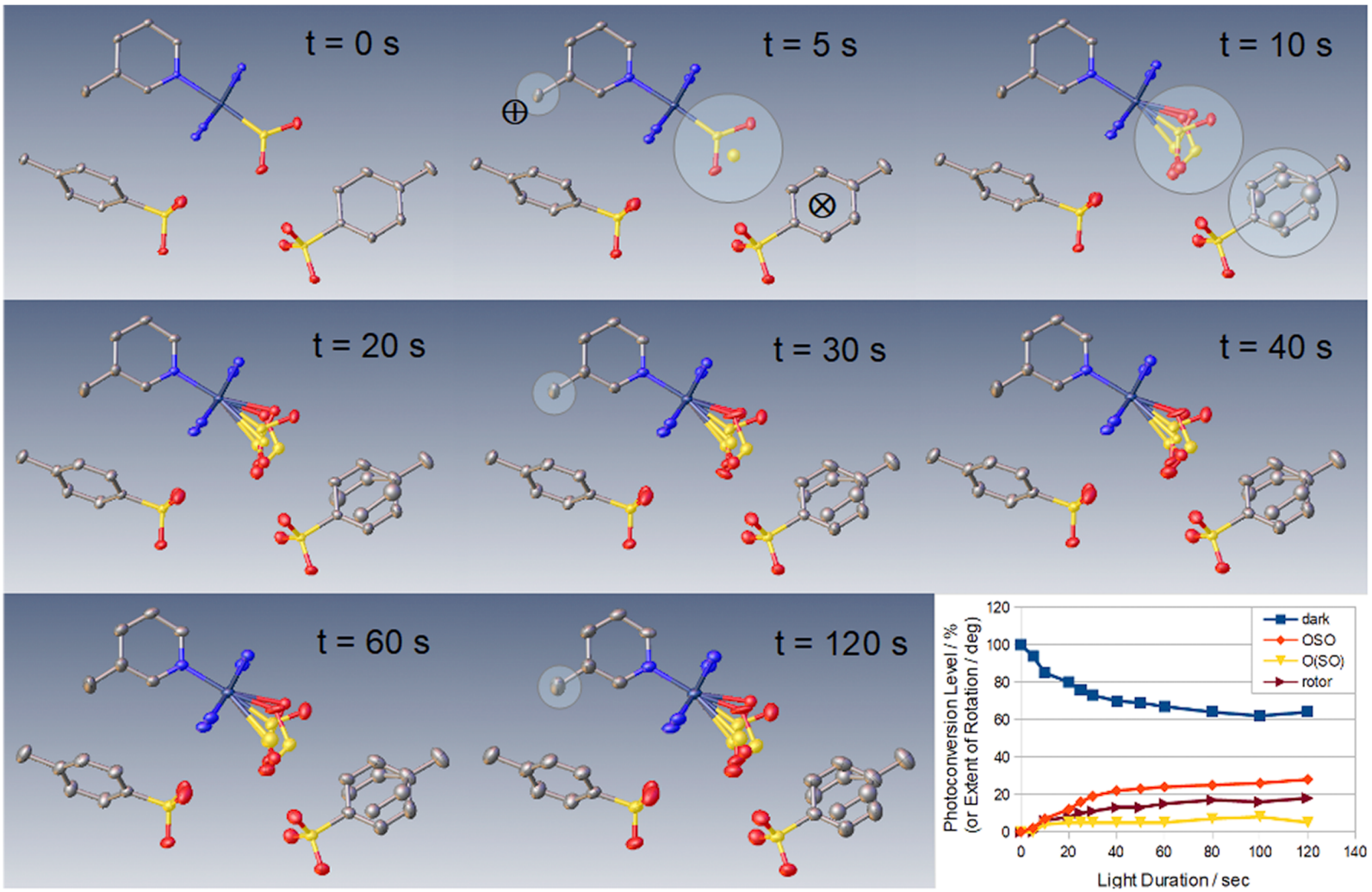
ACA RefleXions

American Crystallographic Association

Structure Matters

Number 2

Summer 2021



Advances in Photocrystallography

Jacqueline M. Cole

2021 recipient of the Warren Award

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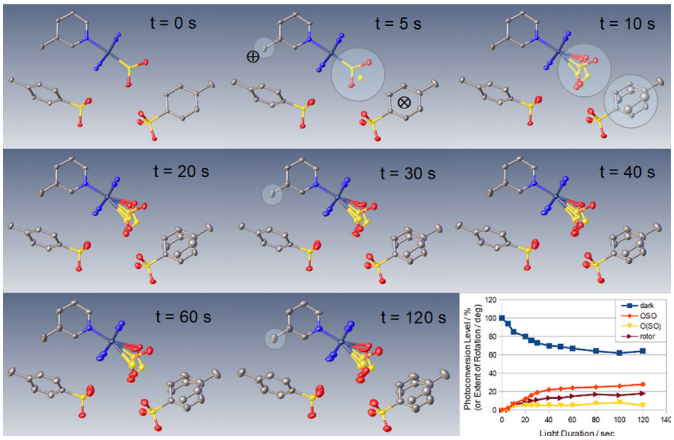

About the Cover:
2021Warren Award: Jacqueline M. Cole

A time sequence of eight crystal structures of the complex, [Ru(SO$_2$)(NH$_3$)$_4$(3-methylpyridine)]tosylate$_2$ as its dark-state S-bound SO$_2$ ligand progressively photoisomerizes as a function of t seconds of 505 nm light from t = 0 – 120 s. The heaviest element of the light-induced O-bound OSO photoisomer (sulfur) can already be refined after 5 s of light exposure. The anisotropic displacement parameter (ADP) of the carbon atom in the methyl substituent (Me) of the 3-methylpyridine ligand also starts to become more elongated at t = 5 s, which exhibits libration and this continues to grow throughout this entire time sequence (see small circled highlights). Me librates in the direction that points into the center of the arene ring of the ring rotor, within the periodic framework of the crystal lattice (the trajectory lies perpendicular to the page, as shown by the head (+) and tail (X) ends of an arrow). By t = 10 s, this arene ring has started to rotate as a consequence of this interaction with Me as well as its proximity to the protruding oxygen of the eta1-OSO photoisomer, enough of which has now formed that it can be distinguished and refined crystallographically (see large circled highlights). The plot in the bottom right panel shows that the photoconversion levels of the rotated ring and both photoisomers (a small amount of a side-bound (OS)O photoisomer is also refined) continue to grow with time, while that of the dark-state S-bound SO2 configuration decreases. The graphic was created by J. M. Cole wherein all structures were visualized using the crystallographic software, OLEX2.

Index of Advertisers

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

Paul Swepston.....paulswepston@me.com

Cover:	Paul Swepston	Book Reviews:	Joseph Ferrara
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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
Summer 2021

David Rose
ACA President

Despite a stubborn third wave of Covid-19 in Ontario, with closed schools and businesses once again, we cannot help but be optimistic. Vaccines are starting to make inroads in many parts of the world, including the US and UK, and, while Canada is lagging behind, progress is accelerating. It is time to start looking ahead to make sure the momentum in Structural Science and other areas of research is maintained. We know that the next pandemic is just around the corner.

There are several lessons that I am taking away from this experience. One is how evident it is that we are one global population. In the final weeks of 2019, we saw how quickly an infectious agent can spread throughout the world, despite early warning signs; such signs cannot be ignored again. We saw how decades of foundational research in Structural and other sciences was able to pay off in the remarkably quick development of vaccines. We also learned as the vaccines rolled out, the importance of broad, international distribution; the regionalization and hoarding of doses is likely one factor contributing to the evolution and spread of variants, prolonging the pandemic in all parts of the world. One sociological area that deserves intense study is how the anti-vax and anti-science industries have been so successful in their communication effectiveness, more so, even, than fact-based sources. Such movements will surely delay the recovery around the world and effective counter-approaches will be critical in limiting the severity of future pandemics. Similarly, the communications industry has not helped, by sensationalizing and exaggerating incredibly rare vaccine side-effects. The W.H.O. has identified 'vaccine hesitancy' as one of the most serious present global health threats. Professional scientists of all stripes can no longer sit within the ivory tower, but have the responsibility of providing effective, reliable communication to the public and policy-makers.

In our discipline of Structural Science, we, of course, need to continue to build the foundations of new frontiers. Progress is already underway in understanding the drivers of mutations leading to variants of the virus. Molecular studies are deciphering how such mutations are leading to higher infectivity and virulence. As vaccinology evolves, structural studies in materials and nanotechnology will lead to more practical, less expensive, and higher stability products. Structural Biology is contributing to vaccines with higher cross-reactivity against coronaviruses and other pathogens. New approaches to broad-spectrum antiviral pharmaceuticals are already underway, including intriguing approaches to host-based therapies, where the host mechanisms that are critical for infection can be regulated. These approaches rely on structures of molecules of all sizes. Underpinning all these is that none of these rapid advances would have been possible without decades of fundamental, discovery research; the importance of continuing strong discovery research at the beginning of the innovation pipeline must be appreciated and celebrated.

