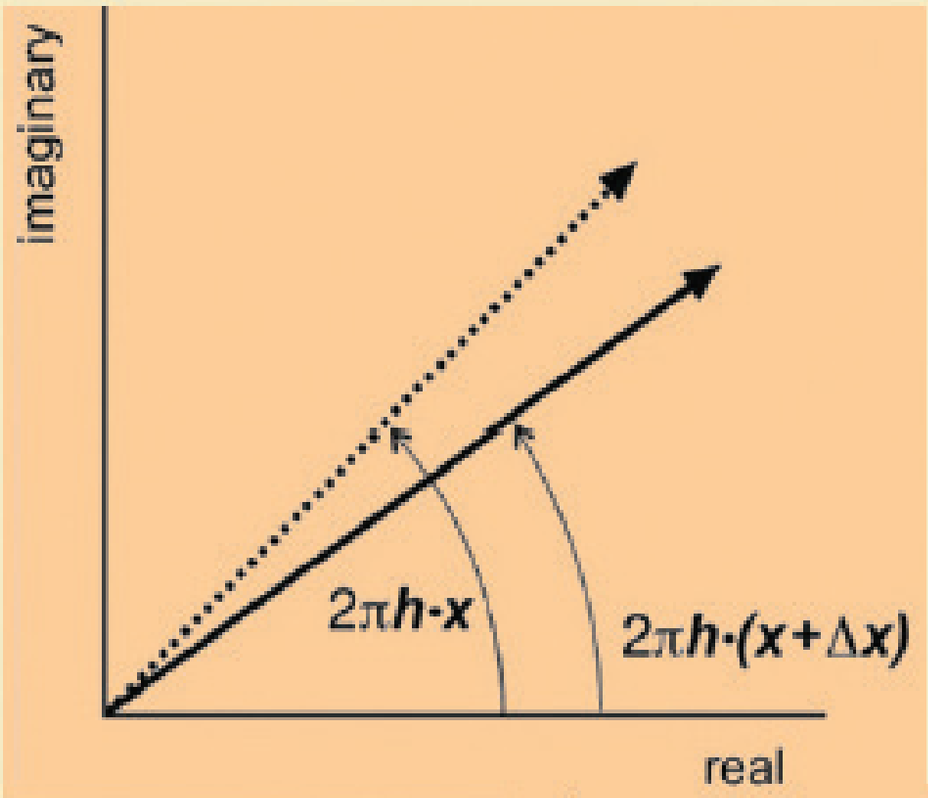
ACA RefleXions

American Crystallographic Association
Structure Matters

Number 1

Spring, 2019

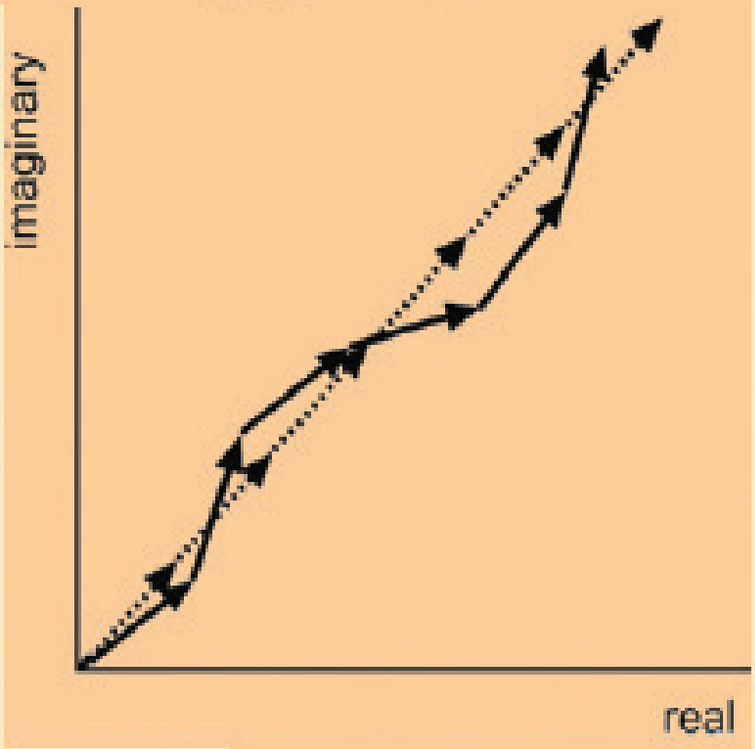


the wobbling vector corresponding to a fluctuating atomic motion leads to an understanding of the effects of uncorrelated atomic motions on Bragg scattering.

$$\langle \cos(2\pi h \times \Delta x) \rangle$$

the Debye-Waller factor, DWF =

$$(\exp(iq - u))^2$$



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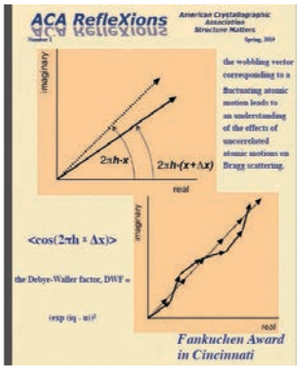
Joseph Ferrara
2019 ACA President



Eaton (Ed) Lattman won the Fankuchen Award for 2019. The cover images are described in the 'What's on the cover' page 2.

Jane Shelby Richardson receives 2019 Alexander Hollaender Award in Biophysics

Stephen Halley White Named as 2018 AAAS Fellow

2019 ASBMB Young Investigator Award to Christine M. Dunham

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Deadlines for contributions to *ACA RefleXions* are: February 1 (Spring), May 1 (Summer), August 1 (Fall), and November 1 (Winter)

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President's Column

Joseph Ferrara

In my column for the winter edition of Reflexions I had asked for volunteers for three ad hoc committees: Strategic Planning, Awards Oversight and By Laws Review. I hope that by the time I write my summer column these committees will be fully formed and moving forward with their remits. Lisa Keefe will be chairing the Strategic Planning Committee and we will be submitting another Venture Partnership Fund proposal to AIP to support strategic planning activities for the ACA as well provide a roadmap for other member societies. I want to remind everyone that we get out of the ACA only what we put in, so I am asking again for volunteers for these committees. You can contact Kristin Stevens or me to let me know your interest.

I am happy to report that the process of moving bookkeeping to headquarters is complete and appropriate generally accepted accounting principles (GAAP) are in place. By the time you read this, we should already have a couple of Budget versus Actuals reports complete and I look forward to letting you know how we are doing in my next column.

Stephan Ginell and Vivien Yee have done a fantastic job with the program for the 2019 Annual Meeting, which is being finalized and for which a preliminary draft appears later in this issue I am ecstatic that Michael Rossmann has agreed to give a lecture on his career in structural science at the opening ceremony. I was lucky enough to hear Michael give an earlier version of this talk as a webinar years ago and I know that it will have improved with age. I am also very happy to report the "Symposium Transactions—Data Best Practices: Current State and Future Needs" has proven to be a very popular session. In fact, it is so popular that non-speaking participants will be allowed to publish papers in the special issue of Structural Dynamics devoted to the Symposium.

This past summer Krystle McLaughlin attended an AIP workshop titled "How to Achieve Diverse, Equitable, and Inclusive Professional Meetings." Krystle's report to Council described some methods we can use to improve the inclusion, diversity, equity and accessibility of our annual meeting. One of the ways to promote inclusion is to eliminate harassment. The ACA has a Code of Conduct (https://t2m.io/PwFTAXrX) and I would remind everyone to review this document, especially before attending the annual meeting. We also are exploring bystander and awareness training to reduce the chance of bad behavior as well reporting mechanisms to bring transparency in the event of bad behavior.

In December, Lisa Keefe and I attended the Council of Scientific Society Presidents Leadership Workshop in Washington, D. C. For over 45 years, this group has advocated for science in Congress and provided a forum for member society leaders to learn how to better govern their societies. At the December workshop, both Lisa and I were elected to act as Members-at-Large of the CSSP Executive Board and will participate in future workshops. One of the most useful working groups is the one for society best practices. Council is implementing some of the best practices Lisa and I learned in December.

I will like to remind everyone that nominations for the Patterson, Rognlie, Etter Early Career and Wood Science Writing Awards and ACA Fellows are open until April 1. It is vitally important that the members participate in the nomination process by selecting peers for the awards and recognition as an ACA Fellow. The nomination form may be found at https://t2m.io/CqQmGHEi.

What's on the Cover

In the spirit of the upcoming Fankuchen Award lecture by Eaton Lattman, the cover provides a heuristic view of the physical basis of the effects of temperature on Bragg reflections. The upper panel shows the idealized scattering from a single atom j at fixed position x (hatched arrow), and the instantaneous scattering from the same atom displaced by thermal motion by an amount Δx. The vector is rotated by an angle $2\pi h\Delta x$. The lower panel shows the scattering from lattice-translation copies of atom j in a few adjacent unit cells (hatched arrows). It also shows scattering from those same atoms subject to random and independent thermal displacements Δx (solid arrows). It is clear that the tipsy walk taken by the sum of the solid arrows around the idealized direction of the hatched arrows yields a shorter overall length, thus decreasing the amplitude of scattering. It is also clear from the figure that this decrease goes up with increasing values.

This figure has been redrawn from Protein Crystallography: A Concise Guide, by Lattman and Loll.The accompanying article in this issue shows that this scattering vector-based discussion yields quantitatively the Debye-Waller factor.

INTERNATIONAL WOMEN'S DAY 2019

This year RefleXions will honor International Women's Day (March 8) by including contributions from various scientists celebrating the achievements of women in the field of crystallography. Some of these contributions are personal and some of them are historical in nature; some of them emphasize achievements and some of them also address the challenges that women continue to face in science. Hopefully the need for a more gender-balanced world will be recognized through these stories.

Dorothy Hodgkin: Britain's only female Nobel scientist deserves to be on the new £50 note

Elspeth Garman
Prof. of Molecular Biophysics, University of Oxford

Republished from
THE CONVERSATION

Dorothy Crowfoot Hodgkin may be the most famous British scientist of whom most people have never heard. As such, she would be a very appropriate face for the new £50 note, on which the Bank of England wants to feature a picture of a scientist.

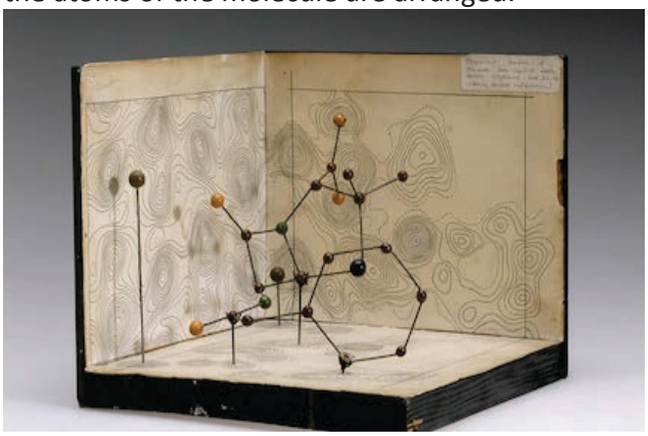
Hodgkin was the foremost leader and innovator in her field, and the major impact of her work led to her becoming the only female British scientist to win a Nobel Prize (so far). The 1964 award recognised her work in chemistry using a technique known as X-ray crystallography to find out the three-dimensional shapes of penicillin (1945) and vitamin B_{12} (1955).

Accurate knowledge of the shape of penicillin was absolutely pivotal in understanding how it could overcome bacterial infections. As as result, Hodgkin's work is still extremely important in the development of new antibiotics, which are currently badly needed as some bacteria have developed resistance to existing drugs.

Hodgkin's work also had an enormous impact on the treatment of diabetes. In 1969, after 35 years of enormously tenacious and brilliant work, she solved the 3D shape of the insulin molecule. Insulin is an important hormone used by the body to process sugars in food, and understanding its structure has helped untangle the mechanism of its action, with critical implications for human diabetes control.

Key to Hodgkin's work was the technique of X-ray crystallography, a way of working out how a complex molecule is arranged in three dimensions. The way we find out this 3D shape is by growing tiny crystals (usually less than a tenth of a millimetre) of a substance so that its molecules are all lined up in an orderly array. We then hit this array with a very intense beam of X-rays and capture the resulting "diffraction pattern" of spots that indicate how the molecules interfere with the beam.

By capturing patterns from each side of the crystal and doing some fairly complicated mathematics, we can eventually get the average of the shapes of all the molecules, highlighting all the common features. This gives us a picture of the density of electrons in the molecule in 3D space, which we can use to show how the atoms of the molecule are arranged.



Hodgkin's model of penicillin. Wikipedia, CC BY-SA

In 1935, Hodgkin, along with her mentor J.D. Bernal, discovered that it was absolutely essential to keep the crystals wet with the liquid they are grown from ("mother liquor") while X-raying them. If the liquid dries out, the molecules start to lose their ordered arrangement, and when hit with X-rays, they don't give a clear pattern of spots.

Hodgkin's pioneering work in crystallography gave birth to a whole new field that applied the methods she developed to large biologically important molecules, including DNA and proteins. We now know the 3D shapes of over 139,000 biological molecules, and all the information is stored in a completely open access

database called the Protein Data Bank.

In this way, Hodgkin's legacy is multifaceted. She was not only an exceptional scientist but also was, and continues to be, an inspirational role model to generations of researchers in the UK and elsewhere, both male and, very importantly, female.

I was thrilled to meet her in 1991 soon after I had changed research fields from nuclear physics to structural biology, and I had the opportunity to discuss the latest developments in crystallography with her. She inspired me to stay in the field and make my career in it, and I know many other scientists on whom she had a lasting positive influence.

She was also very active in standing up for her core beliefs as a pacifist. For 12 years she was president of Pugwash, an organisation founded in 1957 dedicated to reducing the danger of armed conflict and which sought peaceful solutions to global security threats. She even inspired her former student Margaret Thatcher, who reportedly kept a portrait of Hodgkin in 10 Downing Street, despite their differing politics.

Her life was a shining example to many so it would be entirely appropriate for us to honour her great scientific achievements, and help give her the public recognition she deserves, by putting her image on our new £50 notes.

Elspeth Garman

A brief history of my career

Connie Rajnak

I did not know anything about crystallography until 8 years after I graduated from Kalamazoo College. I was working for The Upjohn Company at the time, in a microbiology lab in the "Control" division, and taking classes at Western Michigan University (WMU) towards a MA in mathematics. I was married and had three children, aged 9, 71/2, and 2. Dave Duchamp, a crystallographer recently graduated from Caltech, needed a research associate and my name came up in a computer search of Upjohn employees because of my physics background, (at Kalamazoo College I majored in physics and philosophy), and because of my mathematics studies at WMU. When Dave explained what crystallography was about I was enchanted;

never in my wildest dreams had I ever thought that I could find a local job that satisfied my love for puzzles and patterns and mental challenges. (This was in 1966, when solving small molecule crystal structures still had a few challenges.) I transferred to the Research Division and learned crystallography, more or less as an apprentice to Dave. The first ACA meeting I went to was in New Orleans, in 1970, and I was charmed by the welcoming and congenial atmosphere where one could just stand around after the sessions and be invited to join one or another group for dinner. The meetings were small enough that even if you were a stranger, the assumption was that sooner or later you would be an acquaintance. Even well known, important scientists, whose work I had only read about, were friendly towards new people. At the 1972 meeting in Albuquerque, I very nervously presented a paper, and found the response forgiving and respectful. After a couple of years I divorced my first husband. Around '74 or '75 I was promoted to the scientist track at Upjohn. Except for a sabbatical at the Naval Research Lab in 1985-86, I spent my entire career working for the Upjohn Company in Kalamazoo.

The people who influenced my scientific development most before Dave Duchamp were my high school math and physics teacher, Carson Neifert, and at Kalamazoo College, professors Allen Buskirk in physics and Luike Hemmes in philosophy. From a very early age I had a desire to understand how the world is structured. When it became fashionable in the pharmaceutical industry to conduct team-building exercises and formulate mission statements and study motives, I was mildly surprised to find out that some of the other scientists gave as their primary motivation that they wanted to find a cure for some disease, for example, or that they desired recognition, - for me the first thing always was simple curiosity.

In the early years, my time at work was spent solving small molecule structures and writing computer programs to run diffractometers, analyze data, etc. We worked closely with the chemists and, because chemists were quite paternal towards their compounds, they were supposed to publish first, though always we crystallographers were co-authors. Once in awhile, for exceptional structures, we would get around to publishing a second paper that gave the complete crystallographic results, but as there was no pressure to publish, we often neglected to do so. I always presented papers or posters at ACA meetings, but often that research never made it to a publication. During the 1980s, there were tremendous advances in structure-solving computer programs, especially in direct methods, and the number of small molecule structures that were difficult to solve gradually diminished until in the latter part of the decade the challenges had more and more to do with understanding function in terms of structure - what made drug molecules bind to receptors and what was their mode of action. Structure based drug design became my primary interest, and I focused on central nervous system drugs. Benzodiazepines were in this category, but ultimately I zeroed in on compounds that bound to the dopamine and serotonin receptors. For several years in the 1990s, I felt as though I was in crystallography heaven because at Upjohn researchers had developed a marvelous database that kept track of all biological tests -- including binding at the various receptors - on every compound synthesized at Upjohn as well as other drugs on the market. Making my research even more interesting, these tests categorized compounds as agonists or partial agonists or antagonists. There were also many subcategories of receptors; dopamine D2, D4, and so on; 5-HT1a, 5-HT2c, etc. (serotonin is 5-hydroxy tryptamine). It was a complication for drug design that the drugs marketed for Central Nervous System disorders that exhibited binding to dopamine and serotonin receptors were not at all selective for particular receptor subtypes, so at that time it wasn't possible to know which subtypes might control depression, or anxiety, or psychoses, or insomnia, or hunger.

Also during this period in my career, the way that research was done at Upjohn changed for the better. The company introduced "project" teams. I was on the CNS team, but there were a number of other teams. The idea was to have chemists, cell biologists, biochemists, drug metabolism scientists, computer people, and crystallographers all represented on the team that aimed to find drugs for central nervous system disorders. Every scientist on the team reported pertinent research to the project team leader and reported administratively to a section head. Sections were organized by discipline. I thought the CNS team worked extremely well together, but sympathized with colleagues who had less satisfactory teams, as success naturally depended on the personalities of the various team leaders and section heads. From 1995 on the company endured a number of mergers, but very high quality research continued in spite of the considerable organizational distractions.

My personal contribution to research did not go as well. I retired in 2001, very disappointed that I had not been able to achieve my goal of designing, in partnership with a chemist, a compound that uniquely fit the requirements of any one of several pharmacophores that were known by then. All the chemists, when deciding on a new series of compounds to synthesize, studied the patent situation first. If something could not be patented, there was no point in working on it. For my part, I did not know chemistry well enough to know if it was even feasible to put, say, a hydroxy group or a phenyl group here or there on a

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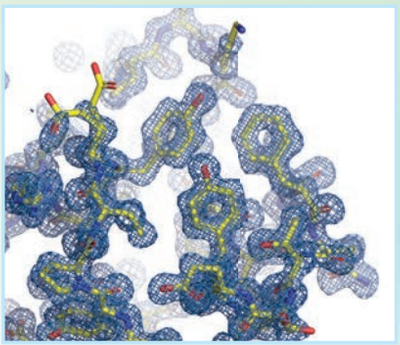
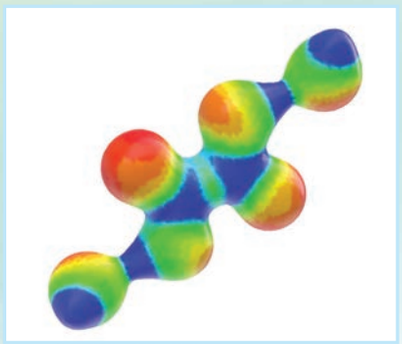


Density maps from a ten minute thaumatin dataset solved by S-SAD phasing



Electron density from a 0.37 Å quantum crystallography measurement of oxalic acid

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compound already synthesized, much less to change the basic ring structure. Furthermore in my final year it seemed that our crystallography lab might be inundated with structure requests from non-Kalamazoo chemists that were not related to my main interest. I consoled myself that retirement would not isolate me altogether from science and from my colleagues in crystallography because I was just coming off the ACA council and knew that I would be able to co-edit the ACA Newsletter because of my experience in editing the newsletter '91- '93. At that time I had adapted it from the admirable ACA Newsletter edited for many years by Jenny Glusker to a desk-top publishing program version. The ACA Newsletter in black and white became the ACA RefleXions news magazine in color. Originally I co-edited this with Judy Flippen-Anderson and we attempted to make our Co-Editor jobs easier by adding other volunteers to the RefleXions staff. We had a staff Photographer, a News and Awards section editor and a Books section editor, and we recruited for an Opinions section editor.

