated or influenced the nature and effectiveness of its plagues.

*Plagues of the Earth* begins with a brief introduction in which Harper dictates his strategy for leading the reader through the intertwined histories of humanity and its diseases. He provides critical contextual information, such as the meaning of the "paradox of progress," which he revisits repeatedly throughout the book. He also provides a historical roadmap for the history of globalization in the context of the evolution of infectious diseases,

breaking it into six separate periods: prehistoric globalization, Iron Age globalization, peak Old-World globalization, the Columbian Exchange, fossil-energy transport, and the age of jet plane travel.

Harper uses this roadmap of periods of human globalization, and subsequent microbial globalization, to break *Plagues of the Earth* into four parts based on the predominant change in human culture that happened in the given historical period it covers. Each part has three sizable chapters presenting information in predominantly chronological order--like any engaging historical writer, Harper injects critical context where needed without bogging down the narrative.

Part I, *Fire*, starts at the very beginning, both in terms of human history and in terms of any reader's general understanding of human diseases. Harper answers some fundamental questions like "What is a parasite?" and "What is a pathogen?" Before digging too deeply into the different diseases that have plagued humanity, and some that continue too, Harper lays as firm a foundation as he can, explaining that the pathogens that negatively impact humans fall into five evolutionary groups, or taxa: viruses, bacteria, protozoa, helminths (worms), and fungi. From the start, Harper reaffirms his motivations, informing the reader that due to their limited impact on the course of human history, and by corollary the limited impact of human history on the spread of fungal diseases, fungi will largely be left by the wayside---except, as Harper notes, in their capacity to infect plants, which has had dire consequences for human agriculture (think: Irish potato famine). If you are only here for the fungi, skip to Chapter 11.

Part II, *Farms*, describes the impact of the shift from a hunter-gatherer society to a predominantly agricultural one in conjunction with its impact on increasing potential vectors for the spread of human diseases. One disease readers might recognize from more recent history, tuberculosis, also known as consumption, makes an appearance. This

respiratory bacterial infection has been plaguing humans for thousands of years--and still does today, with over 10 million people contracting it annually and 1.5 million succumbing to it.

Part III, *Frontiers*, covers the periods of global expansion and colonization of the last 600 or so years. In it, Harper carefully teases apart the highly contested “virgin-soil” hypothesis, a theory popularized by Jared Diamond’s *Guns, Germs, and Steel*. The idea of European immunological superiority triumphing over indigenous populations is, as Harper makes quite clear, critically and evidently fraught in describing the demographic disaster that defined the era of exploration.

Part IV, *Fossils*, brings us into the modern age, with the advent of fossil fuel usage spurring the Industrial Revolution and all the technological advancements that have followed. As always, the paradox of progress has been a separate plague on humanity--the idea that advancements which bring our society and culture forward ultimately weaken its defenses against pathogens that literally spread overnight. Four hundred years ago, the fastest anyone could cross land was by horse. Disease spread was limited by the speed with which its human and animal vectors could traverse great distances. Now, global jet plane networks enable the spread of pathogens from continent to continent in a matter of hours.

You might be sick and tired of reading about human-borne diseases in this time of ongoing global pandemic and I wouldn’t blame you for thinking *Plagues Upon the Earth* is worth passing on. Unlike most books of its kind published in the last year or so that capitalize on the renewed popular fascination with pathogens spurred by the current coronavirus pandemic, *Plagues Upon the Earth* doesn’t end with some contrite conclusion designed to make you feel better about a world that seems to be falling apart at the seams. But given its narrative context, *Plagues Upon the Earth* is almost, even the teensiest bit comforting. Pandemics like COVID-19 are nothing new in the

greater context of human history.

Harper makes clear that for as long as there have been humans, there have been bacterial, viral, and parasitic diseases that prey on evolutionary vulnerabilities in our species. Some of our earliest pre-human ancestors had parasitic worms (and some of us still do); the “so-called Middle Ages,” as Harper puts it, had Black Death (bubonic plague); some of our grandparents and great-grandparents and great-great grandparents had the H1N1 influenza A virus; and we have severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2). Although every pandemic is new and terrifying in its own way, the similarities across the ages can be oddly comforting--or of course, completely disconcerting.

