



Ken Hedberg Oral History Interviews, September 29, 2011

Title

“Returning to Oregon State College”

Date

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Location

Valley Library, Oregon State University.

Summary

Interview 3 begins with Hedberg's memories of Ava Helen Pauling. From there he recounts his acceptance of a job offer from Oregon State College, his return to Corvallis, and the process by which he set up his research program at OSC. In this, he describes his designing and building an electron diffraction apparatus, the techniques that he has used to study molecules over the years, particularly interesting molecules that he has examined, and his teaching work at Oregon State.

Hedberg also delves into his wife Lise's work at OSU, including the anti-nepotism rules that sometimes presented problems. He also discusses the evolution of computer use in the OSU Chemistry Department and provides a description of the "final folders" that are an ultimate outcome of his work determining compound structures.

Interviewee

Ken Hedberg

Interviewer

Chris Petersen

Website

<http://scarc.library.oregonstate.edu/oh150/hedberg/>

Transcript

***Note: Interview recorded to audio only.**

Chris Petersen: Last time we pretty much finished up with Caltech, but one thing I realized I forgot to ask you about was any memories that you have of Ava Helen from that time period?

Ken Hedberg: Of Ava Helen? Only peripherally because I saw her together with her husband fairly frequently, and she of course was always present at the open houses they held, occasionally. These open houses some of the faculty, and so on, were invited, not very many of the students though. I saw her there, and I saw her a lot of course, later on, when she and Linus came to Oregon State, but at the time that I was at Caltech I saw her with Linus a great deal and that's about all.

CP: When did you make the move to OSU, and what made you decide to make that move?

KH: When did I come to OSU? Well, I don't know - have I mentioned at all the circumstances under which I experienced the opening here?

CP: The opening?

KH: At Oregon State?

CP: No, no.

KH: Well, I had been working at Caltech for many years after my doctorate and, well many, five or six, and I was actively engaged in research, and I was stopped in the hall one day by Carl Nieman, who was a distinguished organic chemist and who I knew quite well.

He said, 'Ken I received a letter from a former colleague of mine and that I went to graduate school with at Wisconsin who is now at Oregon State, and he said they have an opening there and he wondered whether I had anybody who would be interested, or we here at Caltech had anybody who might be interested. I just thought I'd mention it to you in passing because I remember that you were an Oregon State undergrad.'

So I, at this time my wife was pretty unhappy in California, in Pasadena, because of the air pollution. Our first son, our son was about to be born and she didn't want to raise him in that environment, so, I said yes I'd better explore this. And so I wrote then to E. C. Gilbert who wrote back that indeed they did have an opening, and one thing followed another and it turned out that my wife and I were going to drive north to Oregon to visit my parents, who lived at that time in Astoria, and I said to Gilbert that I would stop en route and talk with him and members of the faculty and discuss the opening.

Then I got another letter from a guy named Bill Caldwell, William E. Caldwell, who let me know, on no uncertain terms, that the reason this was a job was because he had managed to get the President of the University, A. L. Strand, to commit to two new faculty hires in chemistry. It turns out that at that time, well, let me put it this way - Earl Gilbert and Bill Caldwell were not on the best of terms. Gilbert was a department chair and Caldwell was a professor who did almost did no research on site but had some mining claims and some other things and was kind of a more open, free handed, back slapping type, a member of the country club and he knew A. L. Strand fairly well. And he complained that the freshmen at Oregon State and incoming students were not being given proper instruction because there weren't enough professorial staff involved in [5:00] this, just graduate teaching assistants and so on. He managed to convince Strand that perhaps there should be some positions set up, and these would, people of course, would be nominally responsible to Caldwell since he was running the whole program. The main purpose of, the main task of these people were going to be that they would sort of ride herd on all the teaching assistants. They would patrol the laboratories, make sure that the teaching assistants were doing their job, they would of course have some responsibilities themselves, but in the freshman program they would hold recitations and they would in this way be responsible for laboratories and then, as I mentioned, patrol the laboratories regularly. So I immediately sensed that there was something, there was a bit of an adversarial relationship between Gilbert and Caldwell. Gilbert of course was interested in hiring somebody who could also increase the research potential of the faculty. Caldwell wasn't in the least interested in whether these guys could do any research or not, he just wanted them as sort of majordomos.

So I learned all of this in more detail when I came and talked with Gilbert and talked with Caldwell. I also had more numerous conversations with other members of the faculty, people who have passed on now: Tom Norris, Wendell Slabaugh, everybody that was on the faculty that I had known before. After concluding all these interviews, we drove on down to my parents, came back to California; I had told Gilbert who was still the guy who was officially in charge of the hiring that I would think it over and I'd let him know. So after I got back to Pasadena I thought for a long time about this and decided that the conditions of this job were such that I found it unlikely to be able to get my research program going at Oregon State in a reasonable length of time, so I declined the offer, which was \$5,500 for nine months, or nine months but payments spread over ten months.

Well, my wife was very unhappy about this because she liked Oregon - it's more like Oslo where she grew up in Norway. As she put it, there was water in the rivers up in Oregon and trees in the forest, she couldn't see that in LA. We drove across a bridge one place and I pointed out to her that this was the San Gabriel River. She looked down and there was no water it was just a gully a dry wash, and we went through the San Gabriel forest on the outskirts so that there's nothing but sage bush - that's the source of her comments. At any rate she was very unhappy about this, and a few days later I got a call from Gilbert saying he was very sorry to receive my letter, he had very much hoped that I would accept the job, and he said he wondered if they were able to increase the starting salary a little bit would I reconsider? And I said - at this time home life was a little frosty because Lise was so disappointed. So I said, 'OK, I'll do that.' Have I told you any of this at all? No, ok. So, the offer came back and he said we can pay you \$200 or \$300 more per year. That's maybe 5% or 6% increase.