In 2002 when Pharmacia was bought by Pfizer, the research division was disbanded - no more research in Kalamazoo. Now even the building that I worked in is gone. However, thanks to the ACA I could take my connections home with me. I continued for several years to do the Co-Editing, and go to meetings (my way was paid by the ACA). Eventually, I re-married and moved to a house I share with my husband Stan. I gave up my Co-editorship in favor of the fun part, and I am now the ACA Covers editor. My way to meetings is NOT paid. I still have piano lessons however. It doesn't seem to be a problem for people who graduated from WMU's excellent jazz program to come to my house because I have a very fine class A Steinway piano.

Connie Rajnak

A simple career path

Marian Szebenyi

My crystallographic career has been very straightforward, one could say boring. I've been supported all along the way by several (male) mentors, beginning with my father, who taught chemistry at Tufts. He encouraged my desire, from an earlier age than I can remember, to pursue a career in science. My mother was an alumna of Bryn Mawr College, which was mainly why I chose to go there. I didn't think about it at the time, but attending a women's college neatly avoided any gender-based favoritism among students. I did a double major in chemistry and physics, with a vague idea of working in the general area of solid state physics.

For graduate school, I went to U. Conn, not because it offered the best science but because its rural location was better for the horse I had received as a graduation present. My advisor, Lew Katz, was a crystallographer studying complex inorganic oxides, so that's what I did. We used a Picker diffractometer controlled by a Teletype with a paper tape reader to collect data, and processed it using punch cards and a central IBM 370 computer – submit a deck of cards in the evening, get results in the morning, for one refinement cycle per day. Luckily the datasets were fairly small, and at that time it was enough for a thesis to analyze a few inorganic structures. That's what I did and came away with a PhD in Physical Chemistry in 4 years, as well as a husband who had been a fellow grad student (in engineering, not chemistry).

I had also acquired expertise in Fortran programming, necessary in the days before the availability of plug-and-play crystallographic software; the knowledge came in handy when a brief search for a job in industry failed to pan out. Taking a slight detour from science, my husband and I moved to New Jersey and took jobs in a computer service company, which (oddly for a business of that sort) used Fortran programs for inventory control and so forth. Although it paid the bills, this employment was pretty unsatisfying, so after a couple of years I realized I had to get back into science. Keith Moffat at Cornell was looking for a post-doc in macromolecular crystallography, and I got the job. After some preparation (taking a course in Biochemistry and learning some new software - still in Fortran, and mostly needing local modifications), I worked on solving the structure of a small protein (calbindin, a relative of calmodulin); preliminary results came out in 1981, and a refined structure in 1986. After a few years as a post-doc, Keith asked whether I wanted to move on. I said "No, I like it here" and became a Research Associate (at the time, this was an easy transition, not the more formal process that it is now).

Fortuitously, this was a great time to be at Cornell, as the Cornell High Energy Synchrotron Source (CHESS) was coming on-line and was available for developing synchrotron-based crystallography. Keith and his group were heavily involved, especially after the MacCHESS (Macromolecular diffraction at CHESS) grant was funded by NIH in 1984. We helped Michael Rossmann take the data that he used to determine the first structure of an animal virus, and were early developers of protein Laue diffraction. We were able to take a 120 psec Laue exposure of a lysozyme crystal (using an early undulator and running the storage ring with a single circulating bunch of electrons).

In 1990, Keith moved to Chicago to develop a beamline at the new Advanced Photon Source, while I stayed at Cornell (Chicago was still not a good place for my horses, and I didn't want to live there either), supervised by a succession of MacCHESS directors. Somewhere along the way I was promoted to Senior Research Associate (again, it was considerably simpler at the time than it is now). I continued to do some crystallography but focused mostly on beamline development, especially software. We collaborated on detector development, with Area Detector Systems Corp. and, particularly, with Sol Gruner and his group at Cornell. In 2008, the then MacCHESS Director, Quan Hao, left and there was uncertainty about future funding, so I was asked to become Interim Director. As it turned out, the funding came through (it's still ongoing), but there was no hurry to hire a permanent Director and I slid into the position, which I still occupy. Luckily, the administrative duties are not too onerous (being shared with the PI on the MacCHESS grant, Rick Cerione, and some administrative staff), and I can keep doing at least software development and the occasional crystallographic structure.

So, that's the story of a simple career in academic research in crystallography. With the help of Lew Katz, Keith Moffat, Sol Gruner, and others, I've managed to keep doing research in a great environment and avoiding (mostly) the administrative duties that plague people who get too successful. My husband has been very supportive; he's been happy to stay in the Ithaca area, and is now retired, after going through various jobs, including some at Cornell. We're still together after 46 years.

Marian Szebenyi

Women in crystallography

Helen Berman

I feel very lucky to be in a field in which women have played such a prominent role. I learned this first hand when as an undergraduate at Barnard College I was given the opportunity to work in the laboratory of Barbara Low at the Columbia's College of Physicians and Surgeons. Barbara was one of Dorothy Hodgkin's first graduate students and determined the structure of penicillin. At Columbia she built up a lively research group. Every day after commuting for more than one hour from Brooklyn to Manhattan, I marched into the cold room, mounted a crystal in a capillary and using precession photography determined the unit cell dimensions. Then once a week Barbara would invite us into her office and teach us the fundamentals of diffraction, symmetry, and the phase problem. She made sure we went to seminars and I remember hearing Dame Kathleen Lonsdale talk about her science and her life. What a privilege! After one year there was no doubt in my mind that I wanted to be a crystallographer. Looking back I realize how important it was that I had a strong and brilliant woman mentor with whom I maintained a friendship until she passed away last month.

I went to graduate school at the University of Pittsburgh where I studied with George Allan Jeffrey. In 1969 I went to the Institute for Cancer Research, Fox Chase Cancer Center where I worked with Jenny Glusker who was also former student of Dorothy Hodgkin. During my years at Fox Chase, I became very active in the ACA and worked with many other women crystallographers who did the same. In 1989, I moved to Rutgers University where I expanded my research and also became the Director of the Protein Data Bank. In my many roles at the university, I had the opportunity to mentor students, post docs and staff and hopefully give to them what my teachers gave to me.

It is often said that there were more women in crystallography than in other sciences. This perception comes about perhaps because so many of the first women crystallographers made such outstanding contributions to the field. And, in addition to their scientific excellence, they provided role models for different ways of doing science and how to approach the work-family balance. They showed us there is no one right way to deal with the inevitable challenges in both of these arenas and with perseverance, good luck and good mentoring we can succeed.

Helen Berman

Women in Crystallography Through the Eyes of the CSD

Amy Sarjeant

Working for the Cambridge Crystallographic Data Centre (CCDC), enables one to get a sense of the contributions women have had to the field of crystallography since nearly the very beginning. Last year, my colleague Suzanna Ward spoke at the European Crystallographic Meeting about the role of women in crystallography, and she found that it's instructive to delve into this topic from the perspective of the Cambridge Structural Database. I think it's safe to say that there isn't a woman out there practicing crystallography who herself was not inspired by another woman in the field. It's remarkable to see such a strong pres-

ence of women in crystallography from leadership positions (last year's ACA council saw women in four of its five roles) to Nobel Prize winners (Ada Yonath and Dorothy Hodgkin to name two).

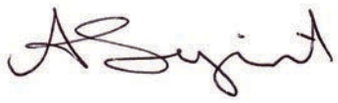
Over the years there have been quite a few women who have inspired me, both on personal and more abstract levels, to pursue a career in this field. Of course, working for the CCDC, my thoughts immediately turn to Olga Kennard, who along with JD Bernal, started building the Cambridge Structural Database. In the early days, when creating the CSD involved punch cards and knitting needles, many of the editors were women and the database was released in book form. But over time, Olga developed the CSD into the valuable resource it has become today and established the CCDC as a centre of excellence in data curation and structural chemistry research.

Olga Kennard wasn't the only female crystallographer to study under Bernal. Dorothy Crowfoot Hodgkin took her first X-ray images of crystalline proteins in Bernal's lab. Hodgkin's first three entries in the CSD date back to 1933 – a year that saw only 34 structures added to the database. Of course, she later went on to win the Nobel Prize for her crystallographic work. Along the way, Dorothy herself inspired many well-known female crystallographers such as Jenny Glusker, Eleanor Dodson, and Helen Stoeckli-Evans who all have made contributions to the CSD. Looking through the rest of the Bragg research family tree, one finds Kathleen Lonsdale whose earliest structures in the CSD date back to 1925. For reference, the first structure in the CSD dates from 1923, and in the years from 1923-1925 only 8 structures were published, four of which were Lonsdale's (under her maiden name of Yardley). We also find Isabella Karle who has nearly 400 structures in the CSD spanning the years 1961-2012.

These women went on to inspire many other female crystallographers – certainly too many to recount in this short article. However, we can also consider pioneers like Rose C. L. Mooney who, while only having one structure in the CSD, is considered the first female crystallographer in the US. Peggy Etter who inspired many structural chemists, worked on 127 structures in the CSD. Her contributions to the field of crystal engineering and her mentorship of students are commemorated every year at the annual ACA meeting through the Etter Early Career Award. Looking through our ACA fellows brings to mind such recent luminaries such as Helen Berman who helped found the PDB and who has 70 structures in the CSD and Marilyn Olmstead who has supplied a whopping 1889 structures by my last count. Connie Rajnak has contributed around 150 structures to the CSD. Winnie Wong-Ng has over 30 structures in the CSD, and many more to other structural databases. Virginia Pett, who is so instrumental in curating the ACA's History Portal has added nearly 20 structures to the CSD and Janet Smith contributed about 10 structures as well. And of course, we remember Judith Flippen-Anderson who inspired so many of us within the ACA community and the more than 500 structures she has in the CSD.
Two of the top-ten all time contributors to the CSD are women, Alexandra Slawin and Judith Howard. As of 2018 they had contributed 3350 and 3047 structures, respectively. There are many other women crystallographers whose work doesn't feature in the CSD, but who deserve recognition as pioneers and inspirations, such as the ACA's first female president, Elizabeth Wood, for whom the Wood Science Writing Award is named. Another of these women is Rosalind Franklin who did so much for protein structure determination, and the elucidation of the DNA structure, yet never quite got the recognition she deserved in her lifetime. While it's impossible to know with certainty the number of women contributors to the CSD, it's safe to say that the database would not be nearly the size it is today without the research efforts,

both past and present, of a large number of women scientists who chose to pursue a path in crystallography. Please accept my apologies for leaving your favourite female crystallographer or mentor off this list. But be consoled that whoever she is, she has had a profound impact on structural science simply by carrying the torch first lit by our earliest crystallographic ancestors.

My thanks to Suzanna Ward, Clare Tovee, Caroline Davies and Matthew Lightfoot for their help in assembling the data presented in this article.



Women in the Early Days of Crystal Structure Analysis

Jenny P. Glusker

The scientific study of the three-dimensional structures of molecules began in the early 1900s, soon after diffraction analysis indicated that, if materials could be crystallized, their X-ray diffraction pattern could, after intensity measurements and subsequent mathematical analysis, give a three-dimensional picture of the molecule instead of the two-dimensional formula that chemists had become used to. The value of this new knowledge was well appreciated and many physicists, including William H. and Lawrence Bragg, J. D. Bernal, Linus Pauling, Lindo Patterson and Jose Donnay set up programs to do this type of analysis. Many chemistry and physics students found this such a fascinating theme for study that they applied to work in crystallography laboratories. Among these were many women students such as Kathleen Lonsdale (who found that the benzene ring is hexagonal and planar), Dorothy Hodgkin (who established the chemical formulae of penicillin, vitamin B_{12} and insulin), Rosalind Franklin (who worked on the structures of DNA, coal and animal viruses), Olga Kennard (who initiated the Cambridge Structural Data Base), Helen Megaw (a mineralogist), Isabella Karle (who investigated and described "direct methods" of structural analyses for general scientific use), Gabrielle Donnay (mineral structure), Ada Yonath (ribosome structure) and Eleanor Dodson (crystallographic computing). Each of these made highly significant scientific discoveries , two won Nobel Prizes and many inspired women students who have also contributed important results in X-ray crystallography.

One of these scientists, Barbara W. Low, Professor Emerita at Columbia University, died on January 10, 2019, aged 98 years. She was born in Lancaster, Northern England on March 23, 1920 and studied chemistry at Somerville College, Oxford University with Dorothy Hodgkin as her main tutor; Barbara Low obtained a B.A. degree in 1946 and stayed for graduate research in Dorothy's laboratory. Barbara was a major contributor in the determination of the molecular structure of penicillin. This was in the early days of structure determination by X-ray diffraction of crystals, and was hard work because there were so many experimental data to deal with and computational equipment was just beginning to be used for such types of scientific research. This structure determination was highly significant because the chemical formula was not known. The antibiotic activity of penicillin, which had originally been found by Alexander Fleming in 1928, was being studied in Oxford, as well as at several industrial companies in Great Britain and the United States. By 1939 the action of penicillin on bacterial infection was confirmed and studied in Oxford University, England by Howard Florey (a Rhodes Scholar from Australia), Norman Heatley and Ernst Boris Chain. Florey was investigating how to administer penicillin to patients who had bad infections, and Heatley was working on finding good methods for extracting penicillin from natural sources. The antibiotic was first used on a patient in 1943, although several doctors reported that they had already successfully used various kinds of bread molds(tested and stored in their basements) to treat infections.

Ernst Chain, working on the purification of penicillin, eventually managed to crystallize the sodium salt and gave Dorothy some crystals, the ones that Barbara worked on. The chemical formula, not known at that time, was eventually found by collaborations between Dorothy Hodgkin and Barbara Low at Oxford with Charles William Bunn and Anne Turner-Jones at Imperial Chemical Industries (its Alkali Division in Winnington, Northwich). The steps in the structure detrmination are described in detail by Georgina Ferry (1).

It turned out that the chemical formula of penicillin was not the expected thiazolidine-structure (favored by many senior chemists at the time) but contained a four-membered beta-lactam ring structure that is very active and therefore appropriate for the action of penicillin (which chemically interferes with cell-wall structure in bacteria). To satisfy questioning chem-

ists Dorothy and Barbara were able to show that their crystals of penicillin, which they confirmed had the beta-lactam formula, were indeed biologically active; they were not thiazolidenes that had been damaged (and therefore converted to beta-lactam structures) by X-ray exposure.

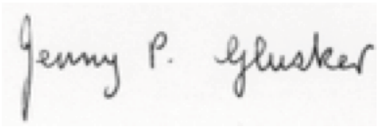
This work was published in 1949 (50 years ago) in an article entitled "The X-ray Crystallographic Investigation of the Structure of Penicillin," by D. Crowfoot (Hodgkin), C. W. Bunn, B. W. Rogers-Low, and A. Turner-Jones" in a book entitled "The Chemistry of Penicillin," by H. T. Clarke, J. R. Johnson and R. Robinson (Princeton University Press.) The Nobel Prize in Chemistry 1964 was subsequently awarded to Dorothy Crowfoot Hodgkin "for her determinations by X-ray techniques of the structures of important biochemical substances," and penicillin was one of these substances (2). Finding this chemical formula in the middle of World War II was a very significant event and led to the possible chemical synthesis of the compound and the design of more active derivatives. Penicillin became available at a time that was essential for the treatment of wounded soldiers during the war, and saved the lives of many injured soldiers.

After obtaining her D. Phil. degree from Oxford University, Barbara came to the United States and continued with structural studies in Linus Pauling's laboratory at Caltech in Pasadena, California. She became interested in the structure of polypeptide chains, influenced by then current structural studies of helical folding in proteins by Linus Pauling and Robert Corey. Her primary interest was the π-helix (with Baybutt in 1952) in which each N-H group forms a hydrogen bond with a C=O group of an amino acid five residues earlier in the polypeptide chain. This π-helix is found in about 15% of proteins. It may affect the stability and bonding properties of that part of the polypeptide chain. Addition or deletion of a single amino acid can interconvert alpha- and π-helices and may be important in evolutionary changes of protein function. Barbara gave a talk about it at the "Pasadena Conference on the Structure of Proteins" in 1953.

After her position at Caltech Barbara moved to Harvard (1948 - 56) and became an Assistant Professor of Physical Chemistry where she was among the first to introduce structural studies of crystalline proteins into the United States. She then moved to Columbia University of Physicians and Surgeons in 1956 where she continued studies of protein structure, especially insulin, and the copper-carrying enzyme ceruloplasmin. Her work on neurotoxic proteins from the venom of the black-banded sea krait, which are inhibitors of the acetylcholine receptor, led to useful information on the structural basis of their binding site on the receptor.

Barbara Low, as a researcher and teacher, has made several important discoveries in biochemistry and medicine. She was appreciated for her careful research in the early days when X-ray diffraction studies were difficult and her later investigations on larger molecules have contributed to the greater efficiency of structure determination and our understanding of chemistry and physics today.

(1) Georgina Ferry. "Dorothy Hodgkin: A Life." Grant Books: London (1998).
(2) Sharon Bertsch McGrayne. "Nobel Prize Women in Science. Their Lives, Struggles, and Momentous Discoveries." Carol Publishing Group, New York, New York (1993).



Ask Now What Crystallography Can Do For You…

Claire Murray
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The Oxford English dictionary definition of a scientist is quite an open and inclusive statement, wherein we are defined as "A person who is studying or has expert knowledge of one or more of the natural or physical sciences." However, it is a curious fact that the scientific community continues to be one of the most exclusive in the world. We claim to be rigorous, methodical and unbiased, and yet we have collectively constructed a culture in which very few can survive and even fewer can even get in the door. A direct illustration of this is provided in the most recent report available from the National Science Foundation titled 'Women, Minorities and Persons with Disabilities in Science and Engineering: 2017'. There is a very stark contrast between the resident population in the United States (Figure 1) and the academic population in science and engineering in the United States (Figure 2) and we should all have serious questions about why there is such a disparity and what we can do to address it.

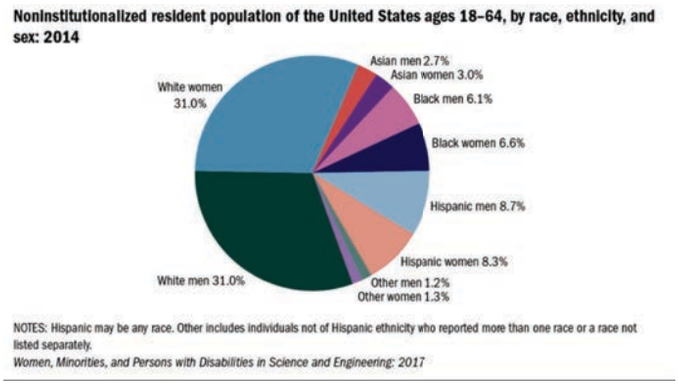

Figure 1 - Resident population in the United States (1)

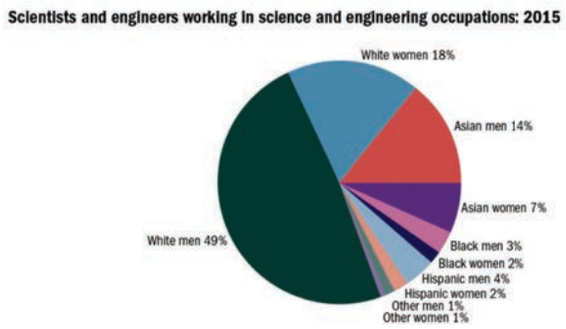

Figure 2 - Academic population in science and engineering in the United States (1)

The field of crystallography is somewhat unusual amongst our peers given the relatively high number of women who started out in W.H. Bragg's group. The 11 women and 7 men were the vanguard for our science but multiple datasets indicate that we are not immune from the issues facing our fellow scientists:

- This article written by Helen Maynard-Casely, Christine Beavers, Amber Thompson and I for IUCr crystallites blog highlights discrepancies between the gender of attendees and plenary or invited speakers for the past few IUCr meetings: http://blogs.iucr.org/crystallites/2018/03/07/women-in-crystallography-we%E2%80%99re-not-just-historical/.
- Building on this, for the last ACA meeting, 22% of invited speakers and 29% of attendees were women. Between 2012-2018, when there was a plenary session, 25% of these sessions were presented by women.
- Gender representation for the 107 ACA awards presented to date currently stands at 17.17% Women: 82.83% Men. Whilst data for the award nominees were not available, these ratios are concerning given the number of outstanding women crystallographers who are working or have worked in the United States - see Figure 3 for a detailed breakdown.

