SCIENCE HISTORY INSTITUTE

ROALD HOFFMANN

Transcript of an Interview
Conducted by

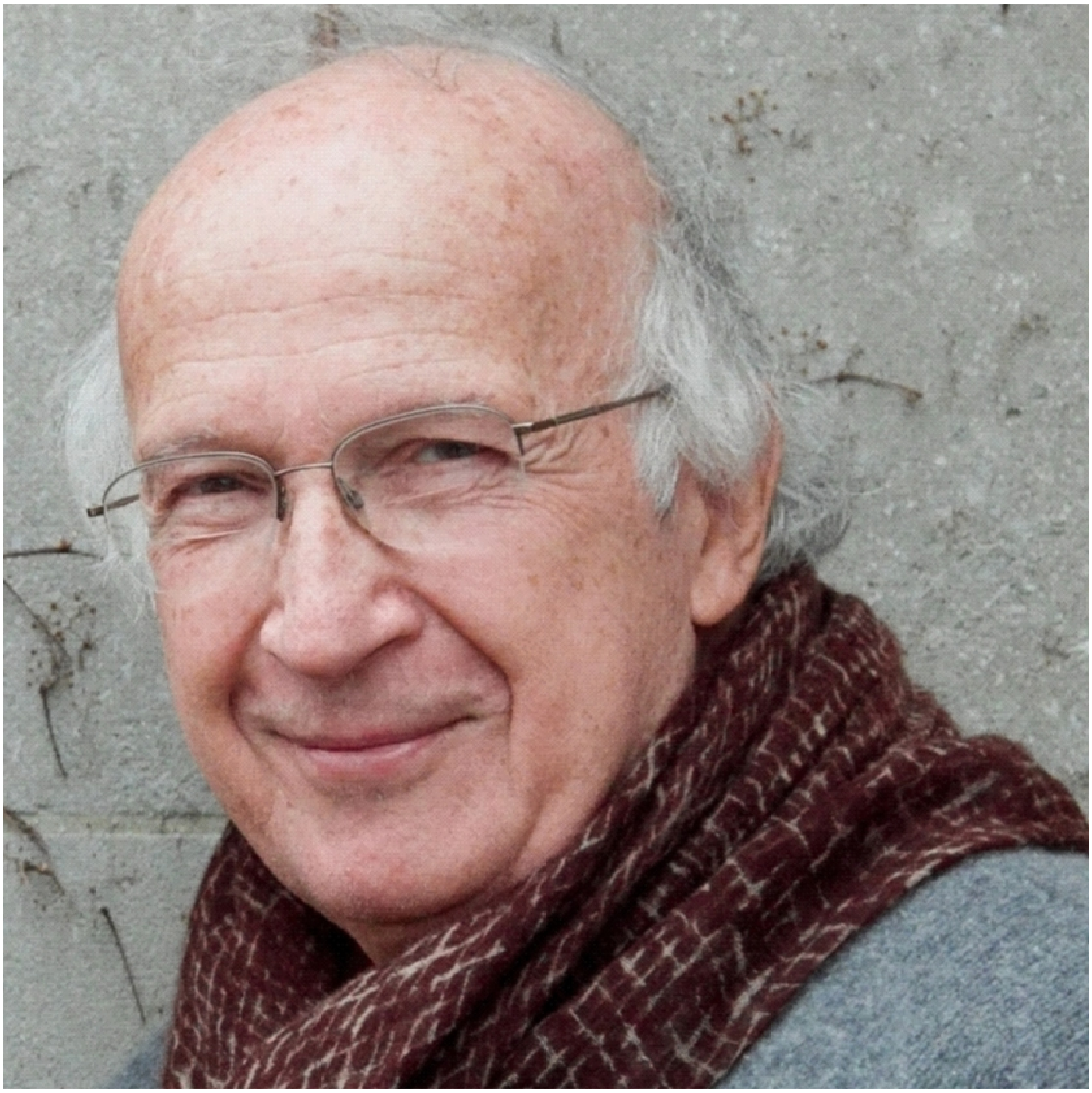
David J. Caruso and Carsten Reinhardt

Cornell University, Ithaca, New York and
Chemical Heritage Foundation, Philadelphia, Pennsylvania

on

16 and 17 October 2014 and 21 March 2015

(With Subsequent Corrections and Additions)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Roald Hoffmann

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Roald Hoffmann, interview by David J. Caruso and Carsten Reinhardt, Cornell University, Ithaca, New York, 16 and 17 October 2014 and 21 March 2015 (Philadelphia: Science History Institute, Oral History Transcript # 0925).

Science History Institute

Chemistry · Engineering · Life Sciences

ROALD HOFFMANN

1937	Born in Złoczów, Poland (now Zolochiv, Ukraine) on 18 July

Education

1958	BA, Columbia University, Chemistry
1960	MS, Harvard University, Physics
1960	PhD, Harvard University, Chemical physics

Professional Experience

	Harvard University
1962-1965	Junior Fellow, Society of Fellows
	Cornell University
1965-1968	Associate Professor, Chemistry
1968-1974	Professor, Chemistry
1974-1996	John A. Newman Professor Physical Sciences
1996-2008	Frank H.T. Rhodes Professor of Humane Letters
2008-present	Frank H.T. Rhodes Professor of Humane Letters Emeritus

Honors

1969	American Chemical Society Award, Alpha Chi Sigma
1969	Fresenius Award, Phi Lambda Upsilon
1969	Harrison Howe Award, American Chemical Society, Rochester Section
1970	Award of the International Academy of Quantum Molecular Sciences
1971	Member, American Academy of Arts and Sciences
1972	Member, National Academy of Sciences
1973	Inaugural Recipient of the Arthur C. Cope Award in Organic Chemistry, American Chemical Society (co-recipient)
1974	Linus Pauling Award
1978	Member, International Academy of Quantum Molecular Sciences
1981	Nichols Medal of the New York Section of the American Chemical Society
1981	Nobel Prize in Chemistry
1982	ACS Award in Inorganic Chemistry
1983	National Medal of Science

1983	Foreign Fellow of the Indian National Science Academy
1984	Foreign Member of the Royal Society
1984	Member, American Philosophical Society
1985	Foreign Member of the Royal Swedish Academy of Sciences
1986	Dickinson College Award
1986	National Academy of Sciences Award in Chemical Sciences
1988	Foreign Member of the Societas Scientarum Fennica
1988	Foreign Member of the Academy of Sciences of the USSR
1990	Priestley Medal
1991	N.N. Semenov Gold Medal, Academy of Sciences of the USSR
1994	Centennial Medal of the Graduate School of Arts and Sciences of Harvard University
1996	Pimentel Award in Chemical Education, American Chemical Society
1997	Inaugural Elizabeth A. Wood Science Writing Award, American Crystallographic Association
1998	Jawaharlal Nehru Birth Centenary Award of India
1998	Corresponding Member, Nordrhein-Westfälische Academy of Sciences
1999	Honorary Member of the German Chemical Society
2000	Member, Deutsche Akademie der Naturforscher Leopoldina
2002	Honorary Member of the Chemical Society of Japan
2006	Gold Medal of the American Institute of Chemists
2010	Member, Mexican Academy of Sciences
2018	Member, Real Academia de Ciencias

ABSTRACT

Roald Hoffmann was born Roald Safran in Złoczów, Poland, in 1937. His father, Hilel Safran, was a civil engineer and his mother trained as teacher. Between 1939 and 1941, Złoczów was under Soviet occupation; when the Nazi Wehrmacht reached Złoczów in 1941, they rounded up the Jews of the town and many men and boys were killed. Roald's family went into hiding, then into a labor camp. His father bribed the guards to allow Roald, his mother, and several other family members to leave, but was himself executed soon after for leading a plot to break additional prisoners out of the camp. Roald's family spent the remainder of the war in hiding. At the end of the war, the family moved to Krakow, Roald's mother remarried, and they acquired the surname Hoffmann from bought identity papers they used to emigrate to Prague and, eventually, to the United States.