And so, I asked Pauling what he thought about all of this, and he invited me to come up to his home one evening and after hours, [10:00] 5 o'clock or so, can't remember exactly, so I went up to 4500 Fairpoint, whatever the street number is. At his house we sat on the veranda and discussed the job. I'd been very active in research at Caltech and had a number of published papers, lots of things going, and I expressed to him my fear that I was not going to be able to get my research program going at Oregon State because it involved a construction of apparatus. You saw that apparatus. I had to build that by hand - there were extremely limited machine shop facilities, nothing in the chemistry department at all, and I didn't see how I could get that instrument built at Oregon State.

So I expressed all of this to him and told him that the actual number of hours that I was expected to be in contact with students was something like 15 or 16 hours a week, just in the hands-on contact. See that's about 30%, no a little bit more than that, 35% of the total time, not counting preparation or anything of that sort. And Pauling sort of leaned back in his chair, we were sitting side-by-side looking out over the valley and the swimming pool and he says, 'Well, I don't know,' he says, '15 hours,' he says. 'When I was at Oregon State I was teaching 40 hours a week.' That was the year that he was a sophomore and had been asked to handle a course for young women in home economics, who were taking chemistry as a requirement. That's where he met his wife Ava Helen; at any rate that's a story you know.

So anyhow he said, 'I think that Oregon State will not be a first class institution for research in my time and probably not in yours.' These are his words. He says, 'on the other hand that's not really important in a bigger sense,' he says, 'if you can get your program going, Lise will be very happy there, Oregon is a wonderful place to live, as you and I know.' He says, 'I don't know - I think it might be worthwhile giving a chance. I think you could make it go and you'd be very happy there.' So, with that encouragement, I called Gilbert up and said, yes, I would accept the offer.

My wife of course was delighted at this because at this time our son had just been born and we lived in Pasadena, down below, not far from Caltech and the smog would roll in the morning at about 11 o'clock and she'd take the baby in, close all the doors and windows, keep them closed until about 4 in the afternoon when the winds reverse their directions and swept all the smog back out to sea again, and she could open things up. It was pretty hot too so I had a hose in this garden cottage that I put on the roof and turn on the water to keep it cool during the time that she was, so to speak, 'incarcerated.' Anyway, that Fall I told Gilbert that I wouldn't be able to come in the Fall, by the Fall term, but I could come January 1.

CP: What year was this?

KH: This was January 1, 1956, so this was all 1955, this conversation. So, come January we drove north, after Christmas, in times of a huge storm that actually led to flooding - this was a fine way for my wife to be introduced to the worst part of Corvallis. You don't know anything today about how it was then, but we drove up to Eugene, got up to Junction City and it turned out that the 99W was closed because of water on the roads. There was a bus going 99E to Albany and I, with

our car, the baby in the back, and Lise and I in front, we followed this bus very carefully up, sometimes water almost up to the hubcaps of the car. Got to Albany and then it turned out that the road from Albany to Corvallis was OK, it wasn't underwater yet, but the road from [15:00] Corvallis south from 99W was under water. By that we managed to get to Corvallis. By prearrangement we had rented a house of a faculty member that was going to be away for 3 months, so we had a place to move into immediately, all furnished, very nice house on Chintimini, over there against the hill, well, you know where it is. It was very nice and it turned out that everything was flooded the following day or two in Corvallis. You could hardly get around at all. Then it turned cold later on, the snow came and so on. So, that was my introduction to Corvallis.

I showed up to work on one of the early days and Gilbert told me, oh, they had a kind of a bonus to give me and that was that I was going to be assigned to teach a course, a graduate course, in physical chemistry to organic chemists, largely, and others. Well, this sounded like a bonus to him but for somebody just coming there, I mean, this was lecture three hours a week and I had never done this course before so I had all those lecture notes to prepare, as well as the stuff I was expected to do under Bill Caldwell's regime. So I had a very, very busy time and with a newborn in the house, and my wife trying hard to accustom herself to life and new place with a new baby and a husband who was up to his ears in work, it wasn't very easy. I was pretty discouraged at the end of that term and as the term drew on I took care to write down on a piece of paper divided into days and hours of the day for a week, each week, how much time I was actually spending in duties connected with teaching. By connected with that meant connected in with students one on one, preparation, including evening hours and everything else, and I was averaging, that first term, 56 hours a week, only in teaching related duties. So my fears about getting my program started in the research side were well born out by that first experience.

Of course, I was expected not only to have a program going, get my research going, but I had to build this apparatus which meant that I had to design it, sit down with - I think I showed you just briefly with folders of those drawings in there. I had a drawing table in my office so I spent a lot of time with drawing these things, and then Professor Yunker in physics, they had a fine physics shop, and I went across to see and he agreed, he saved my life actually, to allow one of the people in physics, I think they had 3 or 4 machinists, who would be assigned to my job. He would do everything and he and I would be in one to one contact all the time. He reserved the right to take this man off for any projects that physics needed of course, since he was employed by physics and using the physics facilities. That worked out just beautifully. It took a long time to get the apparatus built, 3 or 4 years, but it was finally done and put together and we managed to make it go. Ed Yunker's facilities and his kindness are really responsible for getting me off the ground at Oregon State.

CP: So, describe the apparatus a little bit for me.

KH: Sorry?

CP: Describe the apparatus for me.