*Jeanette S. Ferrara, MFA*

## Review: *Our Oldest Companions: The Story of the First Dogs*



**By Pat Shipman**  
**ISBN: 9780674971936**

Pat Shipman’s *Our Oldest Companions: The Story of the First Dogs* is a delightful pre-or-post-holiday read that

digs into the history of the earliest relationships between humans and dogs. Shipman, an anthropologist by training, works to unravel a fairly convoluted evolutionary narrative that has been problematically oversimplified for centuries.

She acknowledges the predominantly Eurocentric influences on the generally accepted understanding of how our canine companions came to be “domesticated,” and sets out to break that down, starting with the issue of the word “domesticated.” Shipman declares in the preface that she does not like the word because it is used both too broadly and too narrowly which results

in an inaccurate general understanding of what the term truly means. “There is also a widespread assumption that domestication benefited humans but not the other species that were our partners in this endeavor--and that belief is wrong, too,” she claims.

Shipman cites the zebra as an example of an animal that was targeted for domestication--and given the domestication of the horse and the donkey, one might suspect successfully--which was in fact a failure. Despite photographic evidence of zebras leading carriages or with saddles, the historical record shows that they regularly rebelled--kicking any vehicle of transport attached to them to pieces, bucking under a saddle, and biting their so-called domesticators with great frequency. Dogs, like any animals that have been domesticated, have made an active choice to cooperate in the process with their human partners, Shipman explains. It is with this logical assumption in hand that Shipman digs in.

She starts with a chapter titled “Before Dogs,” where she delves into the most well-known ancestor of the modern dog--the wolf. The main point Shipman hammers home is that wolves are not dogs, and vice versa. There are distinct biological and behavioral differences, and the oversimplified narrative that modern dogs are simply descendants of domesticated wolves is one Shipman works to replace with a more reasonable and well-explained theory of modern dog domestication in the following chapters.

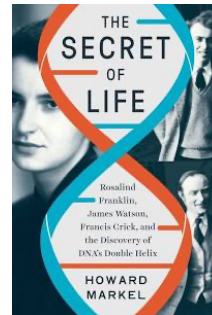
The next few chapters have question-based titles: “Why a Dog? And Why a Human?”, “What is Dogginess?”, “One Place or Two?”, “What is Domestication?”, and “Where Did the First Dog Come From?” In each of these chapters, Shipman concisely and concretely answers the titular question, laying the groundwork for the foundational knowledge the reader will need to better understand future chapters as they dive even deeper into the development of the relationship between humans and dogs. You’ll

have to pick up the book to find out the true history of the domesticated dog for yourself.

Our Oldest Companions is decidedly well-written and engaging. Shipman does an excellent job writing such that any reader with little or no prior knowledge or understanding of the subject or any related subjects should be able to easily comprehend her work. Whether you are a dog-lover or a casual anthropology enthusiast, Our Oldest Companions is sure to be a pleasant read.

*Jeanette S. Ferrara, MFA*

### **Review: The Secret of Life: Rosalind Franklin, James Watson, Francis Crick, and the Discovery of DNA’s Double Helix**



**By Howard Markel  
ISBN: 9781324002239**

The first thing you might notice upon picking up Howard Markel’s latest book, *The Secret of Life: Rosalind Franklin, James Watson, Francis Crick, and the Discovery of DNA’s Double Helix* is that he gives Rosalind Franklin top billing--even though she infamously was not included as a winner of the Nobel Prize for the discovery of DNA’s double helical structure. The second thing you might notice is that Maurice Wilkins--Franklin’s colleague at King’s College London--receives no billing at all, despite sharing the aforementioned 1962 Nobel Prize in Physiology and Medicine with James Watson and Francis Crick. Both of these critical decisions convey a great deal about the tone with which Markel approaches the convoluted and complicated academic history behind one of the most critical scientific discoveries of the 21st century.

Markel’s book reads like a detailed, fleshed out script for a documentary mini-series on the

discovery of DNA's double helical structure. He leans into this screenplay metaphor, titling the first chapter of the prologue "Opening Credits" and the final chapter "Closing Credits." He begins by setting the scene for discovery of the DNA double helix back in 1953, in a passage that seems to play a sort of homage to Watson's claims about the moment as he expressed them in his wildly problematic and wholly inaccurate 1968 memoir *The Double Helix*. But Markel immediately takes a step back, making it clear this is not some kind of Watson homage sequel to *The Double Helix*, but in fact a deconstruction of its false truths. Of Watson's supposedly truthful narrative about the discovery of DNA's double helix and how it all played out, Markel makes a strong claim: "it never happened."

