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Remembrances of Bob Stewart (1936 - 2015)

It's hard to imagine the crystallographic world without Bob Stewart. Bob was a role model and friend for all of us who were part of the Pittsburgh crystallographic community. During my years in Pittsburgh (1967-1970) he was, along with Bryan Craven, arguably the most dynamic character on the local scene. All the rest of us were

working on structure determination, but Bob was trying to use 'the X-ray diffraction experiment' (a term he used frequently) to see the features of the electron density we had all learned about in our undergraduate chemistry courses: bonding electrons, lone pairs, and the like, which were ignored in the work the rest of us did. What he was doing was a hell of a lot neater than the spherical atoms we used in the standard crystallographic representation.

That was cool, but this description fails to present Bob as he was. I remember him especially as the founder of the 'Friday afternoon seminar' that he hosted at the Craig Street Inn. Over beer and his Camels and my Gauloises cigarettes, he would hold forth on topics that ranged from Science, to his graduate school days at Caltech with Norman Davidson (when he drove around LA in his MGA, Reginald), to his postdoc back home in Seattle at the University of Washington. It was under Bob's tutelage at the Craig Street Inn that I learned to combine beer and Science, a combination that wound up working very well for me in later life.

At the Craig Street Inn, Bob sometimes talked about his undergraduate summer studentship at Los Alamos: He told the story of having a meal with a guy who worked on developing nuclear weapons. Bob asked him how he could work on these horrible things; the response was, "Well, Bob, I've got a philosophy." "Really?" Bob asked, "What is it?" "People are just no damn good!"

It was fascinating to listen to Bob talk about his early life, particularly his birth to a whore on the Seattle waterfront and his adoption by a wealthy man. He described going back to the orphanage as an adult and the official there said, "I remember you. You crawled up on my lap, looked up at me with those big blue eyes, and said, 'That goddamn sonovabitch Roosevelt'." Bob had been parroting his mother, because FDR was supposed to be helping poor people, but his mother felt she had not received the help that she deserved. Bob talked about how shortly after Pearl Harbor he had been on a boat in Puget Sound with his adoptive father, and had passed a Japanese gardener, whom he had started to cuss out. His father admonished him that Pearl Harbor had not been the gardener's fault, giving him the impression that his father was not a racist. He was wrong, which he learned the hard way when he was disowned for joining SNCC.

Bob took a sabbatical with Ted Maslen in Perth in 1971-1972. I didn't see Bob during that year, and didn't recognize him when I ran into him at the Kyoto IUCr (IX) in 1972. He had joined Ted's running group, and after a year of that kind of exercise he had temporarily lost a huge amount of weight. I attended his talk at the meeting and was impressed but not surprised when Berthaut got up afterwards and said that Bob had laid out a route that would define the area for years to come.

Of course, Bob worked out the hydrogen atom scattering factor, including the fact that the electron is partly to be found in the bond to another atom; this was just after the then-current edition of the *International Tables* had gone to press, so he was cited in every crystal structure that was reported until the next edition of the *Tables* was published many years later; in its era, that paper was the most cited paper in the chemical literature.

There is a syndrome to which Bob unfortunately succumbed in later life. This was not recognizing when good was good enough. He simply stopped publishing (often taking his name off papers) at the required rate, because he was unsatisfied with the results. It was ironic that even then, when I went to Pittsburgh Diffraction Conferences held in Pittsburgh, I'd go up to Bob's office and couldn't get in to chat with him: He was always too busy holding forth to an audience of wall-to-wall bodies on his thoughts about accurate electron densities. Bob was still the guru, even when he was not publishing or being funded.

At Caltech, Bob was with Davidson as he was switching from physical chemistry to molecular biology. I think Bob was the last physical chemist that Davidson produced. I was fortunate that one of Bob's lab-mates, a molecular biologist, became my dean during my highly vulnerable assistant professorship, certainly not harming my shot at tenure. Between that time and my Pittsburgh era, Bob wrote huge numbers of letters for me, resulting in postdocs, fellowships, and a chance at an independent position.