KH: Well, the apparatus is what is called an electron diffraction unit. It consists of, the essential feature of it is, an electron gun that will produce a well collimated beam of electrons at a potential of about 60 kilovolts. So it's a very energetic beam on the scale of the way chemistry operates. [20:00] That beam is admitted into a large vacuum chamber. In my apparatus the whole thing is mounted vertically, so the beam comes down into this vacuum chamber, and at the bottom of the beam, let's say, is a detecting surface, which is in my case photographic film. In those days it was photographic plates but now is photographic film, and this photographic film is 8x10 inches square and is perpendicular to the beam and is moved into position by a mechanism that I built into the apparatus. And the apparatus is designed to study the structures of molecules in the gas phase by diffracting this beam of electrons from them. So we have a long nozzle that protrudes into the apparatus with a tip that passes, that stops just about a millimeter short of where this very fine, high powered electron beam is coming down. And in this nozzle, which is a tube with a fine tip on it, you admit a gas into the chamber - the gas shoots out the nozzle tip, intersects the electron beam at right angles and produces what is called a diffraction pattern. This diffraction pattern consists - well what happens is of course it's recorded on this photographic film underneath the nozzle and perpendicular to the beam so the diffraction pattern is recorded on this is a set of diffused rings varying in intensity, and the spacing of these rings and their shapes of the pattern contain all the structural information about the length of the interatomic distances of the molecule.

We take these patterns and we analyze them, and out of that we can deduce the intimate details of the structures of these molecules in the gas phase that is essentially, it's the structure of a single molecule because they're so far apart they don't

interact with one another as they shoot into the apparatus. That's what I was charged with, or what I wanted to build, and what I finally got going for all those years. It's still running.

CP: For 55 years.

KH: Yeah, and it is running and right now and running beautifully. We just did an experiment last week; beautiful patterns we got from a new molecule we were interested in. It doesn't take long for the experiment, it's quite interesting. The technique has developed enormously since the days when I first entered the field at Caltech as a graduate student. Now the experiment that lasts, this diffraction pattern, you expose a photographic film to the diffraction pattern for only 2 or 3 minutes, and you might want to make 5 different films or 10 different films. So all totaled you can do the entire experiment in a day, if you push it, everything. That's all, a day, that you need for what might be for a graduate student a year and a half of work analyzing it. So the apparatus mostly sits unused because we can quickly gather all the data we need. So I've had a lot of visitors who come, use the apparatus, and if I had a technician I could supply all the diffraction data for every group in the world, if this technician did nothing but take diffraction pictures of the substances involved.

Now it may be a little more complicated because these are gas phase molecules, we admit them into the chambers as a gas, but that doesn't mean that they have to be a gas as you look at them, you can put them on the table. The fact is that you've got to get them into the gas phase in order to make this experiment work. Well we had a set of ovens and heated nozzles so they can heat these things up and get the vapor. C60 that we worked on of course is very intractable, has no vapor pressure at all to speak of. So, we had to heat this substance [25:00] in an oven to 800 some odd degrees Celsius in order to get the tiniest bit of vapor from it, but that was sufficient to give us a diffraction pattern and we were able to determine the structure of this material, which was a carbon-like powder on the table. We have all sorts of auxiliary apparatus which allows us to produce gas molecules from lots of different circumstances. So it works very nicely, I'm very happy with it.

I should add as a postscript to all this is that this technique was very powerful through the '40s and '50s and '60s and even in the '70s, but there were other techniques that have developed in the meantime too. So there are fewer and fewer laboratories in the world doing this work. When I came to Oregon State and got mine going there were about, there were only two laboratories in the United States that did this kind of work; mine and a laboratory at Michigan. There were other people who were, well there was another apparatus built, it worked for a while but not very long. There was one at Texas that was built similarly, but it was built in the physics department and its interests there was not the same as the interests that chemists have. It worked for a while and then it stopped. Later on, there were apparatuses in Britain. There was one at Edinburgh, and later on, and still extant, is one in Reading, England. There was one in Germany, they were very active in Germany, and when I first started there was one in Belgium and one in Holland, and several in, at that time, the Soviet Union, and two or three laboratories in Japan - all of them had an apparatus and could do experiments. All of those are gone except the apparatus in Reading.

The apparatus in Germany, by the way, the man who was the professor who was in charge of that laboratory retired. His name was Heinz Oberhammer and his apparatus has been transferred to an inorganic chemist who is using it as a kind of an auxiliary to his main work, which is the preparation in interesting inorganic compounds. And as a part of that he wants to know what their structures are. The apparatus in Reading is still extant, but the man who was in charge of it before has now retired, and the woman that was working with him has a permanent position in the university, but she's heavily involved with teaching and has very little time to work with it.

There were two important laboratories in Norway, I didn't mention them earlier. Both of them are now gone as far as apparatus is concerned. There isn't any further support, in that in science, decisions are always made about where you are going to put a limited amount of funds, and in Norway its now determined that this particular area of research will not be supported anymore by the university in the sense that they will hire technicians and professorial type people to do this kind of work. And I fear that will probably be the case here at Oregon State too. So we don't know. Its plain fact is it's not judged by what's going on in the world of chemistry today, cutting edge stuff, a lot of the things going on today have been shifted more to larger molecule biological things: synthetic, organic chemistry, new materials - things of that sort. Not the kind of basic science [30:00] that I was involved with for all those years.

Anyway, I came to Oregon State, got it built and I've been here ever since doing this kind of research. That's what it's all about. I had great fun.

CP: So what were the techniques that you used to analyze the diffraction patterns initially?

KH: Well, yes, that's a good question. I don't know how much of the technology I'll go into but essentially you're faced with this photographic film, if you hold it up to the light you see this beautiful pattern of circular rings of varying intensity, very diffuse, easily recognized going out from a central point. All the information about the structure of the molecules contained, as I said earlier, in the spacings and the shapes of these rings. The question then that you're really asking is, how do you go from that to determine how molecules put together? Well, it turns out that these rings are related to the structure of the molecule by some, according to theory, in rather a simple way. I'll keep it as simple as I possibly can.

