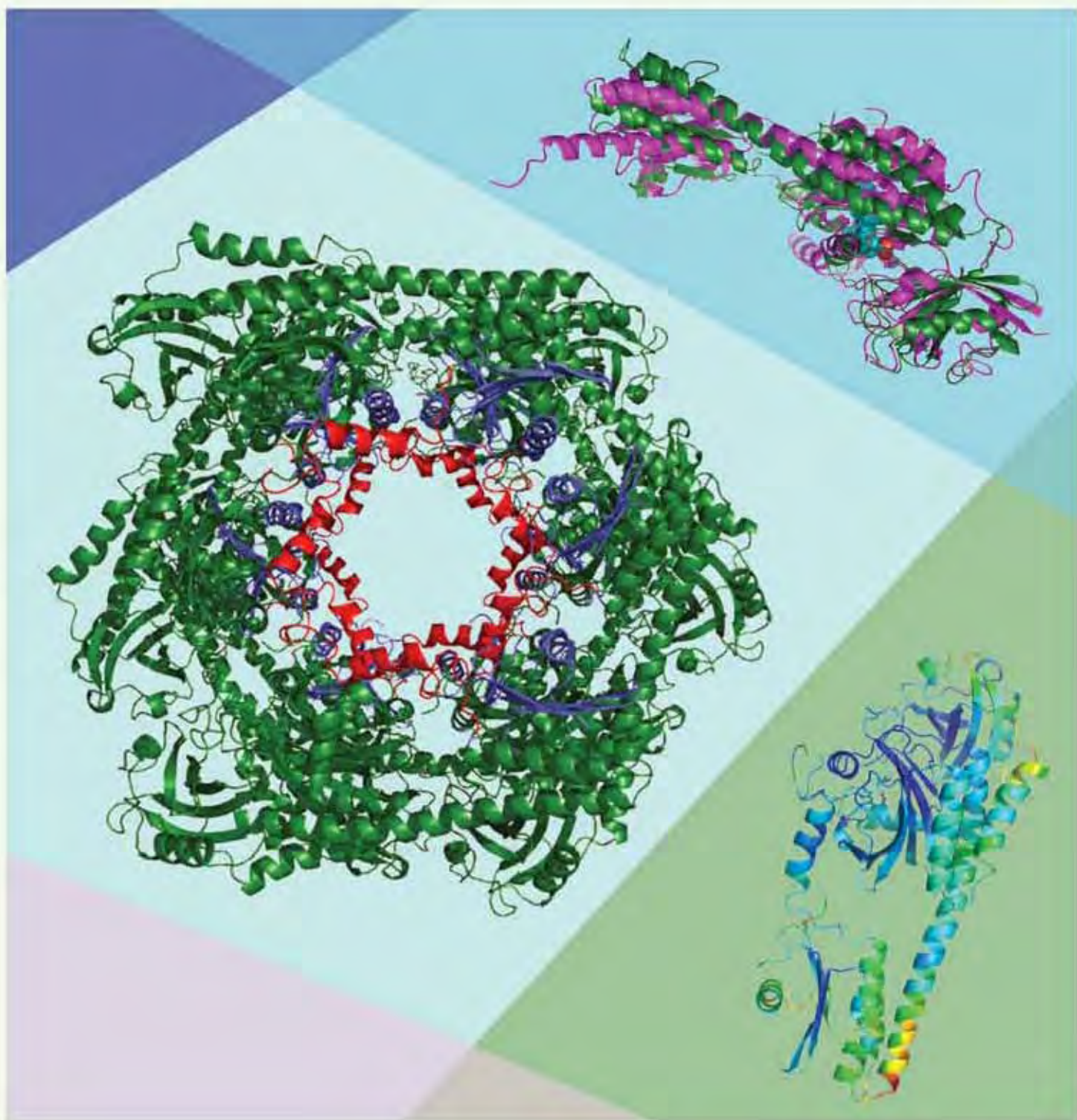


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American Crystallographic
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Number 1
Spring, 2011



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Cover: Keith Moffett will receive the Patterson Award at the 2011 ACA meeting in New Orleans. The images are from his research group, see On the Cover, page 5.



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When I attended my first ACA meeting some forty years ago I never dreamt that one day I would be writing this column as your President. It's truly a privilege for me to be able to serve the ACA, which I have regarded as my scientific home ever since that time when I was a brand-new postdoc.

By coincidence, that first ACA meeting I attended back in 1970 was held in New Orleans – a wonderful site and also the venue for this year's annual meeting, which will take place from May 28 through June 2, 2011. Your New Orleans Program Chair Chris Cahill is planning an outstanding scientific program. Highlights will include a full-day ACA *Transactions*

Symposium, Time-Resolved Studies and Photochemistry (AM) and Charge Density (PM), on Monday, May 30. Inspired by the research of former IUCr and ACA President Philip Coppens, the *Transactions* Symposium is cosponsored by the Small Molecule, Synchrotron, and General SIGs. ACA's Canadian Division is planning a session on Evolution of Powder Diffraction Software in honor of their late colleague Lachlan Cranswick. Also featured in New Orleans will be the presentation of the 2011 Patterson Award to Keith Moffat, the 2011 Wood Science Writing Award to Daniel Nocera, and the 2010 Trueblood Award to David Watkin. David unfortunately was unable to join us last summer in Chicago, and we are very pleased that he plans to be with us in New Orleans to receive his award. See page 34 in this issue for additional information on the exciting program planned for New Orleans.

As Judy Kelly reported in this space in the winter 2010 *RefleXions*, last October Council decided to change the format of our annual meetings and to go from a five-day (Sunday-Thursday) meeting format with four parallel sessions each morning and afternoon to a four-day (Sunday-Wednesday) meeting format with five parallel sessions each half day. The Saturday prior to the start of the meeting will as usual be set aside for workshops. Our 2012 Boston meeting will be our first meeting to use the new, shorter format. Controlling costs, along with time savings for our members, were important factors in Council's decision to opt for the shorter meeting format.

2011 promises to be a very exciting year for ACA and for crystallography. In addition to our New Orleans ACA meeting, the XXII IUCr Congress and General Assembly will take place in Madrid, Spain, August 22-30, 2011, and many of us are looking forward to seeing our international colleagues in Madrid. ACA milestones for 2011 will include the selection of the first group of Fellows, who are in the process of being chosen by Council under the new ACA Fellows Program. We will keep you posted on this and other developments as the year goes forward.

This year we welcome three new members on the ACA Council. Our incoming Vice-President is George Phillips, and David Rose returns as our Canadian Representative. Jamaine Davis joins Council as an ex-officio, non-voting member representing the Young Scientists' YSSIG. Two Council members have completed their terms in 2010: Past-President Bob von Dreele, and Canadian Representative Jim Britten. ACA is extremely grateful to Bob and Jim for their years of service. On a personal note, I want to add my thanks to all of our colleagues on Council including especially my predecessor as President, Judy Kelly, for their work and dedication. My own job this year will, no doubt, be much easier because of all of their outstanding efforts.

ACA's success is, of course, due in large measure to our extremely dedicated professional staff in the Buffalo Headquarters: Director of Administrative Services Marcia Colquhoun, Membership Secretary Crystal Towns and, in the past, former staff members Patti Potter and Jen Shepard. Every year at our annual meeting, I'm sure that we're all impressed by the hard work over many long hours that the staff puts in to make sure everything runs smoothly. Of course, their demanding work goes on behind the scenes year round. While we on the Council rotate through our positions, it is the ACA's staff that provides continuity and enables ACA to be such an invaluable resource for you, our members. We all owe Marcia and Crystal a tremendous vote of thanks!

As I write this, early in February from snowy New York, our spring meeting in New Orleans looks especially attractive. We hope that as many of you as possible will attend. The ACA has worked hard to keep costs down, so don't forget to register by March 31, the early deadline. The booking deadline for the conference rate at the Sheraton New Orleans is April 15. A limited number of specially discounted hotel rooms is available for students and postdocs, on a first-come, first-served basis – so please be sure to get your reservations in early.

See you in New Orleans.

Tom Koetzle

Cartoon courtesy of Nick D. Kim. Nick Kim is an analytical environmental chemist currently working for the Waikato Regional Council. He is an honorary lecturer at the University of Waikato in New Zealand.



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Thank You Letter from Bernice Stewart

Kudos to the three individuals who composed the memorials of Jim Stewart which were published in the winter issue of *Reflexions*. Bruno Morosin, Winnie Wong-Ng and Syd Hall collectively captured the essence of my late husband's attributes and interests. Their memories of Jim honor him and deserve to be acknowledged, my reason to thank all of them for their splendid write-up.