After graduating from Stuyvesant High School and exploring interests in the humanities and in chemistry as an undergraduate at Columbia University, Hoffmann went to Harvard University for a graduate program in chemical physics, planning to work with William E. Moffitt. Moffitt's death led Hoffmann to Martin Gouterman, then to William Lipscomb. In graduate school, Hoffmann continued to pursue a variety of academic interests, attending a summer school in Sweden where he met the woman he would marry, and spending a year in the Soviet Union on a government-sponsored exchange program. Upon his return, he settled into theoretical chemistry work focused on boron hydrides with Lipscomb and completed his PhD within a year.

Offered assistant professorships at Cornell and at several western universities, Hoffmann instead accepted a Junior Fellowship at Harvard, which afforded him three years to pursue research without any teaching responsibilities. He decided to apply the extended Hückel method he had developed for the boron hydride calculations to organic molecules. R. B. Woodward brought the frontier orbital explanation for the electrocyclic reaction to Hoffmann's attention. Hoffmann describes how the ensuing work on orbital symmetry brought together theoretical chemistry and organic chemistry, and spurred a significant change in the chemical community's perception of chemical reactivity.

In 1965, Hoffmann took up a faculty position at Cornell University. He describes the role of computers in his work, both at Harvard and at Cornell, and the importance of the Ithaca community, which encourages socialization across departments and disciplines. The remainder of the interview focuses on Hoffmann's approach to establishing and leading a research group, his interactions with colleagues, his second period of collaboration with R.B. Woodward, and the experience and impact of winning the Nobel Prize. He also discusses his writing projects, which include poetry, plays—including *Oxygen*, which he cowrote with Carl Djerassi—and popular works exploring science and religion. Throughout the discussion, Hoffmann returns to the themes of building bridges between branches of chemistry, between chemistry and physics, between science and the humanities, and between academia and the public.

INTERVIEWER

David J. Caruso earned a BA in the history of science, medicine, and technology from Johns Hopkins University in 2001 and a PhD in science and technology studies from Cornell

University in 2008. Caruso is the director of the Center for Oral History at the Science History Institute, president of Oral History in the Mid-Atlantic Region, and editor for the *Oral History Review*. In addition to overseeing all oral history research at the Science History Institute, he also holds an annual training institute that focuses on conducting interviews with scientists and engineers, he consults on various oral history projects, like at the San Diego Technology Archives, and is adjunct faculty at the University of Pennsylvania, teaching courses on the history of military medicine and technology and on oral history. His current research interests are the discipline formation of biomedical science in 20th-century America and the organizational structures that have contributed to such formation.

Carsten Reinhardt served as the Science History Institute's president from 2013 to 2016 (then the Chemical Heritage Foundation). He is currently a professor of the history of science at Bielefeld University, Germany. Reinhardt has extensively researched and published on the impact of chemistry on society through topics including the history of industrial research, the emergence of instrumentation, and chemistry's links to physics, biology, medicine, and technology. Reinhardt has received many awards and fellowships, including being named a fellow at the Max Planck Institute and a visiting professor in the Department of Philosophy, École Normale Supérieure, Paris. Reinhardt was an Edelstein Fellow at the Institute in 1998–1999 and at Hebrew University of Jerusalem in 1994.

ABOUT THIS TRANSCRIPT

The Center for Oral History, Science History Institute, is committed both to preserving the recording of each oral history interview in our collection and to enhancing research use of the interviews by preparing carefully edited transcripts of those recordings. The preparation of interview transcripts begins with the creation of a verbatim typescript of the recording and proceeds through review and editing by staff of the Center; interviewees also review the typescript and can request additions, deletions, or that sections be sealed for specified periods of time. We have established guidelines to help us maintain fidelity to the language and meaning of each recorded interview while making minor editorial adjustments for clarity and readability. Wherever possible, we supply the full names of people, organizations, or geographical locations mentioned during the interview. We add footnotes to the transcript to provide full citations for any publications that are discussed, to point to extant oral history interviews, and to clear up misstatements or provide context for ambiguous references in the transcript. We use brackets to indicate the addition of material that was not in the audio, and bracketed ellipses to indicate the deletion of recorded material. The transcript also includes time stamps at five-minute intervals. We omit without noting most instances of verbal crutches and all instances of nonlexical utterances. We also make small grammatical corrections where necessary to communicate interview participants' meaning. Finally, staff of the Center create the abstract, chronology, and table of contents. With the availability of online full-text searching of our transcripts, the Center for Oral History opted to discontinue the practice of preparing a back-of-the-book index for each oral history transcript in 2020.

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INTERVIEWER: **David J. Caruso**
Carsten Reinhardt

LOCATION: **Cornell University**
Ithaca, New York

DATE: **16 October 2014**

CARUSO: So, today is the sixteenth of October 2014. I'm David Caruso with Carsten Reinhardt, and we're doing our first session of an interview with Roald Hoffmann here at Cornell University. Thank you again for agreeing to sit down with us.

HOFFMANN: Sure.

CARUSO: As I mentioned to you, what I'd like to do is start at the very beginning and hear a little bit about life in Poland growing up. You were born in 1937. So, I'd like to hear a little bit about what your family was like, where you lived, things like that.

HOFFMANN: Yes. So, the first years of my life were difficult, not of my own doing, just geopolitical circumstances at the time. I was born in July 1937, in a town called Złoczów, [as] it's pronounced in Polish, now Zolochiv [in Ukraine]. [. . .] When my mother was born before World War I, it was Austria-Hungary. And when I was born, Poland. Then it became the Soviet Union. Then it became the Ukraine. And not only did it change hands, that little piece of the world, but it went through [. . .] two and a half waves of what would be called ethnic cleansing in the process. Not an easy part of the world. I was born in a Polish Jewish family. The family was in a typical degree of assimilation of Polish Jews in that time. My last name was not Hoffmann. I'll come to tell you that story. [But my first name was from the beginning Roald]. I was born as Roald Safran [. . .] Roald is my real name—even the name reveals a story of assimilation and something about Jews in Poland at that time.

So, my uncles are named Abraham [Rosen] and Samuel [Rosen]. [Another uncle] was named Friedrich [Rosen]. My father's name was a Hebrew name, Hilel [Safran]—that is also my son's name—and my mother's name was Clara [Rosen]. There is no way that they, good Socialists and Communists that they were, were going to name their son Abraham or Samuel. So, this is a story of generations. [My] grandparents were observant Jews. [My] parents were quite the opposite—Socialists. [. . .] They were both born in 1911, so that's sort of just to set the stage. They were [. . .] not that rebellious. So, I got a Hebrew name, which is Israel, and the diminutive was Yisrul in the Ashkenazi dialect. My aunts and uncles [until they died] would call me Rulush, which was a diminutive for Yisrul.

So, [my parents] were looking for some name that vaguely sounded like Yisrul, Israel, but which was not a biblical name. [. . .] You couldn’t give your son the name of a Polish saint, so Thomas or Michael was out. You looked for secular heroes. So, there are a lot of kids in that time, for instance, boys, were named Emile after Emile Zola, who was a secular hero. And Roald [. . .] was after Roald Amundsen, the Norwegian explorer. That was a good, safe, secular name—[polar exploration was most newsworthy in the Europe of the time]. Now I’ve desperately looked for a romantic connection between my mother and Roald Amundsen, **<T: 05 min>** but he died ten years before I was born. [My mother told a story about choosing my name], which I didn’t believe until I heard it corroborated by someone else. [She said my father and she] were looking for a name, and there was this magazine article on the tenth anniversary of Roald Amundsen’s death, and they thought it was a good name. I thought this was weird, but then I met Roald [Z.] Sagdeev, who is a Russian physicist who came to this country, [who is five years older than] I am, and he told me the same story, [about his mother reading an article about Roald Amundsen]. So, there was a little corroboration [and, though he was born elsewhere, a similar story].