Every interatomic distance in a molecule creates, in effect, on this film, a pattern that consists of nothing more than a sine wave going from the middle out. Now a sine wave just goes up and down, up and down, up and down all the way out to the end of the photographic plates. So if you have a diatomic molecule, all the rings in their intensity would look like a sine wave, just from the beginning—up down, up down, up down—the spacing would be identical between them, aside from some geometric factors that I don't have to go into. So all you have to do is measure the frequency—oh, I should say that the farther apart the two atoms are that are giving rise to this sine wave, the greater the frequency in the sine wave. So two atoms that are far apart like this give a sine wave that goes up and down very rapidly, two atoms that are very close together will give a sine wave that has a very long wavelength. So you'll see very few rings. So all you'd have to do is to measure the spacing between these rings, and that is related by theory to how far apart the atoms are. Now that's the case for a diatomic molecule and they have one sine wave. The diatomic molecule vibrates and so the atoms are not rigid, they are moving back and forth away from one another like two balls on a spring, and of course that means the distance isn't constant.

Well, it turns out according to theory to a good approximation, this sine wave, instead of having constant amplitude all the way up, dies off due to this vibration. So you measure the dying off of the sine wave and that tells you how big the amplitude of this vibration is. So we learn about two things: the distances between the atoms on the average and we learn about how much they're moving with respect to one another by measuring the damping off of the sine wave. Well of course there aren't many diatomic molecules left to study; but every problem, or rather the theory I mentioned, applies to just pairs of atoms. So if you have a molecule that has more than just two atoms in it you're going to have more than two distances, more than one distance. Every pair of atoms in the molecule gives rise to one of these sine waves. So carbon dioxide is a linear molecule, it's a carbon-oxygen bond, and that gives rise to a single sine wave that goes out. There are two of them but they have exactly the same distance so there are two sine waves right on top of one another. Then you have the distance between the oxygen atoms that's twice as big. So it generates a sine wave also, which has a frequency twice as great to first approximation as the frequency in the carbon-oxygen because the distance is twice as long, and that gives a sine wave that oscillates with twice the frequency in the first one and they're on top of one another. So the pattern is no longer a [35:00] simple sine wave, but a collection of two sine waves. If you know how to separate out the sine waves and measure their frequencies then you know exactly what the structure of this molecule is. So if CO₂ were bent like NO₂ is, NO₂ would be entirely similar, but there you would find the distances between the oxygen atoms is not twice the distance between the nitrogen and oxygen because it's a triangular molecule, like this. So that oxygen-oxygen distance would not be moving at twice the frequency of the enol, so you can immediately determine that distance and determine the nitrogen-oxygen distance and by comparing, you know, what the bond angle is in the molecule.

This simple account can be applied to molecules that are very, very complicated. The entire problem then is just to separate out what these different sine waves are, construct yourself a model that will account for all of the distances, and then you have the structure of the molecule. It is, in practice, considerably more complicated than I'm telling you, but that's essentially the features of the whole thing.

Now you asked how we do this. Well, we have to measure the frequencies and to do that we have a scanner that is called a microdensitometer. The film is placed on the bed of this microdensitometer and the film and the apparatus that I have, we have a mechanism that rotates the film around its center. The purpose of this is that you're averaging the information around the entire circle that is, if the densitometer consists of a beam that passes through the film, and a detector that measures how intense the light beam is as it come through the film. So when the ring is intense the light beam that comes through is much reduced, and when the film is more transparent the beam that comes through there is more intense. So you get a recording of the blackness of the film; so this thing translates and we have an electronic data accumulation

system that measures the intensity of the blackness of the film as a function from the center upward. And that gives us digital data, and that's what we actually work with to analyze. So, that's essentially it and without having you in the laboratory for a week I can't tell you much more that would make it clearer I don't think. So, any other questions about that?

CP: How would you decide which molecules to study?

KH: Yeah, well, this largely comes from your own, in my case my own interest, lets say, or the principle investigator's interest. Now if we take C60 for example, that was big news at the time it was discovered and I know a former student, named Bob Johnson, who was working at IBM, in San Jose. They had managed to create or had a sample of this stuff. Now, in the beginning it was very rare. I mean, you could get it in milligram quantities and the sample I actually worked with I think had 300 milligrams in it. It was a little bit of black powder in a vial, and at the going market prices that was \$5,000 worth of samples. Well, Bob wrote to me and he asked me, how could we do this? Could you do this work? I said 'well, it's very exciting we should try.' So they supplied the sample. Several people and IBM were involved in this project and they sent me up here. So we got the sample and we managed to, [40:00] it was very exciting because I didn't know whether we were going to be able to get a pattern from this stuff at all, because it was refractory, you know we had to heat it so hot, and the oven that we had it in was so hot it was glowing red in the apparatus.

Now, fortunately, the film that we used is not very sensitive to red light. Secondly, I was able to build a shield around the nozzle that protected the film from almost all of the glow. As I heated it up I could see it glowing bright red in there and then I would close up the window to the apparatus and turn off the beam, the electron beam, and quickly move the plate in position, open up the beam and expose this. I could not see evidence of any - we have a fluorescent screen in there that we can see patterns for most molecules. At the time of the experiment I couldn't see anything on this fluorescent screen other than a very faint glow from the screen, so I didn't know whether we were getting anything or not. So we made two or three of these exposures and I took the film into the dark room and I couldn't believe my eyes when I saw how beautiful the pattern was. You couldn't have predicted it would be like that or that you would even get one from seeing there was no evidence.

Normally, when I run stuff in the apparatus, I put the main beam through a slot on the fluorescent screen so I can see the scattering all around it and I can see it, you know, it will look like this on the black thing, somewhat reduced. I can see we're getting scattering. Couldn't see that with C60 and, yet, there it was, an absolutely beautiful pattern. It was very exciting.

CP: Was that a complicated analysis?

KH: Was it what?

CP: A complicated analysis?