Perhaps most exciting are the implications that these new areas will have on other, equally devastating health problems. Cancer vaccine studies are getting a boost from all we are learning from the pandemic. Studies of pathogenesis and infection will surely be relevant to the serious and growing antibiotic multidrug resistance problem. Even climate change has taken on a whole new importance as we understand its impact on wildlife and human population migration, urbanization and cross-species transmission of pathogens.

Finally, perhaps most exciting from the point of

view of our Society, is the convergence of critical contributions from all aspects of Structural Science on the pandemic response. Though largely immersed in Structural Biology and Chemistry for my career, I have become even more sensitized to how important areas such as materials, nano- and micro-particles, computational science and others are in coming together to address major global issues. Where would we be without the technical developments of our commercial partners bringing new, more powerful capabilities into our laboratories?

I invite you to continue with me on this exciting journey of the contributions of Structural Science to making our world safer and addressing new global challenges. Our embracing the convergence of all aspects of Structural Science within the ACA family can only accelerate that impact.

David Rose

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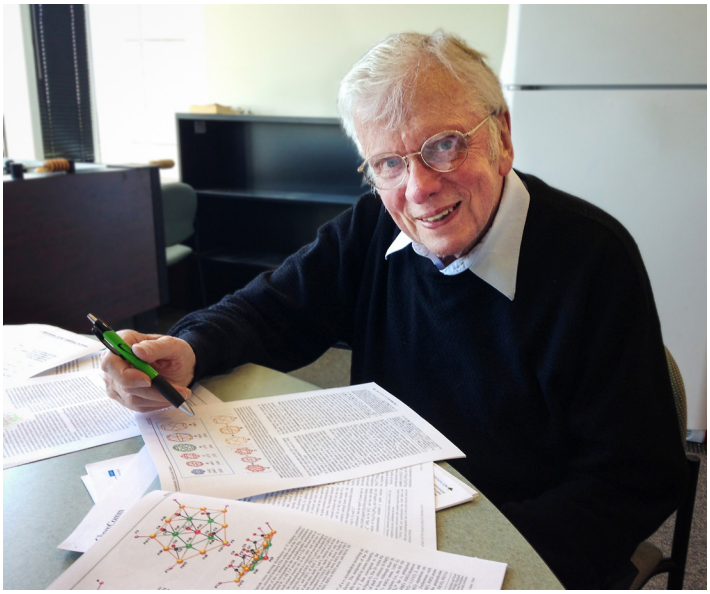
Rembrances of Larry Dahl



Lawrence Frederick Dahl, Professor Emeritus of Chemistry at the University of Wisconsin – Madison, passed away unexpectedly on March 20, 2021, at the age of 91. In 1978 he was named the R. E. Rundle Professor Chemistry and in 1991 he was named a Hilldale Professor of Chemistry. His research focused on inorganic chemistry, with an emphasis on the synthesis of well-defined transition-metal cluster compounds, analysis of metal-metal bonded molecules and the application of X-ray crystallography to characterization of these and related compounds.

Larry Falvello: It is a special experience when you meet a well-known scientist and leader in his field, after having known him only from afar through his publications and status among chemists. This was the context in which I first met Larry Dahl.

By the mid-1970's Larry Dahl had become a main figure in the growing field of transition metal cluster chemistry. As a graduate student elsewhere, following the literature as closely as possible, as was done in those days, I regarded Larry as one of the heroes in the field. With that as a backdrop, I was a newly-arrived post-doc in College Station, Texas, when, in 1981, I met Larry in person for the first time. He was going to give a seminar, and someone had told me that Larry would speak beyond the scheduled time. He did indeed; but he kept my attention, as he would do countless times in later years.

Larry had a lot to say. His unassuming nature did not project the enormity of his achievements as a scientist, but those achievements came through when he talked about research. Larry was one of the pioneers in using x-ray diffraction as a first-line approach to identifying newly synthesized compounds. In the early days of cluster chemistry, each new synthesis produced an unexpected product. As noted by Paolieri et al., only with rapid structure analysis (rapid as per the standards of that time) could enough information be accumulated to permit some degree of order to be imposed in explaining existing results and further to permit the prediction of new products (*J. Clust. Sci*. 2019, 330,1623-1631). Larry Dahl was prolific in the preparation and structure analysis of new clusters. Indeed, in his autobiography, F. A. Cotton wrote that "Paolo [Chini] and Larry Dahl were the two patriarchs of metal atom cluster chemistry."

I always tried to invite Larry as a speaker at ACA meetings, in the sessions that I organized or co-organized (usually with Alberto Albinati), addressing the science that benefits from crystallography. The running title of those sessions was "Important Science from Small-Molecule Structures." Larry could be counted on for an enthusiastic presentation, which was invariably scheduled as the last talk in the session, an informal mechanism for letting him continue overtime.

In the session report for this session in 2015, I described for our increasingly younger audience, something about this older but animated speaker: "*Larry Dahl, ACA Fellow, member of the National Academy of Sciences and winner of the 2010 F. A. Cotton Award in Synthetic Inorganic Chemistry (an ACS national award), closed the first session with an energetic presentation of his work on hetero- and homometallic clusters ligated by CO and* PR_3*. These clusters can be formed by up to*

165 metal atoms." That would be the last time that Larry would speak in one of those sessions. But after decades of working with clusters, he still had something new to present.

When Larry finished his session-closing talk right on time, for a moment I wondered if all was well. The next day he would demonstrate that at 86 he was still a step ahead of things. I was sitting next to Larry at a session that included a talk about metal-metal bonding (a field in which I had worked), and specifically the quadruple bond. The speaker mentioned the first system that had been characterized by Cotton in 1964, some fifty years earlier, as having a quadruple bond, namely the dianion $[Re_2Cl_8]^{(2-)}$ -- which the speaker identified as Re_2Cl_8. Larry nudged me and said, "He forgot the *Two Minus*." That first quadruple bond, in common with Larry's clusters, was a milestone in the advance of modern inorganic chemistry; Larry had been a key player and a keen observer through it all.

That was Larry. When I was a graduate student following the literature, he was a far-away pioneer, the lead author on the by-lines of scores of important papers. Forty years later, his enthusiasm for, and mastery of, the old and the new continued unabated. And in the intervening years, he was always ready with a kind word, a useful suggestion or new results that would make a long lecture interesting from start to finish.

Ilia Guzei: It is hard to believe that Larry, who only a few short weeks ago requested a printed copy of his paper on the structure of $Fe_3(CO)_{12}$ for discussion with a colleague, is no longer with us. Larry knew how to enjoy life, had an unfailingly positive attitude, and remained enthusiastic about science to the very end. I met Larry at the outset of the 21st century. This was when his large metal cluster research experienced a very productive phase after the advent of electronic two-dimensional X-ray detectors. Herein I would like to share what it was like to be in the company of this bright and accomplished scientist.

Larry spent his entire career at UW–Madison. Therefore, naturally, when I joined the UW–Madison Chemistry Department we spent many hours talking science and crystallography. Larry would regularly stop by to share news, ask about the latest developments in the X-ray lab and X-ray world, and sometimes reminisce. Many people and events were mentioned, but remarkably, Larry never had anything negative to say about anyone. He did, though, say that in the olden days, when he hired undergraduates to estimate intensities of reflections recorded on film, women were always better "spot judgers" than men! Larry would remind me that in 1957 his startup package was $4000 and that the proposals of the current new hires were so advanced that were he to apply for a position at UW–Madison today he would probably not get it. It was surprising to hear that from a fellow of the National Academy of Arts and Sciences (1992), the New York Academy of Sciences (1975), the American Crystallographic Association (2015) and laureate of multiple awards and lectureships. Larry never mentioned any of his awards and titles. A few years ago, when we were helping him move his office, we discovered a box full of awards and plaques. He was not interested in looking at the contents at all - but he would not part with his collection of chemistry journal subscriptions. One of Larry's awards was the F. Albert Cotton Award in Synthetic Inorganic Chemistry bestowed in 2010. Larry used to say that he was happy that "Al did not pursue large cluster chemistry." He appreciated being mentioned by name in Prof. Cotton's autobiography as a patriarch of metal atom cluster chemistry, along with Paolo Chini.