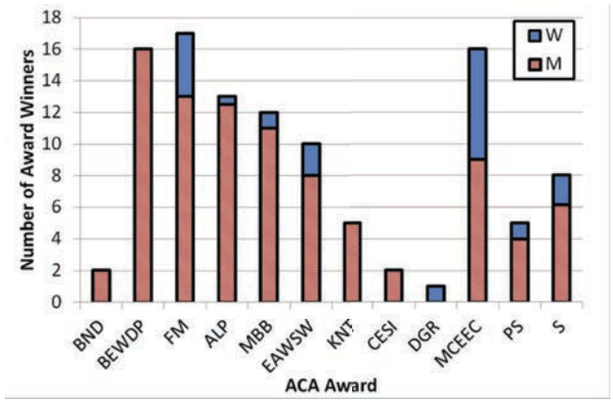

Figure 3 - Women and Men ACA Award Winners, taken from the ACA website.

[Abbreviations: BND = Bau Neutron Diffraction, BEWDP = Bertram Eugene Warren Diffraction Physics, FM = Fankuchen Memorial, ALP = A.L. Patterson, MJB = M.J. Buerger, EAWSW = Elizabeth A. Wood Science Writing, KNT = Kenneth N. Trueblood, CESI = Charles E. Supper Instrumentation, DGR = David G. Rognlie, MCEEC = Margaret C. Etter Early Career, PS = Public Service, S = Service]

think we all can feel a bit helpless sometimes in the face of these problems and serious structural changes are required in organisations around the world to address some of the bigger issues. However, the truth is that you are a lot more powerful than you might realise. The following are some suggestions for big and small ways for us all to use our power to make our community more inclusive and welcoming for everyone.

1. Challenge Yourself

- Do you know what your biases are? Check out Project Implicit, which will help you identify them: https://implicit.harvard.edu/
- How many assumptions do you make about a person based on very little evidence? Think about how frequently we allow meetings or talks to run over, assuming that no one has caring responsibilities or medicines that they need to take. Whether as a conference chair or as a meeting organiser, you have the power to ensure that you end on time. Or how about the assumption that women have better handwriting than men and therefore should take meeting notes? These low-level assumptions slowly build up and hamper the relationships we have with our colleagues and their ability to progress in their career.
- When you lecture, who do you mention? We have great crystallographers who are women that we should absolutely be mentioning when we talk about our science. Unfortunately, however, they are often written out of the history of our science. This directly impacts on students' perceptions of who can be a scientist and this is something I have

seen in action in high school classrooms in the UK and Ireland. Benzene appears on both curricula but Kathleen Lonsdale's name does not appear, even though her experiment is described in many text books. Thanks to a grant from the Royal Society of Chemistry we are currently evaluating the extent of gender bias and we would love to hear your suggestions for who is missing from the curricula: http://bit.ly/ChangeChemistryCurricula.

- Language Matters. Consider how you write reference letters for students and colleagues. Plenty of studies have been done on the text in the letters, and the following is particularly concerning: "it is notable that recommenders used significantly more standout adjectives to describe male candidates as compared to female candidates, even though objective criteria showed no gender differences in qualifications." "It is likely that evaluators place higher weight on letters that describe a candidate as the most gifted, best qualified or a rising star (2)".

2. Challenge Colleagues

- Be an active bystander. Learn to read the situation and step in if appropriate. It is so important to be an ally and to help create a positive environment for everyone.
- Discussions and language of 'tokenism' are extremely unhelpful as this contributes to inferiority complexes and to the perception of women as inferior scientists. Please try to shut down these conversations firmly.
- Who are the chosen ones? Challenge conference organisers, journal editors, politicians, university boards, session chairs, heads of departments… Ask them whether they have thought about Gender Balance and point them in the direction of Prof. Jenny Martin's article on exactly this (3) or the recent statement on gender balance by the European Crystallographic Meeting in 2018 (4). The IUCr is also addressing this and their IUCr Gender Advisory Committee is currently looking for some committee members - apply to Prof. Jenny Martin and please spread the word: jlm@griffith.edu.au. Another important area to address is codes of conduct, which should also be investigated as they provide a clear statement to attendees of conferences that discrimination, harassment and bullying will not be accepted, and that there are consequences for these behaviours.

3. Celebrate their Science

We have a strange history with respect to how we discuss the work of women scientists. Too often the topic of family and children are mentioned in places where men scientists rarely (if ever) will have the same things mentioned. As an example, take a look at some of the articles about the lives and work of some of your favourite women and men scientists. They jar when you realise that men are not framed in the same way at all. This is something we are hoping to address in the International Year of the Periodic Table through #IYPTCrystals/@IYPTCrystals on Twitter and online where we are actively aiming to ensure that we highlight the work of men and women equally (5). Also, returning to the topic of prize nominations mentioned earlier, get out there and nominate! The deadline for the ACA awards is 1st April 2019: https://www.amercrystalassn.org/awards.

Essentially this all boils down to being kind to each other, which is no bad thing in a world full of uncertainty and change.

(1) National Science Foundation, National Center for Science and Engineering Statistics, "Women, Minorities, and Persons with Disabilities in Science and Engineering: 2017", 2017, Special Report NSF 17-310. Available at www.nsf.gov/statistics/wmpd/

(2) T. Schmader, J. Whitehead, V.H. Wysocki, "A Linguistic Comparison of Letters of Recommendation for Male and Female Chemistry and Biochemistry Job Applicants", Sex Roles; 2007, 57(7-8):509-514. DOI: 10.1007/s11199-007-9291-4

(3) J.L. Martin, "Ten Simple Rules to Achieve Conference Speaker Gender Balance", PLoS Comput. Biol., 2014, 10(11), e1003903. DOI: 10.1371/journal.pcbi.1003903

(4) Statement on Gender Balance at ECM31, 2018. Available at https://ecm31.ecanews.org/en/statement-on-gender-balance.php

(5) CCDC and BCA, International Year of the Periodic Table, celebrated through crystals, 2019, Available at https://www.ccdc.cam.ac.uk/Community/educationalresources/PeriodicTable/

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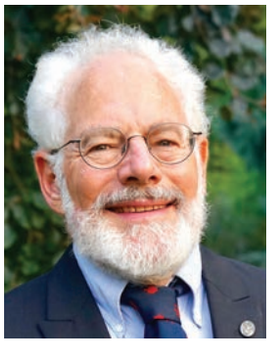

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Saturday, July 20 - Wednesday, July 24, 2019

Important Deadlines

Travel Grant Application Deadline: March 29, 2019
Abstract Deadline: March 29, 2019
Early Registration Deadline: May 31, 2019
Hotel Reservation Deadline: June 28, 2019

ACCESS UPDATED MEETING INFORMATION:

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Abstract submission - Meeting registration - Full call for papers
Sponsorship opportunities
Information for exhibitors

Abstracts accepted online only
(*at least 40% of all talks will be from contributed abstracts*)

Preliminary Program ACA 2019 Annual Meeting July 20 - 24, 2019

Saturday July 20, 2019		Sunday July 21, 2019			Monday July 22, 2019			Tuesday July 23, 2019			Wednesday July 24, 2019			Thursday July 25, 2019
Workshops		**Sessions**	**Session Chairs**	**SIG**	**Sessions**	**Session Chairs**	**SIG**	**Sessions**	**Session Chairs**	**SIG**	**Sessions**	**Session Chairs**	**SIG**	
Morning		**Morning**			**Morning**			**Morning**			**Morning**			**Morning**
Workshop	**Session Chairs**													
		PL1 - K. Trueblood Award: Brian Toby & Robert Von Dreele			PL2 - Fankuchen Award: Eaton (Ed) Lattman			PL3 - Bau Award: Bryan Chaikoumakos			PL4 -Margaret C. Etter Early Career Award: Efrain Rodriguez			PLN2020 - 2020 Planning Meeting
WK1 - Advanced Structural Characterization of Nanomaterials	Thomas Proffen Katharine Page	T1 - Transactions—Data Best Practices: Current State and Future Needs	Nick Sauter John Rose. Talapady Bhat	BPDAA, CryoEm, BioMac, Light Sources, General Interest, Small Angle Scattering, Industrial, Small Molecule	2.1.1 - Structure in Cancer Biology I	Elizabeth Goldsmith John Tainer	BioMac, Canadian Div.	3.1.1 - Structure in Cancer Biology II	John Tainer Elizabeth Goldsmith	BioMac, Canadian Div.	4.1.1 - Central Dogma in 3D: the Legacy of Tom Steitz	Phoebe A. Rice Miljan Simonovic	BioMac	
WK2 - Accelerating your Career Development	Chelsy C Chesterman Korey Carter Kenneth Childers	1.1.1 - Macromolecular Structure Under Physiological Conditions	Richard Gillilan Aina Cohen	BioMac, Small Angle Scattering	2.1.2 - Micro-Electron Diffraction	Tamir Gonen Gerd Rosenbaum	CryoEM, BPDAA	3.1.2 - Time Resolved Macromolecular Structure Determination at X-ray Free Electron Lasers	Marius Schmidt Christopher Kupitz	Light Sources, BioMac	4.1.2 - Radiation damage in X-ray crystallography and cryo-EM	Dominika Borek Gerd Rosenbaum	Light Sources, Cryo-EM, BPDAA, BioMac	
WK3 - Introduction to PHENIX for electron cryo-microscopists	Paul Adams	1.1.2 - Cutting Edge Studies using Cryo Electron Microscopes	Rui Zhao Stephen Burley	CryoEM, Canadian Div.	2.1.3 - Diffuse Scattering for Biological Structure and Dynamics	Steve Meisberger Mike Wall	Small Angle Scattering	3.1.3 - Structural biology combining solution SAS and high resolution methods (cryoEM, MX, NMR)	Jesse Hopkins Nigel Kirby	Small Angle Scattering, BioMac	4.1.3 - Cool Structures: Important Science from Small Molecule Crystallography	Karah Knope Louise Dawe	Small Molecule, Service Crystallography, Canadian Div.	
WK4 - Saturday Morning Serial Crystallography: Obtaining Protein Structure from Many Crystals	Jennifer Wierman Aaron Finke Nicholas Sauter Graeme Winter Aina Cohen	1.1.3 - Morphological Characterization of Porous Materials	Lilin He Tao Li. Charl J Jafta	Small Angle Scattering, Materials, Powder Diffraction	2.1.4 - Solid State NMR Crystallography	Manish Mehta, Tomislav Friscic	Small Molecule, Neutron, Materials, Powder, Canadian Div.	3.1.4 - Solid State Supramolecular Chemistry and Crystal Engineering Part I	Wilhelm Maximilian Hützler Dmitriy V. Soldatov	Small Molecule, YSIG	*4.1.4 - In situ and Operando* Characterization of Functional Films	Joe Strzalka Uta Ruett	Neutron, Materials, Powder, Small Angle Scattering	
WK6 - Phase Identification and Materials Characterization Using Powder X-ray Diffraction	Thomas Blanton Graciela Diaz de Delgado	1.1.4 - Crystallography in the Geosciences	Nichole Valdez J. Caleb Chappell	Small Molecule, Neutron, Materials, Powder Diffraction	2.1.5 - Crystal Structure Solution from Powder Data	Fernando Uribe-Romo	Powder, Materials, Neutrons	3.1.5 - Functional Sustainable Materials	Craig A. Bridges Matthew Logan	Materials, Neutron, Powder Diffraction	4.1.5 - Diversity & Inclusion -- Diverse Teams Perform Better	Anna Gardberg Tooba Shamsi Rebecca McAuliffe	Industrial, YSIG	
					2.1.6 - What is a crystal, in time and space?	Joseph H. Reibenspies	Small Molecule				4.1.6 - General Interest II	Brandon Mercado Travis Mitchell Matthew Brown Joe Tanski	General Interest, YSIG	
		Noon			**NOON**			**Noon**			**Noon**			
		SIG meetings			SIG meetings			SIG meetings			SIG Meetings			
		TMT1 - Three Minute Thesis	Chelsy Chesterman Korey Carter Victor Young	YSIG	TMT2 - Three Minute Thesis - Finals	Chelsy Chesterman Korey Carter Victor Young	YSIG							
Afternoon		**Afternoon**			**Afternoon**			**Afternoon**			**Afternoon**			
WK1 - Advanced Structural Characterization of Nanomaterials	Thomas Proffen Katharine Page	T2 - Transactions—Data Best Practices: Current State and Future Needs	Nick Sauter. John Rose. Talapady Bhat	BPDAA, CryoEm, BioMac, Light Sources, General Interest, Small Angle Scattering, Industrial, Small Molecule	2.2.1 - Powder Diffraction in Industry	James A. Kaduk Elena Kabova	Powder, Industrial	3.2.1 - Application of anomalous techniques in macromolecular crystallography	Armin Wagner Toshiya Senda	Light Sources, BioMac	4.2.1 - What is the Meaning of Resolution?	Raquel Bromberg Zbyszek Otwinowski	CryoEM, BioMac, BPDAA	
WK3 - Introduction to PHENIX for electron cryo-microscopists	Paul Adams	1.2.1 - Structure Without Structure [Structural Dynamics Session]	Garrett M. Ginell Gerald F. Audette	YSIG, BioMac, Canadian Div.	2.2.2 - New toys: Sources, Beamlines and Detectors	Ana Gonzalez James Holton	Light Sources, Neutron, Materials, Powder, Canadian Div.	3.2.2 - SAS Contrast Methods in Biology and Soft Matter	Volker Urban Kushol Gupta	SAS, Neutrons, Materials	4.2.2 - Structure Based Drug Design	Thierry Fischmann Kenton Longenecker	Industrial	
WK4 - Saturday Morning Serial Crystallography: Obtaining Protein Structure from Many Crystals	Jennifer Wierman Aaron Finke Nicholas Sauter Graeme Winter Aina Cohen	1.2.2 - Crystallography at Extreme Conditions	Camelia V. Stan Christine M. Beavers	Small Molecule, Neutron, Materials, Powder Diffraction	2.2.3 - Locating and refining H atoms using X-rays, Neutrons, and Solid-State NMR	James Harper Brandon Mercado Yu-Sheng Chen	Materials, Powders, Neutrons, Service Crystallography, Small Molecule	3.2.3 - Home-Built Software and Hardware	Victor Young Larry Falvello	Service	4.2.3 - Cool Structures: Important Science from Small Molecule Crystallography	Jeffrey Bacon Stacey Smith	Small Molecule, Service Crystallography, Canadian Div.	
WK6 - Phase Identification and Materials Characterization Using Powder X-ray Diffraction	Thomas Blanton Graciela Diaz de Delgado	1.2.3 - Understanding Polymer Structure and Dynamics During and After Processing	Thomas Fitzgibbons Ronald Jones	Small Angle Scattering	2.2.4 - General Interest I	Brandon Mercado Travis Mitchell Matthew Brown Joe Tanski	General Interest, YSIG	3.2.4 - Solid State Supramolecular Chemistry and Crystal Engineering Part II	Wilhelm Maximilian Hützler Dmitriy V. Soldatov	Small Molecule, YSIG	*4.2.4 - In situ and Operando* Measurements	Andrey A. Yakovenko	Materials, Neutron, Powder	
		1..2.4 - Magnetic, quantum, and electronic correlated materials	Efrain E. Rodriguez Branton Campbell	Neutron, Materials, Powder Diffraction	2.2.5 - Crystallization on the International Space Station	Marc Giulianotti Ken Savin	Service Crystallography, Small Molecule, General Interest, BioMac, Materials, Powder Diffraction, Neutron				4.2.5 - Sustaining Crystallography Education and Training	Joe Tanski Brian Toby	General Interest, Service Crystallography	
					WK5A - Cryo-EM Workshop I : Image Processing	Cathy Lawson Wen Jiang Michael Cianfrocco		WK5B - Cryo-EM Workshop II : Reconstruction	Cathy Lawson Wen Jiang Michael Cianfrocco					
Evening		**Evening**			**Evening**			**Evening**			**Evening**			
Opening Keynote Lecture		SIG meetings			SIG meetings			SIG meetings			SIG meetings			
		PS1 - POSTER SESSION #1	Louise Dawe David Rose		PS2 - POSTER SESSION #2	Louise Dawe David Rose		PS3 - POSTER SESSION #3	Louise Dawe David Rose		BAN - Banquet			
Opening Reception														
		1.3.1 - Open Exchanges in Crystallographic Education	Andy Torelli Kraig Wheeler	YSSIG, Continuing Education Committee	Young Scientist Mixer			3.3.1 - Would You Publish This?	Danielle Gray Carla Slebodnick	Service, Small Molecule				
					Fellows Reception									
								AMBM All Members Business Meeting						

	Regular Room Rate	Student Room Rate
Cincinnati Marriott RiverCenter	*$159 Per Night* *Plus Customary Taxes & Fees*	*$129 Per Night* *Plus Customary Taxes & Fees*
Embassy Suites Cincinnati RiverCenter	*$159 Per Night* *Plus Customary Taxes & Fees*	*$129 Per Night* *Plus Customary Taxes & Fees*

General Meeting Information

Venue:

All scientific sessions, workshops and poster exhibits will take place at the Northern Kentucky Convention Center, 1 W Rivercenter Blvd., Covington, KY 41011, http://www.nkycc.com/.

Hotel:

There are two hotels with dedicated ACA room blocks: the Cincinnati Marriott RiverCenter (10 West Rivercenter Blvd., Covington, Kentucky 41011) and the Embassy Suites Cincinnati RiverCenter (10 East Rivercenter Blvd., Covington, KY 41011).

We are able to offer discounted room rates because of our commitment to a contract for a minimum number of sleeping rooms at these two specific hotels. We encourage all attendees to support the ACA and reserve a room in the conference block. With your support, the ACA can continue to provide discounted room rates to attendees in the future.

The Northern Kentucky Convention Center is centrally located across the street from each of these hotels and is less than a minute walk away.

Travel:

The Cincinnati/Northern Kentucky International Airport (CVG) is consistently ranked as one of the best airports in the world. Northern Kentucky is within a two-hour flight from 60 percent of the nation's population. Cincinnati/Northern Kentucky is also within only a two-hour drive of the Port Columbus International Airport (CMH), Dayton International Airport (DAY), Louisville International Airport (SDF) and Lexington's Blue Grass Airport (LEX).

Foreign Travelers:

Obtaining a VISA: Advanced planning by foreign travelers is critical. Obtaining a VISA is the sole responsibility of the attendee. Meeting attendees should first determine whether a VISA is needed and if so, applications should be made at least ninety (90) days in advance of the travel date.

Helpful information regarding traveling to the US can be found on the US Department of State: Bureau of Consular Affairs (https://travel.state.gov/content/travel.html) and through the International Visitors Office (http://sites.nationalacademies.org/PGA/biso/visas/index.htm).

If you require a participation letter to the conference to submit with your application, please e-mail your request to: aca@hwi.buffalo.edu. Please include your name, passport #, birth date, mailing address, e-mail address and the title(s) of any abstract(s) that you have submitted for the conference. A copy of the letter will be e-mailed to you.

Financial Support:

Members and attendees are important to the ACA and as such there are a number of opportunities for financial support to attend the meeting:

- Become a member! Discounted Meeting registration fees are available to members.
- ACA Travel support will be available for young scientists from the ACA. Applications for travel support will be available on the ACA's website and should be submitted to the ACA by March 31, 2019.
- More opportunities for travel support from ACA partners will be posted on the 2019 Annual Meeting website as they become available. The 2018 meeting provided over $10,000 of travel support from our partners and we hope to continue to provide the same level of support in the future.
- Become a session room volunteer! Registered students and post-docs attending the 2019 ACA Annual Meeting can apply to be session room monitors. Session room monitors operate audiovisual equipment, and room lighting, photograph the speakers (cameras provided), track and record attendance, and perform other tasks requested by the session chairs. Applications to be a session room volunteer will be available on the ACA's website and should be submitted to the ACA by May 1, 2019.
- Volunteer at the front desk! Registered students and post-docs attending the 2019 ACA Annual Meeting can help hand out registration packets and assist attendees with general questions and inquiries. Volunteer for one (1) full-day (7:00 a.m.–4:00 p.m.) and receive half-off regular student/post-doc registration.
- Share a room! This is an option facilitated by the ACA to help those looking to save money on their hotel accommodations by sharing the cost of a hotel room. The ACA only assists in facilitating contact between roommates and does not guarantee room availability. Further, attendees/roommates are responsible for making their own hotel reservations. Check out the ACA's website for information on sharing a room and to find a list of attendees looking for roommates.

Program Information: All attendees will receive a hard copy of the program book, but the full set of abstracts will only be available online.