KH: Well, it turns out, if you pick up a soccer ball and you look to see how the things are put together, there are hexagons in it and pentagons in it. They are put together in a completely symmetric way and it turns out that buckyballs are on a soccer thing, the length of the stitching in a soccer ball, it's a little hard to describe, there are bonds that link two six-member patches together and stitches that link a six-member to a five-member, and those two bond lengths are different in C60 itself. Those are the only two parameters that are necessary to determine the structure of C60. Assuming that it is a soccer ball, that's the assumption that you make and that was well characterized by NMR spectra and other things. So we knew it was a soccer ball type but we didn't know what the length of these bonds were. So if you then have, the only thing that changes, it doesn't change the shape, it only changes the size of the six-member and five-member ring as you change the length of these bonds.

Well, we had to put together a model. You see, what you actually do in analysis, you have the experimental pattern and then you have to generate a model and compare the pattern that this model gives with the one that you experience experimentally. So you are fitting a model for which you have calculated a pattern and you adjust that pattern to fit the experiment by changing the parameters of the model. So to make this, applying this to C60, the pattern depends only on the relative lengths of those two distances that I mentioned; the one between six-member rings and the one between a six- and a five-member ring. [45:00]

And so my wife then put together the model and you can imagine it's not easy. You have to remember, generate every distance in the molecule from just these two parameters. There are 720 distances in the molecule and she constructed a program that would calculate this model for us, and that was the one we used and tested and it led finally to the fitting and structure of the thing. We published that in Science a couple of decades ago now I guess; lots of fun.

CP: I wanted to ask also about xenon hexafluoride.

KH: Which one?

CP: Xenon hexafluoride.

KH: Oh, xenon hexafluoride. We never actually finished the structure of that thing because a friend of mine, at University of Michigan, had done a very good job, and he was in ahead of us. We worked on other xenon compounds, we did xenon tetroxide, which is four oxygen atoms arranged in the form of a tetrahedron around a xenon atom. That was quite an experience because it was a very explosive compound. We had several minor explosions with it. We had to generate the compound on the apparatus by adding acid to a perxenate, as it's called, a compound which contains xenon but is a salt. And we had to build an apparatus where we could tip this up slightly and add acid to this where upon the xenon tetroxide would be formed and could flow into our apparatus through our nozzle. Several times - the stuff in the gas phase is very unstable - we had several times very minor explosions. Minor in the sense that there was no danger to anybody involved here, but it blew holes in our conducting line right away. So we had that happen several times. That's the only xenon compound that we actually finished the structure of, xenon tetroxide.

CP: Were there other compounds that are particularly memorable or rewarding?

KH: Well, the ones that we've talked about are ones sort of in the public eye. I think in terms of public interest of something very novel, probably not so much. The work that we do I've always tended to characterize in the term used in the old days, which was basic research. It had no really discernable practical application. It was fundamental stuff and there are a lot of fundamental problems in chemistry. For example, chemistry as it is practiced at some level or another makes continuous and intimate use of the concept of the structure of the things you are dealing with. I mean we talk about the structure of proteins for example. We talk about the structure of almost everything in organic chemical structures, when he lectures on the board. So we were involved in determining structures but what we were doing was actually measuring these structures to very high precision. We're not just making a ball and stick drawing, we're looking at the distances between the atoms and trying to deduce from this how these distances might be related to the reactivity of the molecule and things of that sort. How the intimate details of the structure, distances - well let me put it this way, size and shape of the molecule are related to its reactivity.

I can give you one example of this that most people don't know about but a very common chemical compound in nature is nitrogen dioxide that comes from combustion and internal engines under high temperatures and so on. Well, nitrogen dioxide [50:00] is a triangular molecule, the nitrogen at the apex, and two of these nitrogen dioxide molecules come together and they form a dimer that has, its called dinitrogen tetroxide. A remarkable thing of this is that these two molecules come together and fall apart, come together and fall apart just so easily. If you have NO₂ in the gas phase you have N₂O₄ in the gas phase also, as you change the temperature and pressure the amount of one of these with respect to the other changes. Well, N₂O₄ is very hard to, it falls apart so easily, it's very hard to measure structurally, but we undertook that job. The way it was done is that we got a sample of NO₂ and the reaction for the decomposition or dimer, or dedimerization is extremely rapid. It just falls apart immediately, or comes together immediately. Well, if you cool it down, the stream down, what happens is you get more and more of N₂O₄, as you heat it up all of this is decomposed right away because of the thermal effects. So what we did was cool the sample, cool the oven, I mean, sorry, the nozzle, way, way down. Well, way down below zero Celcius, run the stuff through it, and we got beautiful pictures of N₂O₄. Then we heated up a little bit, we could see all the characteristic distances from that molecule beginning to disappear as the higher we heated it the less of those we had. We got it to a hundred and some odd degrees as nothing but NO₂ present.

Well, the structure of N₂O₄ turned out to be very interesting. It turns out that there is an extraordinarily long N-N bond. The bonds between atoms in typical compounds tend to be more or less the same. For example, saturated hydrocarbons have carbon-carbon bonds, and I can tell you right away it will be 1.54 or 1.535 angstroms to within a hundredth of an angstrom in no matter what compound you look at. Well, there's a characteristic N-N bond too and N-O bonds, and it

turned out that this N-N bond was very, very long. So much so that by simple criteria that Linus Pauling had produced one time, it's only the order of a tenth as strong as a normal single bond. So that accounts for why it falls apart very easily. But one thing that's characteristic of single bonds is that the two ends of the molecule can rotate around like this, you see they're not fixed like this because the bond is so weak. To our intense surprise that's not the case in N_2O_4 . It's a flat, planar molecule no matter how long its bond is.

So what is it that holds it flat, you say? Well, it's not, single bonds don't hold things flat. Why is this flat? Well that was the interesting question of the time and it turns out that the structure of the NO_2 part of the N_2O_4 molecule is almost identically that of the separated NO_2 . That is, bringing the two together to make the dimer doesn't change the structure of the ends at all. Normally, if you bring them together, if you take two monomers and bring them together, these will change somewhat in angles and distances. Not with N_2O_4 . Well, these are puzzles that are just lots of fun to think about and solve. And so this kind of research is the thing that characterized what Lise and I have done most of our career here. We have all sorts of different systems that pose different, basic, chemical questions, and we look at molecules to try to find out what we can learn about these basic chemical questions; answers to them from studying the structures [55:00] of maybe even a series of several molecules that have some things in common some things different to see how the differences and, so on, effect the properties of the molecules. So, that's what we do.