Larry was a great lecturer and it was always a pleasure to listen to him. He was, however, known for lecturing past the end of a time slot. In the Chemical Crystallography course that he taught for many years (and into his emeritus years), he would lecture past the usual time slot into "reciprocal minutes." At this point it would be appropriate to mention that in the era of slide presentations, which predates me, 1 Dahl was a number equal to

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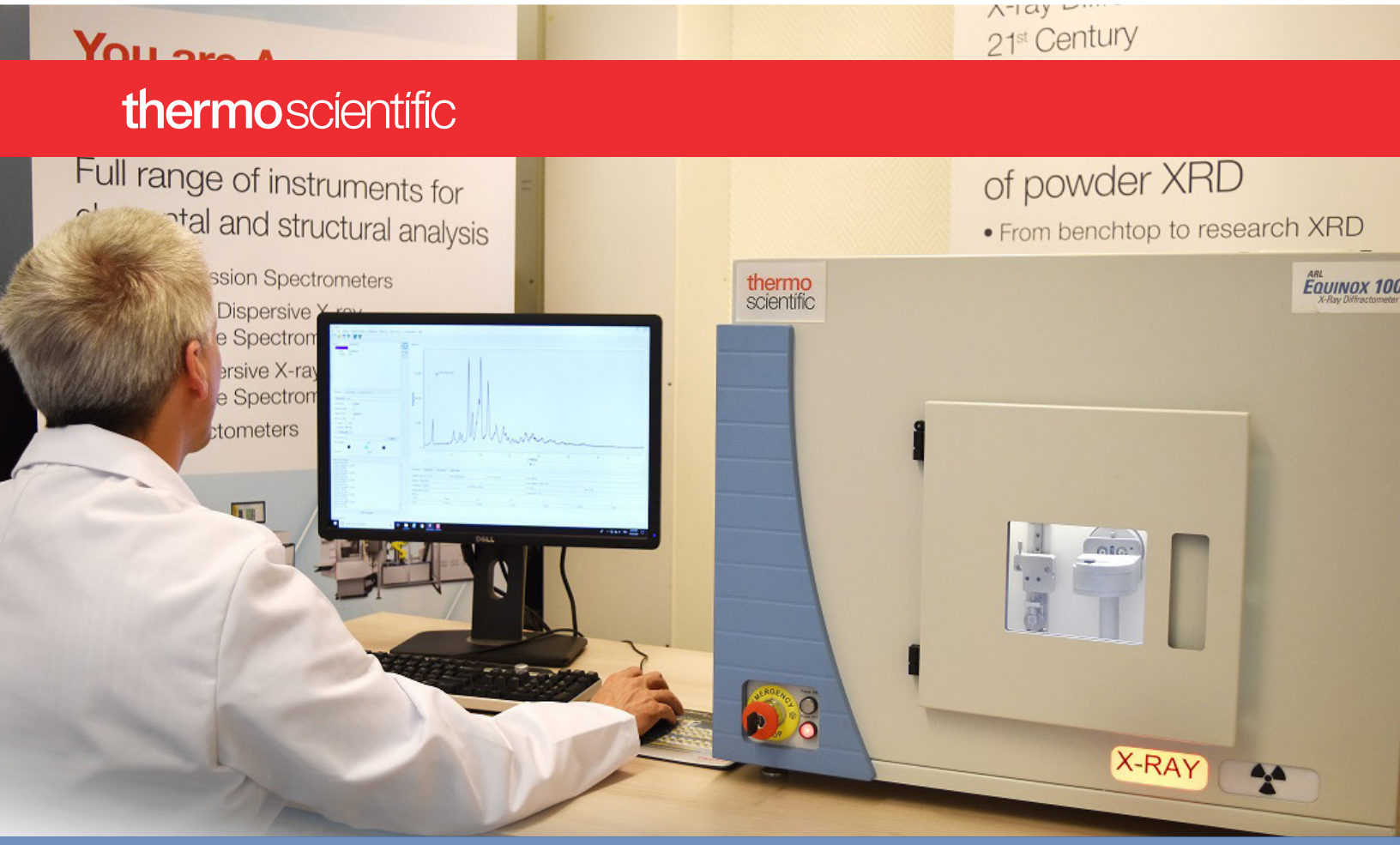

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80, exactly the number of slides a slide projector carousel holds. Professor Dahl was known for his comprehensive style of lecturing and he typically showed many slides in his lectures, sometimes as many as 1 Dahl. I learned about that during the 2009 scientific symposium in Larry's honor when Prof. Dahl turned 1 Dahl years of age.

An exceptionally good writer with a distinct style and excellent command of the English language Larry described his chemistry thoroughly, and his papers are a delight to read. Once Larry told me that some of his colleagues believed that in his articles he put the abstract in the title and the paper in the abstract, but he was all smiles about it and concluded by saying "That's the way I like it." He praised his co-workers, giving the lion's share of credit to his collaborators, and on his articles students and co-workers were the lead authors, though the majority of writing and manuscript editing was done by Larry. Whereas I always valued his input, I feared getting my drafts back because they would have nearly more red ink than the original black. The only way to overrule his language advice was to ask him to show the manuscript to his wife of 63 years Prof. June Dahl. If June reverted a certain phrase back to the original, Larry would concede. Larry preferred to spell things out and I was taught that brevity was talent's sister, thus in the end a good compromise would be reached. Larry did not just read papers in his field, he also read papers referenced in those papers and references therein, and because he read articles printed on paper, he would eventually run out of surface space in the office. But that suited Larry just fine – he enjoyed staying with the students in the outer office.

Larry's science was integrated into various aspects of his personal life. For instance, the largest Pt/Pd carbonyl clusters synthesized in the Dahl lab found their way onto the license plate of Larry's Honda: **PT52CO** [in 1991, unpublished?], **PD145CO** [in 2002, for complex $Pd_{145}(CO)_x(PEt_3)_{30}$)], and **PTPD164** [in 2010, for nanosized $(\mu_{12}\text{-}Pt)Pd_{164-x}Pt_x(CO)_{72}(PPh_3)_{20}$ ($x \approx 7$)].

While Larry did not live to see the newest chemistry tower completed at UW-Madison, he did see the latest Bruker diffractometer added to the X-ray lab. The instrument is named after Larry and that will ensure that our data will be of the highest caliber, just as the name suggests.

Bruce Foxman: Over the years, I've had an overwhelming feeling that Larry Dahl was one of my 'mentors from afar.' There were large time gaps in our friendship as we led busy lives, but it was always clear that Larry was interested in what other inorganic chemists and crystallographers were doing, and clearly interested in doing whatever he could to encourage and help. I first met Larry very briefly when I was a senior undergraduate chemistry major at Iowa State University in 1963-64. His former Ph. D. supervisor, Bob Rundle, had tragically and suddenly passed away at 47, in October 1963, and Larry (then an Asst. Prof. at Wisconsin) was a candidate/interviewee for the open position. He gave a wonderful talk, as did two other superb scientists in ISU's regular seminar series around that time, Al Cotton and Stan Piper. All three were in my application packets for graduate school. In the end, I chose Al Cotton. A few years later I saw Larry again, when he gave a talk at MIT, and Al sent 3 or 4 of us to lunch with Larry; that was a wonderful, enjoyable experience – we asked oodles of questions about $Fe_3(CO)_{12}$ – which I will never forget (more about that later). About two decades would pass before we met again: this time at the RSC's International Symposium on 'Molecules, Clusters and Networks in the Solid State', held at the University of Birmingham in July 1986. When I introduced myself to Larry he claimed to remember the lunch 20 years earlier; Wow! He certainly knew how to make a young person feel important! I was already 44 at that time, but delving into the new area of radiation chemistry: Larry offered praise and encouragement.

Time flew by, and our next meeting, a very important one for me, was another two decades down the road. My mentor, Al Cotton, had received

the G. C. Pimentel Award in Chemical Education, an ACS award, based on his successful book, Chemical Applications of Group Theory. As part of the award, Al would be giving a lecture at the ACS meeting in Atlanta in March 2006; he was aware of a space group tutorial that Jerry Jasinski and I had written. Al thought that our approach was novel enough that I should get some "prime-time exposure" in the middle of his lecture: I quickly agreed to do it, and it went well. After the talk, I saw Larry rushing toward me, and he exclaimed that he really enjoyed the talk, and wanted to buy me dinner and discuss the teaching of crystallography. Done deal! From that point on, we saw each other regularly…at least once a year, most often at the annual ACA meetings. Larry was particularly helpful as I tried to come to grips with Al Cotton's untimely death in 2007. Larry was always "there" with uplifting personal words and succinct and impressive discussions of great science.

Quite apart from what we learn from personal interactions with famous scientists are the many things we can learn from the papers that they write. My friends and I in grad school were quite excited about the first Wei and Dahl communication (*J. Am. Chem. Soc.* 1966, 88, 1821-1822), and spent many hours discussing the paper. Three years later the full paper (*J. Am. Chem. Soc.* 1969, 91, 1351-1361) came out; I was then a Research Fellow at the ANU in Canberra, but luckily they got JACS by airmail! What an exciting read that was and still is (!); reading that paper set a standard for how to think about very tricky problems in those days… (and today too!), and helped me develop a critical approach to structure determination. The recent contribution by Larry, Chuck, Ilia and Evgueni (*J. Clust. Sci.* 2014, 25, 205–224) summarizes the whole story, told in the masterful Dahl style. Larry's papers and his oral presentations - and the incredible enthusiasm in each talk - are among the very best science and the very best scientific writing and speaking that I know. He is in my thoughts on a daily basis, an unforgettable, warm, helpful, creative and brilliant human being.