This three-word sentence really establishes Markel's thesis, if none of the other editorial choices gave a clear enough hint. He's taking *The Double Helix* and pulling it apart, debunking all of Watson's inaccuracies, self-aggrandizements, unflattering and questionable portraits, and overall devil-may-care approach to the truth of the narrative. Many of the chapters begin with an excerpt from *The Double Helix*, only to be followed by a comprehensive, reference-filled explanation of what really happened--leaving it up to the reader to connect the dots between Watson's "truth" and the facts of history.

But true to his thesis, it would be almost disrespectful to everyone else involved in the discovery of DNA's double helix to simply write a book about James Watson's multi-splendored flaws as a narrator, researcher, and a human being. So Markel goes back to the beginning, giving the reader the context they might need--which Watson of course excludes from his tale--about the history of human understanding of genes and DNA. He starts with Gregor Mendel, and doesn't circle back to the main action until chapter 4. Then he offers each key player--Crick, Wilkins, Franklin, Pauling, and Watson--a chapter-long biography, a character portrait of their lives up until they started

working on the DNA problem in 1951.

Part III, entitled "Tick-Tock, 1951," is where things start to get interesting. For the next twenty chapters, including Parts IV and V, Markel digs deeply into the ins and outs of British academia in the early 1950s. He makes it clear that Rosalind Franklin was wronged. There is of course, the argument that she couldn't have won the Nobel Prize because it can't be awarded posthumously. But what Markel hammers home is the delicate imbalance of political power in the academic circles in which all these players ran. Watson and Crick's discovery was critically dependent on an x-ray diffraction pattern collected by Franklin--which was distributed to them without her knowledge or consent. Certainly, Franklin had passed away by the time the prize was awarded--but whether or not the discovery could have happened at all was dependent on an altogether unethical, unprofessional, and immoral breach of academic conduct.

Markel rounds out the book with two short chapters--which are perhaps the most juicy and compelling of the whole work. He describes his ventures to Stockholm, Sweden to gain access to the Nobel Prize nomination letter archives--what he finds there I'll leave for you to glean for yourself. And finally, he ends where he began--with Watson--the only living player today. Markel's portrait of Watson today is no more flattering or endearing than his historical depiction. And Watson's reaction to any mention of Rosalind Franklin--and how he cheated her out of the recognition and respect she had earned and deserved--paints a vivid picture of the chauvinistic climate of an earlier time--and calls into question some unsettling parallels with today's.

*Jeanette S. Ferrara, MFA*

## The Centennial of Insulin

The Nobel Prize in Physiology or Medicine in 1923 was awarded jointly to the Canadian physician Frederick G. Banting (1891-1941) and the British biochemist and physiologist John J. R. Macleod (1876-1935) “for the discovery of insulin”. This was a remarkable achievement in many ways, first and foremost because the new drug provided a reliable treatment for diabetes that has literally saved millions of lives since it became available. The Nobel Prize itself was given to Banting and Macleod less than two years after their original research was published early in 1922 and they were both first-time nominees, which was also unusual.

The story of the structural elucidation of insulin is also quite interesting. It was only in the early 1950s that the English biochemist Frederick Sanger (1918-2013) determined the exact sequence of 51 amino acids present in insulin (*i.e.*, its primary structure). This was an outstanding accomplishment at the time since the structure of insulin was quite complex, consisting of two separate peptide chains linked by two disulfide bonds and a combined molar mass of ~5808 Da. For his work on the structure of proteins, especially that of insulin, Sanger was honored with the Nobel Prize in Chemistry in 1958, a particularly competitive year since there were 85 nominations, including multiple ones for future Nobel laureates such as Melvin Calvin, W.F. Libby, Georg Wittig, R.B. Woodward, Karl Ziegler, and Giulio Natta.