CP: So, you've got your apparatus constructed, do I presume your teaching load decreased some?

KH: Well, in due course, in those days the chemistry department consisted of four divisions. It was organic, inorganic, physical, and analytical. They were pretty clearly defined. People were in these divisions in accords with the kind of research they did. Well, there came an opening in physical chemistry and Gilbert, as chairman, told me immediately that, when that opening occurred he was going to move me into that division. Well, this was two or three years later. The two jobs were filled; this monitoring of the laboratories that brought me here, Caldwell's efforts, the other person was Tom Parsons. Tom Parsons was in chemistry for a while but moved into administration and finished his career here as an administrator.

Well, I moved into physical chemistry, Gilbert, and I became a physical chemist. My teaching responsibilities changed a lot. I no longer rode herd on the TA's but I still taught general chemistry, but I also began to teach courses regularly in physical chemistry. So my contact hours went down but the amount of time I spent working certainly didn't because now I had a contact hour before were just, I knew the experiments in freshman chemistry the kids were doing and I could walk through and make sure that they were getting the proper attention and so on. Now I had to prepare lectures and courses I hadn't lectured in before, and so, the contact hours went down but the amount of time spent teaching didn't diminish for quite a while. But never the less, my apparatus was coming along.

I was very lucky when I came here because I had all the money I needed to build this. I got some money from the Research Corporation before I arrived, I applied for that at Caltech, and I came with a Sloan Foundation grant which was five years of money that I used for summer support when I wasn't teaching and that I condoled fully to drawing up parts for my apparatus and so on. And then I got NSF support too, so I never lacked for funding. The main thing that I had trouble with is the time, in the early days, not in the later days. So things have turned out, later days and teaching loads gradually began to fall into a, how do I want to put it, a range that was consistent with what was being taught at other institutions with which we competed. So there was still a lot of teaching but it was the kind that was really lots of fun.

CP: What was the environment in the department like back then?

KH: It was very collegial, is that the word? We were all very friendly with one another; I mean socially I had friends in physical chemistry, organic chemistry, and we saw one another at analytical chemistry and dinner parties. We did lots of things together; New Year's Eve parties and so on. It was, in my opinion, a lot more cohesive than it is at the moment, and at the time a lot more cohesive at Oregon State than many institutions. In many institutions there is a kind of a very wary attitude or outlook from one divisional type to another [1:00:00] and sometimes even within the members of the division. You have to realize that university teaching, university careers can be very competitive, especially those that depend a good deal on research that you do as well as on your teaching. And so you read about this all the time about the press of people that are competing for, even publicly sometimes, priority in some major discovery. But we never had any of that in chemistry; we just had a very good time. It's been a fine place.

CP: At what point did Lise start working at OSU?

KH: That's a history that is very interesting. Lise decided - did I mention how we met? Well, when we came to the States she was a scientist and we worked together at Caltech she was actually paid at Caltech and we worked in electron diffraction there, both of us together on the same project, did several things there. Then we came to Oregon, she was very busy of course with our son who was only three months old when we arrived. So she did no work at all at that point except - well that's not quite true because we did manage to find some babysitting for a few hours a day now and then when she could come to the university - but she was never away from home more than two or three hours at a time then. A couple of years later our daughter was born so then we had two kids at home. So by and large she worked only sporadically until the kids got into nursery school, she could then drive them up, they were on Orchard Street here in the university nursery school which has changed its location I think somewhat. But the kids would go there and she would come to the laboratory and then when their session was over she would pick them up and go home. We lived very close to the Jefferson School, so until both of them got into school, she was home most of the time, but managed to put in several hours per week working on our projects.

Then when the kids went to Jefferson School, you know, she could, the morning the kids would get dressed, I would go off to work, the kids would get dressed, school would start, they would run out the front door, go over to the school and we had let the teachers know what phone to call. Then Lise would get in her car and drive over to the university and we would work until about 2:30 or so and she would get in the car and go home, park the car and get in the house and the kids would run out of the school and come back. They never knew she actually worked because as far as they were concerned she was there when they left and there when they came home. But she was able to work about half time then.

She was paid by a line item in the budget for grants that Lise succeeded in getting. Then we also had joint grants and then she's very good at mathematics and she was hired at the computer center to be working on, she was very good at programming and she was kind of a liaison with chemistry and programming in the computer center; where we still had centralized computing. Then we had one rhubarb. It went something like this. Gilbert had retired and Burt Christensen had become chairman. Lise had been working on my grant for the line item in the budget for her salary. The proposal had been - department chairmen have to sign the proposal, Bert did that, so it was funded. And then he [1:05:00] decided one time that she could no longer work on the grant after her, after the present year was over, academic year. And so she wrote him a letter and pointed out that she had line item for a salary, it was never explained what the reason was. And he responded and she wrote again and he didn't respond.

It turned out, in retrospect, that he was greatly afraid that there would be some negative feeling about a man and wife working together in the chemistry department because at that time there were, it was not unheard of, but it was a little unusual. The thing is though, she was not being paid on state funds at all and she was an expert in the field in which there were no other west of the Mississippi you see.

Well, he persisted in this, so we finally went over together to the Dean who was Vern Cheldelin at that time. I knew him very well for years. I said, 'Vern, look, this is a situation,' he said 'well why didn't you tell me this before?' I said, well, Lise said this too, 'Well, we were going through channels. Our issue wasn't all with you, it was with Christensen.' So, he looked at this and said well, he says, 'she can certainly work on the grant.' The proposal, by the way, had been signed by Bert and now he was refusing to continue our funding even though we had signed the agreement. So he overturned this, but then he said, 'If Lise wants to work in the future she'll have to have her name on the grant, not just work on your grant.'