It goes without saying that Jim was a pioneer with his far-sighted recognition of the need for transportable programs so that crystallographers would no longer be strapped to the restrictions imposed on them by the diversity of existing software systems. His enthusiasm for computing and the fun he had with it was contagious to his collaborators to whom he always gave credit first, short changing himself in this act. He excelled as a teacher, was an avid environmentalist, read widely - such that after 57 years of marriage my mind would still be boggled by the extensive amount of information he had stored on any subject. He was always able to find common ground to start an interesting conversation with anyone he met.

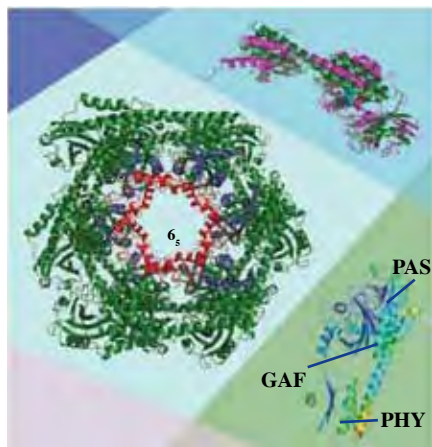
His graduate students adored him and he would always "adopt" them as part of our family. Saturdays would be oil changing day in our back yard along with lessons about how to repair minor glitches in their cars (always the teacher!). I would prepare lunch for the participants and we would eat together as a family.

Above all, Jim was a non-pretentious man, totally lacking in signs of arrogance. I always told him that instead of McDonald, his middle name should have been McHumble. Need I say more. Again I thank the three contributors to Jim's memories for their most favorable assessments of this wonderful and unique person. I was fortunate to have had him in my life.

Bernice Stewart

Editor's note: We received this in handwritten form from Bernice after the winter RefleXions published memories of her husband Jim, pp 8-9.

Images from 2011 Patterson Award winner, Keith Moffat



The lower right image shows the crystal structure of the Q188L mutant of PaBphP-Photosensory Core Module from a PNAS article by Xiaojing Yang, Jane Kuk, and Keith Moffat.¹ Its ribbon diagram is colored by the main-chain rmsd values between the structures of Q188L [Protein Data Bank ID 3G6O] and PaBphP-PCM wild type (PDB ID 3C2W). The other two images are from the supporting information for the same article. The view at left shows the molecular packing of PaBphP-PCM-Q188L in the crystal lattice in space group P6₅. The core of the PHY domains (blue) and their arm regions (red) form a cylindrical solvent channel centered along the 6₅ screw axis, resulting in disorder and therefore poor side-chain density in the PHY domain. The PAS and GAF domains and all helical bundles are colored in green. The image at upper right shows the global structural differences between the same PDB ID 3C2W wild type (green) and a magenta colored cyanobacterial phytochrome from *Synechocystis* species 6803.² Cph1-PCM (PDB ID 2VEA), specifically the long helical bundles at the dimer interface.

Phytochromes are red-light photoreceptors that regulate light responses in plants, fungi, and bacteria by means of reversible photoconversion between red (Pr) and far-red (Pfr) light-absorbing states. The Q188L mutant of the *Pseudomonas aeruginosa* bacteriophytochrome (PaBphP)-PCM exhibits altered photoconversion behavior and different crystal packing from the wild type. Two distinct chromophore conformations in the Q188L crystal structure were observed that were identified with the Pfr and Pr states. The Pr/Pfr compositions, varying from crystal to crystal, seem to correlate with the light conditions under which the Q188L crystals are cryoprotected. All known Pr and Pfr structures were compared and using site-directed mutagenesis residues were identified that are involved in stabilizing the 15Ea (Pfr) and 15Za (Pr) configurations of the biliverdin chromophore. Specifically, Ser-261 appears to be essential to form a stable Pr state in PaBphP, possibly by means of its interaction with the propionate group of ring C of the bilin chromophore. A "flip-and-rotate" model was proposed that summarizes the major conformational differences between the Pr and Pfr states of the chromophore and its binding pocket.³

Static crystallographic studies of signaling photoreceptors such as phytochromes are an essential precursor to time-resolved studies. Such studies will explore the questions: how is the signal generated by absorbing a photon of red or far-red light transmitted from the chromophore, across the chromophore binding domain and ultimately to the output domain (not shown in these structures), a histidine kinase? How is the activity of the kinase thereby modified? In short, how do these signaling photoreceptors really work?

(1) X. Yang, J. Kuk and K. Moffat (2009), *Conformational differences between the Pfr and Pr states in Pseudomonas aeruginosa bacteriophytochrome*, *Proc Natl Acad Sci USA* 106, 15639-44. (2) L.O. Essen, J. Mailliet, J. Hughes, (2008) *The structure of a complete phytochrome sensory module in the Pr ground state*, *Proc Natl Acad Sci USA* 105, 14709-14. (3) This paragraph was adapted from text in (1).

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The *RefleXions* editors, Judy and Connie are hoping someone will volunteer for the position of

Opinions Column Editor

In the past our *Opinions* columns have featured two subjects: **Intelligent Design / the Evolution debates** and **Global Warming**. We can supply sources for both of these, and the column could consist of updates from these sources - or - the *Opinions* editor could choose another subject and put together something different. Please contact Connie Rajnak (conniechidester@earthlink.net or Judy Flippen-Anderson (acarefleXions@gmail.com)).

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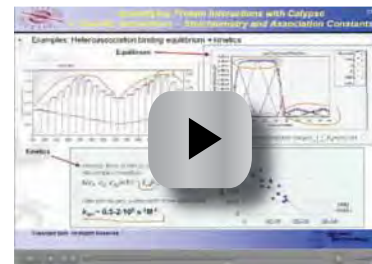
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USNCCr Roster cont'd next page

Bernard (Bernie) Simon Borie Jr. died 30 November 2010 at the age of 86. Borie was widely recognized for his pioneering work on diffuse x-ray scattering theory and in particular for the Borie-Sparks method of determining chemically-specific atomic displacements in short-range-ordered alloys. He received his BS in Electrical Engineering from the University of Louisiana Lafayette, and, following service in the United States Navy during World War II, obtained an MS in Physics at Tulane University and a PhD in Physics at MIT. Bernie studied under B. E. Warren at MIT and remained a strong advocate of the “Warren approach” throughout his career. His work was distinguished by clarity and elegance. When writing his popular book on x-ray diffraction, Warren solicited help from students and former students to write the chapter on dynamical diffraction. Bernie Borie’s eminently accessible extension of the Darwin method was selected over the more traditional methods summarized in the classic dynamical diffraction review by Batterman and Cole.

After graduating from MIT, Bernie completed a Fulbright Fellowship at the University of Paris and then hired into the Metals and Ceramics Division of the Oak Ridge National Laboratory where he served as group leader of the X-ray Diffraction Group. At Oak Ridge, his work on diffraction theory provided insights into materials structure/property relations. Materials systems of interest included short-range ordered TiZr, CuAl, and CuAu alloys as well as oxide thin films. Throughout his career he pushed the frontiers of diffraction theory with an abiding interest in thermal and static displacements and in methods to accurately extract this information from x-ray diffraction patterns. For example, the Borie-Sparks theory of diffuse x-ray scattering grew from earlier work by Borie that exploited distinct symmetry in the diffraction pattern of short-range-ordered alloys arising from chemical order and chemically-specific static displacements. By assuming that the atomic form factor had weak momentum transfer dependence the Borie-Sparks method was able to use 3 dimensional reciprocal-space maps to recover static displacements in binary alloys. These methods are still used at neutron facilities and were later extended with anomalous scattering methods made practical by the emergence of synchrotron x-ray sources.

In addition to his pioneering work on x-ray diffraction theory, Bernie was a gifted teacher, and taught x-ray diffraction theory internally at ORNL, at the University of Tennessee, and as a visiting professor at Cornell and U.C. Berkeley. Ultimately Bernie Borie’s pioneering approaches for the analysis of diffuse x-ray scattering data and his clear writing and teaching have inspired research that continues to the present day.



Gene E. Ice

Gene Ice is Acting Director of the Material Science & Technology Division at ORNL

2011 USNCCr cont'd

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Preservation Hall celebrates its Golden Anniversary throughout the year 2011.

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It is with great sadness that we report the death of one of our dearest ICDD friends and founding fathers, Ludo Frevel. He passed away on Saturday, 15th January, 2011, at Bickford Cottage of Midland, Michigan. Born in Frankfurt, Germany, 31st May, 1910, Ludo recently joined the rank of "Centenarian", celebrating his 100th birthday among friends and family.