As described in more detail in a previous *RefleXions* column (Winter 2019), the renowned protein crystallographer Dorothy Hodgkin (1910-1994) worked for nearly 35 years to solve the crystal structure of insulin, which she finally completed in 1969, five years *after* getting the Nobel Prize in Chemistry.

The postage stamps illustrated in this note are among those issued in 2021 to commemorate the centennial of the discovery of insulin by Banting and his assistant Charles Best (1899-1978) while working in the laboratory of Macleod at the University of Toronto. This milestone in the history of medicine is certainly worth remembering every November 14<sup>th</sup>, which is Banting’s birthday and (since 1991) World Diabetes Day, now celebrated in more than 160 countries and territories.

Daniel Rabinovich





## Puzzle Corner

For Winter, we have a new Crystoquote puzzle, answers to the previous puzzles, comments on the car wheel symmetry puzzles and mention of those who provided solutions.

### Crystoquote #12:

Letter substitution yields a quotation by a well-known crystallographer.

RX LOPZ OV XYZ DAJVOVS,  
JZROUOVS XYRX XYZ QRQZJ XTQZ  
SAOVS OVXA AVZ COKZ AL XYZ  
JZRKZJ NRC VAX ZDZJSOVS AV XYZ  
AXYZJ NRC VAX XYZ YRQOZCX  
ZWQZJOZVTZ.

ZJOT SRIZ

### DISORDERED

Fill the boxes correctly to arrive at the right place

IDLY	Y L I D
PYRONET	E N T R O P Y
DERNHOGY	H Y D R O G E N
NASTIGCK	S T A C K I N G
MACERATE	R A C E M A T E

Answer:

C R Y S T A L      P A C K I N G



### Solution to Crystal Connections #21: Round things with rotational symmetry

1. Painted on barns in Pennsylvania Dutch country. Hex Signs
2. Cars have four of them. Wheels
3. Typically found on doors of crystallography labs. X-ray Warning Sign
4. Posted on labs with BSL-2 rating or above. Biohazard Warning Sign
5. Sand painting created by Buddhist monks in order to be ritualistically destroyed. Mandala
6. Circle Limit III, Path of Life, and Snakes, for instance. Circular M.C. Escher Prints
7. Used to control a watercraft's rudder from its helm. Ship's Wheel
8. At the end of a rope, thrown to a drowning person. Life Preserver
9. In Gothic cathedrals, stained glass structures radiating outward like flower petals. Rose Windows
10. Ice  $I_h$ , photographed by Wilson Bentley and much later by Kenneth Libbrecht. Snowflakes

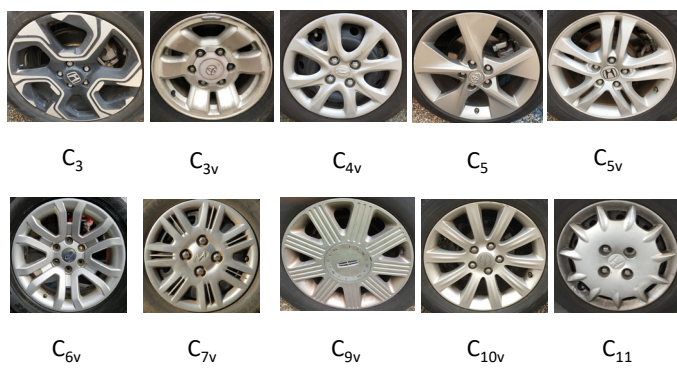
### Observational Symmetry Puzzles:

1. What is the most common order of rotational symmetry (idealized, neglecting manufacturer's logos, bolt holes, valve stems, etc.) for automobile wheels? How common are other orders? Take a guess, observe for a few days, and let me know what you find.

**Answer:** In my experience, fivefold rotation symmetry is by far the most common, likely because most wheels are held on by five nuts, followed by sixfold. 10 is common and 7 is surprisingly common. 3 and 8 are less common, while 4, 9, and anything over 10 are uncommon. I have seen as high as 40-fold. Pictures of some examples with their point groups are shown.

2. How common are wheels without mirrors in addition to the major rotation axis? Those that don't are, of course, chiral. Are the left-side wheels mirror images of the right-side wheels (i.e. are these cars meso or homochiral, wheel-wise)? Again, guess and then observe.