Złoczów was not a shtetl. It was a typical town of that period, twelve thousand people, ethnically mixed. [. . .] The population was about one-third Ukrainian, one-third Polish, and one-third Jewish. And they coexisted somehow. The Ukrainians viewed the Poles as invaders, and they were, in a way, [if one went] back hundreds of years. And there was a Jagiellonian [Polish] castle [Castle Zamok] lording over the town, part of the history of that period.[1]

The Jewish community was very well-established. There are a number of people in the world who’ve come from that community. It was, for instance, the home of Yechiel Michel [Epstein], the Maggid of Złoczów, one of the first followers of Baal Shem Tov [Rabbi Yisroel ben Eliezer], the founder of the Hasidic movement. It was also the home of Moyshe Leyb Halpern, who was a great [twentieth-century] Yiddish poet. And an interesting photographer, Arthur [H.] Fellig, better known by his name Weegee, a photographer of crime scenes in New York. [. . .]

[Złoczów] was a small town in the province [whose] chief town was Lwów [Poland]. [In German/Austrian it was called Lemberg, in Ukrainian, Lviv]. Lwów was where my father went to school, at the Lwów Polytechnic [University]. There [were at that time] restrictive laws on the number of Jews in the professions, the so-called *numerus clausus*. The Polish government was, to varying degrees, anti-Semitic in that period, but still, [overall], it was a very open place for Jews.

[For instance], my father went to Lwów Polytechnic. A classmate of his, I found out later, was a distinguished Polish chemist, Bogusława Jeżowska-Trzebiatowska. Lwów

[1] The Jagiellonian dynasty was a royal dynasty that reigned between the fourteenth and sixteenth centuries, over several central European countries.

Polytechnic was also very well-known in mathematics—Banesh Hoffmann, and a few other mathematicians were [there. My father] got an engineering degree from there. My mother studied education at the University of Vienna. We had relatives in Vienna. [. . .]

My uncle Samuel studied dentistry in Lille, in France. He went out because there weren't enough places for Jews to study dentistry in Poland. The [gravitation towards] Austria was a natural one, since part of our family, after the First World War, went to Austria, and [then remained there]. There was a lot of motion across Europe.

My father was a civil engineer. My mother was a teacher, but never taught. They were born in 1911. My mother has a story. My mother had a very difficult life, [separated from her parents during the first World War for three years]. She lived to a very ripe age of ninety-four, a strong woman, and very important in our survival. And I've recently written a play, **<T: 10 min>** [. . .] about my mother and me.[2] We just had a German premiere of it in, of all places, Bayreuth. [A Japanese production is coming].

REINHARDT: What is the title of it?

HOFFMANN: It's called in English, *Something That Belongs to You*. It's an autobiographical play about my mother and me. [. . .] A translation will be published soon by a small [press] in Germany. Our relations to Germany, I'll come back to a little later. Of course, it's tied up with the war.

CARUSO: Just to ask quickly—

HOFFMANN: Yes.

CARUSO: Your parents, I'm assuming they were children of war as well, right? They were . . .

HOFFMANN: Yes. And I was going to tell you the story of my mother and World War I. So, my mother was born in 1911. World War I breaks out [in] 1914. She's one of, at that time, three children; there were two more to come later. Their mother, my grandmother, [Feige Rosen], is taking them on a train from Złoczów west to Lwów. She gets off the train at Lwów [to get some food], and there is an Austrian attack at that moment. The front line separates her from [her] three young children. My mother's three years old at this time. [The children are left] with a Ukrainian nurse—I tell the story in the play. The nurse did everything in the world [for them], was wonderful. [. . .] The Red Cross takes the children to an orphanage in Vienna, in a convent,

[2] Roald Hoffmann, *Something That Belongs to You*. (Dos Madres Press: Ohio, 2015).

and [there] the three children remain for three years, 1915 [. . .] to 1918, in this convent. Their parents [do not know] if the children are alive until the oldest child, [Abraham], remembers the name of a relative in the United States. It's crazy. [Through that relative the parents are reached. They] find out only in 1918 that the children are okay.

CARUSO: Wow.

HOFFMANN: Imagine a young child, age four years old, separated from her parents.

My mother has good memories of that convent. [. . .] And she still bore a scar. One of the nuns was carrying in some soup for dinner in a hot pot, and my mother ran to the nun to give her a hug and got burned by the soup. She had the scar from that, from Vienna in 1916. [Some years later, she returned to Vienna to study.] We have a wonderful picture of my mother as a student in front of a rather Aryan-looking sculpture in front of the University of Vienna.

[My] parents were not religious. They were professionals, as I've mentioned. It was a good time. [My] grandparents [. . .] on my mother's side, [Wolf and Feige Rosen,] owned a store. It was called a *galanterea*, [selling] sewing trinkets and [supplies], fabrics. On my father's side, there was someone who dealt in lumber, as far as we can make out. Of the four grandparents, only one survived the war, my mother's mother.

So now comes the story of the war. For us, the first two years, '39 to '41, were not so bad, [nor were they for the Jewish population in our town]. The Nazis invade Poland in September '39. There is the Molotov-Ribbentrop [Pact, leading to a] division of Poland.[3] The Soviets come into our part. That was the cure **<T: 15 min>** from Communism for my parents' [generation]. How anyone could be a Communist living one hundred miles from the Soviet-Polish border is beyond my understanding. But [there] were [Communists among them], because that's what progressive young people were. Not just in Poland, but in France [and elsewhere in Europe].

From that generation, and some of the survivors in our family, came the founders of the state of Israel, [the people who settled] the kibbutzim. And my stepfather's sister, [Sabina Kornreich], was one of the founders of the oldest socialist kibbutz, Mizra. I have an uncle who had another story. He's my father's brother, [Yehuda Safran], the only surviving relative on my father's side; he had emigrated to Palestine in '35. He was a Jewish boy who liked to ride horses; Jewish boys did not ride horses in those days. So, he went to Palestine, where he could ride horses freely. And he became a police officer under the British, a mounted policeman, which was, again, not a profession many Jews took. But the moment the state of Israel was founded, all of a sudden there was a need for policemen, especially policemen who spoke Arabic, as he did. And so there is another story there.

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[3] The Molotov-Ribbentrop Pact was a neutrality pact between Nazi Germany and the Soviet Union, signed in Moscow on 23 August 1939. The Pact provided a written guarantee of non-belligerence by each party towards the other, and a declared commitment that neither government would ally itself to, or aid, an enemy of the other party.

REINHARDT: What language did you speak at home?

HOFFMANN: At home, the languages were Polish and Yiddish, were my mother languages. I cannot speak either one of them well [today]. But those were my mother languages. They were [spoken] interchangeably. [. . .]

So, ’39 to ’41 we had the Soviets. In general, the Soviets treated the Jews fairly well. They treated the Poles not so well. They treated the Ukrainians worst, because they perceived the Ukrainians, correctly, as nationalists and opposed to the [Union of] Soviet Socialist Republics. And there is a terrible story there at the end of the ’39 to ’41 period, where the NKVD [People’s Commissariat of Internal Affairs] imprisons, at the castle [above Złoczów], six hundred members of the [. . .] Ukrainian intelligentsia of the town: the doctors, the lawyers, the teachers. And in the week they have in [June] ’41, before the Nazi Wehrmacht reaches us, they proceed to kill [all] the Ukrainians. Because some members of the NKVD were Jewish in that period, that caused an exacerbation of already existing Ukrainian anti-Semitism, which led to terrible things in the first week of that invasion. I talk about that in that play also. The play is autobiographical, though the names are changed.