Well, I can't remember much of the details following that but it turned out that Christensen was about to retire. There were circumstances here that I don't need to go into, but anyway he was going to retire and a new man was going to come. And I was on a national committee at the time and there was a former friend of mine at Caltech named Dave Shoemaker who was on the same committee. And Dave and I - I mentioned to him, he was from Idaho of course and had gone to Reed College, and we had gone to Caltech together, he finished a little earlier than I did. I said, 'Dave, we need a new department chairman.' He was chairman of the committee I was on, I saw how good he was at administering things. 'Would you by any criteria even consider coming back, maybe be considered as our department chairman?' There was a lot of talk about this, he decided that, yes he might like that. He was at MIT at the time. So we invited him out and he was offered the job, and he liked Oregon, you know it was very similar to where he grew up and went to school in Portland. But one of the criteria for him coming was that his wife would be able to work. Here was another man and wife

team. She was a crystallographer as he was. And MacVicar was a chairman at this time and one of the conditions for him coming was that his wife be allowed to work. And he said, 'Oh, by the way, Ken and Lise have the same problem.' And so MacVicar came around to Dave and says, 'That's no problem.' He says, 'I've looked this all up,' he says. 'Two members of the same family cannot work, not only in the same department or in the same institution but in the entire system of higher education, except under unusual circumstances.' And he said, this is MacVicar's words so Dave relayed them to me, 'I regard a man and wife scientific team as an unusual circumstance.' So Dave came, his wife was allowed to work with him, and at the same time, Lise was allowed to work with me.

The really remarkable and most interesting thing about this, there was one small attempt to cover the tracks here, [1:10:00] and that was that Clara Shoemaker was responsible to me and Lise was responsible to Dave for monitoring purposes. But of course Dave came around and says, 'Well, how's Lise doing?' 'Fine,' I said. Then he says, 'How's Clara doing?' I said, 'Oh, fine.' That was that - that was the monitoring. Of course that all disappeared in the end. But in retrospect it's pretty funny. So, that's how we were able to continue.

CP: So Lise did a lot of computer work?

KH: Oh, well, yeah, but not just computer work. She's a special expert in programming, that has evolved during the ages that we've been here, but she is responsible for all the basic materials that we use in our research, even today. Some of these programs have been modified by others and even added to by others. The basic thing she is responsible for...it's very funny.

CP: Can you reflect on the early days of using computers in your work?

KH: Computers and work?

CP: Computers in your work.

KH: In my work. Yes, when I left Caltech we had some IBM office machines and we were able to operate them using IBM punched cards. We had a very, for the time, very efficient system for doing the calculations necessary for our work in electron diffraction. When I came to Oregon State we didn't have this IBM set up here at all, but the mathematics department had managed to, the applied aspect of mathematics here, was very interested in computers and the central computer - my IBM had been developed a few years earlier - and there was a computer that they managed to buy in mathematics that's called an Alwac 3E they sold a few of these things and we had one here. It was set up and running in mathematics in the basement. It was a tube machine, it was a huge thing with tapes, vacuum tubes - transistors hadn't been invented yet, at least were not available in a device like this.

So we wrote together. I did programming when I first came here, there was no compiler for this machine so we had to write things in machine language and I learned enough to do that and wrote the very earliest programs in machine language so it would run on the Alwac 3E. Well, the Alwac 3E, as our analytical scheme improved, the programs got more and more lengthy as far as that machine was concerned. The machine by this time was beginning to teeter a bit and there were some graduate students over there in mathematics that managed to know what tubes to interchange and exchange to keep this thing running. But we had to run our early programs in such a way we couldn't rely on the machine because it would make errors due to faulty hardware. So we wrote our programs in such a way that we could run them twice and if we got the same answer we could continue to the next stage and Lise and I wrote those programs.

Then after a while - and by the way I had some money and to use the machine you had to pay, so I at one stage gave them a few hundred dollars from one of my grants [1:15:00] against future computing so they could buy vacuum tubes to put into this machine, believe it or not. Arvid Lonseth was the chairman of mathematics at that time, very nice guy. A couple of years later it turned out that statistics had gotten ahold of an IBM machine. It was running on punch cards but it had a compiler and so we moved to that—that was a central computer. They charged also, but it was a much better machine, 1410 I think it was called. Then things progressed around here, we were still doing central computing. There was a central computing center that was set up and they bought a CDC machine. That CDC machine was better still, faster, and by this time we had altered our programming so that we could access the machine remotely through a telephone line and we had a teletype terminal in the laboratory. So our data could be put out on punched paper tape and that punched paper tape could

be fed into our terminal and carried over to the computer. We thought this was, boy we were really ahead of things here, it was great.

Then it turned out there was heavy demand for that machine and the amount of storage we needed for some of our programs was huge and they didn't have enough of it, see. So we were limited to how much storage we could use in any of our programs. So Lise very, very cleverly took our biggest, most demanding programs and created it to operate with overlays and so on. That is, instead of saving something she determined what would be needed and wrote the program so succeeding stages could write right over this stuff. So this occurred and that way the program became very efficient as far as space is concerned. Then we still needed space, so I talked to them over there and they said, 'Oh you can have more space after the hours of such and such.' So we would set our stuff to run on this machine at later time.