Ludo earned a doctorate in physical chemistry from Johns Hopkins University, followed by two years of study at the California Institute of Technology with structural chemist and Nobel laureate, Linus Pauling. He joined Dow's Spectroscopy Laboratory in 1936, where he worked as one of Dow's pioneer chemists for 39 years. Upon retirement, he was one of Dow's top scientists and was the first Dow scientist to have the title Research Specialist. Until 2005, he served as a consultant to Dow Corning Corporation. He held 60 patents and authored or co-authored 446 technical papers, publishing his most recent paper at age 95.

Ludo's work in x-ray powder diffraction and catalysis, particularly in the petrochemical industry, is known worldwide. He was also recognized for his method of purifying ethylene to make polyethylene. However, the accomplishment he was most proud of was his work on the purification of butadiene for synthetic rubber.

Ludo's association with the ICDD spanned many decades. His pioneering work began with his vital contributions to the 1938 Hanawalt, Rinn and Frevel paper entitled, *Chemical Analysis by X-ray Diffraction - Classification and Use of X-ray Diffraction Patterns*, published in the Analytical Edition of *Industrial and Engineering Chemistry*. This work, which supplied tabulated diffraction data for 1,000 chemical substances and included the indexing and comparison methods for identifying materials, is considered by most diffractionists to be the classic work in qualitative identification of multiphase polycrystalline materials. This work directly led to the creation of the Powder Diffraction File™, and the tabulated data were the genesis of Set 1, published in 1941.

As an active member, Ludo served the ICDD in many capacities. He published one of the first papers on the use of computers in both the searching and matching steps of crystalline phase identification. From 1978 through 1996, he assumed various leadership roles by serving as a member of the Board of Directors; as such, he performed the duties of Member-at-Large, Consultant to the Board, Chairman, and Past Chairman.

Over the years, Ludo was honored for his contributions to the x-ray analysis field as well as those to the ICDD. The ICDD established the J.D. Hanawalt Award for excellence in powder diffraction in the early 1980s. Ludo was named as the first recipient - a title well deserved! For his long and meritorious service to the ICDD, Ludo was designated as an ICDD Distinguished Fellow in 1984.

Ludo's commitment to the education of young scientists was exemplified in his establishment of the Crystallography Scholarship Program. To encourage promising graduate students to pursue crystallographically oriented research, he founded the Crystallography Scholarship Program in 1991. Administered by the ICDD, the program's name was changed in 2000 to honor Ludo as its founder. In addition, Ludo contributed significantly to the scholarship fund and actively solicited funding from private and academic sectors to sustain the program. As of January 2011,

the **Ludo Frevel Crystallography Scholarship Program** has awarded

122 scholarships totaling over \$282,000. During his lifetime, Ludo mentored many scientists especially those working in x-ray diffraction at both The Dow Chemical Company and Dow Corning. Those who had the pleasure of working with Ludo remember him for his brilliant mind and passion for science. He was always willing to teach others, share ideas, and discuss methods, with a wonderful combination of gentleness and enthusiasm.



Ludo is survived by his three children, Mary (Kadish), Gordon, and Kurt; two grandchildren, Lesley Kadish, and Laura McConville; and two great-grandchildren, Hayden, and Maxwell. He was preceded in death by wife, Ruth; parents, Ludwig and Carrie; and his brothers, Raoul and Karl.

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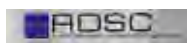
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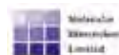
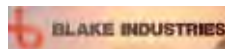
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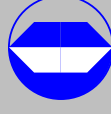
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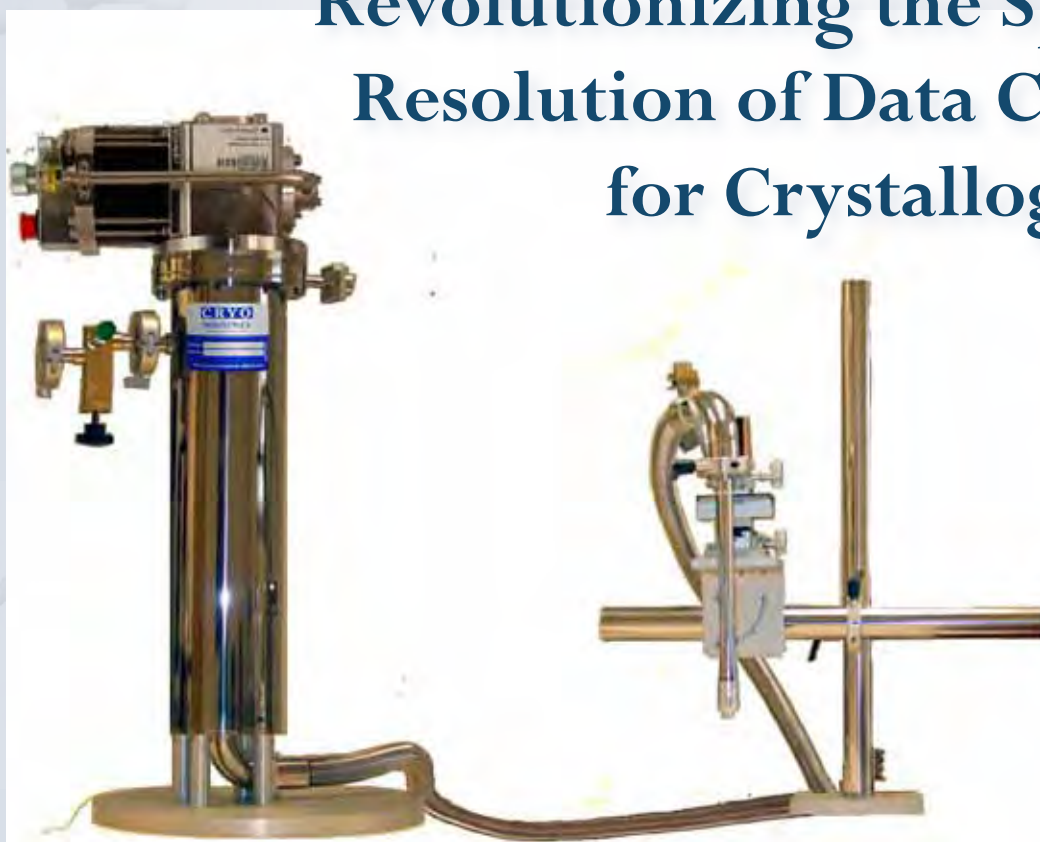
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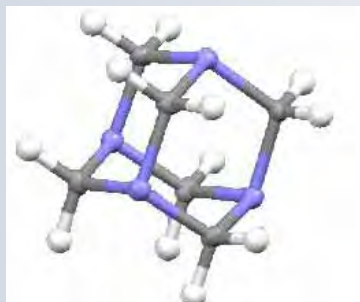


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From Papertape Input to 'Forensic Crystallography': A Short History of the Program PLATON

from the Kenneth N. Trueblood Lecture by Ton Spek

A.L. Spek is an Emeritus Professor at the Bijvoet Centre for Biomolecular Research, Utrecht University, The Netherlands

I was born 24 years later than Kenneth N. Trueblood (1920-1998) whose name is associated with the prestigious Trueblood award that I proudly received in Chicago. Notwithstanding a one generation age difference, I share with Ken doing software development during the early and adventurous days using, from the current perspective, rather primitive computing facilities. I have been fortunate to have met him and other early software developers at various meetings. In the following I will sketch my more than 40 year journey in small molecule crystallography that culminated in the development of the program PLATON that implements much of what I have learned on the way including the Shomaker & Trueblood TLS rigid-body model. PLATON in its structure validation incarnation turned out to be instrumental in the recent uncovering of a massive and saddening fraud case involving papers published in *Acta Cryst.* Section E. Nobody was expecting such a thing to happen on such a large scale in the non-competitive chemical crystallography world.

My scientific CV is simple: I studied, obtained my PhD and worked until my official retirement in November 2009 at the same university. Back in 1966 I started as a student in crystallography in the Laboratory for Crystal and Structural Chemistry at Utrecht University that was at that time headed by A.F. Peerdeman. Peerdeman was the successor of J.M. Bijvoet who had retired in 1962. He was co-author of the famous Bijvoet, Peerdeman & van Bommel *Nature* paper on absolute configuration determination. After WWII, Bijvoet had started a new laboratory in a stately house (used by the Gestapo during WWII) close to the center of the city of Utrecht. Part of the house was his private domain. After his retirement, he still kept a pied-a-terre in the former private quarters for when he was in Utrecht to look-up literature in the library for a book he was writing. As a student, I shared the family bedroom - in its double function as student room. We were expected to find a place elsewhere to work when Bijvoet was in town. The laboratory moved in 1973 to a new building in the university campus outside the city.