**Answer:** Wheels in point groups without mirrors are less common than those with mirrors, but they are common. All four wheels on cars with chiral ones seem have the same handedness, perhaps to avoid the additional cost of manufacturing mirror-image wheels to satisfy crystallographers. Pictures of both sides of a homochiral-wheel automobile are shown. All wheels have  $C_5$  symmetry with the same handedness.



### Comments on the previous puzzles:

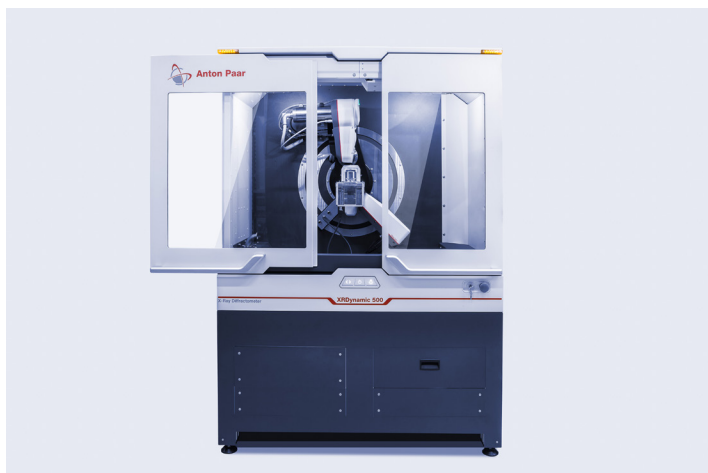
Marian Szebenyi provided the solution to Crystal Connections #21, and she also suggested the crystal packing DISORDERED puzzle, for which I thank her. I received no feedback about the car wheel symmetry puzzles.

As always, I will be pleased to see your solutions and also your ideas for future puzzles. Volunteer Guest Puzzlers are especially welcome!

Frank Fronczek – [ffroncz@lsu.edu](mailto:ffroncz@lsu.edu)



### Driving XRD: Anton Paar launches powder diffractometer XRDynamic 500



Anton Paar introduces its own powder diffractometer after supplying non ambient XRD attachments and pioneering the SAXS sector for many years. XRDynamic 500 is a fully automated multipurpose X-ray powder diffractometer for the laboratory combining unbeatable data quality with up to a 50 % increase in measurement efficiency. XRDynamic 500: Driving XRD.

The core of XRDynamic 500 is the unique TruBeam™ concept which includes a large goniometer radius offering best-in-class measurement resolution for high-quality XRD data. Also, the beam path is evacuated – a first amongst laboratory powder diffractometers – to minimize air scattering and maximize signal-to-noise ratio. Together, these two features eliminate compromise between measurement speed and data quality. Excellent data can now be collected

under standard conditions.

TruBeam™ delivers flexibility and convenience for the user via fully automated X ray optics together with automated instrument and sample alignment routines. Automatic switching between up to three different beam geometries at the click of a button allows measurement of different samples with different instrument configurations without any user input.

The high degree of automation along with component recognition and simplified workflows in the XRDrive control software make XRDynamic 500 both easy to use for beginners and flexible for advanced users, reducing the risk of potential errors. Even novices can collect high-quality XRD data without the need for extensive training.

XRDynamic 500 is a true multipurpose diffraction platform enabling collection of data on many different sample types for various analytical tasks. Whether the sample is a powder, a solid, or a nanomaterial, a prime measurement solution is always possible via an extensive range of components and sample stages. This includes the latest pixel detector technology from CERN and Anton Paar's world-leading non-ambient XRD attachments, which function with a built-in control unit and optimal non-ambient infrastructure in the radiation-safe instrument enclosure. A dedicated SAXS configuration with fully evacuated beam path from source to detector delivers data with the quality of a stand-alone line-focus SAXS instrument with a  $q_{min}$  of  $0.05 \text{ nm}^{-1}$  for advanced nanostructure analysis.

For more information and technical specifications, see [www.anton-paar.com](http://www.anton-paar.com)



## Cryogenic eCryoTag Sample Tracking System

MiTeGen announces the release of the Cryogenic eCryoTag Sample Tracking System. This system is the next generation of tracking samples in cryo-EM and crystallography.