Then of course that was the time that Lise, one of the times Lise was hired to be working over there. Then central computing of course began to gradually disappear as PCs came in and right away - well before that happened in chemistry we determined that we needed a computer locally and we managed to get a grant, several of us pooled our knowledge and resources and made our proposal and we were able to buy a VAX and Lise then converted all of our programs to run on the VAX and that was tremendous. We had lots of programs including plotting ones, we had a plotter also that would work just fine. Then of course the VAX began to be phased out and we had a PDP 11 in our laboratory, finally, Lise and me. Some of our stuff ran on that; this was all very clutzy stuff. The PDP 11 used large disks, like this, and floppy disks that were 8 inches or 10 inches in diameter. Then the PCs began to appear on the scene. At one stage or another I could see that there was going to be no expertise around at all that knew anything about PDP 11's. Everything was going to be going to PCs. So if we wanted to keep current and not be high and dry and if something happened to the PDP 11 nobody would know what to do. So we converted all of our stuff to run on PCs and all of our data, all through the years had been stored on these disks on the [1:20:00] PDP 11. Well, we hired a guy to convert all the stuff on the PDP 11 onto disks in a format that could be used on smaller, well smaller but faster, PCs. These were all on floppy disks like this. Well, pretty soon those disappeared and we had to convert them to some other medium and so we took all of this stuff and copied them all over on to CDs that are now like this and I have a host of things on CDs, but also a whole pile of stuff on these floppies all cataloged and I've maintained on a couple of the PCs in my laboratory a floppy disk drive that will still accept these old ones. There's no reason to change the data to anything else, but now we've gone to extremely fast computers. A calculation that on the Alwac 3E would take us two days we can now do in about ten seconds, something like that. They're so fast now and the storage is so enormous, you know, I can get a program going and I will hit Return, and I can't get my hands in my lap before all of the information is on the screen again. It's been a total revolution.

In the midst of all of this, some place back, we had a special Tektronix scope which could feed data in, it would plot things for us, we could see it on the screen here, and my son later went on to an electrical engineering degree at Stanford and is a software engineer at Microsoft now. When he was in high school he loved these computers and he could program also. So he played, believe it or not, a big role in some of the very early developing because when he was at Stanford he would come home and say, 'Well, what do you need now Dad?' He's still interested in that.

I should say one other thing - our kids were kind of interested in science and so Eric and Lise and I published a paper together on work. He had actually worked in the laboratory and this was a paper by Hedberg, Hedberg, and Hedberg. It was published in the *Journal of Chemical Physics*, and a few years later my daughter was interested. We published a paper, another one by Hedberg, Hedberg, and Hedberg, but I never managed to get the two kids to the laboratory at the same time. So we could have four Hedbergs on a - one time I called up the journal editor of *Chemical Physics*, a man named Willard Stout, way back when. I said, 'This is Ken Hedberg,' and he said, 'Oh! Of Hedberg, Hedberg, and Hedberg?' Apparently he had noticed this. Anyway, that's more or less the story of computing.

CP: OK, well the last question for today, I'd like you, when we were over at your office we'd seen the final folders, could you explain what the final folders are so we can have that on record?

KH: What the final folders are? There are several stages in the analysis of a structure and they begin with the raw data that we get from using this microdensitometer on the films or plates. These raw data are the first things that go into the folder. Now, a lot of things happened to be done to that raw data because, after all, you're taking what is a continuous curve and you are sampling it at very small intervals along and so you have points that correspond to this. Now when this plate or film moves across the densitometer it goes across the middle and back out on the other side. So, we scan [1:25:00] the film from one outside to the other but all the time it's rotating, which means that half of the film should be identical to

the other half, half of the trace should be identical to the other half. But since you're sampling by points you can't make sure that these points are identical. So you have to do something, as we call, find the center. So we have a program that compares the two sides of this and determines where the center is and then it takes the data on one side and add on the other and interpolates, if necessary, between the points; adds them all together to give you a scan. That's all in there, finding the center. So we have the curve and counts, we have the curves that find the center and then we have the data which are just numbers. We want to convert them to something that has a common basis, and because of the properties of the densitometer a very black film can give you the same range of numbers that a very light film can, but there's obviously a lot more scattering in one than in the other. So we have a way of converting this information to, let us call it, absolute density. Its not really that, but really puts the two curves on the same scale in terms of darkness and so on.

Then we have a number of programs that are designed to convert this - there is a difference between the blackness of the film and the intensity of the scattering. Now you can get a sense of this where, for example, if you take a film and expose it for a second you get a certain darkness. Expose it for two seconds and you get another darkness and of course if in the right range the blackness of the second would be - if you exposed twice as long under identical conditions - the blackness would be twice as great. Or clearly the longer you expose the less the photographic film is going to respond. So pretty soon it gets black and it doesn't matter how long you expose it; its not going to get any blacker. So the curve that relates blackness to intensity is not linear. We have to find out how, we know how non-linear it is in terms of how dark the film is, so we have corrections for that. We have a whole host of corrections that are built into this that is designed to take the data from the film and put it into a form which compares with, mathematically, with a theoretical function that we can calculate. There are many steps in this process. Each one of these steps builds up to this point.

Then, when we've got all of that, we do a number of calculations, the most important of which is the final fitting procedure. It's called a least-squares adjustment. This is the program that fits the final model to the experimental data and the result of that is an output in the folder that shows the fitting quality of this. And then there are often plots of the curves at various stages of this procedure, so it all moves into the line printer output, which those days we called the final folder. It might be anywhere from two inches thick - well, anywhere from an inch thick, to three inches thick, say. And that's what you saw in those line printer folders. Now we have almost the same thing, nowadays, but it is all done on 8.5 x 11 stuff you see, when we're doing hard copy that we'll want to look at. But now we'll actually put all of this stuff on a disk, on a CD. We have folders on the computer for molecules that contain all the information we want, [1:30:00] and then subfolders and subfolders.

And I take these, the major folder I'll just copy the whole thing over onto a CD and I'll give it a name for the molecule and everything we want now we can put on this CD—look in there and we can find it right away. So it's the hard copy stuff that you saw in the laboratory really is stuff that we stopped generating maybe twenty years ago, and the later stuff is all in, either in folders or on devices like CDs. I read recently somewhere where they were saying CDs were going to disappear also, so maybe it will all be on a thumb drive now, who knows. [1:31:04]