The Crystal Palace, as the laboratory was often referred to, was also the home of the first generations of computing platforms within the University of Utrecht (Zebra and Electrologica X1

respectively). In 1966 computing had moved to a new university computing center elsewhere in the city. Computing was from then on until the early 1970's done on an Algol language specific X8 computer from the Dutch company Electrologica which isolated us from the FORTRAN world elsewhere. Nearly all crystallographic software had to be developed in-house. FORTRAN programs such as ORTEP and later on MULTAN could not be used. You had to be a software developer as well as a crystallographer in those days. Processing on the X8 was essentially a one job at a time operation with all input via paper tape and output over a line printer or Calcomp plotter. Computing jobs were run by an operator during daytime shifts. Most of our serious crystallographic work had to be done during the once-a-week 13 hour nightshift when we as crystallographers had the university computer to ourselves. Half of the staff and students stayed overnight to run their own jobs in turn. We scientists were all, at that time, also programmers and computer operators. A block-diagonal least squares cycle might take one hour and an E-map ten minutes. The preparation of programs and program input was done on a so-called Flexowriter. This very noisy electrical typewriter was also often used as output medium. Editing was done with a pair of scissors to cut out unwanted material from the source code or data and adhesive tape to glue a substitute into the paper tape. A lot of time was spent on optimizing memory and execution time requirements. Program and data had to fit in sixteen thousand machine words. One of my early achievements was the creation of an alternative algorithm as a practical substitute for an elegant piece of code by a professional programmer, bringing execution time down from many hours to one minute.

My supervisor, Jan A. Kanters, gave me what turned out to be an interesting assignment to work on. He handed me a batch of white crystals with unknown composition, code named M200. The assignment was to find out what the composition and structure might be, using single crystal

x-ray techniques only. In hindsight his assignment very much determined the rest of my career. Preliminary investigations done with film data suggested the centro-symmetric space group $P1\bar{1}$. A 2D Patterson synthesis based on laboriously collected integrated zero layer Weissenberg intensity data subsequently suggested a light atom structure. This blocked any further analysis with the 2D data. Eventually a three-dimensional data set was collected with an Enraf-Nonius AD3 diffractometer that was operated via an instruction patch panel and setting angles for reflections on paper tape. The latter tape had to be created on the X8 on the basis of an orientation matrix. This was a two week data collection for an eleven non-hydrogen atom compound! It took me half a year to finally solve the structure with the 3D data assuming equal scattering type atoms. The laboratory had a tradition in Direct Methods (Paul Beurskens, Ad de Vries, Jan Kroon, Henk Krabbendam). However, all available software failed to solve my structure. These were pre-MULTAN days! In the end I had to write my own Direct Methods program that solved the triclinic structure and subsequently many other unsolved structures

that were hanging around in the lab. AUDICE, as the program was named, was one of several Symbolic Addition Method programs that were developed in that period. Its specialty was that at the start of the evaluation of the triple product phase relations with strong indications for a positive sign, 27 symbols were assigned to strongly interacting starting reflections rather than just three as was the case in many other approaches. The number 27 is not arbitrary but represents the number of bits of X8 computer words. Eventually, by eliminating 24 symbols based on multiple symbolic 'indications', 8 solutions were produced with figures of merit. The structure analysis showed that the triple bond in the original dicarboxylic acid had reacted with the methanol solvent of crystallization. The crystal structure of M200 was published subsequently. Unfortunately attempts to publish the algorithms that were used in the program AUDICE in *Acta Cryst.* were blocked by a referee requirement that performance be compared with that on non-ALGOL (so-called real ..) platforms. That was a killer at that time. Anyway AUDICE was superseded by the program MULTAN (FORTRAN) when the University eventually moved to a multi-user Control Data FORTRAN standard mainframe in the early 1970s. The complete structure determination process that took over half a year has now been automated. M200 is solved and refined in a matter of seconds on current hardware such as my MacBook Pro with the SYSTEM-S tool in PLATON when run in the so-called *No-Questions-Asked* mode.



Multiple meetings and schools were organized in the 70's with Direct Methods (software and theory) as the major subject. Examples are the NATO schools in Parma, Italy (above) and York (UK), the schools in Erice, Italy in 1978 (see at right), and the meetings at the Medical Foundation (Buffalo) and Göttingen (Germany). The CECAM workshops on Direct Methods in the early 70's were important and inspiring. They were held in Orsay (near Paris) around a big European IBM-360 with lectures by Herbert Hauptman (5 weeks (!) that brought together people working on current issues related to Direct Methods). Among the participants were Gabriel Germain, Peter Main, Ricardo Destro, Davide Viterbo and Henk Krabbendam. The program MULTAN was finalized there including interfaces to high end interactive graphics. Coming from the limited X8 & paper tape world into the multi-processing, FORTRAN and punched card world was a culture shock.

In 1971, a national single crystal service facility was set up in Utrecht, with me to make it all happen. I kept that position for 38 years until my emeritus status in 2009. The project is now continued by my former co-worker Martin Lutz. My last postdoc was Maxime Siegler, now staff crystallographer at John Hopkins University. The program PLATON is a side product of that national facility. A lot of free time went into it as a job related hobby. Its development has never been explicitly funded! Work on PLATON started in 1980 in order to manage the analysis of the growing number of structure determination projects. It was to replace an earlier ALGOL suite of programs and was designed to interface with SHELX76. The idea was to produce with a single 'CALC ALL' instruction an exhaustive listing of all relevant derived geometry, including ring puckering analysis, least-squares planes etc., to be handed over to our clients as a structure report. Over time numerous additional tools have been added based on our service needs, our local research and valuable ideas from external users. PLATON has become, in combination with SHELX(L/S), DIRDIF and SIR one of the major working horses of our national service.

PLATON has been purposely designed as a single program, as independent as possible from external libraries. The tools available in PLATON are shown as clickable options on the opening window of the program. Examples are ADDSYM for detection of missed symmetry, TwinRotMat for automatic twinning detection, SQUEEZE for handling disordered solvents, SYSTEM S for guided/automated structure determination, FLIPPER as a new approach for solving the phase problem and CHECKCIF for structure validation.

Reporting structures in the correct space group is a major issue. Dick Marsh has reported numerous cases where a description in a higher symmetry space group was in order. Yvon LePage published an excellent algorithm (MISSYM) for detecting possible higher symmetry elements in a structure. The actual implementation of that additional symmetry is left to the analyst. ADDSYM also implements that step and provides the proper space group name and associated transformations. In that way, the complete CSD can be examined automatically

for possible missed symmetry cases. In response to one of Dick's space group error papers, I wrote to him to ask whether he was



interested in my list of structures needing detailed inspection. He was indeed and was amused to find out that one of his previously published corrections was 'Marshed' again in that a still higher space group symmetry was found.

The SQUEEZE tool was created to make possible the publication of the structure of a pharmaceutical that was already hard to crystallize. The structure exhibited infinite channels filled with disordered solvent. The tool consists of two parts. In the first part the solvent accessible volume in a structure is identified. In the second part that volume is used as a mask on the electron density found in that region. Iterative back-Fourier transformation of that density provides the solvent contribution to the calculated structure factors.

A busy author or referee can easily miss problems with a structure. Increasingly, black-box style analyses done by non-experts are being published. The number of referees and experts available for detailed examination of the exploding number of structure reports is quite limited. It is easy to hide problems from the experts with a ball-and-stick style illustration. Sadly, fraudulent results and structures have been identified in the literature that contaminate the assumed solid information archived in the CSD. Automated Structure Validation as a solution for this problem was pioneered and 'pushed' by Syd Hall as editor of *Acta Cryst.* Section C with the creation of the CIF standard for data archival and exchange (Hall et al., (1991) *Acta Cryst.* A47, 655-685. He also encouraged George Sheldrick to adopt CIF for the then new SHELX97 refinement program. Subsequently he made CIF the *Acta Cryst.* Section C submission standard and set up early CIF checking procedures for submitted CIF's. I was invited to include PLATON checking tools such as ADDSYM and VOID to search for missed solvent accessible voids. Over time several hundreds of new ALERTS were introduced on the basis of issues I detected as *Acta Cryst.* Section C Co-Editor. Validation was made into a standard WEB-based tool by the IUCr Chester staff and strongly imposed by the next Section Editors George Ferguson and Tony Linden. The validation scheme has been very successful for *Acta Cryst.* Sections C & E in setting standards for quality and reliability. The missed symmetry problem has effectively been solved for the IUCr journals though unfortunately not yet for other journals. There are still numerous 'Marshable' structures published as Dick Marsh keeps showing although most major chemical journals now have implemented some form of a validation scheme.