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2021 ACA Meeting Transactions Symposium

Function Follows Form: Celebrating the 50th Anniversary of the Protein Data Bank

Organizing Committee: Stephen K. Burley, David Rose, Natalie Strynadka, Rui Zhao

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Plenary: **John Rubinstein** - Sick Kids Hospital Toronto, Canada

Plenary: **Squire J. Booker** - Penn State, State College, PA

Plenary: **Rafael M. Couñago** - SGC/UNICAMP, Brazil

Plenary: **Erica Ollman Saphire** - La Jolla Institute for Immunology, La Jolla, CA

Nobel Lecture: **Frances H. Arnold** - CalTech, Pasadena, CA

Keynote: **Wayne A. Hendrickson** - Columbia, New York, NY

Plenary: **Chris Sander** - Harvard Medical School, Boston, MA

Plenary: **Eva Nogales** - UC Berkeley/HHMI, Berkeley, CA

Plenary: **Andrej Sali** - RCSB PDB/UCSF, San Francisco, CA

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PART 2
Saturday, July 31st

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2021 Awards

Sunday August 1st

Julia V. Zaikina: Margaret C. Etter Early Career Award
"How to discover new solids containing alkali metals: predictive screening, facile synthesis and in situ studies"
Sunday, 8/1/2021 @ 11AM - 12 PM ET

Monday August 2nd

Wah Chiu: M.J. Buerger Award
"CryoEM Structures of Macromolecules"
Monday, 8/2/2021 @ 11AM - 12 PM ET

Tuesday August 3rd

Jacqueline M. Cole: Bertram Eugene Warren Diffraction Physics Award
Molecular Engineering of Single-crystal Optical Actuators
Tuesday, 8/3/2021 @ 11AM - 12 PM ET

Registration

The ACA 2021 Annual Meeting will be 100% virtual with the entire meeting being streamed live with the ability for questions and answer sessions in real time. Once registered, you may attend any sessions and/or events that you wish (excluding workshops).

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Sessions

For a full ist of sessions please go to:
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Workshops

WK1: Characterization of Soft Materials Via Small Angle Scattering: Applications of Scattering for Polymer Systems
Monday, August 9, 2021 | 1:00 PM ET - 5:00 PM ET (PART 1)
Tuesday, August 10, 2021 | 1:00 PM ET - 5:00 PM ET (PART 2)
Wednesday, August 11, 2021 | 1:00 PM ET - 5:00 PM ET (PART 3)

WK2: Introduction to Hydroxyl Radical Footprinting Methods for Structural Analysis of Proteins and Complexes
Monday, August 9, 2021 | 12:00 PM ET - 4:00 PM ET

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WK3: Fundamentals of Single Particle Cryo-EM
Tuesday, August 17, 2021 | 12:00 PM ET - 6:00 PM ET (PART 1)
Wednesday, August 18, 2021 | 12:00 PM ET - 6:00 PM ET (PART 2)
Optional Reception: August 18, 2021 6:00 PM ET

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WK4: Managing and Using National Cryo-EM Facilities
Monday, August 16, 2021 | 12:00 PM ET - 6:00 PM ET
Optional Reception: August 18, 2021 6:00 PM ET

WK5: MicroED of Small and Macromolecules
Thursday, August 12, 2021 | 1:00 PM ET - 5:00 PM ET

YSIG Speed Mentoring

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This year, the ACA/YSIG will hold a special Zoom meeting with volunteering ACA mentors and younger ACA mentees. Forming private group chats between ACA mentors and mentees, this will give everyone an opportunity to ask questions about getting into the structural sciences! (e.g. crystallography, CryoEM, MicroED, NMR, Molecular Modeling and more).

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Poster Session & Exhibit Show

The ACA will be holding FOUR virtual poster sessions. Poster sessions are organized by the Poster Chairs and feature presentations covering a range of crystallography topics. Poster presentations may not seem as prominent as oral presentations, but they offer a terrific opportunity to interact with other scientists in your field in a structured way. Make sure to stop into the dedicated breakout rooms of our exhibitors!

Poster Session #1 Saturday, July 31st

Confirmed Exhibitors

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Poster Session #2 Sunday, August 1st
Exhibitors Coming Soon!

Poster Session #3 Monday, August 2nd

Confirmed Exhibitors

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Poster Session #4 Tuesday, August 3rd
Exhibitors Coming Soon!

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2020 U.S. Crystal Growing Competition

"The crystal growing project was fun and really worth my time. All I have to say is, I thought mine was going to be the smallest one and the worst one, but in the end, mine was big and clear. Therefore, if you are upset, never give up, try your best, and always give your best. Thank you so much for letting me participate in this! IT WAS AMAZING!!" --Tanner Horton, 5th grader in Laura Osborn's class at Sand Hill Elementary School in Guyton, GA.

A lot changed in 2020, but not the US Crystal Growing Competition (USCGC, http://www.uscrystalgrowingcompetition.org/)! Once again, thousands of kids, parents, and educators from all over the country participated in the #2020USCGC! Of course none of this would be possible without the tremendous efforts of the regional coordinators Fernando Uribe-Romo (University of Central Florida, UCF), Michael Nippe (Texas A&M University, TAMU), and Karah Knope (Georgetown University, GU), all their wonderful students, and mine too! And a special thanks to USCGC Assistant Tasha Benedict (University at Buffalo, UB), who really went the extra mile this year to help keep the contest running smoothly!

The 2020 USCGC once again began during National Chemistry Week in mid-October and concluded in early December. Hundreds of kilograms of alum went out, and over 110 crystals were sent back to Buffalo!

The 2020 judges included many veteran judges: UB Professors Ekin Atilla-Gokcumen (Chemistry), David Lacy (Chemistry), and Luis Velarde (Chemistry), and Andrea Markelz (Physics). And the contest welcomed back veteran judge and support technician extraordinaire Travis Nelson (Geology). The contest also welcomed two new judges: UB Professors David Heppner and Andrew Murkin.

Figure 1. 3rd grader Mason Doll from Valentyna Bardakova's class in Manhattan School Plus (New York, NY) won 1st place Overall. (Photo credit: Catherine Doll)

Winners were dotted all across the country! For grades K-8, 3rd grader Mason Doll from Manhattan School Plus (New York, NY) won 1st place Overall ($200) – That's two in a row for Valentyna Bardakova's students (Figure 1)! Alexandra Rupert and Phoebe Keiser (both 7th grade) from Mike Grove's class at Mifflin County Middle School in Lewiston, PA won 2nd place Overall ($100, Figure 2). And Leslie Zunk, homeschool student in 6th grade from Erick, OK took home 3rd place Overall ($50, Figure 3). Highest quality in grades K-8 went to Laura Osborn's K-5 team at Sand Hill Elementary in Guyton, GA ($100).

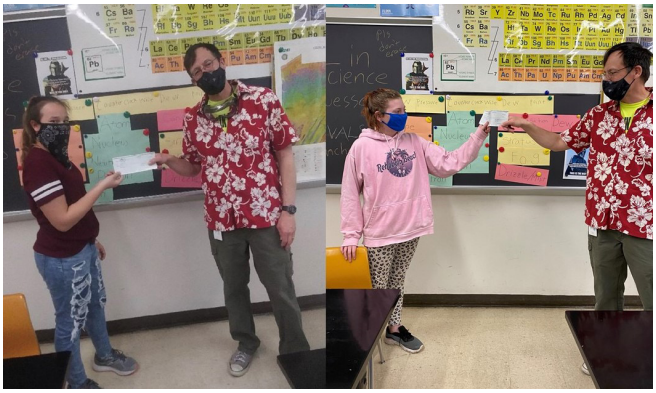

Figure 2. 7th graders Alexandra Rupert (left) and Phoebe Keiser (right) from Mike Grove's class at Mifflin County Middle School in Lewiston, PA won 2nd place Overall. (Photo credit: Alexandra Rupert and Phoebe Keiser.)

"With greatest thanks for opening the world of science to all who dream." – Catherine Doll, parent of Mason Doll who also shared with me that Mason was partly inspired to grow crystals because his great uncle, Aleksei Vasilevich Shubnikov (in Russian it is spelled А. В. Шубников) was a Russian

Figure 3. Leslie Zunk, homeschool student in 6th grade from Erick, OK took home 3rd place Overall. (Photo credit: Liz Zunk)

crystallographer! How cool is that!

In the 9-12 grade division, 1st prize Overall ($200) went to Sarah Evans's 11th grade Lew-Port Lancers General Chemistry Class from Youngstown, NY. 12th grader Micah Trevino, from Bradley Miller's class at Kearney High School in Kearney, MO won 2nd place Overall grades 9-12 (Figure 4). Lea Wilson, Kennedy McCormick, and Jillian Beebe from Dawn Kelley's class at Lyme/Old Lyme High School in Old Lyme, CT won 3rd place Overall (Figure 5). Another pack of Dawn's students took home 1st place quality: Thomas Moore, Matthew O'Leary, Malcolm Speirs, and Sebastian Burgio.