[. . .] We had nowhere to run. We were trapped. That is the story of Polish Jewry in general. [. . .] Many Jews came over from the German-occupied part to where we were, in the Soviet-occupied part. So, the Jewish population of the town swelled [. . .]—and then there was nowhere to go. [. . .] The escape channel to, let’s say, Palestine, was [difficult, thousands of miles away], clouded in illegal immigration. [. ..] It was not a good time.

REINHARDT: Did you know about *Sondereinsatzkommandos* in West Poland?

HOFFMANN: Yes. [. . .] We have, unfortunately, firsthand experience of that.

June 22, 1941, the Nazis invade the Soviet Union. It takes them a week to reach us [in Złoczów]. **<T: 20 min>** [The Polish army is defeated]; the Soviet army retreating, blew up bridges, communications. That [actually] plays a role a little later on [in our story of survival].

[. ..] In that first week, SS [*Schutzstaffel*] Einsatzgruppen followed the Wehrmacht, and essentially organized killings in the various towns with a Jewish population, of which there were many. In our case, it was SS Einsatzgruppe C, and also [the SS] Wiking division, which was a division made up of Scandinavian mercenaries. [. . .]

They [set up at] the castle. The Ukrainian police and Ukrainians rounded up the Jews, brought them to the castle. This castle, which is now a peaceful tourist site, [had become] a terrible killing ground. That castle was used as an NKVD prison. In that castle were six hundred and fifty or more Ukrainian [prisoners], who were killed by the NKVD between June 22 and July 1. They were buried there in the courtyard of the castle.

The Jews [brought to the castle] were first made to dig out the newly buried Ukrainian corpses, who were then properly [buried]. We know the numbers because their families buried them. And then two [thousand] to three thousand Jews were killed up there. It was still largely men and boys. They let the women, by and large, go. In that roundup were caught my grandfather Wolf and my uncle Abraham [Rosen]. [Rosen was my mother's maiden name.] Wolf was killed, Wolf Rosen. Abraham crawled out from among the dead. To the end of his life—he eventually came to the United States—he carried a [fragment of a] so-called dum-dum bullet [embedded in his arm]. So when he went through [security controls], he set off alarms in the airport.

We were hiding in [our house in Złoczów]. We had somehow prepared a secret hiding place in the attic, [walled off], and I have a memory of going into that place, [crying along the way]. So, now comes the worst part of the war for us. The really difficult part of the war was July '41 to June '44. In June '44, American soldiers are landing at Normandy on D-Day. For us, the war was over. We were freed [then] by the forces of evil, meaning the Red Army. [. . .]

[Returning to our story], we stayed [until] the end of '41 in our house. A ghetto was being organized. [It was decided that it was better to be in a labor camp, and that we entered in 1942.] The labor camp was called Lackie. The story of the labor camps is not well told yet. The reason is that they were not killing camps, extermination camps. So they somehow didn't capture the public attention, [a terrible thing to say]. There were hundreds of them. There were typically a hundred to five hundred Jews and other people in a slave labor situation. No one was killed outright [in these camps], though people were beaten, [and many] died from typhus and typhoid.

Usually, the camps were run by one or two Germans, in our case a very **<T: 25 min>** sadistic man named Herzog, who, after the war, fled to Egypt. The guards were German hangers-on, [collaborators], Romanians, Ukrainians, Latvians, people from other places. [. . .] There weren't supposed to be any children in the camp, but you bribed the guards, you had children in the camp. [The guards] were venal but bribable. My mother was beaten by Herzog. She had some scars from that too.

My father was valuable to the Germans because he had, as a civil engineer, built some of the bridges and culverts and roads in the area. I have pictures of him doing that. Fortunately, we have photographs from before the war, which we saved in that attic [in town].

[My father was then] able to move in and out of the camp. The only documents we have from that wartime period are in fact the passes that my father was given, which say "the Jew Hilel Safran is entitled to travel between Złoczów and Lackie and such." It was an Austrian construction company that was using the slave labor. People were moving from town to town, repairing the [roads. It was 1942]; I was, at this point, five years old, [my parents were] thirty-one. They're young people. They're organized in socialist Zionist groups. [The one they were in was called Hashomer Hatzair]. Those groups were politically active and formed some nucleus of a resistance movement. One of my uncles, [Frank (Fromcie) Rosen] was in the forest in a partisan group. The partisan groups are a terrible story, because they were Jewish, Polish, Russian, Ukrainian partisans who were often busy killing each other rather than fighting the Germans. [. . .] They usually had abandoned Russian weapons.

A couple of people [who] escaped from the concentration camps came back with a story of what [was happening in them—the mass killing was beginning. The camps] most active in our part were two great killing camps, not Auschwitz, but Sobibór and Bełżec. A couple of people escaped, jumped out of trains, came back, told the story. No one wanted to believe it. No one. It's not only that [President Franklin D.] Roosevelt didn't want to believe it; it's the Jews who were on the ground there who didn't want to believe it. They were told they were going to [work in the west. And] nobody wanted to believe such a terrible story.

But the socialist youth movement tried to organize something, and my father began plotting an attempt to break out of the camp. [They needed] weapons. He got access in and out [of the camp], and in his briefcase he smuggled in weapons—at the end of '42, beginning of '43—into the camp, from my uncle in the forest. Meanwhile, he was talking to some people around, Ukrainians. Everyone was looking for a place to hide. He found a Ukrainian schoolteacher, the only educated man in a small village called Uniow, [now Univ], about thirty kilometers from Złoczów [. . .]. The [camp population was working nearby], and there they found this man who would be willing to hide us. [He was Mikola Dyuk, his young wife was Mariya Dyuk.]

[Dyuk agreed] initially to take in four people. Eventually there was my mother and me and an uncle and an aunt. My father was going to join us after the breakout **<T: 30 min>** from the labor camp. Let's see. The fifth person [who came in was eventually my uncle Frank Rosen, who was in the forest initially]. My father would have been the sixth. We bribed the guards [in the camp] and walked out at night to this hiding place [in Dyuk's house] in January '43. I'm five and a half. My father remains in the camp. [. . .] In June '43, the attempt to break out [of the camp] is betrayed by another Jew, and the two leaders, my father and another person, are arrested, tortured, and killed in [Złoczów], June 30, 1943.

News of that reaches us by letters. There was actually a system of communicating. Two letters came describing the killing. My mother cried. She didn't want to cry for me, but she told me about [my father's death]. We're in an attic the first year—five people. The attic [is under a] peaked roof. The attic was used to store books for the school. It's a one-room schoolhouse. On the bottom [floor] is the schoolhouse for this village. This village has two hundred people, and maybe thirty children. And those children all go to this [school] with one teacher. The teacher and the family live in back of the house. In between are two storerooms, one sometimes rented out, a passageway. In front is the one-room schoolhouse, on a dirt road, [the only road] in the village.

In the attic, there are the five of us—first four, and then my uncle comes in. Each day [the schoolteacher] brings up food, he takes away slops. We stayed in that house for fifteen months, from January ’43 till June ’44. We moved [to the first floor after a year]. We barely survived the first winter. The attic has cracks. It’s not [insulated]; air comes in. I could watch the children playing [at recess] through a window [without glass] with slats at one end in the schoolhouse.

Among the children playing are three Jewish children. I didn’t know this till 1980. [. . .] At the end of the road there was a monastery of the Greek Catholic Church, the dominant Ukrainian denomination there. Those three children are in an orphanage there with false identities. One of them becomes, later, the foreign minister of Poland, who was very active. He was the head of the Peace Studies Institute [Stockholm International Peace Research Institute] in Stockholm, [Sweden]. Adam Daniel Rotfeld.