The IUCr has recently gone one step further with FCF-validation. *Acta Cryst.* is unique in requiring that reflection data have to be archived for published papers in computer readable format. This is standard in the bio-crystallography world but surprisingly not in chemical crystallography. When validation of the structure factor data is included then sloppy and even fraudulent practices become obvious. Errors are easily made and unfortunately not always discernable from fraud in the absence of deposited reflection data. It took some time to discover a pattern of systematic fraud. Wrong element type assignments can be caused as part of an incorrect analysis of an unintended reaction product. Alternative element types can also be (and have been) substituted deliberately in order to create 'new publishable' structures. Reported and calculated R-values differing in the first relevant digit (!?) have been detected, obviously meant to 'clean up' the validation list of ALERTS. Until recently, nobody seems to have looked seriously at the other structures published by the authors of a strangely incorrect structure. Doing so, and as part of the testing of FCF validation software, a large fraud was detected with papers published in *Acta Cryst.* Section E around 2007. Over 100 structures have now been retracted and marked as such in the CSD. A whole series of 'isomorphous' (often chemically impossible) structures was detected for an already published (correct) structure. The data sets of different structures could be shown to be identical. Similar series have now been detected for coordination complexes (transition metals and lanthanides). **How could referees have let those pass?**

Recently, it was realized that there is an 'age-concern' issue in that many software developers are retiring with only a limited next generation. IUCr Computing Schools organized in Siena in 2005 (see below), and in Kyoto (2008) addressed this issue. Lachlan Cranswick was the major force in that project.



From left: Ton Spek, Tony Linden (current Section Editor of *Acta Cryst.* C), George Ferguson (previous Section Editor), and Aggie Spek in Zurich.

Finally I would like to thank the selection commission for this award; my former co-workers in the project over 38 years and in particular my successor Martin Lutz; Louis Farrugia for following my frequent updates of native UNIX PLATON with his MS-Windows implementation; the users of the software for communicating new ideas and bug reports; Lachlan Cranswick, who sadly is no longer with us, for promoting my software, and my wife for enduring me with my notebook.

Ton Spek

The Puzzle Corner column introduced on page 19 of the Winter 2010 issue of *ACA RefleXions* invited/challenged readers to identify a participant at an international crystallographic meeting held in the 1960's or 70's. The unknown was third on the left of a photograph thought to have been taken at an IUCr related gathering in the USSR, as it was then, or a related eastern European country. The resulting lack of response was possibly related to the combination of decades passed since the photo was taken together and the international nature of those present, resulting in too difficult a choice.

We now offer a group photo taken much more recently at an ACA meeting – the editors think they know all the names, but not when or where. Readers might find it amusing to name the participants also (we promise to publish the names in the next issue). Your answers will have lasting institutional value in addition to any diversion they might provide because many photographs in the ACA archives presently contain unidentified participants that we hope you will identify.



On page 37 of the winter 2010 *RefleXions*, the twelve faces above were printed, without names, as a puzzle-challenge for readers. The editors knew some, but not all of the names. Their names are (l to r) : Amy Sarjeant, Thomas Proffen, Donnie Berkholz, Donald Raymond, George Oh, Branton Campbell, Jennifer Gehret; below: Elena Zlateva, Ju He, Donnie Berkholz, Nicholas Deifel, Balendu Avvaru. All these photos were taken at the Poster Sessions in Chicago.

On page 42 of the winter, 2010 *RefleXions* the eleven faces below were printed, Their names are: top row, (l to r): Luchita Doucette, Mario Rosa, Krystal McLaughlin, ??? ????. 2nd row, l to r: ???, Ritcha Mehra-Chaudhary, Argentina Becker, ???, ???, ???. All these photos were taken at the Mentor-Mentee dinner in Chicago.



Two additional puzzles were submitted by Edgar Meyer:

≈ Name the last crystallographer to appear in a Hollywood movie.

≈ Which science fiction book references Martin Buerger's *X-Ray Crystallography*?

With the kind agreement of the *BCA's Crystallography News'* Puzzle Corner editor, Carl Schwalbe, the following is a reprint of their March 2009 puzzle.

Sometimes a person's name is turned into an adjective. Mathematicians, physicists

and musicologists seem particularly keen to do this, and "-ian" is the usual ending. It may be applied as a simple suffix as in Bohm - Bohmian; Freud - Freudian; Keynes - Keynesian; Lagrange - Lagrangian and Laplace - Laplacian:

Sometimes when this happens the accent is changed; for example Darwin - Darwinian or Mozart - Mozartian

And sometimes, along with the change of accent, the pronunciation of the final vowel is lengthened as in Abel - Abelian; Beethoven - Beethovenian; Hamilton - Hamiltonian; Mendel - Mendelian or Wagner - Wagnerian.

Or -- the adjective may end with -c instead of -n as in Galvani - Galvanic; Napoleon - Napoleonic; Ptolemy - Ptolemaic and Volta - Voltaic.

Crystallographers don't seem to do this. We discuss Bohmian interpretations of quantum mechanics but not Braggian interpretations of diffraction. We use the Hamiltonian to calculate our wave functions but not the Pattersonian to calculate our vector maps. So we ask our readers:

- (1) Can you name any crystallographers-turned-adjectives?
- (2) Can you name other important people-turned-adjectives, especially if their suffix has a different structure?
- (3) Can you formulate rules for the whole business?

The answers to all puzzles, or at least the ones the editors know, will be in the summer issue of *ACA RefleXions*.

Sidney Abrahams

The editors welcome puzzle responses. Please contact Judith Flippen-Anderson, acareflexions@gmail.com or Connie Rajnak, conniechidester@earthlink.net. Thanks from the editors to Frances Bernstein, who supplied many of the answers to our winter issue puzzles.

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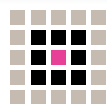
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You have solved a new structure. How do you describe it to a non-scientist? A few key words are necessary: atoms, bonds, shape, size - but they are not sufficient. You need to show a picture or model - this implies an artistic representation.

Science is material - art is spiritual. Both are profoundly creative, peering into the depths of nature and of the soul. The scientist-artist must strike a balance, first for him/herself, then for the viewer. And how many ways are there to describe a molecule, an atom? Overlapping wave functions? Electron density maxima? Sum of van der Waals radii? Connectivity? Chirality? Iconic abstractions? A confluence of spheres? While graphical representations are visually appealing, their lifetime is limited and devoid of the sense of touch. Sculptures are the answer, but herein lay distinct challenges; it also takes courage to make a scientific sculpture.

Max Perutz was not pleased with the worm-like shape of the backbone chain in the first myoglobin structure ("hideous") but observed "like many other things in nature, myoglobin gains in beauty the closer you look at it"; aesthetics are part of our heritage. Someone referred to a protein structure as looking like a lumpy potato. But then, compare a lumpy de Kooning sculpture to a polished Brancusi; some of Jean Arp's sculptures appear 'molecular'; -other examples may come to mind.

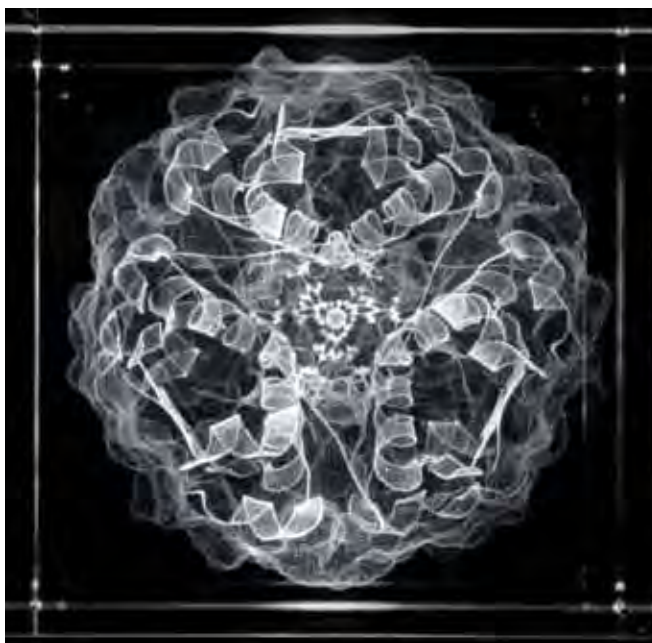
Often, the artist does not know how the art-piece will be received; an internal aesthetic balance of complexity and simplicity is essential. The crystallographer who spent years on a structural study may take umbrage at an artist's necessarily simplified representation. While a small rotation can give a graphical image a different appearance, the sculpture can be inspected; an enduring sculpture can be inspected, touched.

The least of our structures enforces the edifice of the scientific literature, occasionally yielding information initially overlooked in publication. In context, even our best structures are deposited and reprints safely filed, seldom to be seen by the general public. Imagine then how your most significant structure could be sculpted and displayed for the world to see, ponder, and yes, admire. *ars longa - vita brevis*.