Tomislav Friščić

While I am writing this, we are still deep in the throes of Winter. As 2019 is getting into full speed and preparations for the Annual ACA meeting, this year in Covington, Kentucky, are underway I would like to highlight a few important meetings of ours taking place in Canada. The first one is this year's embodiment of the traditional powder X-ray diffraction workshop. The 12th Canadian Powder Diffraction Workshop in 2019 will take place in Trois-Rivieres (Quebec), hosted by Jacques Huot (Université de Québec à Trois-Rivières, UQTR) and Patrick Mercier (National Research Council) from 8-11 May. The first announcement can be found on the webpage of the Canadian National Committee for Crystallography (CNCC):

https://xtallography.ca/index.php/xtal/meetings/cpdw-12/

This year, the workshop will be strategically organized just before the GAC-MAC-AIH Geosciences meeting, which will take place in Quebec City, 12-15 May 2019. For more information for people with geoscience interest, check out the meeting webpage:

https://gacmac-quebec2019.ca/overview/

I am also tremendously glad to tell you that this year will also see the 6th installment of the Crystal Engineering and Emerging Materials Workshop of Ontario & Quebec meeting (CEMWOQ-6). The meeting this year will stay in Montreal, and will be organized by Ashlee J. Howarth, Marek Majewski and Louis A. Cuccia at Concordia University, from 30 May to 1 June 2019. This meeting is unique in Canada, and perhaps in North America, by the fact that it brings an exciting program on crystal engineering, materials science and crystallography, with absolutely no registration fee! This year's Plenary and Invited Speakers have just been announced, and include Andrew Cooper from the University of Liverpool, UK, Dominik Cinčić from the University of Zagreb, Croatia, Michael Wolf from the University of British Columbia, Anna Gudmundsdottir from the University of Cincinnatti, USA, Murallee Murugesu from the University of Ottawa, and a number of other high-flying researchers. To register (did I mention it was free?) and more information, please visit the meeting webpage:

https://www.concordia.ca/artsci/chemistry/cemwoq6.html

The CEMWOQ-6 meeting is strategically placed just before the most important Canadian chemists' meeting, the 102nd Annual Meeting of the Canadian Society of Chemistry (CSC), which will be taking place in Quebec City, 3-7 June 2019 and is organized by Western University. This meeting will also feature events of interest to the community of crystallographers and crystal engineers, notably the Dynamic Molecular Materials Symposium, being organized by Kathryn Preuss and Dima Soldatov at the University of Guelph, and Stephen J. Loeb at the University of Windsor. For more information on the 102nd CSC meeting, check out the webpage of the conference:

http://www.ccce2019.ca/

For this postcard from Canada, I would like to highlight two eminent members of the crystallographic community here in Canada, Hanna A. Dabkowska at McMaster University, and Miroslaw Cygler at the Department of Biohemistry, Microbiology & Immunology, University of Saskatchewan.

Hanna Dabkowska is a Research Scientist whose interests are focused on challenges of crystal growth and characterization of oxide materials. Her research demands expertise in crystal growth by Optical Floating Zone Method, Growth from High Temperature Solutions, as well as Top Seeding, Czochralski, Directional Solidification and Bridgman Techniques, which leads to fantastic crystalline samples of high-melting oxides such as different cuprates, including superconducting materials, ferrites, germanates, tungstates, vanadates, and many more, often including rare earth elements. Hanna received a M.Sc. degree in Chemistry from the University of Warsaw in Poland, and a Ph.D. degree in Physics from the Institute of Physics of the Polish Academy of Science. She was employed as an Assistant Professor at the Institute of Physics, Polish Academy of Sciences until 1990 when she joined

McMaster University as a Research Scientist. During this time (1979, 1980, 1985) she also periodically worked in the Crystal Growth facilities in Clarendon Laboratory, University of Oxford (UK), and was a visiting scientist at the Crystal Growth Laboratory in Moscow State University in Russia (1976). For her work she twice received the Award of the Secretary of the Polish Academy of Sciences, and was a three times recipient of the British Council Scholarship.

Her work and unique expertise are critical for the studies and understanding of properties of these technologically highly important materials, enabling the synthesis of high quality crystalline samples for magnetic, neutron and other types of studies. In that context, she has also provided educational and guiding materials, for example chapters on crystal growth in the Handbook of Crystal Growth, Vol. II (Elsevier, 2015), Springer Handbook of Crystal Growth, Defects and Characterization (Springer-Verlag, 2010), Elementary Crystal Growth (SAAN Publishers, 1994) and more. She often works with her husband, Antoni Dabkowski and they both have a great time doing so. Obviously they are a dynamic team and an inspiration to the younger generation, as both their children have also decided to pursue a path in Science.

Figure 1. (a) Hanna Dabkowska, McMaster University, current Vice-President of the IUCr; (b) some of the single crystal oxide samples grown by Hanna and (c) Hanna and Antoni with the research group at McMaster Laboratory. Photos provided by Hanna Dabkowska, and more can be found on her website: www.bimr.ca/people/hanna-dabkowska.

However, Hanna Dabkowska is also particularly notable in Canada and internationally for her services to the crystallography community, as she served from 2005 to 2011 as a Member of the Canadian Co-Data Organisation, and in the period 2005-2011 was also the Chair of the Commission of Crystal Growth and Characterization of Materials in the International Union of Crystallography (IUCr). From 2011 until 2017 Hanna served as a Member of the Executive Committee of the IUCr and was elected Vice-President of the IUCr in August 2017. In the same period, Hanna also held other important posts with the IUCr, such as Chair of Calendar Committee, Executive Committee, IUCr (2013-2016) and since 2013 is also Secretary of the Executive Committee of International Organization for Crystal Growth (IOCG)

Miroslaw Cygler (Figure 2a) is presently a Professor and a Tier I Canada Research Chair at the Department of Biochemistry, Microbiology & Immunology, University of Saskatchewan. He obtained his Ph.D. in Crystallography from the University of Lodz in Poland, and later spent two years as a Research Associate at the Division of Biological Sciences, National Research Council (NRC) in Canada, working with one of the pioneers of crystallographic computing, Dr. F.R. Ahmed. He subsequently joined the laboratory of Dr. W.F. Anderson at the Department of Biochemistry, University of Alberta in Edmonton, focusing on protein-nucleic acid interactions. In 1987, he moved to the Biotechnology Research Institute, NRC in Montreal to organize the protein crystallography laboratory. There he headed the Macromolecular Structure Group, achieving the rank of Principal Research Officer. In 2011, he moved to the University of Saskatchewan, home of the Canadian Light Source (CLS) synchrotron. His current focus is on structure and function of protein complexes, with an emphasis on proteins involved in host-pathogen interactions,

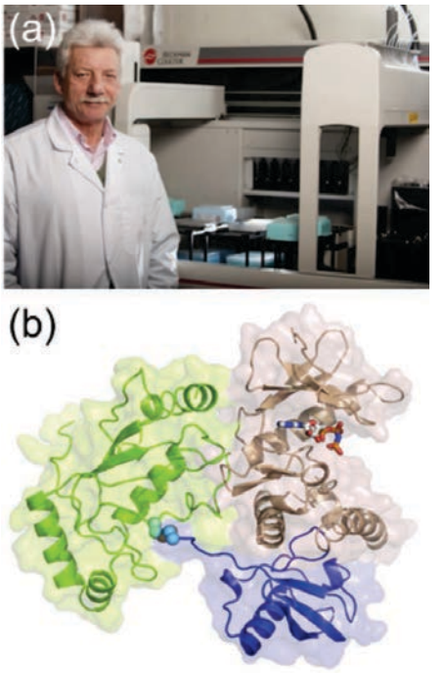


Figure 2. (a) Miroslaw Cygler in the laboratory and (b) structure of a complex between the effector kinase OspG and the UbcH7 ubiquitin conjugating enzyme with ubiquitin. Obtained from the Cygler laboratory website: www.usask.ca/research-groups/cygler/index.php.

molecular machinery for assembly of iron-sulfur clusters and polysaccharide degrading enzymes. He is a member of the Editorial Advisory board of the journal Protein Engineering, Design and Selection, and a recipient of the NRC Outstanding Research Achievement Award, the CLS Allen Pratt Memorial Award, and was recently honored by being elected a Fellow to the Canadian Academy of Health Sciences. Throughout his career, Miroslaw has strongly focused on structure-function relationships of proteins, with a primary focus on molecular mechanisms of action.

There are a number of significant contributions resulting from Miroslaw's work, and I am particularly fascinated by exploration of the bacterial and mitochondrial machinery for the assembly of the Fe-S cluster essential cofactors. Whereas the structures of individual components of this molecular machine were previously known, it was the work of Cygler in 2010 that provided the first crystal structure of the desulfurase-IscU Fe-S scaffold complex from E. coli and also the desulfurase-TusA complex, which delivers sulfur for tRNA modification (see: Shi et al. Structural Basis for Fe-S Cluster Assembly and tRNA Thiolation Mediated by IscS Protein-Protein Interactions. PLoS Biology, 2010, 8, e1000354). These structures showed that the sulfur, in persulfide form, located at the tip of a long loop can be delivered to different locations around the periphery of the active site, and that the iron-sulfur scaffold protein binds with the end containing 2Fe-2S assembly site directed toward the active site of the desulfurase. His recent work on eukaryotic assembly complex (see: Boniecki et al. Structure and functional dynamics of the mitochondrial Fe/S cluster synthesis complex. Nature Commun. 2017, 8, 1287) suggests the two eukaryotic-specific components, ISD11 and ACP play a regulatory role, connecting the Fe-S cluster assembly with respiratory chain and lipid synthesis in mitochondria. Another recent set of exciting contributions from the Cygler laboratory resulted from the focus on host-pathogen interactions (Figure 2b), especially on the structure and function of effector protein – virulence factors injected into the host cell via secretion system machineries. The Cygler team has determined the structures of ~20 effectors and identified for some of them their cellular targets, leading ongoing functional studies in the Cygler laboratory, as well as in collaboration with leading groups in the field. He has shown, for example, that some bacterial effector kinases are activated by binding to cellular targets rather than by phosphorylation of the activation loop. This work is making an impact on understanding the molecular foundation of pathogen infection mechanisms, and some of recent published work includes: Grishin et al. NleH Defines a New Family of Bacterial Effector Kinases. Structure, 2014, 22, 250, D'Costa et al. Salmonella Disrupts Host Endocytic Trafficking by SopD2-Mediated Inhibition of Rab7. Cell Rep. 2015, 12, 1508 or Xu et al. Crystal Structure of the Salmonella Typhimurium Effector GtgE. PloS One, 2016, 11, e0166643.

I would also like to highlight Miroslaw Cygler's work on the structure and function of lipases, which led to a discovery of the Ser-His-Glu catalytic triad (Schrag et al. Ser-His-Glu Triad Forms the Catalytic Site of the Lipase from Geotrichum Candidum, Nature, 1991, 51, 761),

which was observed independently and at about the same time by Joel Sussman and colleagues in acetylcholine esterase. This key paper changed the paradigm of the hydrolytic serine proteases active site, by showing that the third partner of the triad does not have to be an aspartate - but that a glutamate can equally well play this role. The lipase and acetylcholine esterase displayed the same fold, shared in part by three other proteins whose structures were determined in the same year, and named the alpha/beta hydrolase fold. The description of this fold, and comparison of the five structures, was provided in another seminal paper The Alpha/Beta-Hydrolase Fold, Protein Engineering 1992, 5, 197. This fold was later identified in many other proteins, and is now considered one of the most common folds in protein structures.

The Cygler laboratory has made a number of other significant contributions in context of protein structural biochemistry, but the available space in this column is too short to describe them all. However, I invite you to check out Miroslaw Cygler's work on the mechanism of the bacterial cell surface O-antigen length determination (for example, see: Tocilj et al. Bacterial Polysaccharide Co-polymerases Share a Common Framework for Control of Polymer Length, Nat. Struct. Mol. Biol. 2008, 15, 130), the extensive work on the structural genomics of E. coli as a bacterial model organism (for example, see: Cygler et al. Bacterial Structural Genomics Initiative: Overview of Methods and Technologies Applied to the Process of Structure Determination Methods Mol Biol. 2008, 426, 537), results on the crystal structure of the lumenal fragment of calnexin, the prototypic protein of the endoplasmic reticulum quality control system (seeI Schrag et al. The structure of calnexin, an ER chaperone involved in quality control of protein folding, Mol. Cell, 2001, 8, 633) and the work on the molecular mechanism by which cysteine protease proenzymes are inhibited by their propeptides (for example, see: Sivaraman et al. Crystal Structure of Human Procathepsin X: a Cysteine Protease with the Proregion Covalently Linked to the Active Site Cysteine, J. Mol. Biol. 2000, 295, 939).

Finally, if you wish to know more about our Canadian National Committee for Crystallography and its activities, a lot of information can be found on the exciting and often updated webpage that has been put up and is constantly improved by Louise Dawe at Wilfrid Laurier University:

http://xtallography.ca/

So much from Canada in this issue of ACA Reflexions. As always please feel free to contact me on my e-mail address tomislav.friscic@mcgill.ca with any comments, critiques or suggestions of topics, and information of the events or people that you think should be highlighted in this column.

Keep warm!

Thomas Steitz
2009 Nobel Prize Winner in Chemistry

On October 9th of the past year Tom Steitz passed away in his home in Brandford, Connecticut, after fighting pancreatic cancer. Tom was a Sterling Professor of Molecular Biophysics and Biochemistry, and a Professor of Chemistry at Yale, where he had been on the faculty since 1970. He was also an investigator for the Howard Hughes Medical Institute.

Born in Milwaukee, Wisconsin, he graduated in 1962 from the Lawrence University in Appleton, Wisconsin. He received his Ph.D. in biochemistry and molecular biology from Harvard University in 1966 under William Lipscomb's mentorship. After his postdoctoral research at the Laboratory of Molecular Biology at the University of Cambridge he had a short stint as assistant professor at the University of California at Berkeley before coming to Yale.

Tom's scientific contributions focused on structural characterization of biomolecules involved in the central dogma of biology: the process going from genes to protein. His most renowned work – for which he shared the Nobel price of Chemistry in 2009 – is of the first structure of the ribosome large subunit, in collaboration with Peter Moore. The structure was solved in the year 2000 at 2.4Å resolution, a remarkable achievement considering the complexity of the molecule, with 27 protein chains in addition to the 2 RNA strands, one of them more than 2,900 nucleic acid long. The ***s***tructure paved the way to understanding at a structural level

the synthesis of proteins, as well as paving the way for elucidating how several antibiotics work upon binding to the ribosome.

There are too many landmark structures that Tom solved in his career to mention here. Among them are the first structure of a DNA polymerase and the first structure of a tRNA synthetase complexed with its cognate transfer RNA and ATP. A particularly note-worthy structure is that of the HIV reverse transcriptase. At the time the nucleoside analog reverse-transcriptase inhibitor AZT was the only treatment. A structure of the compound bound to the protein could spearhead the developments of new generations of inhibitors, and many Laboratories around the world entered the race to be first to solve the structure of the enzyme at high resolution, a race that ultimately Tom won. The structural work impacted the discovery of new generations of medicines.

Thierry Fischmann
Merck & Co., Inc., Kenilworth, NJ, USA

Photograph courtesy of the Yale School of Medicine

Remembering Håkon Hope

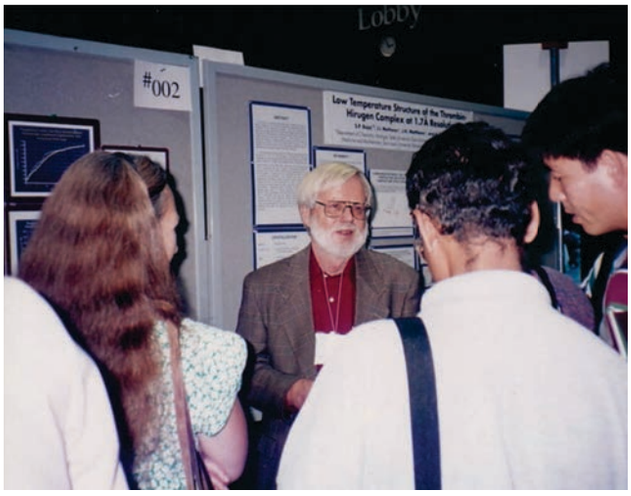
Håkon Hope

Håkon Hope, professor emeritus of chemistry at the University of California - Davis, passed away on November 22, 2018, at the age of 87. Håkon Hope has been called the Father of Cryo-crystallography and his work is recognized as resulting in a transformation of macromolecular crystallography. Following are the remembrances of several of our community who knew Håkon well.

Ada Yonath: Prof. Håkon Hope was an exceptional scientist who made seminal methodological contributions. His insights and experimental design were decades ahead of his time. As such, he advanced not only my research beyond my

wildest expectations, but also made extraordinary contributions to the entire field of structural biology.

I met him first when I was a student. Håkon was collaborating with Fred Hirshfeld on on accurate charge density distribution, focusing on very small molecules. We, the students, were ridiculing: "Håkon and Freddy know the location and charge of each portion of each electron at each fraction of time, in all two-atom molecules"…. Who could imagine that he would even consider ribosomes? That he would challenge the extreme deterioration of ribosome crystals during data collection at ambient (or slightly cooled) temperatures, as performed until the late eighties, kept at controlled humidity in glass capillaries. To reduce or eliminate this terrible damage, which actually led me to consider stopping the ribosome-structure project, Håkon suggested applying his unique cryo temperature procedure, which greatly reduces internal thermal vibrations. It required uniform flash freezing (thus did not allow capillaries) by dipping the crystals, which contained about 2.5 M salts, into an inert viscose solution. It sounded impossible, but Håkon did not give up. He came to Israel for almost a year, during which we sacrificed almost 100 crystals… The result is well known. It is among his most exciting key achievements. Thus, his bold attitude led to the development of what, almost instantaneously, became routine worldwide. Not only several ribosome structures were determined at atomic resolution, over 50,000 new and significant structures were elucidated at cryo temperature, many of which were not suitable for traditional data collection methods.



Sue Byram: Professor Håkon Hope was a mentor and a friend, and directly responsible for my joining the single crystal diffractometer company Syntex Analytical Instruments, which later became the X-ray group at Bruker. I was writing crystallographic software at National Research Council in Canada with Eric Gabe when I moved back to the San Francisco Bay Area near Stanford. I asked Eric for suggestions on working in crystallography, and he said "contact Håkon Hope at UC Davis."

That's a bit far away from Stanford, I thought, but I rang up Håkon. In his typical whimsical fashion, Håkon explained nothing further than to say "contact Carl Djerassi at Stanford." Hmm, thought I, I'm not sure what that is all about. With some trepidation I rang up the great Professor Djerassi and explained who I was to his Administrative Assistant. The next day I was invited to visit Syntex Analytical Instruments and offered a software position working for Bob Sparks. Professor Djerassi, unknown to me but well known to Håkon, was the Director of Research at Syntex and was Bob Sparks' boss' boss. Thank you, Håkon, for the rest of my career!

For decades, Håkon kept us all in line crystallographically and linguistically. He regularly read and offered improvements to our manuals, and was central to the design of our low temperature devices. We spoke often and met regularly at ACA, ECM and IUCr meetings, often with his wife Sally and children Erik and Mollie. I much admired their multi-lingual family – Håkon spoke only Norwegian with the children, while Sally spoke English with them. Quite an achievement for all of them.

Marilyn Olmstead: My interest in crystallography was first sparked by Tom Dunne, my senior thesis advisor at Reed College who had been a post-doc with F. A. Cotton in 1963 and had determined a structure of a cobalt complex. Then Larry Dahl, a member of my Ph.D. thesis committee at the University of Wisconsin, assured me that I would love crystallography and besides, "women were good at it." However, my research up until then had nothing to do with crystallography. I decided to follow that crystallography interest a few years after moving to UC Davis with my husband, Alan, in 1969. I was hired as a half-time lecturer in the Department of Chemistry. Since I had experience

with computers and computer programming, I was able to convince newly appointed associate professor Håkon Hope to take me on as a part-time post-doc.

What I recall about Håkon in those early days was how much more he knew than I did and how he enjoyed impressing me with his superior knowledge. I was a willing subject. I did love crystallography. He and his assistant, Karen Swanson, taught me everything I needed to know to solve my first structure, starting from the Weissenberg camera and then to the new green machine, the 4-circle Picker diffractometer. His pride and joy was the low temperature apparatus that he had built, able to collect data at an amazing 85 K. Not only was he a gifted experimentalist, his knowledge of theory was far more advanced than anyone needs to know today. I still have copies of his lecture notes from 1978, filled with integrals and operators. He wrote a Fortran program that would read in reflection data and output the seven reflections with the most statistically significant Bijvoet differences. Those seven reflections would then be carefully remeasured, including their Laue equivalents, and the absolute configuration determined. It worked most of the time.

I have an assortment of other memories. We had champagne glasses in the X-ray lab in order to celebrate the determination of each new structure. He ate canned tuna directly from the can for lunch. He ate a pomegranate by chomping down directly on the fruit, not caring about the seeds and juice spilling everywhere. Bruce Noll and I still chuckle about that scene today. He clearly believed that, because he was Norwegian, he was a first-class cross-country skier.

His knowledge of crystallography and passion for the science was passed down to his students, colleagues, and both small molecule and protein crystallographers worldwide. The Department benefited a great deal from the strong program in crystallography he initiated. The legacy he left behind will not be forgotten. I am so very glad he came into my life.