Figure 4. Wow! Check out all of the winners from Dawn Kelley's class! These teams won 3rd place grades 9-12, highest quality 9-12, and Coolest Crystal! (Photo credit: Dawn Kelley)

"*I learned that persistence and examining the crystal and its growth consistently is the best for growing a proper crystal. We should participate next year as it is a very fun and competitive contest. The crystals are amazing to watch grow and crystallize in their solutions.*" – Awesome feedback from one of Dawn Kelley's students.

The 'Best Teacher Crystal' was won by Bradley Miller from Kearney High School in Kearney, MO (Figure 5). And once again the competition for

Figure 5: Micah Trevino (left, 12th grade) and Bradley Miller (right, teacher) from Kearney High School in Kearney, MO. They won 2nd place Overall grades 9-12 and Best Teacher Crystal, respectively. (Photo credit, Ray Weikal and Michelle Lawrence)

Coolest Crystal was fierce! In a real squeaker, the 'Snowman crystal' sent in by more of Dawn's students, Grace Coverdale, Prudencia Kennedy, and Evan Montville, took first (Figure 4). They barely edged out the "super dark purple – nearly black crystal" sent in by Gwenyth Hall from Provo, UT (Figure 6). She attends Wasatch Elementary but grew her crystals at home! It's always so fun to see what happens when kids and their imaginations combine with crystals!!! (Figure 7)

Figure 6. Runner up for Coolest Crystal, Gwenyth Hall from Provo, UT. (Photo credit: James Hall)

"*I even had to have the staff at the school vote on which crystals they thought were the best to send off.*" – Bradley Miller describing how he gets school staff

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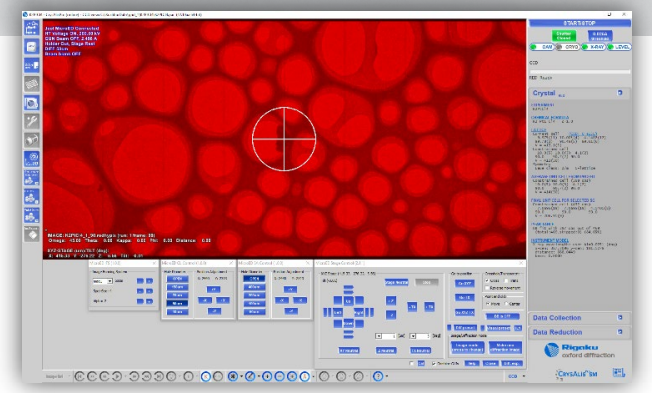

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involved in selecting the best crystals to send into the contest!

"I liked learning how the crystals form and seeing other people's crystals." – Gwenyth Hall, Runner up Coolest Crystal.

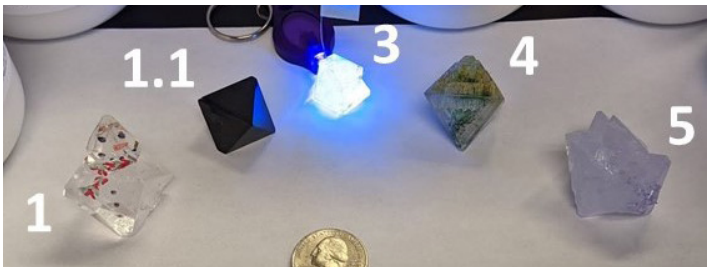


Figure 7. Top 5 Coolest Crystals (Photo Credit: Jason Benedict)

This year all of the winners were announced Academy Award Style on Tiktok:

K-8: https://www.tiktok.com/@benedictlabs/video/6923377783670443270

9-12: https://www.tiktok.com/@benedictlabs/video/6923377443613019397

Teacher/Coolest: https://www.tiktok.com/@benedictlabs/video/6923377892739108101

Please check out all the winners and some great participant posts on the contest website and at #2020USCGC on Twitter!

The USCGC helps raise public awareness of the importance of crystal-based research and the organizations, including the ACA, that promote and support these important activities. The USCGC gratefully acknowledges the support of our sponsors: ACA, National Science Foundation, Ward's Scientific/VWR, Pritzker School of Engineering at the University of Chicago, Bruker AXS, Rigaku, Krackeler Scientific, Cambridge Structural Data Centre, the Western New York section of the American Chemical Society, the Departments of Chemistry of UB, GW, UCF, and TAMU. Please consider making a tax-free donation to the 2021 contest! For more information, please visit the USCGC website or e-mail Jason Benedict at jbb6@buffalo.edu.

Jason Benedict

ACA HISTORY

AMERICAN CRYSTALLOGRAPHIC ASSOCIATION

History Project Update

Virginia Pett

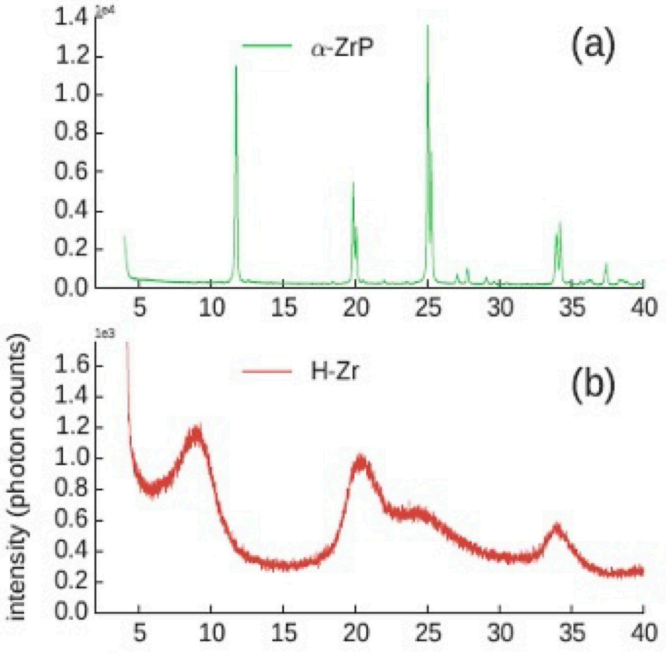
Award Video

Simon Billinge

Simon Billinge won the 2018 Warren Award. His lecture was titled "A series of fortunate events: how the atomic pair distribution function method went from niche technique to mainstream and beyond." Thanks go to Jeffrey Bacon for making the video of this lecture from the raw camera recordings. There were some technical difficulties that Jeff had to overcome.

Billinge introduces "crystallography for the 21st century" by contrasting the natural materials in use 100 years ago with the engineered materials of today. These modern nanomaterials are complex and inherently nonperiodic. Diffraction patterns from (a) crystalline material and (b) nanocrystalline material are compared below. The broad peaks in the nanocrystalline material result from diffuse scattering, giving information about the variations from unit cell to unit cell.

Billinge describes how diffuse scattering measurements and the pair distribution function (PDF) can be used to characterize real materials that do not form perfect crystals. The technique is very much like powder diffraction, except that



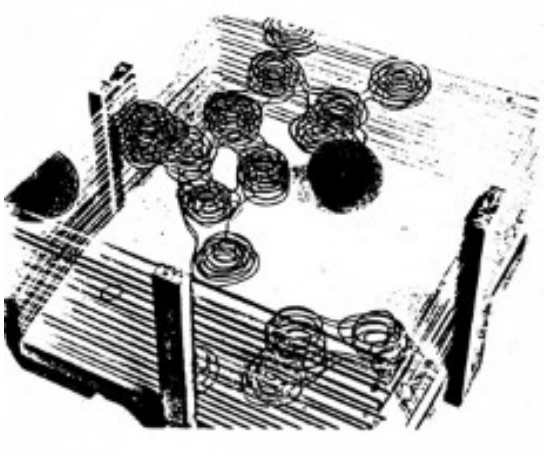
extremely short wavelengths are used to probe a much wider section of reciprocal space. Early on Bertram Warren and Rosalind Franklin made use of diffuse scattering and the PDF to study real materials, but the intensity and available short wavelengths of synchrotron radiation make this approach much more effective now. Both Takeshi Egami (2003 Warren Award winner) and Nozomi Ando (2020 Etter Award winner) have explored applications of diffuse scattering and the PDF.

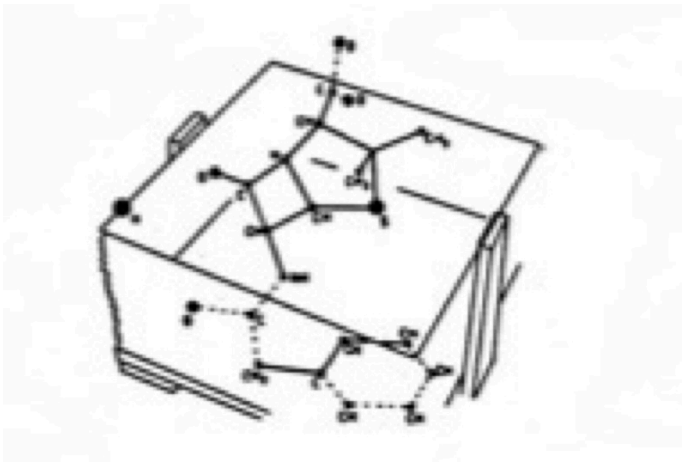
For more information on PDF and its applications, also see Billinge SJL. 2019 The rise of the X-ray atomic pair distribution function method: a series of fortunate events. *Phil. Trans. R. Soc. A* 377: 20180413. http://dx.doi.org/10.1098/rsta.2018.0413.