CARUSO: Can I ask what were you doing in that attic for fifteen months? I mean, was it just getting up and surviving every day and going to sleep? You mentioned your mom received her degree in education.

HOFFMANN: I learned how to read. My mother was a schoolteacher. There were actually books up there. There were atlases. I was very good at geography. She would invent endless games, endless games to play with me to keep me quiet. I must have gotten frustrated, but I was a quiet child. I learned how to read there, in Polish. I may have learned some Yiddish also. And we just sat quietly. I could stand up [completely] because I was small. The rest of them, the men, had trouble.

After the first winter, [. . .] the second winter came around, ’43 to ’44, November, December. It was [decided] that we couldn’t [survive] up there. Ukrainian winter is like [winter was in] Ithaca, [New York].

So, we [moved] into a storeroom on the [ground] floor [. . .], one window blocked up. In that storeroom we dug out a bunker underneath **<T: 35 min>** for when the police would come in the house, which happened [every once in a while]. Later in the war, German soldiers were stationed in that schoolhouse. And we would go into the [hiding place, the bunker] we dug out from the earth—I still remember the smell of wet earth. We dug out a place where on a bench five people could sit. [We’d go into that hiding place, and Mikola Dyuk] would move the planks across the top of it, and move a cupboard across that. And that’s where we sat in the worst moments. Otherwise, we [stayed] in [that storage] room, a six-by-ten-foot [space, I am guessing].

That storeroom—the schoolhouse [stood until around 2010]. The attic is there. The attic has been rebuilt. I have been in that attic twice since then, [in 2006 and 2009]. The storeroom on the first floor where we were has been rebuilt into a classroom. The classroom was a chemistry classroom [in 2009]. [. . .] The children there don’t know that I was there. Which tells you something about education of Ukrainians about World War II.

[Mikola Dyuk] had a young wife. They had three young children. The oldest was my age. In June ’44, I was almost seven, when we came out. [. . .] The Russians were advancing. They were stalled near us. [We walked across one night to the Russian lines]. We went to Złoczów. We stayed there, and at this point [. . .] I learned Ukrainian. That was my third language at this point, [when I was seven]: Polish, Yiddish, and Ukrainian.

[. . .] It [became] clear the Soviets were going to take over that part [of Poland]. So we went west to Przemysl, a town which was more clearly in Poland. And then, following the Russian troops, we went to Krakow, [Poland].

REINHARDT: Who is we at that time? Your mother, of course. And you. But your aunt and uncle also?

HOFFMANN: Yes. They had a two-year-old child that was given to a Polish family when we went into hiding. [. . .] It was judged that the two-year-old would not keep quiet in the attic, whereas I would. After the war, they went back to the Polish family, and the Polish family and the child were both killed during the war. [Such terrible] decisions people had to make [in the war].

[One] grandmother [Feige Rosen] and a third uncle [Abraham Rosen], survived in a bunker in the town of Złoczów, and we reunited after [the war]. [. . .] Of about four thousand Jews, about two hundred survived the war in this town. That’s about the dimensions of the destruction of Polish Jewry in general. Of those two hundred, three were children, and I was one of them. The other two are in the United States also. [. . .] We were the largest family group in that town to survive, seven people: a grandmother, four of her children, the wife of one. The wives of the other were killed. And I.

We moved as a family to Krakow, [in early 1945—this is one month after the Red Army goes through Krakow, in January ’45]. I’m now eight years old, it’s time for me to go to school. I had missed the first grade already. [. . .] A deal was made—the only thing functioning in the way of schools is the Catholic church. [. . .] **<T: 40 min>** The future pope is teaching in a neighboring school. My parents strike a deal with the priests and nuns [. . .] that I would be brought up as a Catholic if they let me into the school, because it was time for me to go to school. I still have my report cards from second and third grade. My best grades are in catechism. I had all the experiences that a small Catholic kid—described very well in Fellini’s *Amarcord* movie.[4] How boys talk about which priest should [they] should confess to, because this priest wants to hear dirty stories, and this priest tells you [to repeat] too many—

CARUSO: Hail Marys?

[4] *Amarcord*, directed by Fedrico Fellini, (Pic Distribuzione and Warner Bros.) 1973.

HOFFMANN: Hail Marys to say. So this—typical kid stuff, Catholic kid stuff. I have a picture of me as a First Communion. I was a choir boy in church. I knew I wasn't Catholic, but it didn't matter. I didn't know what I was.

CARUSO: How was it adjusting to life, given what you had gone through?

HOFFMANN: It was easy. In general, children are very adjustable, [and so are parents]. My mother remarried in that first year, a man who had lost his wife in the war, whom she knew from before the war. He was from another town.

I'm going to tell you about the refugee camps in Europe in a moment, but the birthrate in the refugee camps was bigger than anywhere else in the world. There were all these people who had missed six or seven years of their lives. I was in classes with kids who were five, six years older than I was, because everyone was catching up. It was life. One was still scrambling where to go, [what] to do. We wanted to go to America. We had relatives [there]. We almost went to Israel. We almost went later on to Peru, of all places. But many Jews went to South America, because they gave visas, and it was very difficult to get an American visa.

My stepfather's name was Naftali Margulies, Margulies. The Margulies brothers are the ones who sponsored Fritz Haber, right?

REINHARDT: Yes. Yes.

HOFFMANN: But it's not them. It was a good German, Polish, Jewish name, comes from the Hebrew word for pearl, "*margalit*." [. . .]

So, for a year, I was Roald Margulies. Now it's at this point, at the end of '45, as we're about to leave Poland, quasi-legally, that I acquire the name Hoffmann. [How this came about is] a bizarre story, [one difficult for Americans to] understand. You can imagine you could get a false identity during the war to survive, and many people did. Now the war is over. [. . .] Why are we getting this [new] identity? Because we're desperate to get to the United States, and just like immigrants today in Bangladesh, or in Zaire, or in Costa Rica, know the US immigration laws, so we knew about [. . .] discriminatory quotas.[5] We knew that it was better to be a German Jew than a Polish Jew, because of the [quotas which favored German immigrants over Polish ones].

[5] Also known as the Immigration and Nationality Act of 1952, the Act allowed the US government to deport immigrants or naturalized citizens engaged in "subversive activities" and also allowed the barring of suspected individuals from entering the country. The Act specifically, but not overtly, targeted suspected members of the Communist Party.

So now comes another bit of geopolitics. Russian troops go through. [. . .] It becomes clear that the borders of Poland [will shift. The Soviets will take] **<T: 45 min>** Western Galicia, the part we [came from]. [. . .] So, the Poles for their own part, do what they can to discourage the Silesian Germans, who are in the part that Poland's going to take over. Those who didn't run remain. And so there is a priest in Mittenwalde, a little village near Breslau, now Wroclaw, in Silesia. And as part of making life uncomfortable for him, the Poles no longer give him any money to run his parish. So, he invents a business, which hurts nobody. He sells the birth certificates of German soldiers who were killed in the war. Naftali Margulies goes to the village priest in Mittenwalde and becomes overnight Paul Hoffmann, buying a birth certificate of a German soldier. [What] irony. [. . .]

My uncle, the one who was in the forest, an enterprising character, [seems to have been] in the business of forging documents. He forges a wedding certificate between Paul Hoffmann and Clara Rosen, and my father disappears from the picture; we become Hoffmann. And that's the papers under which we eventually come to America. So, our immigration was illegal. So what? Nobody's going to deport me now. Anyway, I was a child. [Nor did we change the name back later].