These sculptors, with different media and emphases, make sculptural images of molecules to bridge the gap from illusion to reality; - see if you like their art.

Bathsheba Grossman

CrystalProtein.com makes protein structures by 3D laser etching in glass blocks. This technology, more familiar as souvenir cubes, is a surprisingly neat hack for rendering intricate data, producing beautiful handheld models of proteins and other subjects. I began by laser etching sculpture designs but soon found that scientific imaging was a more compelling use of the medium, and as I learned more about proteins and adapted my software to work well with them, I found some demand for this as a customized service.



Now it's about 1/3 of my sculpture business, my assistant knows enough about protein imaging to be mistaken for a postdoc, and we're very happy to be able to make these models available. <http://bathsheba.com>
<http://www.symmetrymagazine.org/cms/?pid=1000174>



Estrogen Revealed detail; triple embedment stereo-lithography and caste arcylic, 9" x 3" x 3", 2007.

Mara Hazeltine

My work explores the explosion of information that has occurred since the advent of computerized bioinformatics. I have used many molecular structures that come from data gleaned from electron microscopes or x-ray crystallography. I use digitized data from these structures to fabricate my sculptures by means of stereo-lithography, rapid prototyping, and 5-axis milling. These modern techniques are augmented by traditional sculpting methods such as the ancient lost wax method in bronze, and Japanese garden design. My most current projects use environmental technology to combine minute structures from the nano-world in such a way that a living eco-system of functional underwater sculptures is created.

www.calamara.com

http://www.thewip.net/contributors/2010/05/geotherapy_artist_mara_haselti.html

Contributors:

Bathsheba Grossman

Mara Hazeltine

Julian Voss-Andreae

Byron Rubin

Edgar Meyer

Julian Voss-Andreae

My work explores the nature of life through art. My protein-based works, inspired by life's molecular building blocks, recreate the emergence of three-dimensional bodies from one-dimensional DNA. Utilizing an algorithmic approach as the point of departure, I follow my artistic vision freely to create sculptures that facilitate a broader understanding of nature than the one provided by science alone, and that help to reestablish the Renaissance notion that the natural sciences constitute an integral part of culture.

www.JulianVossAndreae.com

Quantum objects on show. (2009) *Nature*, 462, p. 416.

Angel of the West, commissioned as the signature piece of the new Scripps Research Institute's campus in Jupiter, FL, is a large-scale sculpture based on the structure of the human immune system's key molecule, the antibody.



Byron Rubin

I make anatomically correct models of proteins, DNA, RNA and small molecules that aptly are described as molecular sculptures. These metal sculptures are rendered in a variety of styles at scales from desktop to monumental for either indoor or outdoor installation. The photo at right shows a recent sculpture representing the antibiotic drug, Zocin®. The antibiotic is a combination of two β-lactam molecules. Each is represented in metal as a gold ball and stick model, mounted on a 44 inch high, cherry display case. The sculpture is 16 inches in height. <http://www.molecularsculpture.com>
Perkins, J.A., *The History of Molecular Representation Part 2: The 1960s - Present.* (2005) *J. of Biocommunication* 31 (2), 1-14.



Edgar Meyer

Moving from studying small molecule structures to proteins, I struggled with conceptualizing and visualizing these and other structures in 3-D. After the thrill of watching a new structure emerge from electron density maps, I strove to depict the beauty I saw and felt. Nearing retirement, I was inspired to carve models of molecules in noble hardwoods, so I wrote programs to drive a cnc milling machine. Two museum commissions, especially the polio virus bronzes commissioned by the Smithsonian, helped. Recently, I have been placing images of molecules onto photos of flowers or landscapes and have been using a 7-axis rapid prototyping robot to create precisely scaled bronze sculptures of molecules, thus striving to place man-sized sculptures in public spaces. <http://molecular-sculpture.com/Campus-sculptures/Imagine.html>. *Digital Design of Molecular Sculptures and Abstractions*, (2011). E.F. Meyer, *Leonardo* 44, No. 1, 22-29

Now, judge for yourself; the variety of images is striking, representing the tip of the iceberg from these sculptors. Numerous choices (materials, design, execution, finishing, exhibition) are just part of the artistic component of molecular representations. Technical skill and artistic detail must be matched with scientific sensitivity; Snow's 1959 Rede "Two Cultures" lecture continues to challenge sculptors. Even as we live in the "golden age" of structural biology, let us find ways to exhibit vital nano-scale objects as old as life itself in forms as contemporary as tomorrow.

Newly cast, precisely scaled bronze sculptures of the polio virus capsid and capsid+receptor complex (Hogle Lab, HMS) commissioned by the National Museum of American History (2005) to commemorate the sesquicentennial of polio vaccine.

Using food and cooking to teach science to a wider audience is a growing trend since the appearance of the Food Network. The network draws 44 million viewers to its cable shows and its website posts 2.8 million unique visitors a month, so there is a ready-made audience for science education in the context of food. For those unfamiliar with the topic, the science of cooking is not about nutrition food safety. Rather, it falls under the discipline of molecular gastronomy, a scientific approach to cooking pioneered by French physical chemist Hervé This and Hungarian physicist Nicholas Kurti. A science of cooking course can be very chemistry oriented and multidisciplinary in nature.

Asmorgasbord of courses: There are many examples of courses that successfully utilize the science cooking to teach students chemistry, molecular biology and physics. One of the first courses to combine food and science was taught at MIT and titled *Kitchen Chemistry*. That class, created by Patti Christie, was taught in a small seminar format and combined hands-on cooking with current scientific literature. In a similar course taught at Harvard University, top chefs are brought into the classroom to present molecular cooking to undergraduates. This course teaches about gel foams and the molecular nature of *haute cuisine*. Marcia France at Washington and Lee U. teaches a course that covers science basics in lecture and takes students on field trips to restaurants and vineyards. Brenda Kelly and Brandy Russell at Gustavus Adolphus College teach a four-week course that involves laboratory experiments and covers a wide range of materials from oxidation of food to food color and fermentation. While many of these courses incorporate laboratories into their pedagogical approach, Deon Miles and Jennifer Bachman at Sewanee had a good experience teaching the science of cooking in a lecture-only format.



Joseph Provost teaches a liberal studies course at Minnesota State U. Moorhead called *The Science of Cooking*.

Joseph Provost Adapted from the March 2011 issue of *ASBMB*.

*Editors note: Page 20 of the winter 2010 Reflexions included a book review by Joe Ferrara, *Cooking for Geeks* by Jeff Potter, which also linked chemistry to cooking.*



"Okay - is there anybody ELSE whose homework ate their dog?"

Cartoon, "The Humpback of Notre Dame" courtesy of Nick D. Kim. See page 3.

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A scientist who enlisted Britain's hairdressers in the early hunt for DNA has emerged from the shadows, with a museum exhibition, a blue plaque and a place in the BBC's *History of the World in 100 Objects*.

William Astbury, a brilliant popularizer who also used poached eggs and pigs' ears to gain public interest and funding, took the first x-ray photographs of the "building bricks of life" 15 years before the work of Franklin, Watson and Crick. Long acknowledged by experts, his role was sidelined in the subsequent celebrations, despite a style that endeared him to laymen as well as the elite in the new science of molecular biology.

While laying the foundation of DNA studies, he was corresponding with salon owners such as Muriel Smith of Leeds, a prizewinner at the World Permanent Wave Championships.

Their shared interest was the then fashionable kink in women's hair whose molecular properties were part of Astbury's specialist field. Originally hired by Leeds University to investigate textile fibres, his fascination with their protein structure revealed how molecules change shape when heated and stretched. This discovery was central to perming, because the method fixed significant molecular changes which otherwise returned to normal when the hair cooled and shrank.

The helical shape of hair proteins discovered by Astbury later also proved to be the secret of DNA. "He got pretty close, but there were aspects to the DNA puzzle which he could not have solved in 1938," said Bruce Turnbull, a Royal Society University Research Fellow in chemistry at Leeds's Astbury Centre for Structural Molecular Biology, named in the scientist's honor.

It was not realized at the time that DNA's "building blocks" came in pairs, while the complexity of the helix was disguised as cross-like shapes in x-ray photography. "Later scientists built on his work and his 'pile of pennies' description of DNA was not so far from the answer they correctly described, the double helix," said Turnbull.

The implications of his findings were prophetically described by Astbury's brilliant assistant Florence Bell. She wrote in 1939: "Possibly the most pregnant recent development in molecular biology is the realization that the beginnings of life are clearly associated with the interaction of proteins and nucleic acids."