Ed Stevens: It has been 50 years since I arrived at the University of California, Davis, as a new chemistry graduate student. I knew very little about X-ray crystallography, but the idea that the 3-dimensional structure of molecules could be determined by experiment was intriguing, and I chose Håkon Hope as my research advisor.

Håkon's lab had a Weissenberg camera and a precession camera for unit cell determination, and a Picker 4-circle diffractometer for data collection (state-of-the-art at the time). The diffractometer was not computer controlled, but was automated with an IBM card reader. The card reader would read the h,k,l and 4 setting angles of a reflection to be measured and the values were stored in binary in a large box of electromechanical relays. Motors drove the diffractometer to the given angles, the reflection was scanned, and the background and scan counts were punched on a following blank card.

To determine the crystal orientation, reflections were located and centered manually on the diffractometer, and positions plotted on polar graph paper in order to index the reflections. The orientation matrix was then determined by least-squares refinement of the indexed reflections using the departmental PDP8 computer. With the aid of the university main-frame computer, the orientation matrix could then be used to produce a deck of IBM cards that contained the predicted setting angles of each reflection for data collection. If the crystal orientation changed during data collection, it was necessary to repeat the process, and get a new deck of cards punched.

Data collection required frequent monitoring because the IBM card reader was prone to card jams, and the contacts of the electromechanical relays needed frequent cleaning. For long data collections, at night I slept on a cot in the lab with the hope that the silence of a malfunctioning instrument would awaken me.

After several group meetings where the basic theory of X-ray crystallography was introduced, Håkon gave me the task of writing a FORTRAN computer program for calculating a 3D Fourier summation for acentric structures (we had a program from UCLA that was only valid for centrosymmetric structures). For my Ph.D. dissertation, I measured the experimental electron density distributions of 3 compounds, and I wrote a computer program to correct X-ray intensity measurements for thermal diffuse scattering using crystal elastic constants.

Håkon was passionate about collecting accurate data, and was always eager to demonstrate that, with proper attention to experimental detail, it was possible to measure effects that would be lost in the noise of routine experiments. Examples include his interest in the measurement of electron density distributions and the determination of absolute configurations of structures using MoKα radiation with no elements heavier than oxygen.

Håkon loved to tinker. He invented a glass device for recrystallizing samples that relied on circular convection of a solvent to carry the solute from the heated side to a cooler side where it crystallized. While I was still at UC Davis, he had already started working on an improved nozzle for low temperature data collection that only required a single gas stream. I copied his design while doing postdoctoral research with Philip Coppens in Buffalo, and constructed a similar nozzle that I used for a number of low temperature charge density studies, including two studies of samples that were liquids at room temperature, and one that was a gas.

Now, Håkon is perhaps most noted for his promotion of the technique of flash cooling of crystals of macromolecule samples, and the use of low temperature data collection to limit radiation damage in those samples. As a research mentor, he was always calm, patient, and friendly. He continued to be helpful as my career developed, and I always looked forward to seeing him and having a chance to talk at meetings. Whenever I see the Travelocity commercial with the Norwegian gnome, I am reminded of the twinkle in his eye when he would have some new result or idea to share.

Four generations of crystallographers at UCD: Håkon Hope, Marilyn Olmstead, James Fettinger & Kamran Ghiassi

Martha Teeter: I first met Håkon Hope at the Japan IUCr meeting in 1972. I learned he was a highly respected experimentalist and good with low temperature techniques. Independently, I had been intrigued by the power of low temperature to improve X-ray data of protein crystals held in capillaries. While at Boston University, my graduate student Marc Whitlow and I devised an iso-propanol system for cooling protein crystals on our Syntex P21 diffractometer, using a commercial low temperature device. It had its difficulties.

When I met Håkon again at the Hamburg IUCr in 1984, he had cleverly devised a way to stabilize pyrophoric small molecules for cryo-crystallography using a drop of neutral oil at the end of a fine capillary mounted in a copper pin. With this ingenious method, he could mount the crystal air free, cool it in liquid nitrogen, and transfer it to a nitrogen stream on a diffractometer. He made special tongs with a high thermal mass block to keep the crystal cool from the microscope to the diffractometer.

At the Stanford ACA meeting in 1985, we discussed

applying his method to protein crystals. They lose solvent and decay in air and in the X-ray beam. Ordinarily, we mount protein crystals in capillaries sealed with wax, but that method seemed to interfere with low temperature data collection. The capillary often created turbulence in the cool gas stream, resulting in ice formation.

Håkon and I proposed to cool crystals of the protein I was studying (crambin) to liquid nitrogen temperatures with his method, and he collected diffractometer data to 0.83 Å later that year. It worked beautifully. This was the pioneering first use of his capillary-free mounting technique in liquid nitrogen for protein crystals. Now those techniques are routinely used. He continued to develop these cryo-crystallography techniques and popularize them, extending later work to liquid helium data collection. He worked closely with several synchrotron sites to freely share his experimental procedure and apparatus.

A second example of Håkon's inventiveness and experimental prowess came to my attention in 1987. I was visiting the Weizmann Institute and found that Håkon was also there. He had just created a small glass, double platform support for ribosome crystals grown by Ada Yonath. With this physical stabilization and application of liquid nitrogen to the crystal, they were able to extend the lifetime of ribosome crystals in the X-ray beam. It was this pivotal event, coupled with Ada's persistence in looking for better crystals and large heavy atom clusters, that led her and others to the solution of the ribosome structure and Ada's sharing the 2009 Nobel Prize in Chemistry. She has referred to Håkon as the Father of Cryo-crystallography.

Finally, Håkon delighted in teaching crystallography both in class and in informal conversations. He had accomplished this both at UC Davis Department of Chemistry and at ACA and IUCr meetings, which he had attended since 1968, hardly missing one. He was always advocating for his very high standards of data collection and refinement for determination of accurate structures.

At meetings, Håkon engaged me and others in dialog around accurate structure determination and held others to the high standards he himself used. He challenged many to think about their crystallography, in order to create the best possible structures. He was able to insure this attention to detail on an international level as a member of the IUCr Commission on Crystallographic Apparatus (1974-1984).

Håkon was a brilliant and inventive experimentalist, a caring and highly principled crystallographic educator, and a friend. He is sorely missed in Davis and in the crystallographic world.

Charles Campana: I first met Håkon Hope in 1980, when I joined Nicolet Instrument Corporation in Cupertino, California, as an applications scientist for single-crystal diffraction. The company was founded in 1968 by Bob Sparks and Tom Workman, as a division of Syntex Research. Håkon was instrumental in convincing Carl Djerassi, president of Syntex Research (and Stanford Professor), to fund the development of computer- controlled diffractometers (Syntex P-1, P21, P3/R3, etc.). Arild Christensen, a Håkon Hope postdoctoral fellow, was also hired as a crystallographer at Syntex Research and later Syntex Analytical Instruments, Inc. (SAI).

Håkon Hope established a world-class X-ray crystallographic facility at the University of California – Davis, where he mentored generations of faculty, staff and students. I was a frequent visitor to UCD where HåkonΩ demonstrated his techniques for collecting all small molecule datasets very quickly at 140K. From that point forward, I collected nearly all datasets using the Hope method.

The 1985 Stanford ACA meeting was a turning point in low-temperature crystallography of macromolecules. Prior to that time, low-temperature crystallography of proteins was done on four-circle diffractometers running in cold rooms at 4° F. Håkon Hope and Martha Teeter presented a paper at the Stanford meeting in which they had collected a complete overnight dataset on crambin at 140 K. This experiment defied the conventional wisdom that protein crystals could not be frozen - leading to the development of cryo-crystallography of proteins. 2009 Nobel Prize winner Ada Yonath has called Håkon "The father of cryo-crystallography" and

claimed that none of her research could have been done without Håkon's contributions.

On a personal note, I always enjoyed long conversations, in person or over the telephone, with Håkon. Håkon's discussions were logical, but not always concise. I would never interrupt him, knowing that he would 'rewind' and start over to include all the details of his explanation. Patience in listening to Håkon was always worth the effort!

Paul Swepston: I was attending my first ACA meeting and making my first poster presentation as a graduate student. I was nervous as I stood by my poster for the first time, hoping (perhaps praying) nobody would ask me any questions. Up walks this grizzled looking guy who I assumed was a professor somewhere. He stared at my poster and stared at my poster and stared at my poster and finally asked, in a Norwegian accent, how I had managed to isolate and crystallize the phosphine compound that I was presenting a structure of. I think I must have had a blank look on my face and then looked closely at my poster title and my eyeballs almost popped out: I had inadvertently written the formula for my triphenylphosphine group as "PPH3" rather than "PPh3." The discovery of that mistake led to a rather detailed review of my poster by Håkon Hope. That day he taught me a lesson about the importance of accuracy that I will never forget. The funny thing is that he was the only one to find the mistake during the whole poster session. I think the fact that he took the time to even look at my poster says a lot about his serious interest in helping students.

After that encounter there was never an ACA or IUCr meeting that I did not talk to Håkon and discuss a wide range of topics from the proper way to collect data to the most efficient way to cool crystals. He was one of those people who didn't blindly accept common scientific knowledge. Before Håkon very few people believed that you could successfully collect data on protein crystals at liquid nitrogen temperatures, but his pioneering work in that area transformed protein crystallography. He will be missed but his impact on structural science will be felt for a long time.

Bruce Noll: I met Håkon Hope in my first summer as a graduate student at UC Davis. When I joined the program in 1988, X-ray crystallography was something completely unknown to me. We may have covered it in one lecture of physical chemistry when I was an undergraduate, but that day was lost to me. This meant that Håkon's discussions were as foreign to me as his Norwegian! Fortunately, things became more clear during the lectures of his course. I grew to love the distinctly non-Cartesian relationships of crystals and fell into the X-ray lab as my second home.

Prior to college, I worked a number of years as a mechanic, so I was able to make a trade with Håkon and Marilyn Olmstead. I would help to maintain the hardware if they would teach me crystallography. Håkon always seemed to find a project on Friday afternoons, perhaps polishing the target of the rotating anode generator, or maybe exchanging the water in the heat exchangers for the instruments. So, it was on a Friday afternoon when I was submitting some refinements to the computer queue that Håkon entered the lab. As I was looking forward to spending a little time with friends over a beer or two, I did my best to ignore Håkon's inspection tour of the facility. Out of the corner of my eye, I spied him walking into the enclosure for the rotating anode system. I did my best to look down and focus on my work. I thought I might just get to the pub. Suddenly, over the din of the pumps and fans of the lab, I heard a plaintive "Uh oh, uh oh, uh oh…." I looked over to the enclosure to see Håkon bouncing on his clogs and holding firmly to the cooling-water supply hose for the anode. Water was rushing from the hose! I calmly asked "Do you need help?" and walked to the chiller to turn off the supply. Well, I didn't make it to the pub, but I did spend time with Håkon mopping the floor, crawling around the instrument to soak up all the spilled water, and repairing the water connection. A Haskris chiller can really pump some water!

Håkon and I built a friendship over Macintoshes, spelling and grammar in software and user manuals, and of course, low-temperature devices. His command of languages was second to none, and we shared a disdain for language errors on user interfaces and in documentation. Together we performed a thorough beta test of some second-generation diffractometer software and made pages of notes on the grammar alone. He said we are all scientists, and as such, we should be held to exacting language. Håkon expected a lot from his colleagues

and students. I'd like to think I earned his respect. I always looked forward to seeing him at the annual ACA meeting and will miss his presence.

Sean Parkin: I was Håkon's last Ph.D. student at UC Davis, from 1989 to 1993. Although he formally retired shortly before I graduated, he never stopped working: the X-ray lab was his domain. In terms of experimental skill, Håkon had few peers, and his mastery of the practical was bolstered by a deep understanding. He had two laws of crystallography: 'no two crystals are alike' and 'the highest observable symmetry is P1'. Both 'laws' have subtle hidden meaning, and if you didn't 'get it.' he knew, and judged accordingly. I have far too many fond memories of Håkon from the last three decades that it would be impossible to recount anything but a tiny fraction of them here. Nevertheless, here are a couple that people who knew Håkon well enough might enjoy.

Shortly after joining Håkon, at about the time we were planning a little research project to get me up to speed in the X-ray lab, he suffered an attack of gout. That naturally got us to talking about uric acid crystals. The structure of pure uric acid had been known for years, but a dihydrate, thought to be orthorhombic, remained unsolved. There was even a published recipe to grow crystals of the dihydrate, so although they were extremely thin plates, we had a good dataset pretty quickly. It was also immediately obvious that the crystals were not orthorhombic, but monoclinic – good old P21/c. The structure solved easily but refinement was poor, even after accounting for pseudo-orthorhombic twinning. By that point I was fairly self-reliant in the lab, so even though the uric acid project was incomplete, for me it had served its purpose and was relegated to a back burner. Much later, upon seeing a massively distorted orthorhombic model in Acta B, I had a 'smack my head' revelation, added whole-molecule disorder to the twinned model and showed it to Håkon. The fit was spectacular! Håkon's response was along the lines of "… oh good, I was wondering when you'd figure that out." I use that same dataset as a teaching tool to this day.

In addition to his experimental genius, Håkon excelled in the written word. He always strove for an ideal balance between information density, precision, and readability. He had little tolerance for nonsense, especially if it came from supposed positions of authority. I've long since forgotten the exact context, but a couple of his responses to particularly boneheaded review comments were: "The referee invents situations that have no counterpart in reality, and then argues against them." That was closely followed by: "The utility of a crystal structure determination is not measured by R, but by the scientific insight it provides." Those always bring a smile to my face!

Even after I left Davis, Håkon and I were in regular contact until shortly before his death. On the (too few) occasions that my work schedule took me back

Joel Sussman, Felix Frolow & Håkon Hope

to California, I usually tried to squeeze in a trip to Davis to see Håkon and Sally. On my last visit, in July 2017, we drove over to the Chemistry building to see the changes over the intervening quarter century. The X-ray labs were of course much changed – all modern equipment, many new faces etc. I was, however, delighted to find that Håkon was happily ensconced in the small lab in the annex that I had occupied as a grad student. There were still pictures on the walls and boxes of samples that I left there 24 years earlier! I'll be forever grateful to Håkon for his guidance and friendship over the years. Crystallography, for me, is quite different without him. It is rare for a day to go by when I don't think "… what would Håkon do?"

Kay Onan

Heuristic Views of Classical Results

Adapted from a talk be given in acceptance of the Fankuchen Award, July 2019

Eaton Lattman

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It is a particular honor and privilege to receive an award from one's own professional society, because it comes from colleagues who have a sharp-eyed understanding of what one has actually done. I offer heartfelt thanks to the ACA for this wonderful recognition. I am thrilled to receive this particular award because the roster of previous winners, as well as the award's denominator, form a Who's-Who list of my intellectual heroes in crystallography. For example, Isidor Fankuchen, whose home base was the Brooklyn Polytechnic Institute, had a wonderfully vivid persona. I have memories of attending a seminar there in which Marvin Goldberger from Princeton was presenting very deep work on a potential way of measuring phases by looking at the cross-correlation between signals measured from three simultaneous reflections. The discussion illustrated wonderful contrast between the Brooklyn and Princeton academic styles. Fan – as he was universally known –simply demanded that Goldberger cut through the formalism and make him understand.

As an aside, I now recognize that the ideas presented by Goldberger (Use of Intensity Correlations to Determine the Phase of a Scattering Amplitude, Marvin L. Goldberger, Harold W. Lewis, and Kenneth M. Watson, Phys. Rev. 132, 2764, 1963) are somehow related to the earlier - and initially wildly controversial - introduction of energy interferometry by Hanbury-Brown and Twiss in the area of radio astronomy. The approach broached by Goldberger et al was not realizable by any existing x-ray source in the 1970s, but might repay re-examination in the context of x-ray lasers.

Among the previous winners who have had great influence on me is David Sayre, with whom I developed a close friendship in our later years. I spent quite a bit of my graduate student life rediscovering things that David had figured out a generation before. His landmark paper Some Implications Of a Theorem Due To Shannon is only 362 words long, and has been cited 340 times. It lies at the heart of all current methods in protein crystallography that rely on oversampling the electron density function to assist phasing, e.g., the use of non-crystallographic symmetry. This is by far the most influential paper I know on a per-word basis.

Don Caspar was my joint post-doctoral advisor. He was enormously supportive but a truly deep thinker. Don would address a topic that he had been thinking about for thirty years, and assume you were right there with him. When I came to Brandeis I understood about 10% of what Don said, but by the time I left it was closer to 50%. That I believe was a record.

But enough of reminiscence. The description of the Fankuchen Award recognizes contributions by "one known to be an effective teacher of crystallography." This phrase has inspired me to choose a pedagogical rather than a research theme for my talk: Heuristic Views Of Classical Results. This is shorthand for a series of vignettes in which important crystallographic topics such as Bragg's Law are examined from a non-traditional, sometimes more intuitive, viewpoint that may make them easier to understand or visualize, at least for some people. In this article I would like to extract and slightly expand one of the vignettes in the talk.

The Temperature Factor

In figure 1a the hatched vector represents scattering from the j-th atom in a structure. As is familiar to all of us, the amplitude of scattering is given by the value of the atomic scattering factor f(h), while the phase of the scattering from this particular atom is given by $2\pi \boldsymbol{h}\cdot\boldsymbol{x}_j$, where h indexes a reciprocal lattice point and the $\boldsymbol{x}_j$ are the fractional coordinates of the atom. In figure 1b the scattering from this atom is reproduced on a reduced scale as the hatched vector running from the origin. The other hatched vectors in figure 1b picture the scattering from atoms corresponding to j in adjacent unit cells. Their positions are related to that of atom j by pure lattice translations. The collinearity of the scattering vectors from these translationally related atoms represents a statement of the von Laue condition: atoms related by pure translational symmetry scatter exactly in phase at reciprocal lattice points h. Thus, if there are N copies of atom j in a coherent scattering volume, the intensity is proportional to N^2f^2, where henceforth we suppress the subscript j for economy.

As traditionally used this diagram does not allow for the motion of atoms. It describes an idealized structure. But it is straightforward to introduce this. In figure 1a the solid vector represents the scattering from atom j when it has been shifted by a small amount $\Delta\boldsymbol{x}$ from its equilibrium position. Of course $\Delta\boldsymbol{x}$ varies rapidly and randomly with time, so that in reality the solid vector is moving continually through small, random angular displacements about its equilibrium position. At any instant the projection of the solid vector onto the ideal (hatched) direction is given by $\cos(2\pi \boldsymbol{h}\cdot\Delta\boldsymbol{x})$.

In panel b we introduce random orientational displacements for the set of atoms translationally related to j. Thus, the sum of the solid vectors, which represents the actual instantaneous scattering, executes a tipsy (but not fully drunken) walk along the ideal path given by the line of hatched vectors. It is the components of these solid vectors along the ideal, hatched direction that contribute to coherent scattering.

The scattering amplitude from the real structure is thus given by the projection of the solid vectors onto the ideal direction of the hatched vectors. This directly illustrates the reduction in scattering intensity introduced by atomic motion. The falloff in intensity becomes larger with increased atomic motions $\Delta\boldsymbol{x}$, and with increased h.

We can readily develop a more quantitative view of this scattering falloff. The time-average value of the ratio of the real to ideal scattering amplitude is given by

$$<\cos(2\pi\boldsymbol{h}\cdot\Delta\boldsymbol{x})>$$

where the notation <z> represents the expectation value of z. If we imagine that the values of $\Delta\boldsymbol{x}$ are Gaussianly distributed and are uncorrelated from atom to atom, then we can write that

$$<\cos(2\pi\boldsymbol{h}\cdot\Delta\boldsymbol{x})> = \int \exp(-|\Delta\boldsymbol{x}^2|/2u^2)\ \cos(2\pi\boldsymbol{h}\cdot\Delta\boldsymbol{x})dV$$

where $u^2 = <\Delta\boldsymbol{x}^2>$ is the mean square atomic displacement. This integral is a cosine Fourier transform of a Gaussian, for which the value is another Gaussian, Thus,

$$<\cos(2\pi\boldsymbol{h}\cdot\Delta\boldsymbol{x})> = \exp(-B\sin^2\theta/\lambda^2)$$

which is our old friend the Debye-Waller factor. B is the temperature factor given by $8\pi^2u^2$ in units of $Å^{-1}$. The details of going from $\boldsymbol{h}$ to $\sin\theta/\lambda$ have been glossed over.

Thus, the visual of the wobbling vector corresponding to a fluctuating atomic motion leads to both a qualitative and a quantitative understanding of the effects of uncorrelated atomic motions on Bragg scattering.