Anyway, I become Roald Hoffmann, and with those papers, we buy a visa to go to France. We cross the border in Prague, [Czech Republic]. We declare ourselves stateless. We acquire one of these Nansen passports that were used.[6] And after three months, in Prague, we wind up next in a so-called DP camp, displaced persons camps, refugee camp, in the American Zone in Austria. [The camps were not bad, often old Army quarters.] I'm now nine years old. And we're all the time trying to go somewhere, trying to get visas. These camps were nice. I learned German now, my fourth language.

REINHARDT: How did you manage to survive in the way—where did you have your money from? I mean, how did you manage to—

HOFFMANN: They worked. Everyone worked somehow. In the DP camps, there was work created. But even in Krakow, in 1945, my stepfather got a job. I remember it exactly. He became a representative for a chocolate company whose name you will recognize, Carsten, but not Americans. This is Suchard [Chocolate Factory]. A great European, French or Swiss—

REINHARDT: It's big. Yes.

HOFFMANN: [A great Swiss firm originally. Now] absorbed into Nestlé, I think. [. . .] I remember as a kid, still to this day, [. . .] chocolate coming in aluminum foil wrappers, and

[6] Originally called "Stateless Persons Passports," Nansen passports were internationally recognized refugee travel documents from 1922 to 1938. They are known as "Nansen" passports after promoter, polar explorer Fridtjof Nansen, for which he was awarded the Nobel Peace Prize in 1922.

sometimes the wrappers had legends [or patterns] imprinted on them, and I would collect them. [My stepfather] would bring them home; I had a collection. I don't have it anymore. So, he worked for Suchard, and—

REINHARDT: What was his profession?

HOFFMANN: His profession was businessman. He has a degree from the Handelshochschule in Vienna [Austria]. [. . .] In the United States, [he] couldn't find a job; that education was worthless. But he found himself eventually as an accountant for a Wall Street firm. That's what he ended life as. My mother never worked as a teacher. It was, again, a profession you could not carry very well [from country to country].

CARUSO: What were you doing during these—

HOFFMANN: I was going to school. [. . .] I was **<T: 50 min>** good at school. Now, it's '47, we are in Austria, outside of Linz, and these DP camps were often old Kaserne, military [barracks]. [. . .] The next one we were in [I think] was in the French occupation zone of Germany, [. . .] in a place called Wasseralfingen, near Aalen. [It] was a DP camp, and we were living in the officers' quarters, which were very nice, private houses essentially. [. . .] Oh, the instruction [in the schools] was in various languages. In Poland, it was in Polish. In Austria, the DP camp, the school was run in Yiddish. In the second DP camp, in Germany, the instruction was in German but Hebrew was [also] taught. At this point, I get my first exposure to chemistry. [. . .]

The American occupation forces in Germany, in their wisdom, decide to teach the Germans about democracy. So they produce a series of textbooks for the schools, which are German translations of American books. We should gather some of them. Among those—I'm now ten years old—are the two following books, which I remember. One was a very well-known book, and that is a biography of Marie Curie by her daughter Eve [D. Curie Labouisse], a book that has inspired many young people. [. . .] The second book was a biography of a black American agricultural chemist, George Washington Carver, by—and that's what I don't remember now. [. . .]

These two books are translated into German by the American occupation forces and used in German schools. [. . .] I remember being so interested in Carver, because he's making all these things, inks and plastics and flavors and other chemicals, all from peanuts, soybeans, and sweet potatoes. And I had never seen a peanut or a soybean or a sweet potato, so I had to look up what those were. You could see there'd be a reason I'd be interested in Marie Curie, because she is a Polish heroine. But the idea that the first exposure of a chemist to chemistry comes from a story of a Polish-French woman scientist and a black American agricultural chemist is pretty [amazing]. I didn't decide to become a chemist then, but they were my first recognizable exposure to chemistry.

We moved to another DP camp outside of München [Munich, Germany], in '48, and finally at the end of '48, we get out of the DP camps. We are assigned an apartment in the most wonderful section of München, in the Maximilianstraße, right above the Kammerspiel, opposite the Hotel Vier Jahreszeiten [Kempinski]. You've seen these places.

REINHARDT: I have seen these places. Of course, München was a special city.

HOFFMANN: It was not bombed as badly.

REINHARDT: It was not bombed as badly. But how did it feel for you to live in a German city after all that happened?

HOFFMANN: We were assigned the apartment of a German army officer, **<T: 55 min>** and his wife was still there. She lived in one room, we were given two rooms, our little family of three people. [I] went to a school somewhere, a Jewish school, where everything was taught in Hebrew. My first course in English was in fifth—I was now in fifth class, and I had an English course, taught in Hebrew from a Hebrew textbook. Bizarre. Thus, Hebrew was my fifth language, and English was my sixth.

How did it feel? So, the reactions of the survivors to what happened are very varied. They vary both in a willingness to talk about what happened during the war, or in the suppression of it. And even if they didn't go through the worst times, like Madeleine Albright, our former Secretary of State. Her parents—she claims they didn't tell her [of their origins. This happened—their behavior was representative]. They were representatives of the Czech government in London. [They were Jewish.] But they said nothing of their Jewishness [to her]. There were different degrees of talking about what happened, and there were different degrees of attitudes towards Germany. And I discuss this to some extent in the play. [. . .]

My mother is the important actor in my life, as you can see from this. My stepfather—I didn't get along too well with him. [He was good], but my father I lost when I was five. My mother [. . .] was also the strongest person in her group of siblings. She was the one who kept the family together during the war, after the war, and even in America.

Let me just finish this story. In February '49 we finally get a visa to come to the United States. We leave München, and we go to Queens, [New York], and then an apartment in Brooklyn, [New York], and I grow up in New York City, [New York]. I'm now in sixth grade; I'm eleven and a half. This is 1949. [. . .]

Going back to attitudes about Germany, in the case of our family, the attitudes toward Germany were reasonably tolerant. [Not so about the Ukrainians]—every time anything Ukrainian was mentioned, [my mother] would say, "Those murderers." And even though it was a good Ukrainian who saved us at great risk to his life, there were also terrible stories. The Ukrainians and the Nazis had together killed my grandfather. The Nazis had shipped off my grandfather and grandmother on my father's side, to Bełżec, in '42. The Nazis had killed my father. [. . .] Other Ukrainians hid an aunt, two aunts, who were then given up to the police and were killed.

My mother could not [forget, much less forgive], and her brothers, too—the Ukrainians were people who had gone to school with them. The Ukrainians had betrayed them to the Nazis. [. . .] **<T: 60 min>** And it was very much in reach. It was this SS officer who was running the camp who beat my mother, and she had the scars from that beating. But somehow, the hate of the Ukrainians was [greater]. And this is not untypical of many people. [. . .]

So, after the war, we had one relative who remained in Germany. He actually just died recently. He was a carpet dealer in Dusseldorf, Ephraim Bardach. He was not from Germany originally. He was from Poland. And his story of survival is a remarkable story, too.

[My mother and stepfather and uncles], we had no trouble [. . .] going to Germany. Once in a while I would hear a comment about an older person, when we were in Germany together: "I wonder what he was doing during the war," that kind of a comment. [On matters like] not buying German cars or something like that, I think that's for the most part an American Jewish displaced guilt feeling, for not having suffered.

At home, we spoke—when we first came to America—interchangeably four languages. Initially, Polish, Yiddish, and German, because we had living with us my father's sister who came from Austria, and she spoke German. She didn't speak Polish. I made them speak English. So at one point we spoke four languages interchangeably at home, Polish, Yiddish, German, and English.

My mother did not have strong problems [with Germany]. We even took a vacation one time, a family vacation, where we reunited people from Israel and the ones [who were in] Germany. We did it in Austria, in [the village of] Schruns, a mountain place. [As for me], I've [. . .] had over the years twenty-two German postdocs, [. . .] many of them much more sensitive to what happened in World War II than an American postdoc, for sure, because the education is better about the Holocaust in Germany, much better than anywhere else in Europe. [. . .]