### The system allows users to:

- Track crystallography and cryo-EM pucks and cryo-EM grid boxes at cryogenic temperatures (LN2)
- Help facilities and users easily keep track of their samples
- Add confidence they are collecting data on the right samples
- Cryogenic or Room Temperature scanning compatible

### How it works:

Cryogenic RFID Tags (eCryoTags) are embedded into the various components utilized in sample storage and tracking in cryo-EM and crystallography. These include sample storage pucks, grid boxes, or potentially other components (e.g. canes or dryshippers). The pucks and grid boxes with cryogenic RFID tags (eCryoTags) can be easily read using a simple reading system with a cryogenic compatible wand or via a puck reading station.

Users can correlate the designated ID to their samples. The system is able to be easily integrated into most LIMS.

### Primary system components:

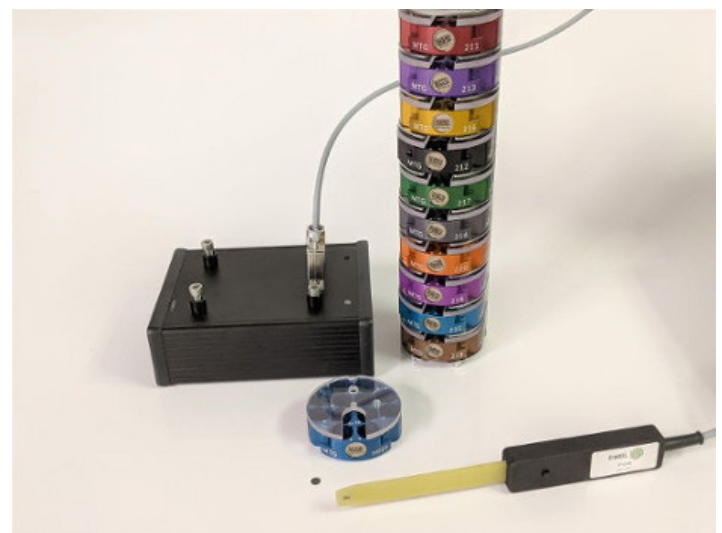
- Tagged sample storage pucks (Cryo-EM pucks, Uni-Pucks, SPINE Baskets) or cryo-grid boxes
- CryoRFID Reader (developed at the European Molecular Biology Lab (EMBL))

### The system has multiple applications:

- Cryo-EM Sample Tracking
- Crystallography Sample Tracking (Beamlines ESRF ID30B and ID30A1 (massif 1) are already CryoRFID ready (equipped with reader). All other MX beamlines at ESRF are ready to be enabled with a reader)
- Other cryogenic sample storage

Developed in Collaboration with F. Cipriani (EMBL) & G. Papp (EMBL)

[Learn More About The Cryogenic eCryoTag Sample Tracking System](#)





**The first installation of Rigaku's electron diffractometer, the Synergy-ED has occurred at Kitasato University in Japan.**