There is one more tidbit to be gleaned from this representation. Atomic motion cannot reduce total scattering; it can only redistribute it. So what happens to the scattering that is diverted from the Bragg peaks? The magnitude of this non-Bragg scattering can be calculated by forming a right triangle in which the hypotenuse is the total scattering f and the longer leg is the Bragg scattering $f\exp(-B\sin^2\theta/\lambda^2)$. In this simplistic view then

$$\text{Non-Bragg} = f^2(1-\exp(-2B\sin^2\theta/\lambda^2))$$

This approach takes no account of correlated motions among atoms, which lie at the heart of actual non-Bragg scattering patterns. Yet, if we substitute for our atom the "concerted unit" as developed by George Phillips we end with an equation that lies at the basis of a powerful and useful analysis.

Some material is this article has been adapted from Protein Crystallography: A Concise Guider by Eaton Lattman and Patrick Loll, JHU Press, 2009.

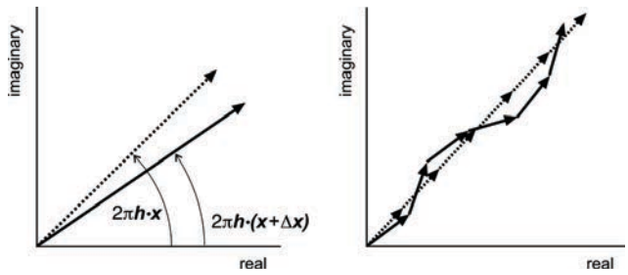

Figure 1. (a, left panel). Hatched line: contribution to the scattering at a reciprocal lattice point h by an atom at equilibrium position x. Solid line: contribution to the scattering by the same atom displaced by Δx. (b, right panel). Hatched lines: scattering by the same atom as in (a), plus scattering from corresponding atoms in a few adjacent unit cells. Solid lines: scattering from the same atoms each displaced by its own Δx. Note that the scattering contributed by the set of displaced (solid) atoms is reduced compared with the idealized scattering from the undisplaced (hatched) atoms. This fall-off corresponds quantitatively to the Debye-Waller factor. See text for more detail.

Isidor Fankuchen

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Nominations for 2020

ACA Awards: Nominations for the 2020 **A. L. Patterson, Dave Rognlie, Elizabeth Wood Science** and **Margaret C. Etter Early Career** awards are due by April 1, 2019. **Nominations** for **ACA Fellows** were also due by April 1.

ACA Offices and Committees: In Fall 2019 we will elect an ACA Vice-President and one person to each of the ACA Standing Committees (Continuing Education, Communications, and Data, Standards & Computing). In addition, the Canadian Division Chair and the Canadian Representative to the ACA Council are up for election this year. To suggest a candidate for one of the above positions, please contact **Kristin Stevens: kstevens@hwi.buffalo.edu**. Full details describing the criteria for all ACA awards and offices can be found on the ACA website.

2019 Dues are Due: Please renew promptly and remember to support your favorite ACA Award Funds.

NOTE: It is now possible to renew online.

ACA website: www.AmerCrystalAssn.org

Send all award nominations to: kstevens@hwi.buffalo.edu

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Answers to this issue's crossword puzzle on page 56.

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ACA Member Named as 2018 AAAS Fellow

In November, 2018, Stephen Halley White, Professor of Physiology and Biophysics at the University of California at Irvine, was named a 2018 AAAS Fellow, an honor bestowed on scientists "in recognition of their extraordinary achievements in advancing science." Stephen White has carried out pioneering work in the field of membrane protein biophysics. In the 1970s he had a long succession of high-impact publications on the physical chemical properties of fluid lipid bilayers that established the foundation for his influential work on fundamental aspects of membrane protein folding, assembly and function. He has received a number of awards, among them the Avanti Award in Lipids from the Biophysical Society in 2009 and the Protein Society Carl Brändén Award in 2014.

2019 ASBMB Young Investigator Award to Christine M. Dunham

Christine M. Dunham, Associate Professor of Biochemistry at Emory University, School of Medicine, has received the 2019 American Society of Biochemistry and Molecular Biology (ASBMB) Early Investigator Award. This award recognizes "outstanding research contributions to biochemistry and molecular biology" by a researcher who has had no more than 15 years of experience after earning their doctorate. Her award talk is entitled "Mechanisms of RNA-mediated translational control."

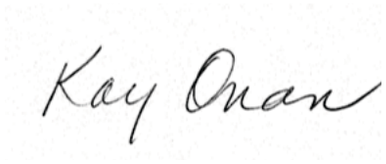
Christine received her BA at Barnard and then her PhD at the University of California, Santa Cruz in 2003, having studied an RNA enzyme. She was an American Cancer Society Postdoctoral Fellow at the MRC laboratory of Molecular Biology at Cambridge, UK, where she studied ribosomal translocation of the tRNA-mRNA helix through the ribosome during protein synthesis. She took a faculty position at Emory University where she is studying the molecular basis for protein regulation and dysregulation leading to gene regulation and stress responses, with focus on the ribosome.

She has received an NSF Early Career Development Award (CAREER), was a Pew Scholar in the Biomedical Sciences, a Burroughs Wellcome Investigator in the Pathogenesis of Infectious Diseases, and received the Margaret C. Etter Early Career Award from the American Crystallographic Association.

ACA Fellow Receives 2019 Alexander Hollaender Award in Biophysics

Jane Shelby Richardson, James B. Duke Professor of Biochemistry at Duke University School of Medicine, is the recipient of the 2019 Alexander Hollaender Award in Biophysics, awarded by the National Academy of Sciences. The award is to recognize "her pioneering work into the understanding of protein structures." In 1969 she and her husband, David, solved the tenth distinct protein structure – ever. Throughout her career Jane Richardson has made innovative contributions to the understanding of biological macromolecular structures, including their description, determinants, folding, evolution and control. A 1981 article provided deep, fundamental insight into how proteins are structured and introduced the iconic Richardson ribbon diagrams that provide such an elegant way of visualizing structure. She continues to work on novel methods of visualizing, analyzing, and improving macromolecular structures.

Jane has been the recipient of many awards during her career including the Emily M. Gray Award from the Biophysical Society, being named a MacArthur Fellow, a Fellow of the American Academy of Arts and Sciences, a member of the National Academy of Science and a member the Institute of Medicine of the National Academies.



Supporting Structural Chemistry in Africa and Beyond

Amy Sarjeant

Back in 2017, I had the privilege of being involved with the Cambridge Crystallographic Data Centre's launch of the Frank Allen International Research and Education Programme, or FAIRE for short. This program allows researchers in developing countries who lack sufficient funding to access the CSD free of charge. It was established to enable users with limited access to research resources the ability to conduct chemical research and to teach chemical concepts using crystallographic data and without relying on costly laboratory equipment. To date, 18 universities have availed themselves of the FAIRE program; 16 of these signed up before or during 2018 and two have joined more recently. Members of the FAIRE program are asked to provide the CCDC with details surrounding the usage of the CSD data and software tools. To date, over 85 people have benefitted from using the software, including faculty, post-doctoral researchers and students. Access to the CSD under the FAIRE program has led to 32 publications in peer reviewed journals and enhanced learning experiences for many students. Research publications spanned topics from metal-organic

coordination analyses to photophysical properties of coordination polymers to synthesis and structure determination of natural products. Clearly access to the CSD is having a positive effect for these users!

A few weeks ago, I had the pleasure of attending the 2nd Pan-African Conference on Crystallography (PCCr2) in Accra, Ghana. While there I was able to catch up with quite a few of our FAIRE users from western Africa. It was great to see how they were getting on with their various research projects and to

listen to their talks as part of the scientific program. One user in particular caught our attention. Dr. Samuel Tetteh of the University of Cape Coast, also in Ghana gave an excellent talk about research that he is doing employing data mining searches of the CSD. His work isn't yet published, so I can't say more about it here, but we were excited to see what questions of structural chemistry and the nature of bonding Samuel is able to answer simply by searching the CSD.

Of course, it's not just users in Africa who are able to participate in the FAIRE program. We've heard from users in Venezuela who have published work made possible by access to the CSD. As early adopters of the program, I was able to meet up with several students from Venezuela at the XVII Congreso Colombiano de Quimica held in Bucaramanga, Colombia in late 2017. It was such a pleasure to meet students who were such deft users of the software and to hear about their research. And it was doubly kind of these students to translate their posters for me when my limited Spanish failed. Another FAIRE group, from the Hanoi University of Science in Vietnam, has produced 11 publications and used the CSD to teach over 30 students.

Being able to meet up with these users at conferences and to hear about the progress they are making in their research is truly a rewarding experience.

UCSD JANA Workshop Summary

Diane A. Dickie

Nearly thirty crystallographers from academia, industry and government labs recently gathered for the 2018 Jana Modulation Workshop organized and hosted by Drs. Milan Gembicky and Curtis Moore of the University of California, San Diego. The workshop was led by Profs. Václav Petříček and Michal Dušek of the Czech Academy of Sciences, two of the co-authors of the Jana2006 software. The participants came from a wide variety of backgrounds, including chemistry, geology and materials science, and their experience level ranged from graduate students to emeriti faculty. More than half a dozen US states, two Canadian provinces and three other foreign countries were represented.

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

Everyone was sent back to their universities or companies with several more datasets to keep practicing on.

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

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

ACA Living History Project Update

Virginia Pett
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After consultation with Council and Kristin Stevens, webmaster Vanessa Reitz has created an attractive ACA History home page that fits the online style of the ACA pages now online with MemberClicks, the new ACA website management system. Vanessa also made a user-friendly history navigation menu. However, while she was reconstructing broken links, Vanessa discovered that a large proportion of ACA History pages are missing from the new site. Fortunately, Kristin had retained our relationship with the old website management system, and all the History pages are backed up. It will take some time to resolve these and other difficulties.

In this issue of ACA RefleXions Ron Stenkamp presents his Living History. After his graduate research with Lyle Jensen at the University of Washington in the 1970s, Ron spent the bulk of his career at the UofW determining both small-molecule and protein structures. He and his colleagues investigated oxygen-binding proteins (such as hemerythrin and rubredoxin) and drug-detoxification enzymes (such as glutathione S-transferase and cytochrome P450) by mutation and ligand-binding studies. In 2000 he and colleagues published the structure of rhodopsin, the light-absorbing molecule in the retina of the eye. This was the first high-resolution structure of a G-protein coupled receptor.

Ronald E. Stenkamp Living History

I attended my first scientific meeting as a junior in high school in 1964. NASA came to Bend, Oregon, to see how astronauts could walk on lava fields in their space suits. Two of us locals listened to several talks concerning the source of the moon's craters, i.e., volcanos or meteorites. I didn't understand much of it, but I thought it was boring, and if that's what scientists did for a living, maybe I'd do something else.

I was already thinking science wasn't very inviting. In response to Sputnik in 1957, science educators had generated special programs and tools to get kids interested in science. In 6th grade, I learned all about hypothesis generation and testing, and I was not impressed. I still have trouble with hypothesis-based science. Making observations and asking questions is what I enjoy doing. Posing hypotheses isn't.

I did well in school, and without planning it, I'd taken and enjoyed all sorts of classes. I greatly enjoyed mechanical drawing, and I'd out-run Mr. Lively's curriculum in Advanced Mechanical Drawing. He generated new projects for me, and engineering looked like a possible field for me, but I wanted a liberal arts education, so when it came time to pick a college, I chose the University of Oregon (UofO) instead of Oregon State University. Besides, the UofO's school colors (green and gold) matched those of my grade school.

The UofO has an Honors College (HC) which provides smaller courses focused on a core curriculum in the humanities and liberal arts. I applied to the program and was accepted. There was also a special center that provided a place to work with the other HC students, and I made many friends there, including my future wife, Larilyn.

Before joining the HC, I had chosen chemistry as my major, based largely on enjoying my high school chemistry class with Mrs. Cruickshank. When I started talking with other HC students about what we wanted to do with our lives, two of

them expressed interest in molecular biology. I'd never heard of that. This was 1966, and Kendrew, Perutz, Watson, Crick, and Wilkins had gotten their Nobel Prizes just four years earlier (1962). (Along with Steinbeck (Literature) and Pauling (Peace)). Molecular Biology was a brand-new field, but the UofO already had an Institute of Molecular Biology organized for interdisciplinary studies.

In the fall of 1966, my college days started with the honors section of freshman chemistry. In the second quarter laboratory class, I had an accident that foreshadowed much of my chemical career. One of our first tasks was to produce a dichromate/sulfuric acid cleaning solution. I made the solution OK, but a few days later, when I lifted the bottle up from my cabinet, I didn't lift it quite enough, and it clipped the stone counter top, about ¼ inch above the bottom of bottle. The bottle broke all the way around, and a liter of cleaning solution hit the benchtop, spilled down the front of the cabinet, and splashed a little on me. The TA quickly got the spill under control, but I spent the rest of the lab period cleaning up the mess.

I had a fair amount of growing-up to do in college. I came from Bend thinking I was a pretty smart guy. It turns out a lot of bright people go off to college, and many of them were a lot brighter and harder-working than I was. It was harder for me to get good grades in college, and this was a big blow to my ego. I grumbled a lot about the lousy teachers in college. Clearly, if they knew how to teach, I would have been doing better academically. Prof. Donald Swinehart was our instructor for freshman chemistry lab, and I talked a lot with him about teaching and learning. He wasn't very sympathetic. He told me about his experience in college where he decided to master a class in spite of the professor. I thought that was outrageous, but several years later, I ended up thanking him for that. In addition to listening to my complaints, Swinehart was willing to let me take reading courses with him where I could learn about special topics I found interesting.

I spent some of my undergraduate years in the library, looking at history of science books and others indicating what science was all about. I was greatly impressed by Pauling's "The Architecture of Molecules", and Roger Hayward's accompanying artwork of molecules looked like mechanical drawings of molecules. Maybe looking at molecular structures could combine my science and mechanical drawing interests?

One feature of the Honors College core classes was that after taking them for three quarters, you had to pass a comprehensive exam to remain in good standing. However, another option was to "challenge" a class by just taking the comprehensive exam. If you succeeded, you could get credit for the class without actually taking it. The exams were given in the spring and in the fall.

The history comprehensive exam was feared by most students who took the course, but I'd always enjoyed reading and thinking about history, so I figured I could challenge the history exam. So, for my summer "fun" project, I did all the readings for the HC history class. That meant I needed to do daily history reading assignments through the summer to cover the material discussed in class during the previous nine months. I borrowed the books and notes from a friend who'd passed the course that year, and I managed to read and study nearly all the assignments that summer. I did well with the fall comprehensive exam, and it promoted my confidence in doing independent study.

My sophomore year was very challenging and caused a lot of self-assessment My basic problem that year was organic chemistry. The first two quarters were about reactions (which I've never understood), but the third quarter had more physical organic content, so my understanding and grades went up for that. But lab was awful. One of my two worst grades was for third quarter organic lab. My lab skills (and luck) were not compatible with qualitative organic. I had one unknown that I could not make derivatives of. Even the prof couldn't do it, and the unknown was a natural product he'd pulled off his shelf. But in a concession to justice, he gave me half credit. Half credit! I had trouble with that class in addition to the intellectual content. And I'm not at all bitter, 50 years later. Further complicating my sophomore year were physics and a second year of math. Overall, by the end of the year, I figured anything had to make the next year better than this one.

After a summer working on a surveying crew (which paid enough to cover half of my school expenses), I returned for my junior year. Physical chemistry was a lot better for me. I could understand much of it, but it wasn't terribly exciting. By the end of the year, I was thinking I still needed to find some chemical field that was exciting and inspirational.

Then a wonderful thing happened. Brian Matthews joined the faculty to do something called protein crystallography. I had decided to stay in Eugene

for summer school, and I arranged with Brian to take a reading class where I could learn about crystallography.

When school started in the fall, I asked if I could do my senior Honors College thesis with him. He agreed and set me to solving a small molecule structure. Bill Simpson's lab was interested in organic compounds with metal-like spectroscopic properties, and they wanted to know what the crystal structure was of one of their compounds. Brian's X-ray lab was just setting up and had an Enraf-Nonius Weissenberg camera, so he had me collect diffraction data for 3-bis(dimethylamino)-trimethinium perchlorate using that camera. There was no film scanner available, so I eye-estimated the intensities on those films. I generated an intensity scale by exposing a single reflection for various lengths of time on a film. This gave a spot with the same shape and extent as those on my data frames. And then I spent several months over a light box determining the relative intensities of the reflections.

At that point, the school year was finishing, and I had to write my undergraduate thesis. Peter Colman joined the lab as a post-doc, and he ended up solving the structure. Soon after, a diffractometer arrived, and a higher quality data set was obtained for refinement. My efforts on this structure got me co-authorship with Peter and Brian and started my publication list.

Of course, while this project was important for my future career developments, other important things went on that year. First, Larilyn and I had to make wedding plans. Second, we needed to figure out what to do with our lives. The main thing we were reasonably skilled at was being students. And it seemed the natural consequence of that was to keep going and get our Ph.D. degrees. To prepare for that, we took three quarters of biochemistry and finally started seeing what molecular biology was about. In addition, we took a fantastic statistical mechanics class (mainly filled with graduate students), and several computer programming classes (assembly language and FORTRAN).

But we still needed to decide on a graduate school. We considered three schools, and Verner Schomaker, the chair of Chemistry at the University of Washington, let us know that protein crystallography was being done in Lyle Jensen's lab, and interdisciplinary research would be OK with Verner. That sounded terrific, and in the spring of 1970, Lyle came to Eugene to give a seminar about his group's refinement of rubredoxin. This was exciting, since it was the first protein to be successfully refined crystallographically. What was more exciting was that after talking with him, he said I should come to Seattle, "and we'll have some fun." I was convinced.

So, in late August of 1970, we got married, went to San Francisco for our honeymoon, drove back north to visit with family in Oregon, and moved to Seattle.

Crystallography was a big deal at the UW. The senior crystallographer was Ed Lingafelter. He'd joined the Chemistry faculty in the late-1930s, straight from being a graduate student at UC Berkeley. He was a physical chemist, and in 1938 or 39, he was joined by his "best" graduate student, Lyle Jensen (one year younger than Ed). Lyle was from Stanwood, a small town about 40 miles north of Seattle. He'd attended Walla Walla College and come to the UW to get his Ph.D. For his thesis, he determined unit cell parameters for a series of long-chain organic compounds. Once he obtained his Ph.D., Lyle joined the Manhattan Project in Chicago and worked with plutonium compounds. He left that position to teach at a church-sponsored college before going to The Ohio State University to work on the physical chemistry of liquid hydrogen. Soon after that, the UW needed additional instructors to deal with the large number of returning GIs, so he came back west and took up an instructorship in Chemistry. In 1948, just after the UW Medical School opened, he talked with the chair of Anatomy who offered him a junior faculty position the next day. Stan Bennett had a very broad view of "anatomy" and thought crystallography and electron microscopy would eventually be important for studying biological structures. Imagine that!

The third senior crystallographer was Verner Schomaker. Verner was a Cal Tech product where he did a lot of electron diffraction of compounds of interest to Pauling. There are many footnotes in Pauling's "The Nature of the Chemical Bond" referring to "V. Schomaker, unpublished results". The story I heard was that Pauling would get interested in some M-X bond and get Verner to use electron diffraction to obtain the M-X interatomic distance. In the mid-1960s, after years at Cal Tech and Union Carbide, Verner became chair of the Chemistry Department at the UW.

By 1970, other crystallography faculty at the UW included G.H. Stout in Chemistry, Jon Herriott in Biochemistry, and Art Camerman in Neurology. Subrata Ghose joined Geology sometime in the 70s. There were many graduate students, post-docs and research associates associated with these faculty, so there were people solving enough structures to support a weekly X-ray seminar. It was a wonderful environment for learning the fundamentals and

cutting-edge techniques in crystallography.

Our first year at the UW was filled with normal graduate school issues. We had coursework to manage, teaching assistantships to master, research groups to join, etc. Larilyn joined Ernest Davidson's quantum mechanical group, and after a bit of negotiation with a new chair of Chemistry, I could work in Jensen's group. (Lingafelter was my official

Ed Lingafelter and Verner Schomaker.

advisor, but Lyle was in charge and made any decisions a supervisor had to make. This qualified me as Ling's "easiest" grad student.)

Lyle wanted me to learn small molecule techniques that I could then apply to macromolecular structures. Accordingly, my first projects in the lab were crystal structure determinations of dipeptides. The first molecule I tried to solve was a chloromethyl ketone of acetyl-leucyl-phenylalanine. I determined the unit cell and space group using Weissenberg and precession photos, and then we (mainly Larry Sieker) used a Picker FACS-1 (driven by a PDP-8, with paper tape output) to collect a diffraction data set. The structure suffers from super-symmetry, but a bigger problem was that the crystal was greatly radiation damaged before we put it on the diffractometer. I didn't solve that structure, but it taught me a lot about crystallographic computing.

Following that, I grew crystals of two more dipeptides and solved their structures. I also worked on two small computational projects having to do with less-than reflections and resolution. Crystallography's appeal for me was (and is) tied up with the idea that solving or refining a structural model is just a big puzzle, and the big question is to see if I understand my craft enough to solve the puzzle. My research efforts have focused on using crystallographic techniques, and not so much on the molecules being studied or the biochemical questions being asked.