My relations with German chemistry have [grown] very strong through these twenty-two young people. Plus something else. Somehow by chance the kind of work I did coincided with the rise in Germany of physical organic chemistry, so that, for instance, the orbital symmetry ideas got often picked up. I'm thinking of people like Rolf Huisgen or Wolfgang Roth or [Emanuel Vogel]. These are people who tested predictions that we made. We had a great interchange [over the years], and I've had no special problems with Germany or Germans.

And what I'm telling you is my mother didn't have, either. I remember very well the last trip we took, my mother and I, to Europe. [At this point, she was] eighty-five. She died at ninety-four. And she has macular **<T: 65 min>** degeneration. [. . .] She doesn't see very well. And I get an award from Society of German Industrialists. [. . .] They have a literature prize. I get this award, and they say, "You can bring your wife." I was separated from my wife at that time, [. . .] so I write to them saying, "Can I bring my mother?" So they said, "Sure." And though they weren't offering to pay for my wife, when they found out it was my eighty-five-year-old mother, they [bought her] a business class ticket. The [organizer of the conference] was Heribert Offermanns, whom you may have met. The meeting is in Baden-Baden, [Germany]. She's treated extremely well. [The German Chancellor, Helmut J. M.] Kohl, was there, and we met Ms. Kohl. My mother was glowing because her son was being honored, and she was very happy. Then at some point—they knew [our] history, so they asked her a little bit about the war. She answered honestly; she said that we suffered a lot because of Germany, but she was very diplomatic, while not mincing her words. She remembered the war [and our family's losses. But] my mother didn't have troubles with Germany.

CARUSO: How was it transitioning to the United States? You mentioned having some English classes, but were you proficient?

HOFFMANN: Not much. On the boat here—we came by boat, on a troop carrier. My first breakthrough in English was a Tarzan comic book that a sailor gave me on the boat here, where I really felt I could read it and understand. I had a cousin here [in the US] who was a schoolteacher, who made sure I wasn't set back, that I wasn't put in some [remedial] class because I didn't know English. I remember very well that sixth grade at PS93 Queens. The schools had numbers in those days, [and this school was followed by] PS16 Brooklyn, in Williamsburg, [New York]. [. . .]

But I still remember my first essay [in that sixth-grade class]. It was an assignment [where] you write a page, and it was about Simon Bolivar. It was American history [class]. A teacher read my essay to the class. That was my [second] breakthrough point in English. I learned quickly.

I went to Stuyvesant High School, a science-oriented school. We took advantage of all the educational adventures America offers. Stuyvesant High School at that time was 70 percent Jewish kids. Today, is it 70 percent Asian-American kids. And you know, they're the same as we were. And the others [at that high school are of minorities and various] immigrant groups. [. . .]

CARUSO: In 1951, that's when you started roughly—

HOFFMANN: Stuyvesant High School. Yes.

CARUSO: I know that when I was growing up, Stuyvesant High School was a school you had to test into. Was it the same policy in 1950?

HOFFMANN: Oh, yes. I had to take a test.

CARUSO: Was there a reason why you wanted to go to Stuyvesant above others?

HOFFMANN: No. I think I took the test also for—there were three elite schools, Brooklyn Tech [Brooklyn Technical High School], Stuyvesant, and Bronx [High School of] Science. Bronx Science was the only one that was co-ed. The other two were for boys [only] at that time. And there was a girls' school, Hunter [College] High School at that time. My sister—I have a sister who was born in the United States, seventeen years younger than I am, half-sister, same mother, different father. **<T: 70 min>** [She went to Hunter.]

[. . .] We lived in Brooklyn and Queens. It was enough of a commute. It would have been too much to go to Bronx Science. [These schools took students from all over]. Stuyvesant was the natural one to go to, if you lived in Queens, as we did at that point.

CARUSO: And so, Stuyvesant is also known for its science programs. Were you interested in science at this point?

HOFFMANN: Yes.

CARUSO: And you had the exposure to chemistry through reading books about scientists. So, I'm curious to know—

HOFFMANN: [. . .] I played with chemistry sets, as many kids [did] in our period. I remember going down to—Gilbert [A. C. Gilbert Company] was one of the manufacturers of chemistry sets. I remember going to the Gilbert showrooms, and I remember buying reasonably sophisticated—not dangerous— chemicals from the local pharmacy. You could do that at that point. I played with chemistry sets. I also had a relative, distant cousin, who was a stockroom clerk at Yeshiva University, and he liberated some old glassware for me. So I had a little bit of a chemical laboratory—not much—at home, I would say around the end of elementary school, around eighth grade.

When I graduate from eighth grade from PS60 in Brooklyn, I get two medals. One is for mathematics, and the other is for attendance. That means I had not missed any classes. [laughter] Hilarious. But the mathematics—[. . .] so Jewish kids from Europe at that time, immigrants in general from Europe, are always ahead of American students in mathematics. And that provides an entry point. The same is true for the Asian immigrants [today]. And the other things come later, though they were important for me.

In Stuyvesant, the only advanced placement [course] I do not take is in chemistry. I take biology, physics, calculus. Why? Because there was a lousy teacher. Usual reason. We knew about it. The other [subjects] had good teachers.

If you had asked me in eighth grade, I would have said I wanted to be a mathematician. By tenth grade, I'm realistic enough to see that there seems to be a talent for mathematics, and I don't have it. That is, there are kids in high school to whom the math comes so easy that I just couldn't compete. I do very well in high school, nine hundred boys in a graduating class, if you can imagine that. Nine hundred boys. Imagine the smoking in the bathrooms that goes on.

I begin to do very [well] at social studies. I get a history award on graduation. I take French, which by now is now my seventh language. I do well in French. No chemistry. But in my high school yearbook, if you look under my picture for what I want to do, it says medical research.

So, [that's] a compromise between what my parents want me to do, which is to become a doctor. Typical aspiration for the Jewish European immigrants then, typical aspiration for the poor Asian-American kids across the hall whose parents want them to be doctors. So, when I was an advisor at Cornell [. . .], [I often had] to instruct these kids to tell their parents gently that they're not going to become doctors.

CARUSO: How was the—

HOFFMANN: Medical research was the compromise. I got conflicting signals about doctors, such—[. . .] doctors don't know anything **<T: 75 min>** except for the specialists. This is a typical European feeling, that specialists are important. [. . .] And second, that doctors don't know anything and they're always trying to cheat you. They're out after money. Well, I'm a smart kid. I hear that. At the same time, there's nobody in the family who was a doctor, [only] one dentist. I don't want to be a doctor, but I say medical research.

In the summer between high school and college, I'm a winner of the Westinghouse Science Talent Search. [. . .] My project was in physics, nothing to do with chemistry. Out of that Westinghouse Science Talent Search competition, now called an Intel Competition [Intel Science Talent Search] I think, I get a summer job at the National Bureau of Standards [National Institute of Standards and Technology] between high school and college, age eighteen, in

Washington, DC. It's now outside of Washington in Gaithersburg, [Maryland]. At that time it was downtown Washington.

I have a friend who has a job at NIH [National Institute of Health], a summer [job]—I go over there, and all of a sudden I get a revelation. The revelation is that many of the people doing research at NIH don't have MDs. They have PhDs. A kid doesn't know this. So, all of a sudden, I realize I don't have to be a doctor. [I go on] to Columbia [University]. I almost went to Cornell, [where I have now been over fifty years]. I [actually] wanted to go to Swarthmore [College], but this is before needs-based scholarship. My stepfather's unemployed at that point; I got into Swarthmore, but we couldn't afford [for me] to go there. At Columbia and Cornell, I get full scholarships. I get rejected at Yale [University]. That's the first of three rejections in my life from Yale. Yale at that time, and Harvard [University] and Princeton [University], are still [. . .] limiting the number of Jews admitted. [. . .] We knew that only two [students from our high school] each year would get into these schools. [Cornell was long past that.]