100 Years of Crystallography

Jenny Glusker

Jenny Glusker gave a 20-minute historical survey in 2012 at the ACA meeting in Boston. The video of her talk is now available for viewing at ACA History online. Shown below, the electron density of the β-lactam ring of benzylpenicillin (Hodgkin et al., 1949), which confirmed the strained four-membered ring structure.





Oral Interview

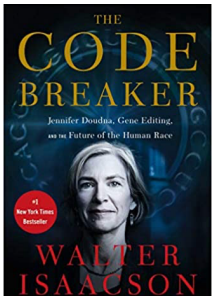
David Hass

The conversation between David Haas and David Zierler of the American Institute of Physics is now online at ACA History. Haas worked with well-known figures in the history of crystallography, and he describes the culture of the various laboratories in an engaging way. He did his Ph.D. at SUNY-Buffalo with David Harker, then a brief interim appointment at the U.S. Naval Research Laboratory with Jerome and Isabella Karle before going to The Royal Institution in London with David Phillips. Phillips suggested that he investigate how to protect protein crystals from radiation damage. Later, at the Weizmann Institute in Rehovot (with Wolfie Traub) he discovered that freezing lysozyme crystals with liquid nitrogen prevented radiation damage. The Six-Day War persuaded Haas to leave Israel for Michael Rossmann's laboratory at Purdue University. There, despite Rossmann's initial skepticism, Haas showed that cryocooling (as it is now called) prevents radiation damage to lactate dehydrogenase crystals. The discovery and subsequent publication made no immediate splash at all and Purdue never sought a patent. Discouraged with academia, Haas went into industry at Philips Electronic Instruments and later set up several businesses of his own (with patent protection!). He never knew until recently that cryocooling became a standard technique in macromolecular crystallography. It's exciting to see how fundamental research becomes crucial, sometimes years later.

People from the Past

Browse through these obituaries at ACA History pages, newly added online by webmaster Robin Payne. The 10 individual stories give us a real flavor of the individuals and what it was like to do structural science in the past.

–Virginia Pett



Book Review: The Code Breaker: Jennifer Doudna, Gene Editing, and the Future of the Human Race

ISBN: 978-1-9821-1585-2
By Walter Isaacson

Walter Isaacson is widely regarded as one of the foremost biographers of our time. Indeed, to have your biography written by Isaacson is considered by many to be a sign that you have "made" it, at least in the cultural zeitgeist intersection of innovation and power where Isaacson's work dwells.

But The Code Breaker falls flat. It is not a statement about the subject matter: Nobel prize-winning chemist Jennifer Doudna is a fascinating woman, and the story of her work with CRISPR even more so. It is a statement about Isaacson's biography of her.

It became clear to me, very early on, that Isaacson had never written a biography of a woman before. He is most famous for his works on Steve Jobs, Leonardo da Vinci, Henry Kissinger, Albert Einstein, and Benjamin Franklin. Most of the issues are subtle, a deep thread woven in the subtext of the book of what at best could be considered tone deafness and at worst could be considered something much more insidious.

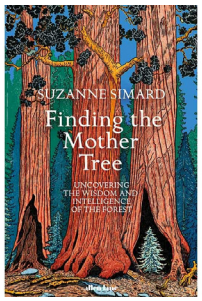
There have been a lot of parallels made—both in the book and in society at large—between Jennifer Doudna and Rosalind Franklin. Franklin, many feel, was robbed of recognition for the Nobel prize award to Watson, Crick, and Wilkins for the discovery of DNA. Others disagree, claiming that Franklin, despite taking the x ray diffraction image that led to the double helical discovery, would not have been able to figure out the structure—an unfair projection at best, a misogynistic one at worst. We'll never know what could have been or would have been, but making such comparisons in the wrong way creates uncomfortable insinuations. Suggesting Doudna's award of the prize was in some way a "correction" of past wrongs or a consolation prize decades in the making for a wronged Franklin both undermines the significance of Doudna's contribution and creates a problematic illusion that the men who contributed to CRSIPR (and subsequently, DNA) somehow made greater contributions than the women. It's a muddled mess, and Isaacson does a terrible job of teasing apart these intricate subtleties especially given the controversy at the center of the CRISPR patent battle.

Isaacson also repeatedly underscores that Doudna is incredibly competitive. This in and of itself is not bad—he claims Doudna herself acknowledges her own character and the impact it has had on her work, sometimes for better and sometimes for worse. But he places a lot of emphasis on the negative impact—such as the deterioration of her relationship with Emmanuelle Charpentier, with whom she shares her Nobel Prize. It is out of place and uncomfortable in the context in which it is presented—as a recurring theme of Doudna's character—a highly competitive person, whose competitiveness is described as a flaw of her character. By comparison, Isaacson discusses Eric Lander, the head of the Broad Institute who was funding Doudna's male competitors in a recent patent battle over using the CRIPSR technology in humans. Lander, who Isaacson alludes to having a, if not personal, genuinely jovial relationship with, is also described as being highly competitive—but it's cloaked in language of endearment and a tone of congenial collegiality. The contrast between how the competitiveness of a man who is not the subject of the book and who is not a scientist who actually worked on CRISPR is portrayed and the woman who is the subject of the book and won the Nobel prize for her role in discovering and developing the technology, is hard to ignore, and makes reading the book a less than enjoyable experience.

If you want a more gripping book about the story of CRIPSR, I would recommend Editing Humanity by Kevin Davies. If you want a better biography

of Doudna, you may have to wait until a new biographer dethrones Isaacson as the historically accurate tale teller of our time.

Jeanette S. Ferrara, MFA



Book Review: Finding the Mother Tree: Discovering the Wisdom of the Forest

ISBN: 978-0525656098
By Suzanne Simard

Suzanne Simard's *Finding the Mother Tree* is a *Silent Spring* for the next generation. Just as Rachel Carson's groundbreaking work illuminated the negative environmental impacts of DDT, so does Simard's book provide readers with an unprecedented glimpse into the lives, minds, and cultures of forests.

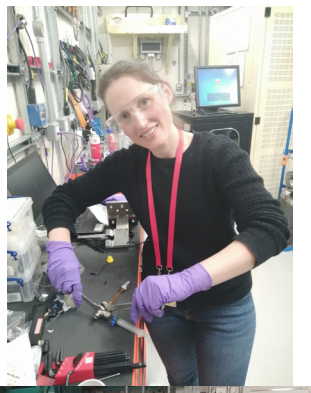
Finding the Mother Tree, like *Silent Spring*, is masterfully written. Dressed in the garb of a memoir, the book is just as much about Simard as it is about her work, but in such a way that serves to underscore her dedication to her research, rather than draw focus away from it. Simard carefully weaves her interpersonal narrative of memories with her hyper-focused academic one, providing readers with a book that makes learning about the complex neural networks of trees seem somehow easy, even though the concept is mind-blowing.

A wonderful read as we ease from Spring into Summer, after devouring *Finding the Mother Tree*, one may find themselves never really looking at forests the same way again.

Jeanette S. Ferrara, MFA

The Judy Flippen Anderson Memorial Journal of Structural Dynamics Poster Prize

The Judy Flippen Anderson Memorial Journal of Structural Dynamics Poster Prize, supported by the American Crystallographic Association and the American Institute of Physics Publishing, is given for excellence in research on structural determination and dynamics of systems, enabled by the emerging new instruments (e.g. XFELs, electron sources, etc.) and new experimental and theoretical methodologies and is open to students (graduate and undergraduate) and post-docs. This was awarded to Bethan Evans a PhD student at the School of Chemical and Process Engineering of the University of Leeds whose poster was entitled "From solutes to crystals: realistic structure models from time-resolved in situ pair distribution function analysis". Her co-authors were Anuradha Pallipurath, Arturs Pugejs, Philip Chater, Helen Wheatcroft, Robert Hammond and Sven Schroeder and the work was carried out in collaboration with Diamond Light Source and AstraZeneca. The judges for this Poster Prize were Christine Beavers and John Helliwell.



X-Ray Windows: To Be or Not to Be

It is unfortunate that beryllium has a bad reputation among the chemical elements, mainly due to its conspicuous toxicity, because the element itself has a number of fascinating properties, including the highest melting point among the alkaline earth metals (1287 °C) and a marked tendency to form compounds with a significant degree of covalent character. Beryllium is used as a moderator material in nuclear reactors, and its mechanical strength and low density (30% less than that of aluminum) have led to various aerospace and military applications. Beryllium-copper alloys containing up to 3% of the light metal ("beryllium bronzes"), despite being more expensive and not as strong as steel, are used for the production of non-sparking metal parts and tools widely used in the oil and gas industries.