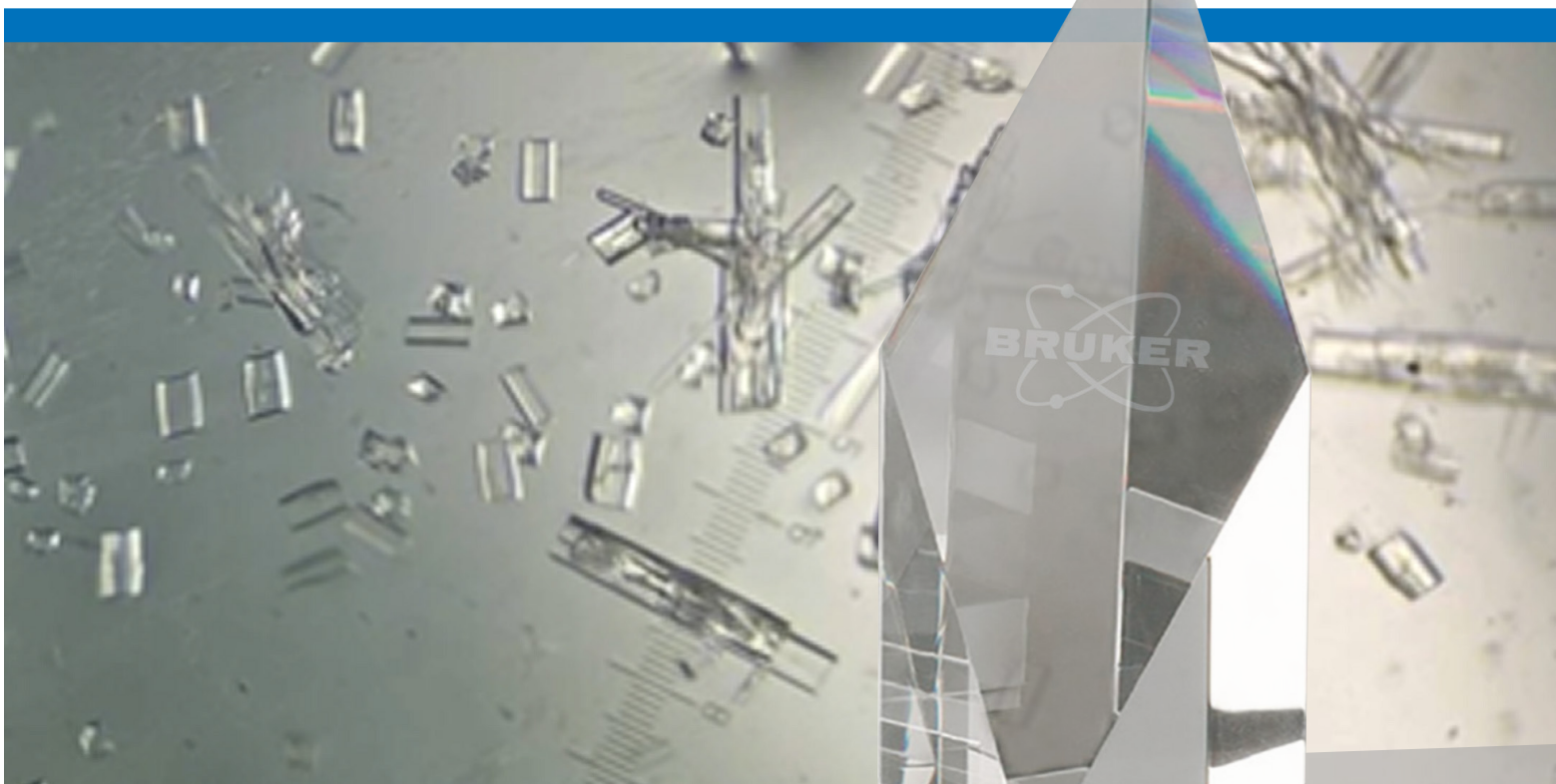


XtaLAB Synergy-ED is a new and fully integrated electron diffractometer, creating a seamless workflow from data collection to structure determination of three-dimensional molecular structures. The XtaLAB Synergy-ED is the result of an innovative collaboration to synergistically combine our core technologies: Rigaku's high-speed, high-sensitivity photon-counting detector (HyPix-ED) and state-of-the-art instrument control and single crystal analysis software platform (CrysAlisPro for ED), and JEOL's long-term expertise and market leadership in designing and producing transmission electron microscopes. The key feature of this product is that it provides researchers an integrated platform enabling easy access to electron crystallography. The XtaLAB Synergy-ED is a system any X-ray crystallographer will find intuitive to operate without having to become an expert in electron microscopy.

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<https://acas.memberclicks.net/corporate-membership>



## The Bruker AXS Co-crystallization award

### ● Bruker AXS will award the **Best co-crystal structure**

Bruker AXS will award the **Best co-crystal structure** based on the new 'Chaperone' approach published by Krupp et. al, Angew. Chem. Int. Ed. 2020, 59, 15875-15879.

The prize is endowed with 1 000 EUR and the submitted structures applications will be evaluated by a Scientific Committee, under the following criteria:

- Structure pushes the limits of the methods (quality time, molecular weight, first time quality crystallization of a high interest molecule)

- Structure fully complies to IUCR requirements and, ideally, it is published

- Data were obtained using a Bruker instrument

Interested parties can register via [www.bruker.com/crystallization](http://www.bruker.com/crystallization) by August 31st, 2022. Chaperones will be made available at cost level.

The award will be presented in October 2022.

[Accept this challenge and stay connected with us!](#)