Bob was *sui generis*. He was a great scientist who was an authentic personality. There are far too few people like Bob in Science, particularly now, when we need more individuals like him. His loss impoverishes the entire enterprise.

Ned Seeman



Bob Stewart (second from left), during a 1996 visit to the author's farm in Denmark. L-R: Syd Hall, Bob, the author, Don Glusker, and Jenny Glusker.

Robert F. Stewart in Memoriam

Bob Stewart's name is intimately linked to the development of charge-density analysis, and it was due to my interest in learning more about this exciting and rapidly developing field that I got to know Bob in 1977. I attended the two-week long Batsheva de Rothschild

Seminar organized by Philip Coppens and Fred Hirshfeld and held at the Weizmann Institute, Israel. Bob's lecture 'Total X-ray Scattering and Two-electron Density Functions' was not the easiest to understand, because it required a good knowledge of both physics and mathematics. The lecture notes from the seminar were published the same year in the special issue 'Electron-density Mapping of Molecular Crystals' of the *Israel Journal of Chemistry* that long served as my reference text for the field. Bob and I met again the following year in Arles, at a NATO Advanced Study Institute on charge-density studies organized by Pierre Becker. Charge-density analysis was a rapidly expanding field and Bob and I met regularly at meetings during the following decade, in which Bob also visited Copenhagen several times. At these occasions I noticed how he enjoyed interacting with the students in the group; he showed great interest in their projects and could always contribute with some clever comments.

I was therefore more than delighted when Bob aired the possibility of spending a sabbatical at University of Copenhagen the first half of 1991. Denmark is a small country, so not only my group but also the whole Danish crystallographic community was happy to have Bob Stewart with us for half a year. I succeeded in getting the necessary financial support to appoint him as a visiting professor with a large apartment in Nyhavn, an exclusive address in central Copenhagen, in an old house owned by the Danish National Bank – a historic house where the Danish author Hans Christian Andersen had lived. Bob arrived in January 1991; it was cold and there was snow in the streets. In Nyhavn we were met by the caretaker of the house, who with great pride showed Bob this fancy apartment with three big bedrooms and fully furnished with the best of Danish design. Bob looked more and more tired, and I could see that he just wanted a bed to relax in and getting a chance to look at the TV to follow the news of the Gulf War. Though Bob enjoyed the apartment and its setting in central Copenhagen, I am not sure that he really felt at home there.

Bob started by giving the prestigious Bjerrum-Brønsted-Lang lecture on February 8, 1991. The lecture is named after three well-known Danish chemists and was instituted by the founder of crystallography in Denmark, Axel Tovborg Jensen. The title of Bob's talk was 'How a Chemist Gets a Charge out of Crystallography'. The title shows Bob's great sense of humor, and it marked well the focus of the new area of research that

Bob was initiating, namely implementing Richard F. W. Bader's theory Atoms in Molecules (AIM), developed for theoretical electron densities, for experimental electron densities derived from X-ray diffraction data. In his talk Bob presented the first results from his collaboration with Wolfgang Jauch from Berlin on MnF_2 . It was clear that AIM had great potential to quantify all the interatomic interactions that make a crystal, and we were keen to use Bader's AIM theory on molecular and hydrogen-bonded systems. VALRAY was the program system that Bob used for the calculations; it originated in Jim Stewart's XRAY System and had been developed in collaboration with Mark Spackman when Mark was a postdoc in Pittsburgh. Claus Flensburg was a master's student in my group when Bob came for his sabbatical; Claus had the responsibility of maintaining the computer systems of the group and served as our computational expert. Claus and Bob hit it off immediately. They discussed mathematics, physics, chemistry, programming, history, philosophy, etc., and Claus soon played an important role in the new developments of VALRAY. Bob enjoyed his sabbatical in Copenhagen in 1991, and when he left it was clear that he had to come back next summer for a couple of months, though it was obvious that it could be difficult to arrange a similar accommodation for him. Bob's sabbatical in Copenhagen was the start of a very fruitful and productive collaboration that was maintained through his yearly visits each summer for more than 10 years; our group knew – come summer, come Bob. In 1993 I was fortunate to obtain a Center of Excellence grant to develop structural biology, at the same time as our developments of AIM on experimental densities had reached a very promising and useful stage, so for the next ten years we maintained the program of charge-density studies parallel to the development of our structural biology program on carbohydrate active enzymes and enzymes in nucleotide metabolism. It is my impression that Bob enjoyed this mixed bag of activities, in which he always participated very actively.