Readers of *RefleXions* may be most familiar with the use of beryllium for the manufacture of X-ray tube windows, which take advantage of the low density and low atomic mass of the metal, and hence very low absorption of X-rays. These beryllium windows were developed in the 1940's and, interestingly, are only 8 to 100 μm thick, which is good enough to withstand the pressure exerted by the air against the vacuum inside X-ray tubes.

Beryllium is commonly obtained from beryl, an aluminosilicate mineral with chemical formula $Be_3Al_2Si_6O_{18}$, which is colorless when pure but typically adopts different colors based on the presence of other chemical elements. For example, the two best-known gem-quality crystalline forms of beryl, emerald and aquamarine, derive their beautiful green and light blue shades from the incorporation of small quantities of chromium(III) and iron(II) ions, respectively.

In the United States, beryllium is not extracted from beryl but from bertrandite, a related silicate hydroxide of chemical formula $Be_4Si_2O_7(OH)_2$, mined almost exclusively in the Spor Mountain area of Juab County in western Utah. ACA members in Utah (I assume there are some!) may be pleased to know that Beryl is also the name of a small town located in the southwestern corner of the state, in Iron County, about 50 miles northwest of Cedar City.

Daniel Rabinovich

Puzzle Corner

For summer, we have a new Crystoquote, a new Crystal Connections and a new DISORDERED puzzle. The solutions to the previous puzzles are also given, along with mention of those who provided solutions and a few comments on the puzzles.

Crystoquote #11: Letter substitution yields a quotation by a well-known crystallographer.

AS TOOUTHODFG OF HUSKOTZZFIUTQWS DGDODTZZS YTK,

RUTGEZS, OFOTZZS TVKOWVODH. DO'K T JVTXODRXZ KHDVGHV.

D OWDGE ATGS FR XK YWF JVHTAV HUSKOTZZFIUTQWVUK

YVUV TOOUTHOVC JS OWTO JVTXOS.

- ***WVZVG JVUATG***

Solution to Crystoquote #10:

Her photographs are among the most beautiful X–ray photographs of any substance ever taken.

John D. Bernal

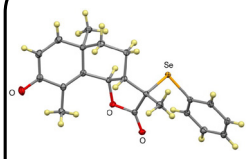
Crystal Connections #20: What do the answers to these clues have in common?

1. **Emily Dickinson wrote a poem about the song of *Icterus galbula*, for which this baseball team is named.**
2. **"And ____ _____, never flitting, still is sitting, still is sitting…" This poem led to the name of a pro football team.**
3. **The author of that poem, who also wrote "The Gold-Bug," which involved cryptograms.**
4. **The _____ _____ _____ groups viruses based on genome replication strategy.**
5. **The "Star-Spangled Banner" was written during its bombardment in 1814.**
6. **In Monopoly, the "B&O" railroad.**
7. **Considered the first research university in the United States.**
8. **The Preakness Stakes horserace is held here.**
9. **The Susquehanna, Potomac, Rappahannock and James Rivers drain into _____.**
10. **Randy Newman song which contains the line "beat up little seagull on a marble stair".**

DISORDERED

Correct these anomalous spellings to resolve the ambiguity

FHOTO	
DEFILER	
RICHLA	
TRAFCO	
KEPS	



x=0.986(8)

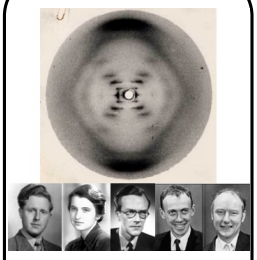
If you report the incorrect absolute structure, the referees will give you…

Answer:

DISORDERED

Win the prize (or not) by correctly sequencing these strands

CHELLIA	H E L I C A L
MYNITHE	T H Y M I N E
GRAMBICED	C A M B R I D G E
SKINIWL	W I L K I N S
FLANKNIR	F R A N K L I N
SWANTO	W A T S O N



The tale of Photograph 51 is

Answer:

T W I S T E D

Comments on the previous puzzles:

In the quote by J. Desmond Bernal, he speaks of Rosalind Franklin's photographs. The people in the DISORDERED photographs are (l. to r.) Raymond Gosling, Rosalind Franklin, Maurice Wilkins, James Watson, and Francis Crick. Gosling, while a PhD student at King's College working with Franklin, prepared the X-ray photograph known as "Photo 51." A number of readers submitted solutions to the DISORDERED puzzle and attempted the extra credit challenge by identifying the five pictured people. Most were not able to identify Gosling, but **Mitchell Guss** (Univ. of Sydney) did, and receives extra credit. **Frances Bernstein** was the first to provide the solution to the DISORDERED puzzle, and **Joel Harp** (Vanderbilt) provided the solution to Crystoquote #10.

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

Frank Fronczek – ffroncz@lsu.edu

MiTeGen
www.mitegen.com

MiTeGen announces the development of a next-generation crystal mounting system that will change how crystals are prepared for X-ray diffraction data collection.

This new system allows users to:

- Mount single crystals or thousands for micro-crystals
- Optimize for serial crystallography or single crystal XRD
- Perform either Cryogenic or Room Temperature diffraction

How it works:

Crystals are mounted onto the supports utilizing a humidified sample loading box. The high-humidity box allows samples to be prepared without unintentional dehydration to the drops or crystals. The supports can then be plunge cooled (for cryo) or sealed (for room temperature work).

The system has multiple applications including:

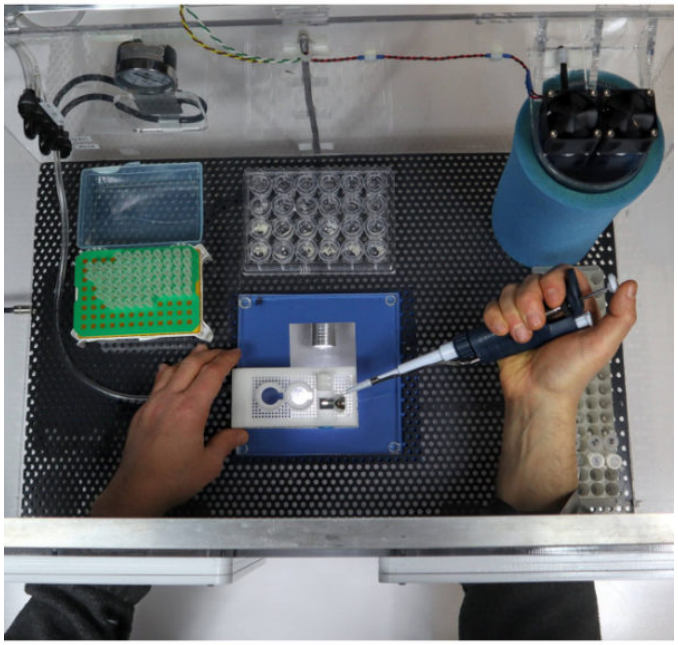
- Conventional Crystallography
- Serial Crystallography
- *In Situ* Crystallography
- Room Temperature Crystallography
- And more

Why did MiTeGen design this system?

"We are excited about the developments we have been making to advance how crystals are delivered to the X-ray beam", says Ben Apker, COO of MiTeGen." We believe that the new sample support system will change how crystallographers prepare crystals for data collection, whether they are doing serial work on microcrystals or using larger single crystal approaches."

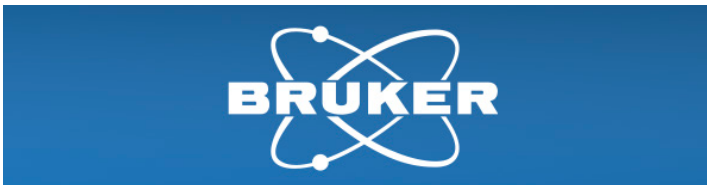
The system is still in continual development and MiTeGen is seeking input from interested parties for further refinement of the system.

Learn More About The Crystallography Sample Supports



- MiTeGen is searching for an X-ray and Cryo-EM Application and Methods Development Scientist. Candidate will work with the CTO, R&D Engineering Manager, and other R&D staff to assist in developing new methods and technologies for biomolecular X-ray crystallography and single-particle cryo-electron microscopy and more - Learn More
- MiTeGen is searching for a Research and Development Scientist/Engineer. Candidate will work for the R&D Engineering Manager and collaborates with the CTO. Takes guidance for daily activities and longer-term efforts from the Engineering Manager and the CTO. Supports other development and production staff in their tasks and in solving issues and answering questions in your areas of expertise and more - Learn More

- MiTeGen is searching for a Customer Sales Assistant who will focus on the development of sales opportunities with scientific customers. This will include outlining scientist-focused sales campaigns, making sales calls to scientists, nurturing opportunities, and providing sales support to a broad range of researchers from academia to industry. The role of Customer Sales Assistant at MiTeGen requires a multi-talented individual who can adapt their skill set to a broad range of areas within our growing organization. An outgoing personality who is detail oriented and loves speaking on the phone will thrive in this role. A background in structural biology or related science is not required, though experience with crystallography or cryo-EM would be a plus! An organized, independent, individual who is able to multi-task and is highly motivated to develop customer relationships, find solutions and adapt to various situations and company needs will find this to be an opportunity to start a rewarding career - Learn More



Chaperone Compounds for Co-crystallization of Organics

Even for highly performing, modern X-ray diffractometers, such as the D8 QUEST ECO, D8 QUEST or D8 VENTURE, the efficiency and quality of a single crystal structure determination is often limited by the availability of good quality samples. This is particularly true for low to mid-range molecular weight organic molecules, where the structure investigation is often motivated by the need to elucidate diastereomers or enantiomers. The absolute structure determination is often only possible after good quality crystals have been grown.