While the research work was of great importance, equally so were the social interactions in Lyle's research group and in the crystallographic community at the UW. Lyle's been recognized by many as a gracious, dignified leader. And those characteristics pertained in day-to-day life in his group. He delegated responsibilities well and made us feel like our projects were ours. He would occasionally come by our offices to see how we were progressing, but almost every day, I went to his office to ask questions and just talk about stuff. I still consider him my "boss", but he was really a friend.

And the supportive environment carried over with the other members of his group. Larry Sieker was the main crystallizer/data collector and for me, the lowly graduate student, he was the number two person in the group. He knew how to get things done and he was as dedicated to doing good science as Lyle was. That was true of everyone in the group, a dedication to doing good work. While several people came through Lyle's group as post-docs and visitors, the major post-docs who educated me about crystallography and computing were Keith Watenpaugh, Ellie Adman, and Jonathan Hanson. I can't express how grateful I am for the things I learned from them and their continued friendship.

I also benefitted from interactions with the other crystallographers on campus through the weekly X-ray seminars. For the presentations of new structures, and there were many of them, there was usually a figure showing the bond lengths and angles for the molecules. What was especially fun was to watch the senior faculty (usually Ling, Verner and Lyle) get interested in comparing the bond lengths and angles to see what the bonding was like. If the presenter was particularly successful, he or she could get the old guys talking and arguing and end up using a substantial portion of the seminar time. I don't remember ever manipulating my talk to succeed at this, but it happened accidentally enough to make it a career goal.

Ling and Verner also were great influences on how I approach problems, but in addition, they were important for my academic progress. The Chemistry Department expected its graduate students to pass cumulative exams to ensure they had a broad understanding of whichever branch of chemistry they were studying. These exams were given twice each quarter on Saturday mornings. If you could pass four of the first six that you took, you became a PhD candidate (and got a pay raise). Or you could pass five of 12 or six of 18. The faculty alternated in producing questions for the exams, so Verner put in

a question for the physical chemistry exam about the structure of diamond. None of us did very well with the question, and he pretty much read me the riot act about it. Since exam-taking is very much a game, we figured we were safe when it came to diamonds and didn't study the structure. Of course, on the next exam, here came another diamond question. This time there was no riot act, but Verner just shook his head at me when we next passed in the hall. After sufficient time, he seemed to get back to thinking I was OK.

Jensen's lab attracted many visitors, especially those interested in crystallographic refinement of macromolecules. Seattle was on the way to Japan and Asia, so we often had people come by for short visits during their travels. I tended to be shy when the famous visitors showed up. I found it hard to talk with these people who were my great heroes. I'm especially irritated that I never worked up the courage to spend more time talking with Max Perutz or Dorothy Hodgkin. Lyle had spent a sabbatical in Cambridge, so he knew Max from that time. And Lyle and Dorothy had competed on at least one small molecule structure. When Max and Dorothy came to visit (probably more than once each), they stayed at Lyle's house. Lyle and his wife, Mildred, held wonderful picnics in their backyard for the visitors and the rest of us. I wish I had an opportunity to re-live those get-togethers. I would work a lot harder at talking with the guests.

While completing my small molecule projects and writing them up, Lyle and I considered several protein problems for my thesis research. The problem that became my PhD project was hemerythrin. This is an octameric, non-heme iron, oxygen-binding protein with a molecular weight of 108,000, found in a few marine invertebrates. It fit with the Jensen group's overall interest in redox- and metalloproteins. Joann Sanders Loehr at Portland State University collaborated with Lyle and Larry and provided protein for a structure determination.

Data collection in Jensen's group was on the FACS-1 diffractometer. Larry oversaw the equipment, and his dedication to keeping the green machine aligned and in good condition, and Lyle's emphasis on precision, were important reasons I managed to solve the structure. The asymmetric unit for our crystal form contained four subunits from two hemerythrin octamers. The structure was solved at 5 Ångstrom resolution using a single mercury iodide derivative and its anomalous scattering signal. There are about 7500 reflections out to that resolution, and the quick step-scan data collection protocol (developed largely by Jonathan Hanson and Keith Watenpaugh) resulted in our collecting 1500 reflections per day.

We lost a large part of our data when the paper tape output messed up. There wasn't time to re-collect it. We still had a printout, so I ended up key-punching about 2000 reflections onto computer cards so I could keep the project going.

Then it was time to use the campus' CDC6400 to generate a difference Patterson map. Ellie Adman had solved a multi-site Patterson in working out the structure of ferredoxin, so she'd set an example for working your way through a Patterson. Still, the major thing I remember from solving the six-site mercury derivative was the sense of desperation that came with computing in the evenings and trying to make sense of the vector map. (Desperation can be a major driving force in research. Sometimes, you just have to get things done.) Subsequently, Lyle complimented me on being able to work through that noisy Patterson map, so I suppose I must have shown a bit of skill in doing it.

In 1975, a low-resolution structure of a protein was a significant result, and because the hemerythrin subunit is a four-alpha-helical bundle, there was a lot to be said about the molecule at low resolution. It was time to write my dissertation.

Once again, I benefitted from having Ling, Verner and Lyle on my thesis committee. Without any special effort on my part, the three of them disagreed on what I should include in my thesis. Should I just staple my small molecule structure papers together and call it a thesis? Should I just write up the hemerythrin structure? Should I combine all of those in a larger volume? When they disagreed, I had room to negotiate with Lyle. I ended up writing up just my hemerythrin work, about a year's worth of my PhD research.

Writing a dissertation in 1975 was considerably different from the current process. First, you had to find a typist who was careful and skilled enough to meet the formatting standards of the Graduate School. The margins were checked with a steel ruler, and edits had to fit within the margins, so re-typing had to be minimized, especially since we paid by the page. Of course, typographical errors had to be avoided, and spell-checking was a human-based process, not a button in a word-processing program.

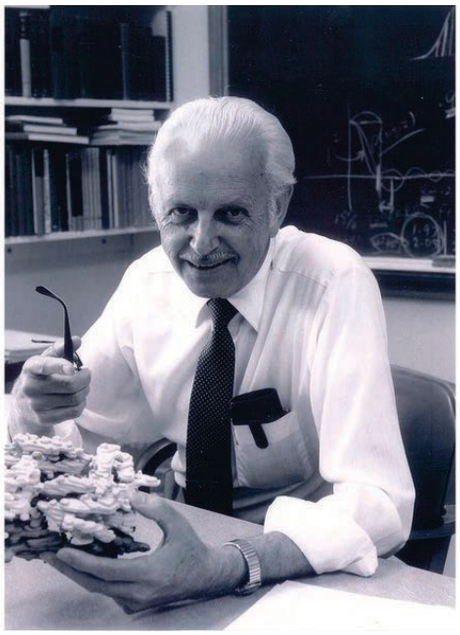
Since it was such an involved process, Larilyn and I decided I should go first, so three months before she finished, I wrote my thesis and got it typed up. It was

71 pages long, and 25 of those were Calcomp plots of the hemerythrin electron density map. We had to submit our theses for approval before scheduling our thesis presentation, and during the two-week waiting period, I built a balsa wood model of the low-resolution electron density map. (See photo below of Lyle holding the model.).

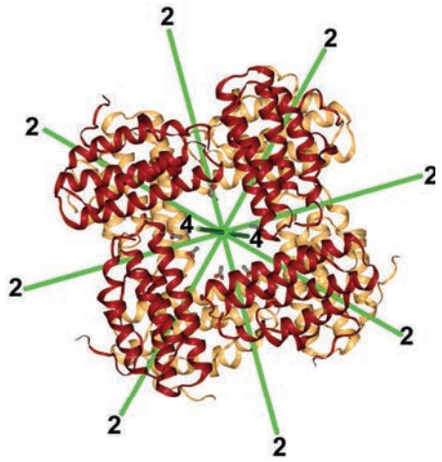
When the big day arrived for my presentation, I was a little nervous. And there was still Verner.

Hemerythrin's octamer has 422 symmetry relating the subunits. I'd built a couple models of the possible subunit arrangement using Styrofoam balls for the subunits. At some point in the presentation, I held up one of the models and stated the symmetry was 422. Verner immediately asked, "What's the symmetry of that model?" Gasp… I quickly answered that the symmetry was higher than 422 due to the spherical balls, and I said I didn't have time right now to figure out the actual point group. And I moved on with my talk. And amazingly, Verner let me go. (Diagram of hemerythrin (PDB 2HMQ) shown at right.)

I've thought of that moment often over the years, and I still think of it as a sort of personal triumph. It signified a time when I was the expert in the room. No one knew as much about my structure as I did. I was invincible (that day). The next day, I started on my path to being more and more confused by things, both scientific and not. I've heard many people, especially Lyle, Ling and Verner, talk about how they just didn't understand this or that thing. With the exuberance and certainty of youth, I thought they must be crazy. They obviously knew more about those things than any of the rest of us did. I now understand what they meant. I will always have more questions to answer. It's part of what makes us scholars and scientists.



Lyle Jensen with molecular model.

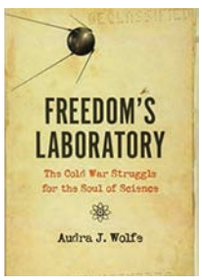


Hemerythrin.

Book Reviews

Freedom's Laboratory: The Cold War Struggle for the Soul of Science

Audra J. Wolfe (ISBN 9781421426730)



Freedom's Laboratory provides a detailed history of science and its role in society during The Cold War. Wolfe takes a deep dive into the role the United States government played in scientific inquiry and discovery around the world in the years following World War II. The Space Race was merely one facet of the heightened, science-related tensions between the capitalist United States and the communist Soviet Union.

Wolfe begins by introducing the concept of scientific freedom, the idea that science is an apolitical subject—or at least should be—which ironically, is a concept fundamentally fueled by the powers that be. In other words, the ideology of scientific freedom was in many ways created by the United States government during the Cold War, and perpetuated both in America and around the world via public propaganda and covert CIA operations. Scientific freedom, like truth in history, seems to be a matter of perspective.

Despite the escalation of tensions between the ideology of scientific freedom and Communism during the Cold War, the disconnect existed even before America entered World War II. JD Bernal, the well-known British crystallographer, published a book called The Social Function of Science in 1939. Bernal criticized the role of American capitalism in curtailing scientific discovery, and proposed that the Soviet approach was the best means of bettering society through scientific advancement. Although Bernal's book sparked intense academic debate at the time of its publication, it provided a crystallized version of an argument that had been cycling in academia for decades, since the revolution that transformed Russia from an imperial monarchy to a communist country.

From Bernal's The Social Function of Science, Wolfe weaves an intricate and often hard-to-follow historical narrative—though that is less of a statement about Wolfe's talent as an author and more of a statement about the subject matter. The history of scientific freedom during the Cold War is a convoluted one, with innumerable players both on the world stage and behind its scenes, from scientists to politicians to world leaders to covert operatives. Wolfe's dedication to providing a balanced history, both comprehensive and concise, is decidedly admirable.

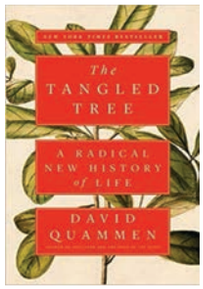
It's a complicated concept, to consider that the very ideal of scientific freedom that defines American research is one contrived and carefully cultivated by our government. Wolfe plays the role of neutral historian, presenting history as a series of factual events, and letting the reader draw their own conclusions, at least until the epilogue.

Wolfe saves the best (or worst, depending on how you look at it) for last, comparing the tensions between society and science in the 1950s and 1960s to those that exist today. It is hard to ignore the glaring parallels between international tensions over fifty years ago and those that exist now—and disorienting to watch the repetition of history unfolding in one's own lifetime.

In the wake of the open-mindedness and supportiveness of the Obama administration, the Trump administration has taken a sharply different tack regarding the relationship between science and the government. Only a few months after our current president took office, scientists across the country gathered in Washington, DC for the March for Science—something Wolfe discusses in her epilogue. It is worth considering the implications of living in a society where marches for political demonstration are not only geared towards basic human rights and equality, but the critical importance of freedom in scientific discovery.

Science, fundamentally, should be a pursuit of fact as proven by rigorous experimentation and results, whereas truth in this time seems to be a relative concept dependent on perspective and feeling. Given the current administration's adamant disregard for fact, or rather, its constant declaration of fiction as truth, it is hard to not understand why science itself—the pursuit of evidence-based fact—is a threat.

Jeanette S. Ferrara, MA



The Tangled Tree: A Radical New History of Life

David Quammen (ISBN: 978-1476776620)

David Quammen's The Tangled Tree is an absolute delight. In many ways, it feels like a biography of Carl Woese, the microbiologist who defined the domain of Archaea in 1977. Despite over 40 years having passed between now and then, Woese's definition challenged our fundamental understanding of evolutionary biology.

But The Tangled Tree is more than just a biography--calling it that does an insult to the work and the writer--it's more like a biographical history of evolutionary

biology. Quammen himself declares in his introduction "this book is about a new method of telling that story [of life], a new method of deducing it, and certain unexpected insights that have flowed from the new method. The method has a name: molecular phylogenetics." The line that follows illustrates the engaging tone Quammen takes throughout the book (and the wordiness): "Wrinkle your nose at that fancy phrase, if you will, and I'll wrinkle with you, but, in fact, what it means is fairly simple: reading the deep history of life and the patterns of relatedness from the sequence of constituent units in certain long molecules, as those molecules exist today within living creatures."

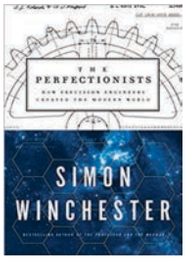
In other words, "molecular phylogenetics" means using patterns in DNA, RNA, and some proteins to determine how life evolved on Earth. This shouldn't come as a surprise. The Human Genome project largely concluded in 2003, and researchers have been charting the genome of various species for quite some time now. Scientists have known for some time now that the key to evolution lies in DNA--it just might not only be ours, but that of other organisms, namely single-celled nucleus-less ones, i.e. Archaea.

The heart of Quammen's book isn't just science--it is scientists. He introduces Woese early on, along with numerous other key players in this history of the history of life, including Lynn Margulis (also known as the first wife of famed astrophysicist Carl Sagan) and Ford Doolittle, a biologist who published an essay called "Uprooting the Tree of Life"--that sought to do just that.

Quammen starts the book itself, post-introduction, where you might suspect he would: with Charles Darwin. He gives a brief introduction to Darwin, his studies and his Origin of Species, but only enough to give quality context to the chapters ahead. Darwin occupies Part I of VII--only eight short chapters in a book of eighty-four. Darwin's work laid the foundation for modern evolutionary biology, and so it must be taken into consideration.

From Darwin, Quammen moves quickly to Crick and others, before settling on Woese in Chapter 11, where he stays for quite some time, straying to others in the field like Margulis and Doolittle, but ultimately always tying the story back in to Woese. You'll have to read the book to find out how--and I highly recommend it.

Quammen's prose is artistic and informative. His presentation and attention to detail flows naturally--it is easy to forget you are reading a work of nonfiction, because the characters and the story are so captivating. His chapters, though numerous, have a fairly short average length--a good metaphor for his storytelling style. Quammen has a lot to tell, and tells it well and concisely. Each chapter ties itself into the narrative neatly, pushing the reader further on. As a reader, you have the context and explanation you need to keep the story and the science moving forward. Should you want more, there is always an extensive index at the end.



Jeanette S. Ferrara, MA

The Perfectionists: How Precision Engineers Created the Modern World

Simon Winchester (ISBN: 978-0-06-265255-3)

Simon Winchester's The Perfectionists: How Precision Engineers Created the Modern World, is a marvelous work of popular science, tracing the history of high-precision engineering from 1776 to present day. Precision engineering is a subdiscipline of effectively all other engineering disciplines. As the name suggests, precision is tantamount. High tolerances, repeatable results, and stability over time are the tenets of the practice.

The book's prologue starts with a delightful anecdote about a young Winchester and his father—a precision engineer to whom the book is dedicated. When Winchester was a boy, his father brought home some gauge blocks (also known as Jo blocks) from work. For those readers unfamiliar with them, these metal blocks are so precisely ground flat that pressing them together makes them impossible to break apart. The only way to do so is not by pulling, but rather by sliding. They are used for measuring things to incredibly high tolerances. The man who invented them was Carl Edvard Johansson, who makes an appearance later

in the book.

Winchester then gives his readers a brief but thorough refresher course on the difference between precision and accuracy. Though often used interchangeably, the two terms mean something vastly different. Winchester presents the classic example of hitting a bullseye. If all of the shots are clustered close together, but not near the center of the target, they are precise but not accurate. If all of the shots are near the center of the target but not necessarily close to each other, they are accurate but not precise. If all of the shots are clustered directly on the bullseye and even on top of each other, they are both precise and accurate. It is an incredibly important distinction in any field, but especially in engineering.

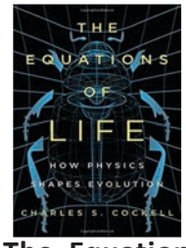
The prologue's combination of a brief, illustrative anecdote and detailed engineering explanation echoes through the rest of the book. Winchester begins each chapter with a contextualizing tale, either from history or from his personal repertoire. Even if the connection might seem tenuous at the beginning, Winchester deftly pivots back to a milestone of precision engineering in each case. He then offers a concise but significant explanation of exactly how precise that milestone's engineering is.

He dedicates each chapter of The Perfectionists to a subject with an increasingly higher tolerance, which not so coincidentally follows a fairly consistent timeline. Tolerance, per Winchester, is "the permissible variation in size from a specified standard allowed for a machined part." He starts with steam engines (tolerance: 10-1), then turns to ship-building (10-3), guns (10-5), screws (10-7), cars (10-10), planes (10-12), lenses for telescopes and cameras (10-13), GPS (10-17), and finally, computer chips (10-35).

In a great moment, Winchester turned to Eli Whitney. Whitney is perhaps best known to schoolchildren across America as the inventor of the cotton gin, but as Winchester so eloquently puts it, he was a "charlatan" of precision engineering. In early 19th century America, reliable weaponry was something of a challenge. Handmade by gunsmiths, rifles were prone to misfires. Something as simple as an uneven surface on the inside of a barrel could mean the difference between shooting someone or being shot at first on the battlefield. Gun repairs could take weeks, as each part had to be fixed by hand. Thomas Jefferson, while a US ambassador to France, became aware of the country's practice of gun-making. The French made interchangeable parts for their weaponry. If something on a rifle failed to perform or broke, it could be easily swapped out for a newer part.

Jefferson pushed for the US to contract someone to make American weaponry following the French system. And Whitney—who knew nothing about the musket-making business—used his connections as an alumnus of Yale to win the government commission. He even went so far as to present his "work" in front of President John Adams and Jefferson, then vice-president, and for lack of a better word, totally bamboozled them.

Winchester's Whitney revelation is one of many such juicy historical tidbits tastefully peppered throughout The Perfectionists. His prose flows effortlessly, and though it sometimes dips too quickly or too deeply into engineering jargon, the ever-self-aware Winchester includes a "Glossary of Possibly Unfamiliar Terms." It spans eight pages from "accuracy" to "wabi-sabi."



All in all, a wonderful read for a fall weekend.

Jeanette S. Ferrara, MA

The Equations of Life: How Physics Shapes Evolution

Charles S. Cockell (ISBN:978-1541617599)

Charles S. Cockell's The Equations of Life does a phenomenal job presenting evolution from a new perspective. Cockell, an astrobiologist at the University of Edinburgh, states in the short preface, "This book explores one line of thinking that tries to make sense of diverse areas of science that straddle the living and the nonliving, the indefeasible links between physics and evolutionary biology." The Equations of Life does just that, and does it quite well.

Without getting overly bogged down in minutiae, Cockell explores the building blocks of life on Earth--DNA, water, and carbon, to name a few of the better known ones--and details how they work, on a physical level. For example, he explicates why having two hydrogens and an oxygen in a water molecule actually matters in terms of evolution and life on Earth. At the conclusion of the book, Cockell briefly extrapolates how life might or might not evolve on other planets, based on how it has evolved here and why it has evolved that way and not another way.

Perhaps one of the best and most illustrative investigations involves the lesser mole-rat, Nannospalax leucodon. The first page of the book immediately following the table of contents features a black and white photograph of this creature, with the caption P = F / A. You might recognize this from a high school physics class, or even a middle school one: pressure equals force divided by area. But what does this have to do with the lesser mole-rat, you might ask? You'll have to read Cockell's book to find out--I don't want to spoil it for you.