Bob often said that he would have liked to study history, and it was only due to his poor language capabilities that he did not continue in this direction. He knew the history of the major countries in Europe well before he came to Copenhagen, and during his many visits he became an expert in Danish history. He enjoyed the Danish national historical museums at Frederiksborg castle and could spend hours watching the exhibitions. The Danish astronomer Tycho Brahe fascinated Bob; Tycho Brahe had his observatory at Ven, a small island between Denmark and Sweden that now belongs to Sweden. Bob visited the island several times and knew all about Tycho Brahe's life and therefore was a bit disappointed about the limited information at Ven.

During Bob's sabbatical we started the study of a compound with a very short symmetric hydrogen bond, methylammonium hydrogen succinate monohydrate, in which we used AIM to investigate the nature of this intriguing interaction. It was a long process that also involved detailed analysis of atomic displacement parameters, and employing neutron diffraction to verify that the hydrogen bond is truly symmetric. I think that Bob was happy with this first result from our collaboration when it was published in 1995. Claus did very well in his master's studies and was granted support from the Faculty of Science for his Ph.D. study,

naturally with Bob as a co-supervisor. Claus visited and stayed with Bob and his wife Janet in Pittsburgh in the summers of 1992 and 1995. Just before he completed his Ph.D. degree Claus visited again in January 1998 having joint birthday celebrations with Bob. Henning Osholm Sørensen and Anders Østergaard Madsen followed in the tracks of Claus Flensburg by having Bob as co-supervisor in their Ph.D. studies. Their research took other directions towards the analysis of anharmonic thermal vibrations and the modelling of hydrogen atoms in charge-density studies. Both enjoyed and learned a lot from working with Bob and visited him in Pittsburgh, Henning in 2002 and Anders in 2009.

Bob was known as a heavy smoker, but when he encountered severe health problems he quit smoking without any problems. However he was not happy with a situation, where he had to look after himself and his medication. I noted that it affected his usual scientific enthusiasm to some degree when he visited me in Grenoble in 2005. As Director of research for life science I had looked forward to share my excitement of the applications of synchrotron radiation in fields like art and archeology with him, but Bob was not turned on by the large facilities and was not too happy with traveling anymore.

Writing e-mails and letters was not Bob's forte, so it was difficult to communicate during the last years of his life. The last time Bob and I met was in 2010 at the ACA meeting in Chicago. He and Janet had travelled from Pittsburgh by train, as they did not like flying anymore. We had a great lunch together refreshing our good memories on collaboration and friendship from the past three decades, and talked about the three great young men Claus, Henning and Anders.

Everyone who met Bob realized that he was a great scientist who took crystallography to his heart and contributed significantly to the development of this field. He also stood out as a scientist of the old school who only wanted to publish things that he felt were done in the 'right' way. Bob was never tempted to follow the hot topics to attract research funding, and only worked on research he found really interesting.

For those of us who had the pleasure to get close to him, Bob became a dear friend, not only for me, but for all members of my family. He participated in all family events that took place during each summer, and my family and I are grateful for the good times we spent with Bob. He is missed not only as an inspiring and enthusiastic colleague but also as a dear friend.

Sine Larsen