Numerous methods have been developed to overcome the 'poor crystal'-bottleneck. Many of these methods make use of a crystalline framework with rather rigid, pre-designed cavities. The molecule of interest, the analyte, migrates into the cavities if major requirements, such as size, electrostatic potential, etc. are fulfilled. However, the proper adjustment of the cavity size to the needs of the analyte requires upfront design and synthetical efforts for the framework or a sequence of trial-and-error experiments. The migration process, often controlled by thermodynamics, can take several weeks and still might be incomplete. As a result, disorder of the analyte is observed in the diffraction experiment, which often prevents the high-quality data set needed for absolute structure analysis.

Recently, tetrahedral adamantane aryl-derivatives have shown an impressively high ability to form co-crystals with many organic molecules, difficult to crystalize by other methods. This approach takes advantage of the flexibility of the substituted adamantanes and is called "Chaperone method". It has been developed by Prof. Richert at the University of Stuttgart in Germany. It is easy to use and can be carried out in-house in very little time and with minimal experimental effort. Only a few milligrams of the analyte are required and added to the Chaperone in a small crystallization vial. After the vial is gently warmed to create a homogenous solution, co-crystals form upon cooling, often in just a few minutes with success rates in the 95% range.

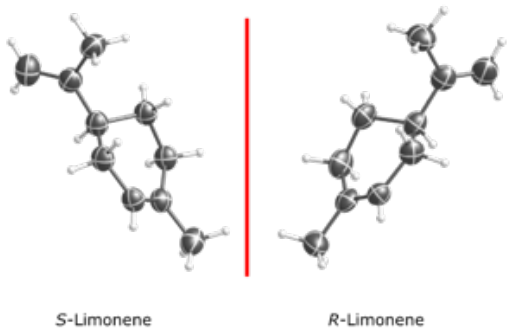


Fig. 1: Absolute structure determination of Limonene using the new Chaperone method (adamantane derivatives omitted for clarity).

In collaboration with Prof. Richert, Bruker has developed a first set of three Chaperone crystallization kits. Each kit contains the adamantane aryl-derivative, crystallization vials, operation instructions, related literature, and safety documentation.

"The ease-of-use and the speed the crystallization takes place are both impressive", Dr. Tobias Stuerzer, head of Bruker's single crystal application labs states. "The Chaperone method adds a powerful tool to the toolbox for organic chemists or service crystallographers. It enables them to get access to those high-quality crystals required for a high-quality structure. In our application lab we have successfully crystallized the two limonene stereoisomers, solved, and refined the structures in less than two hours", Stuerzer continues (Fig. 1).

More information on the Chaperone method is available on Bruker's web page or via your Bruker support contact.

Rigaku and JEOL Launch a Revolutionary Electron Diffraction Platform XtaLAB Synergy-ED: a Turnkey Solution for Molecular Structure Determination for Nanocrystals

Rigaku Corporation (Headquarters: Akishima, Tokyo, Japan; Chairman & CEO: Hikaru Shimura), a leading company producing X-ray analysis instruments, and JEOL Ltd. (Headquarters: Akishima, Tokyo, Japan; President & COO: Izumi Oi), a leading company producing electron microscopes and other analytical instruments, have announced the launch of the XtaLAB Synergy-ED, an integrated electron diffraction platform for the determination of molecular structures from nanocrystals, a joint project that has been underway since May 2020.

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

The determination of 3D molecular structures at the atomic level is a key technique for driving innovation in the drug discovery, synthetic chemistry and material science fields. Single crystal X-ray structure analysis has long been the primary technique used to determine accurate 3D molecular structures for inorganic, organic and protein molecules. By providing highly accurate and reliable molecular structures, X-ray crystallography has contributed to the discovery of new substances, elucidation of biological activity and chemical reactivity, prediction of interactions with other substances, and confirmation of expected efficacy of medicines.

However, in recent years, there has been an increasing need for the structure analysis of substances that only form microcrystals, crystals that are only a few hundred nanometers or less in size. Analysis of crystals of this size is not possible with X-ray crystallography, where the smallest possible crystal dimension is 1 micron, and only

then when utilizing the brightest X-ray sources. In recent years, a new analytical method, MicroED, has been developed that uses electron diffraction on a TEM electron microscope to measure 3D molecular structures from nanocrystalline materials. Researchers developing this technique have relied on customized electron microscopes and a combination of microscopy software for measuring diffraction data, and public domain X-ray crystallography software for data processing and structure determination. Switching a microscope configuration between imaging and diffraction can be time-consuming, making the sharing of an instrument sometimes difficult.

To address these issues, Rigaku and JEOL started a collaboration to develop a dedicated single crystal structure analysis platform for nanocrystals utilizing key technologies from both companies. The result of this collaboration is the XtaLAB Synergy-ED, a dedicated electron diffractometer that is operated by the same control software that is used to run Rigaku's X-ray diffractometers and includes a complete integrated pipeline from sample selection and diffraction measurement to data processing and structure solution. This instrument can easily be installed in an existing X-ray crystallography facility, where researchers and students will be able to easily master the MicroED technique since the software workflow is the same as for an X-ray diffractometer. Having such an instrument installed in an X-ray facility immediately provides structure determination for materials that only form nanocrystals.

DECTRIS

Welcome summer!

Although we specialize in detecting X-ray photons, we are highly interested in catching some light, too! Throughout May and June we have been biking to work (getting tanned), and planning our summer activities. To start with, we are launching the second season of…

Application webinar series

The second edition of the DECTRIS application webinar series features two sessions. The first session starts on June 23rd and celebrates the beginning of summer with contributions on high X-ray energy applications. The other session starts in September and tackles contemporary structural biology. In total, we will be hosting six scientists, two of which come from the USA:

- Dr. Prakapenka (GSECARS, APS) will present the challenges and solutions of collecting high pressure XRD data on samples with various degrees of crystallinity
- Dr. Kneller will introduce the capabilities of a laboratory diffractometer to collect X-ray diffraction data for structure determination of macromolecular samples

How about the other four speakers? Discover them here and book your calendars for exciting discussions!

ACA meeting

By now, you have already submitted your abstracts for the meeting of the American Crystallographic Association. So have we! Dr. Dubravka Sisak Jung will join the session Economics of crystallography, and reflect on the experiments and equipment used at synchrotron sources and in academic and industry labs. Dr. Marcus Müller will focus on detectors used in a laboratory setup, and introduce the hybrid-pixel X-ray and electron detectors. And if you have any follow up questions, you don't need to worry. Direct emailing always works, or just pick up the phone and contact our colleagues at DECTRIS USA.

We wish you an innovative, scientific and collaborative summer!

Escargone

American Crystallographic Association
Statements of Financial Position | December 31, 2019 & December 31, 2020

		2020		2019
Assets				
	Current Assets			
	Cash	$382,576.00	$	153,008
	Accounts Receivable	$0.00	$	2,000
		$382,576.00	**$ 155,008**	
	Restricted Cash	$72,848.00	$	52,555
	Investments	$964,456.00	$	966,074
		$1,419,880.00	**$ 1,173,637**	
Liabilities & Net Assets				
	Current Liabilities			
	Accounts Payable	$9,159.00	$	6,679
	Deferred Revenue	$53,725.00	$	63,695
		$62,884.00	**$ 70,374**	
	Net Assets			
	Without Donor Restriction	$490,245.00	$	517,677
	With Donor Restriction	$866,751.00	$	585,586
		$1,356,996.00	**$ 1,103,263**	
		$1,419,880.00	**$ 1,173,637**	

ACA ACCOUNT BALANCES AS OF 12/31/20

Name	2019 Balance	2020 Balance
Bau	$36,494	$36,494
Buerger	$38,978	$38,978
Rognlie	$60,000	$57,000
Etter/SIG	$70,439	$71,044
Fankuchen	$71,343	$71,343
Patterson	$48,786	$47,286
Pauling	$40,270	$41,305
Supper	$12,661	$12,661
Trueblood	$40,459	$40,459
Warren	$31,994	$32,079
Wood	$54,211	$54,211
Student Travel	$27,396	$31,151
Rosenstein Estate	NA	$250,000
Total	**$533,031**	**$784,011**

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		AIP American Institute of Physics

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