One minor refreshing detail in Cockell's chapter on DNA involves Rosalind Franklin, a brilliant crystallographer whose work helped Watson and Crick discover the molecular structure of DNA. Cockell gives credit where it is due: "When James Watson and Francis Crick, with inspiration from X-ray images made by Rosalind Franklin, proposed a structure of DNA, a monumental step forward was made in deducing the centerpiece of life."

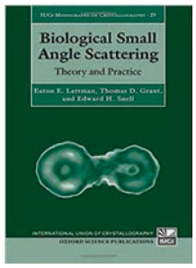
Due credit is something Franklin was denied in her own time and in Watson's autobiographical retelling of history, The Double Helix. Even though Brenda Maddox's Rosalind Franklin: The Dark Lady of DNA came out 15 years ago, and Franklin's contributions to the discovery of DNA have been made better known in the years since her death, some authors still neglect to mention her when the subject of DNA as it pertains to Watson and Crick surfaces in their work. So it's always a refreshing and positive moment when an author like Cockell gives Franklin her dues.

Despite its seemingly complex subject matter, The Equations of Life feels like a highly informative beach read in the best possible way. I could not put it down--Cockell's prose is engaging and fun--a perfect introduction to the fundamental connections between physics and evolutionary biology.

Jeanette S. Ferrara, MA

Biological Small Angle Scattering: Theory and Practice*

E. E. Lattman, T. D. Grant and E. H Snell (ISBN:978-019967087-1)



I've reviewed at least one other book on small angle scattering and this volume really addresses the current theory and practice with sufficient detail for a skilled scientist to successfully begin a study. The book is divided into five parts.

Part 1, the introduction, conveys the basic reasons you might perform a SAS experiment and the results you might obtain: particle molecular mass, radius of gyration, pair distance distribution, compactness and molecular envelope.

Part 2 has three chapters. The first two chapters provide a mathematical description of scattering theory and derives the equations for many of the results listed in the previous paragraph. The last chapter of Part 2 covers topic modeling from SAS data.

The first half of Part 3 delves into the issues of how to prepare samples for data collection, data collection, initial interpretation of results at the time of collection, and interpreting final results. The second half of Part 3 considers various aspects instrumentation both at home and the beamline, special experimental setups, and neutron scattering.

Part 4 looks at some interesting examples of the application of SAS to biological problems. Here the authors provide initial findings from XFELs and describe an interesting concept that many will recognize as an application of the Shake-n-Bake algorithm to the SAS problem. The authors conclude with a short epilogue listing a number of references for operating various software packages.

Part 5 contains an appendix, a list of acronyms, a glossary, a list defining major variables, references, and an index.

* I should disclose I have known two of the authors for many years, there is a picture of a Rigaku system on page 139 and I have no financial interest.

Joseph Ferrara, Ph.D.

Structural Dynamics
co-published by AIP Publishing, ACA

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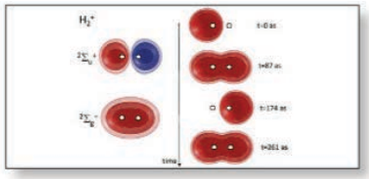

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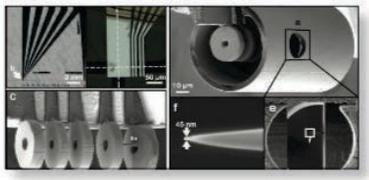

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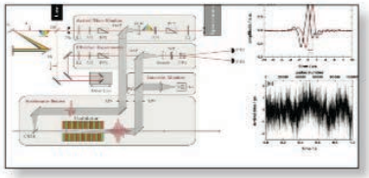

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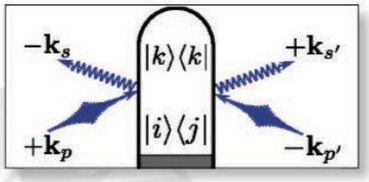

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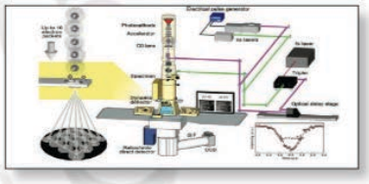

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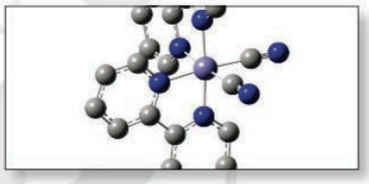

Ligand manipulation of charge transfer excited state relaxation and spin crossover in [Fe(2,2'-bipyridine)$_2$(CN)$_2$]
Kasper S. Kjær, Wenkai Zhang, Roberto Alonso-Mori, Uwe Bergmann, *et al.*
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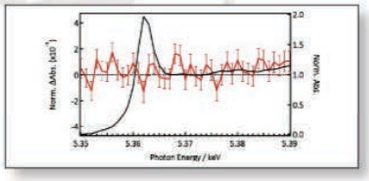

Localized holes and delocalized electrons in photoexcited inorganic perovskites: Watching each atomic actor by picosecond X-ray absorption spectroscopy
Fabio G. Santomauro, Jakob Grilj, Lars Mewes, Georgian Nedelcu, *et al.*
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Perspective: Structure and ultrafast dynamics of biomolecular hydration shells
Damien Laage, Thomas Elsaesser, James T. Hynes
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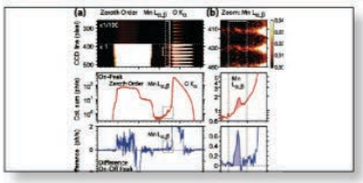

Soft x-ray absorption spectroscopy of metalloproteins and high-valent metal-complexes at room temperature using free-electron lasers
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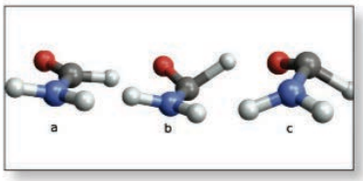
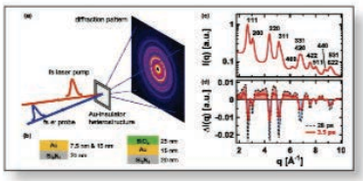
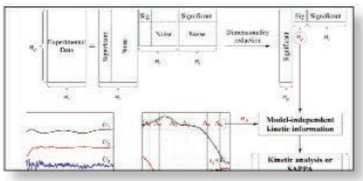


Photoinduced molecular chirality probed by ultrafast resonant X-ray spectroscopy
Jérémy R. Rouxel, Markus Kowalewski, Shaul Mukamel
Structural Dynamics **4**, 044006 (2017), **DOI:** 10.1063/1.4974260



Electron-lattice energy relaxation in laser-excited thin-film Au-insulator heterostructures studied by ultrafast MeV electron diffraction
K. Sokolowski-Tinten, X. Shen, Q. Zheng, T. Chase, *et al.*
Structural Dynamics **4**, 054501 (2017), **DOI:** 10.1063/1.4995258



SVD-aided pseudo principal-component analysis: A new method to speed up and improve determination of the optimum kinetic model from time-resolved data
Key Young Oang, Cheolhee Yang, Srinivasan Muniyappan, Jeongho Kim, *et al.*
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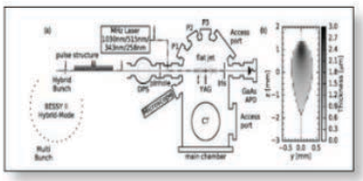
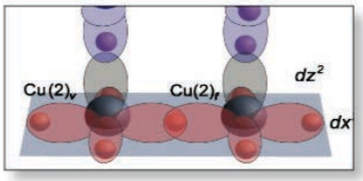
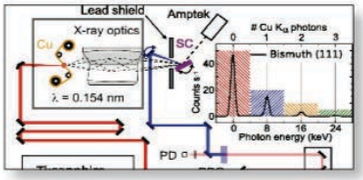


Time-resolved soft X-ray absorption spectroscopy in transmission mode on liquids at MHz repetition rates
Mattis Fondell, Sebastian Eckert, Raphael M. Jay, Christian Weniger, *et al.*
Structural Dynamics **4**, 054902 (2017), **DOI:** 10.1063/1.4993755



Optically induced lattice deformations, electronic structure changes, and enhanced superconductivity in $YBa_sCu_3O_{6.48}$
R. Mankowsky, M. Fechner, M. Först, A. von Hoegen, *et al.*
Structural Dynamics **4**, 044007 (2017), **DOI:** 10.1063/1.4977672



Towards shot-noise limited diffraction experiments with table-top femtosecond hard x-ray sources
Marcel Holtz, Christoph Hauf, Jannick Weisshaupt, Antonio-Andres Hernandez Salvador, *et al.*
Structural Dynamics **4**, 054304 (2017), **DOI:** 10.1063/1.4991355

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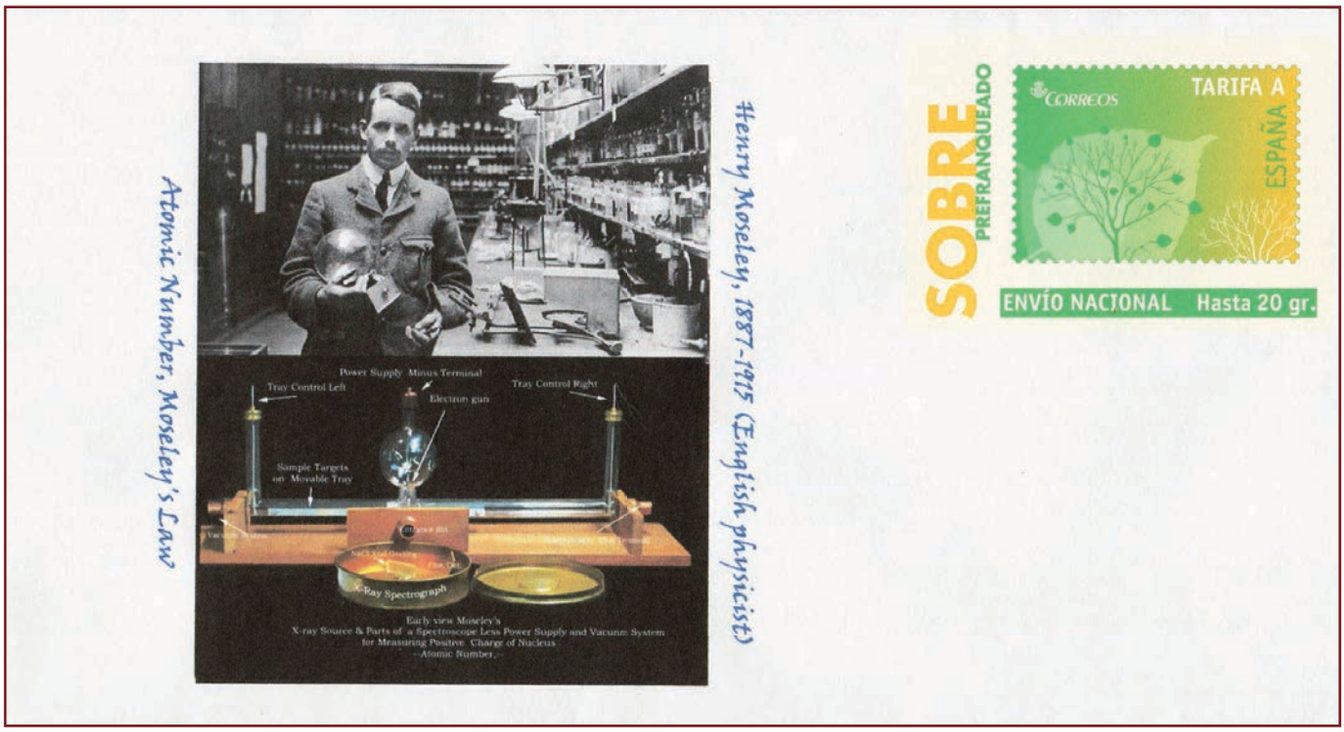
Daniel Rabinovich

2019 - International Year of the Periodic Table

Remembering Henry Moseley

I knew I was going to write about Henry Moseley sooner or later in this column even though no postage stamp honoring the brilliant British physicist (1887-1915) whose life was cut short by World War I has ever been issued. Now that we are celebrating the International Year of the Periodic Table, the timing to remember his critical role in the development of the modern chart of the elements seems to be ideal.

In the fall of 1913, Moseley used samples of ten different metals (calcium through zinc, with the exception of scandium) to discover a rather simple relationship whereby the square root of the frequency of the X-rays reflected by the irradiated samples was proportional to the nuclear charge (or atomic number) of the elements. Moseley's law, as it became known, explained why cobalt (Z = 27) preceded nickel (Z = 28) in the periodic table despite having a slightly higher atomic weight. Significantly, from then on, chemical elements in the periodic table were to be organized by increasing atomic number, not atomic weight as originally advocated by Mendeleev 150 years ago. Furthermore, X ray spectroscopy quickly developed into an essential tool to verify the identity of alleged new entries in the periodic table. Moseley himself recognized the existence of elements with atomic numbers 43, 61, and 75, years before the discovery of technetium (Tc), promethium (Pm), and rhenium (Re) was confirmed.



The pre-stamped envelope illustrated here, printed in Spain and valid for mailing letters up to 20 grams within the country, features the classic 1910 photograph of Moseley in a laboratory during his student days at Trinity College, one of the constituent colleges of the University of Oxford in England, and a picture of the only surviving X-ray spectrometer he used in his seminal experiments, now on display at Oxford's renowned History of Science Museum.

Puzzle Corner

Guest Puzzler Joe Ferrara has provided another challenging crossword puzzle; answers are given on Page #. A new Crystoquote puzzle is also provided, along with answers to the previous puzzles. Comments on the answers to Crystal Connections #15 and mention of those who provided solutions are also included.

Solution to Crystal Connections #15 - Words which are also refcodes

1) The 1875 painting Otoño by Frederic E. Church celebrates this season AUTUMN

2) The symmetry of a wallpaper BORDER is one of the 7 frieze groups

3) We are stardust, we are golden, we are billion year old CARBON

4) Buck, greenback, piastre, 8 bits. DOLLAR

5) Receptacle for unwanted delivery of canned meat? Spam FOLDER

6) South of Toms River, near Double Trouble State Park in the Pine Barrens: FORKED River

7) Take a stare at this spicy dancer: GINGER Rogers

8) Statler is a MUPPET; Waldorf too

9) The Kalpha wavelenth of SILVER is about 0.56 Angstroms

10) His comedy routines included Phonetic Punctuation and Inflationary Language: VICTOR Borge

Comments on the answers:

1) Church (1826-1900) is my favorite American painter, who created such spectacular works as Niagara, Cotopaxi, Twilight in the Wilderness, El Rio de Luz, and Rainy Season in the Tropics.

2) Frieze groups are also called border groups or band groups. They describe two-dimensional patterns with repetition in only one dimension.

3) From the song Woodstock by Joni Mitchell (1970). We are stardust… is an unusually scientifically astute line for a rock song, commenting on the origin of most elements. But billion year old carbon is a bit of an underestimate.

9) CARBON of course contains carbon, but SILVER contains no silver.

Exercises for the reader: How many other elements have 6-letter names? Are any others also refcodes? Can you provide other examples of refcodes which are words? In other languages besides English?

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

Frank Fronczek – ffroncz@lsu.edu

Crystoquote #3:

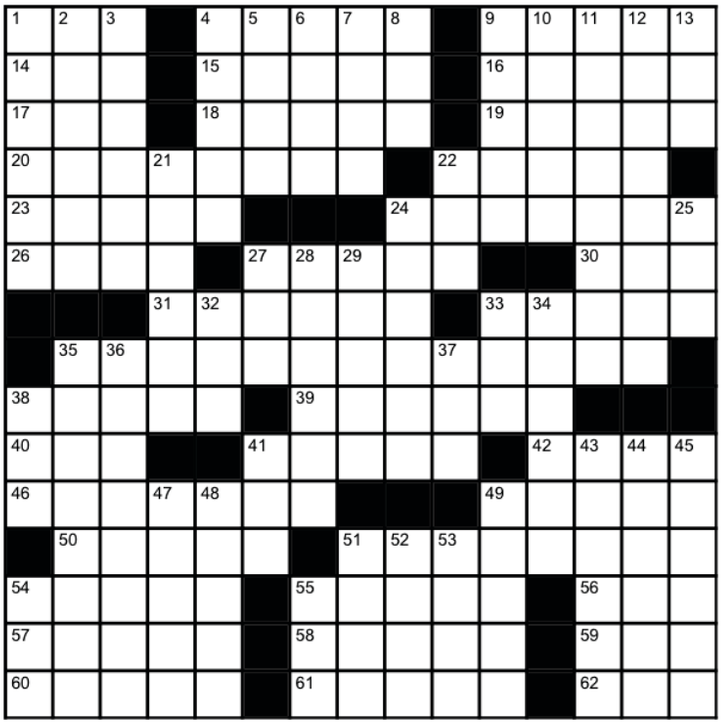
Letter substitution reveals a quote by a well-known crystallographer

HI TEMP, HP HA PGO OYMORPHDIA, DX DKPJHOXA PGEP HCIHPO DKX MKXHDAHPW EIL JOEL KA PD IOU OYROXHVOIPA, IOU PGODXHOA, EIL IOU LOZOJDRVOIPA.
BDOJ FOXIAPOHI

Solution to Crystoquote #2:

I am grateful for the opportunity to give something back to the community which has given me so much.
Judith Flippen-Anderson

Ilia Guzei provided the solutions to the Karle DISORDERED puzzle and to Crystoquote #2. No solution was submitted to Crystal Connections #15.



Across
1. Tax pro, for short
4. 7 7 7, in Paris
9. One side of a 46 across
14. Monopolize
15. Devoured
16. Incongruity in expectation
17. Shorn female
18. Bluefin
19. Waste water
20. Elightening
22. Bud
23. Mister, in Majorca
24. Prom gift
26. Units of work
27. Eat beans?
30. Winner's cry
31. With 46 across, a most desired item.
33. Signs
35. Thought to have done in the Romans
38. Half a Fourier
39. World leader?
40. Cell lengths
41. Forbidden by Islamic law
42. Major processor advance of the early 90s
46. Something with an essentially sharp diffraction pattern
49. Of part of the lung
50. Pallid
51. Sisterhood
54. Fragrant oil
55. Ones who might take you to 44 down
56. Dove's sound
57. Scoundrels
58. Banish
59. Before, before
60. Confuse
61. Late bloomer
62. Type of card (abbr.)

Down
1. France has over 600 types of this
2. Debye-Scherrer ring producer
3. Normal process of life
4. Woodland deity
5. Pin cushion
6. Southernmost Ivy
7. Source of a wood protector
8. Bond, for one
9. Photo 51 shows this type of diffraction
10. Seed covers
11. Molecule with a triple helix
12. Absorbing
13. Wade of Ready Player 1
21. Anatomical cavities
22. Dandy
24. Ridge
25. Printer's widths
27. Old econ. figure
28. Body di-
29. Foxier
32. Often forged items
33. P1?
34. Pm has one
35. Not translated or screwed
36. Descriptor for an object in a 21 down
37. 1/Siemens
38. St. Nick tracker (abbr.)
41. Most Chinese
43. Some Alpine goats
44. State of enlightenment
45. Imaging technique
47. First person future
48. To the point
49. Clinton in 2016
51. How you might study macromolecules in solution
52. Type of map
53. Death rattle
54. Essential oil
55. Where you might find 17 across

DISORDERED

Go directly from the observed letters to the solution

CREDIT	DIRECT
OHMSTED	METHODS
KALLIADO	ALKALOID
SLOWELF	FELLOWS
PHATUNAM	HAUPTMAN

When Jerome Karfunkle shortened his name to Karle, his original name…

Answer:

WAS "DE-FUNKED"

Answers to crossword puzzle on page 37

JUNE 2019

23-28 **11th International Conference on Inelastic X-ray Scattering**.
Stony Brook University, NY
http://www.bnl.gov/ixs2019/

23-28 **Crystal Growth and Assembly. GRC**.
Manchester, NH
https://www.grc.org/crystal-growth-and-assembly-conference/2019/

JULY 2019

20-24 **ACA 2019 Annual Meeting**. Covington, KY
http://www.AmerCrystalAssn.org

28-2 Aug **19th International Conference on Crystal Growth and Epitaxy**,
Keystone, Colorado
http://www.crystalgrowth.org

AUGUST 2019

22-26 **European Crystallographic Meeting,** Vienna, Austria
https://www.ecm2019.org/home/

OCTOBER 2019

10-12 **Latin American Crystallographic Association,** Valparaíso, Chile
https://www.cristalografia.cl/3rdlacameeting

DECEMBER 2019

1 - 6 **Materials Research Society Fall Meeting,** Boston, MA
https://www.mrs.org/Fall2019

JULY 2020

31-7 Aug **ACA 2020 Annual Meeting**. San Diego, CA
http://www.AmerCrystalAssn.org

AUGUST 2020

22-30 Aug **IUCr 25th General Assembly**. Prague, Czech Republic
http://www.iucr25.org

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