Astbury's revived reputation follows a Royal Society initiative to honor "local heroes", which led to an exhibition at the Thackray medical museum in Leeds that ended 2nd January. *Hair Splitting Images - How William Astbury's X-Ray Vision Changed the World* coincided with the BBC's choice of Astbury's x-ray camera in its 100 objects, and a Leeds Civic Trust plaque which was unveiled 26th Nov., 2010.

The trust's director, Dr Kevin Grady, said: "Leeds University was originally founded to further understanding of the study of textiles. Isn't this a remarkable example of where such an initiative can unexpectedly lead?"

Astbury's mastery of fiber structures led to a pursuit of proteins in scores of fields -including poached eggs, where his work on how molecules change shape under heat remains important in today's research on Alzheimer's and Parkinson's diseases. "He

was brilliant on making connections between similar proteins in things which seem impossibly different," said Jim Garretts, senior curator at the Thackray. "He showed how a sow's ear could become a silk purse, made a coat out of peanut fibres and speculated about a day when viruses could be turned into clothing, through work on their protein structures."

Astbury's easy manner may have owed something to his background as a potter's son from Stoke-on-Trent. He would have entered that industry had not scholarships taken him to grammar school and Cambridge University. His lecture on perms to Muriel Swift's adult academy of hairdressing, part of the Leeds Guild of Hairdressers, Wigmakers and Perfumers, was part of a system of keeping in touch with the outside world, as much as with academic papers.

From David Rose: an article in The Guardian: 23rd Nov, 2010, by Martin Wainwright.



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Robin Rogers wins ACS Award

The American Chemical Society will honor **Robin D. Rogers**, U Alabama, with their 2011 **Award in Separations Science & Technology**, which recognizes the development of novel applications with major impacts and/or the practical implementations of modern advancements in the field of separation science and technology. Rogers serves as Robert Ramsay Chair of Chemistry, Distinguished Research Professor, and Director of the Center for Green Manufacturing at the Department of Chemistry at the University of Alabama. His innovation, foresight and influence in the field of separation science is evident in the numerous patents he holds and hundreds of publications he has authored. A pioneer in the use of ionic liquids and green chemistry for sustainable technology, Rogers' seminal findings on ionic liquid/aqueous partitioning kick-started interest in applying ionic liquids to clean separations. One of

the many diverse focuses of his research group is in developing novel strategies for the separation and purification of value added products from biomass, thus reducing energy usage and cost and improving economic viability. Rogers is also founding Editor-in-Chief of *Crystal Growth & Design*.

Administered by the ACS, the **Award in Separations Science & Technology** is sponsored by Waters Corp. Rogers will receive the award at the Awards Ceremony on Tuesday, March 29, 2011, in conjunction with the 241st ACS national meeting in Anaheim, California, where he will also deliver a lecture at the annual Division of Industrial and Engineering Chemistry Separations Science and Technology Symposium.

Chan, Ealick, and Gschneidner elected as AAAS Fellows

In December, the Council for the American Association for the Advancement of Science (AAAS) elected 503 members as Fellows of AAAS. A Fellow is defined as "a Member whose efforts on behalf of the advancement of science or its applications are scientifically or socially distinguished." Among the new Fellows were three ACA members: **Michael Chan** (Ohio State) and **Steven E. Ealick** (Cornell) in the Chemistry Section and **Karl A. Gschneidner, Jr.** (Iowa State) in the Physics Section.

Michael Chan, Professor of Chemistry and Molecular & Cellular Biochemistry, is also the Interim Chair of Biochemistry. His research interests include pyrrolysine-containing proteins, proteins involved in carbon dioxide and methane degradation, membrane-inserting proteins, and bioinformatics.



Steve Ealick is William T. Miller Professor and Director of the Northeastern Collaborative Access Team (NE-CAT) at Cornell University. He studies enzymes involved in purine nucleotide metabolism and pyrimidine nucleotide metabolism, and enzymes involved in thiamin, polyamine, and purine biosynthesis. His group is also involved in the development of tools and techniques associated with synchrotron radiation.



Karl Gschneidner is the Anson Marston Distinguished Professor of Materials Science and Engineering, Senior Materials Scientist in the Ames Laboratory of the US Department of Energy, and Senior Editor of the *Handbook of the Physics and Chemistry of Rare Earths*. His research focuses on the alloy theory of metallic systems and the physical metallurgy of the rare-earth elements.



The three were recognized with the other Fellows for their contributions to science and technology at the Fellows Forum in February during the AAAS Annual Meeting in Washington, D.C. The new Fellows receive a certificate and a blue and gold rosette as a symbol of their distinguished accomplishments.

ICDD Awards now include ACA membership

Established in 1991 by the International Centre for Diffraction Data, the **Ludo Frevel Crystallography Scholarships**, (www.icdd.com/resources/awards/frevel.htm), are awarded yearly to encourage promising graduate students to pursue crystallographically oriented research. All applicants are required to be enrolled in a graduate degree program during the calendar year for which they are applying, with a major interest in crystallography, e.g. crystal structure analysis, crystal morphology, modulated structures, correlation of atomic structure with physical properties, systematic classification of crystal structures, phase identification and materials characterization. Multiple recipients are selected on a competitive basis, each receiving \$2,500. For the first time, this year, the award also includes a one year membership to the ACA. Sadly, Ludo Frevel passed away on 15th January, 2011 (see the obituary on page 17).



2011 ICDD Award Winners

Gokhan Barin, Northwestern U, *Metal-Organic Frameworks Incorporating Copper-Complexed Rotaxane Struts.*

Jeffrey Bertke, U Notre Dame, *Synthesis and Characterization of Azolate Functionalized Metal-Organic Frameworks for the Sequestration of CO₂.*

Sharon Bone, U California, *X-ray Absorption and Scattering Analysis of Hg Sorption by Nanocrystalline FeS.*

Honghan Fei, U California, *Solvothermal synthesis of cationic framework materials, including zeotypes, inorganic extended materials and cationic metal-organic frameworks.*

Hua He, U Delaware, *Single-crystal and high resolution powder x-ray diffraction studies on new antimonides with layered and framework structures.*

Zachary Hudson, Queen's U, Canada, *Triarylboron Compounds for Optoelectronic Materials: Applications in Solid-state lighting and chemical sensing.*

Shmuel Samuha, Ben-Gurion U of the Negev, Israel, *Characterization of the Structure of a New Ternary Phase in Al-Ru-Rh system.*

Pradeep Sharma, All India Institute of Medical Sciences, India, *An approach towards prevention of septic shock syndrome: Structural and functional studies of PGRP and its complexes with various PAMPS.*

Chutchamon Sirisopanaporn, Universite de Picardie Jules Verne, France, *Crystal Chemistry and Electrochemical properties of Lithium Transition Metal Silicates; Li₂MSiO₄ where M are Fe and Mn.*

Vedran Vukotic, U Windsor, Ontario, Canada, *Development of new materials which have application in non-linear optics, ferroelectronics, piezoelectrics, and other technologically important physical properties.*

Andrew Warren, U Central Florida, Orlando, *X-ray scattering of nanometric films and interfaces.*


Julie Wilkerson, U Texas, Austin, *Synthesis, characterization, and study of new luminescent materials based on conducting metal-lopolymers.*

Jeongho Yeon, U Houston, *Investigation of New Polar Oxides: Crystal Structure and Physical Property Relationship.*

The deadline for the next competition is October 26, 2011: www.icdd.com/resources/awards/frevel.htm.

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Galileo Goes to Jail and Other Myths about Science and Religion edited by Ronald L. Numbers, Harvard University Press, 2009, ISBN: 978-0674033276

I don't know what I was thinking when I picked this book up. It is a set of twenty-five essays on how religion has not negatively impacted science. The fourth myth "That Medieval Islamic Culture Was Inhospitable to Science" seemed to have the properties of what I understand to be true so I thought there was promise. Myth 7, "That Giordano Bruno was the First Martyr of Modern Science" just about drove me mad.



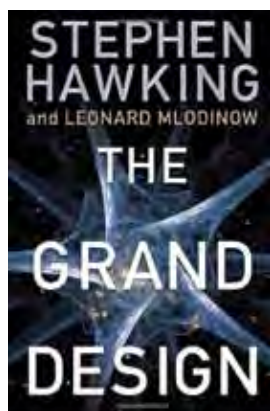
The essayist, Jole Shackelford, makes the following arguments that debunk the myth. If you remember, Bruno was a priest who adopted the Copernican view and taught that the earth might not be the only planet with life, among other things. He was burned at the stake for this. Shackelford suggests that Bruno wasn't the first scientist martyr because he wasn't a scientist, that this form of capital punishment was common practice anyway, and finally, that he was a priest and the Church could do what it wanted with him.

The essays give the appearance of being well researched but I felt as if I were reading a skit by a partisan political pundit purporting to provide a fair and balanced viewpoint.

Moving on to - in my humble opinion - a far more interesting book:

The Grand Design, by Stephen Hawking and Leonard Mlodinow, Bantam Books, 2010 ISBN: 978-0553805376

From a technical perspective this book is a relatively easy read. It has lots of good pictures and no math, except a definition of π similar to the Indiana legislature's old value. However, don't be fooled, as the philosophical implications are profound. The authors start by introducing the question of why does the universe behave the way it does. Next they pass through history and the development of the laws that we think describe the behavior of the universe: Aristotle's, Newton's, Einstein's and Feynman's theories, then string theory and ultimately M-theory, which is a combination of all the theories necessary to describe the behavior of the universe. The difficulty arises in the concepts of free will and causality.



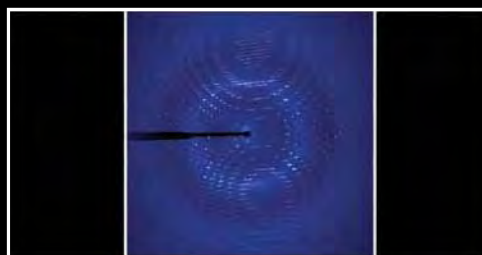
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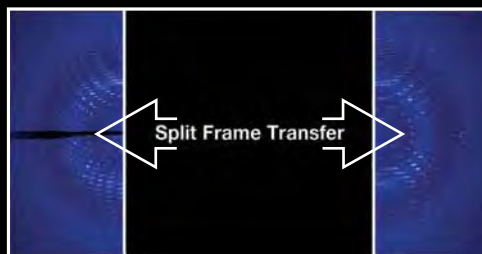
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Step 1: Image is captured on main imaging area



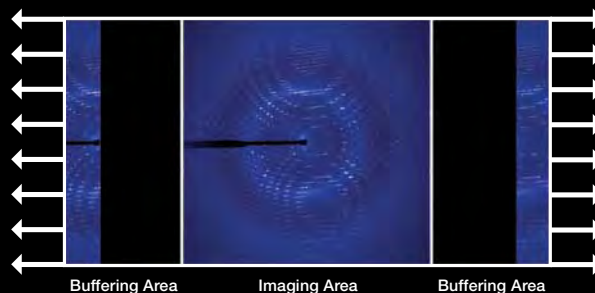
Buffering Area Imaging Area Buffering Area

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The Grand Design, cont'd

have “free will”? Is my typing of this document a series of random probabilities? The other mind bender is the idea that observing an event forces the path of the event to become evident. In other words, observing the present impacts the past. I first came across this concept five years ago in Davies’ Cosmic Jackpot. It still does not sit well.

Proofiness: The Dark Arts of Mathematical Deception by Charles Seife, Viking, ISBN-13: 978-0-670-02216-8



I saw this book at the store and bought it for my wife. We had both read and enjoyed an earlier book by the same author, *Zero*, and I expected this to be just as good. It was better – it is also the first “math” book I have ever read that made me laugh out loud. In all seriousness though, what it does is lay down a basis for interpreting mathematical information in the correct context. As crystallographers, this should be very familiar to us.

But, this ability to interpret numbers applies to society in general, not just scientific inquiry.

Seife first defines proofiness: “the art of using bogus mathematical arguments to prove something that you know in your heart to be true – even when it’s not”. He then cites numerous examples of proofiness that you and I have both experienced in our lifetime.

In Chapter 1, “Phony Facts, Phony Figures” Seife defines distastimation: “the act of taking a number too literally, understating or ignoring the uncertainties that surround it” and provides several examples. In addition he demonstrates the problem with fruit picking data to give the answer one desires.

Chapter 2, “Rorschach’s Demon”, Seife defines causistry “where the fault in the argument comes from implying that there is a causal relationship between two things when in fact there isn’t any such linkage” and randomness in “which one insists there is order when there is only chaos”. Again examples are given, most from *Nature* and one from the *Wall Street Journal*.

Chapter 3, “Risky Business” takes a look at understanding risk. The shuttle program and air traffic safety are one example. If the aviation industry had the same record as the shuttle program there would be 275 airplane crashes a year. This chapter also summarizes nicely the Enron affair and the current financial mess we are in now.

The next two chapters, “Poll Cats” and “Electile Dysfunction” (not a typo!) are very interesting. The former chapter introduces random and systematic error, and how they bias the results of polls. The latter chapter analyzes the 2008 Minnesota Senate election which resulted in a recount in favor of Franken over Coleman, which was really quite humorous, and the 2000 Bush vs Gore recount in Florida. In the end, Seife suggests that the counts in Florida were much too close and a flip of a coin would have adequately reflected the will of the people.

Chapter 6, “An Unfair Vote” should upset you. It details the process of gerrymandering and how redistricting of the type that dilutes the will of the people will happen with the publication of the 2010 census.

Chapter 7, “Alternate Realities” looks at how lawyers and judges are able to turn numbers upside down to win cases that would make no sense to anyone who actually paid attention to the numbers. The O.J. Simpson trial is given as one example of how lawyers confuse juries with bad statistics.

The last Chapter, “Propaganda by the Numbers” is quite interesting. Here Seife reviews the string of victories in Viet Nam that led to the US pullout and why buying a Hummer 3 is greener than buying a Prius.

Three appendices, “Statistical Error”, “Electronic Voting” and “The Prosecutor’s Fallacy” supplement the main text with detailed discussion on the particular topic.

My wife says “believe nothing you hear and only half of what you see”. This book will help you decide which half of what you see to believe.

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Sheraton, French Quarter, New Orleans

Abstract Deadline: The early deadline has passed but late abstracts are still being accepted

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Advance Hotel Registration Deadline: April 15, 2011

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Workshops

Symmetry-mode Analysis
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Organizer: Paul Adams

Award Symposia

Patterson Award in honor of Keith Moffat

*Margaret C. Etter Early Career Award
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Transactions Symposium

*Time Resolved Photochemistry and Electron Density
 In Honor of Philip Coppens on his 80th Birthday*
**Organizers: Peter Lee, Yu-Shang Chen
 and Jason Benedict**

*Evolution of Powder Diffraction Software
 in Honor of Lachlan Cranswick*
Organizer: Peter Stephens

Plenary Lecture

Ned Seeman - Winner of the 2010 Kavli Prize in Nanoscience

Banquet Speaker

Elizabeth Wood Award Honoree: Daniel Nocera

**Travel Fellowships for XXII IUCr Madrid Congress,
 22-31 August 2011.**

This year the USNCCr will be continuing its tradition of providing travel fellowships for young scientists (students, post-docs, and untenured faculty) to attend the triennial IUCr Congress. Applications for travel assistance to the Madrid Congress were due by March 1, 2011 and are currently under review. Successful applicants will be notified in time to meet advance registration deadlines.

Recipients will be expected to submit a short report on their experiences at the Congress that will be published in an issue of *ACA Reflexions*.

NOTE: LATE ABSTRACTS FOR ACA NEW ORLEANS STILL BEING ACCEPTED

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25-29 **MaThCryst School on Fundamental Crystallography**, Mahdia, Tunisia.



SEPTEMBER 2012

9-13 **EMC 2012**, European Mineralogical Conference, at Johann Wolfgang Goethe-University, Frankfurt, Germany.



MAY 2011

21-26 **ACA2011**, Sheraton Hotel New Orleans, New Orleans, LA. **Program Chair: Chris Cahill; Local Chairs: Cheryl Klein-Stevens & Ed Stevens.**



23-27 **2nd Course on Neutron Scattering Applications in Structural Biology**, Oak Ridge, TN. See <http://neutrons.ornl.gov/conf/gcnb2011/>.

July 2011

11-15 **Inter/Micro: 62nd Annual Applied Microscopy Conference**, Chicago, www.mcri.org. Titles & Abstracts due by April 15, 2011; contact Therese Newman, Inter/Micro Coordinator, McKrone Inst. intermicro@mcri.org.

AUGUST 2011

22-29 **XXII Congress and General Assembly of the IUCr**, Madrid, Spain. www.iucr2011madrid.es.



JULY 2012

28-August 1 **ACA 2012**, Westin Boston Waterfront Hotel, Boston, MA. Program Chairs: Bruce Foxman, Brandeis Univ., foxman1@brandeis.edu, and Bruce Noll, Bruker, Bruce.Noll@bruker-axs.com **NEW ! Sessions will begin on Sunday, July 29, and conclude on Wednesday, Aug. 1**

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