I go to Columbia, and the world opens up [for me]. I'm taking pre-med courses. I take introductory chemistry. I take organic chemistry. They're good, routine courses. They're not inspiring. I'm not interested in chemistry yet.

CARUSO: Can I back up just for—I just had a couple of questions. What was the cultural transition for you like? I can imagine being a child who grew up in war-torn Europe and coming to the United States. Were your classmates at Stuyvesant, for example, coming from a similar background, or were they mostly US born and raised?

HOFFMANN: Most of them were US born. [. . .] Where I was in neighborhoods were there weren't that many Jewish kids, in Ridgewood, Queens. But, I never felt any strangeness, somehow. If anything, I assimilate too fast. So I'm intolerant of [the way my parents speak English]—my parents have a job, one in a corset factory, my stepfather. My mother in a bakery as a saleswoman. [. . .] I make them speak English, and I'm pretty cruel about it. I'm not proud of that. I think something has changed in America, and I think the Latino political movement has changed that. That is, it's okay for immigrants not to speak English. That was not true in my time.

REINHARDT: And you knew that?

HOFFMANN: I knew that. I felt it. I was **<T: 80 min>** ashamed of my parents. The assimilation forces were very strong. And it's not just me, I think. Other immigrant groups also felt this in America. It was in the times, and it was what America meant and felt. That has changed.

REINHARDT: When did you become a US citizen?

HOFFMANN: [. . .] At age eighteen, to get a scholarship that I needed, the New York State Regent's scholarship that I needed at Columbia. [. . .]

[END OF AUDIO, FILE 1.1]

HOFFMANN: Yes, that took a long time to tell you the story, because those first years were so traumatic and so eventful in various ways. I mean, several countries, six languages, all before age eleven.

CARUSO: Yes. And, I mean, that's part of why I was curious to know how you transitioned to something that became stable, right? You weren't moving around. You weren't in countries where your people were hated, and—

HOFFMANN: I did not own a book until—I remember the first book. My parents gave it to me in the United States.

REINHARDT: You remember which one?

HOFFMANN: No, I don't remember the book, but I remember the occasion, because I had my tonsils out. So, this was an operation which was overdone in our time. Whenever a kid had chronic colds or something, they took their tonsils out. It was an operation, and I got some book as I was recovering. I remember that. And I was then in seventh grade, so I must have been around thirteen or something like that.

We carried along some precious photos and some other things, but by and large, one moved. Maybe one learned not to be attached [to things] too much. [And as one moved from one place, to another, I would] lose all my friends. [The effect is unlikely to be good], but I don't want to indulge in pop psychology. There is an interesting question [here, to be explored with a psychologist]: what were the effects of that hiding, [the trauma of war?] There are some things I can point to. To this day, I remain afraid of people in uniform, even if the uniforms are harmless. I mean, doormen in an apartment building, if they're wearing a uniform. [. . .]

And I'm also afraid of standing in front of a window at night, [probably because that window in hiding was where people could spot us, give us away]. Outside was danger, and inside, inside [that cramped attic], there was a lot of love. I've sometimes said that it was a cocoon of love. But outside was infinite danger. Unusual things [to experience for a child of six].

So, about chemistry. Let me just trace a little bit.

CARUSO: And, I mean, I was also curious to know what your . . . you mentioned that you didn't do advanced chemistry in high school.

HOFFMANN: In high school. Yes.

CARUSO: I was wondering, what were these science classes like? Was it just standard learning from textbooks? Were you doing experiments? And I'm also partly curious, because I know that the 1950s, you know, the US is really ramping up their investment in science.

HOFFMANN: Yes.

CARUSO: And I think you were—I forget the exact year, but, I mean, is this the right—

HOFFMANN: So, '51 to '55, I'm in Stuyvesant High School.

REINHARDT: And Sputnik.

CARUSO: Sputnik. Yes.

HOFFMANN: And '55 to'58 I'm at Columbia College. The dates are also important with respect to another thing I'll mention.

The science classes [at Stuyvesant] were routine, except that the advanced placement courses were not routine. [. . .] We had teachers [. . .] who held PhDs. [. . .] I had a teacher in English and I had a biology and a math teacher who had PhDs. Those men [and women] had found those jobs during the Depression, when they couldn't get other jobs, and [ended up] teaching. We owe those great teachers to the Depression. **<T: 05 min>** Dr. Brody in math, Astrachan in English. The advanced placement courses were exceptional. [There was an excellent, fun component to the biology labs]. I was very attracted to the biology.

There were the usual kinds of things, the dissection of a fetal pig, let's say, that you would do in an advanced biology course, of a frog and a fetal pig. And the chemistry lab was not particularly well equipped. Rather interesting, the daughter of one of those chemistry teachers used to work for Chemical Heritage Foundation.[7] [. . .]

In college, the courses were routine, and I did not have a really exciting chemistry course in college until my third year. I moved at a rapid pace through the courses. I was eighteen, and I was old at eighteen, to start college, because in New York City in those days, you could skip grades. And I had classmates who were fifteen and sixteen when they started Columbia. I was somewhat in a hurry [for another reason]—my stepfather, as I mentioned, was unemployed. There was some [urgency to finish and it looked like I could do anything], I took twenty-five credits a semester, and I took one summer course, and graduated in three years from Columbia.

In my last year at Columbia, I finally had [two good courses]: a course in statistical mechanics and an introduction to chemical physics. I think they were the one that lured me into theory.

REINHARDT: By whom?

HOFFMANN: Two people whose names are not very well known today. The introduction to chemical physics was George Fraenkel and the statistical mechanics course was by Ralph Halford. I also sat in on a course by a leading theoretical chemist, George Kimball. There is a textbook, [Henry] Eyring, Walter, and Kimball, *Quantum Chemistry*.[8] But Kimball's course was not about quantum chemistry.

What kept me interested in chemistry, were summer jobs, which began between high school and college, and continued for the next three years. So, there were two years in Washington at the National Bureau of Standards, and then there were two years at Brookhaven [National Laboratory]. Out of those came my first two published papers. So they had a significance in my life.

The first paper was on the thermochemistry of a compound in in Portland cement.[9] The second paper was on a low-level counting system for carbon-11 produced in an accelerator at Brookhaven.[10] I went on to work in neither of those fields. The science in the first paper, which was published in the *Journal of Research of the National Bureau of Standards* . . . . The second

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[7] On 1 February 2018, as a result of the merger with the Life Sciences Foundation, the Chemical Heritage Foundation changed our name to the Science History Institute.
[8] Henry Erying, George Kimball, and John Walter, *Quantum Chemistry*, (John Wiley & Sons, Inc, 1944).
[9] E. S. Newman and Roald Hoffmann. "Heats of Formation of Hexacalcium Dialumino Ferrite and Dicalcium Ferrite." *Journal of Research of the National Bureau of Standards* 56, no. 6 (1956): 313.
[10] J.B. Cumming and R. Hoffmann. "Efficient Low-Level Counting System for C^{11}." *Review of Scientific Instruments* 29, no. 12 (1958): 1104-1107.

paper I'm proud of, because this was published in *Review of Scientific Instruments*. I will never publish anything there again in my life. They were experimental papers.

[What were these papers about?] The calorimetry of cement compounds is [pretty] boring stuff in retrospect, but it was new to me. [The second project I had] was in a much more interesting program the Bureau of Standards had about relatively low temperature pyrolysis of hydrocarbons. You take propane and you heat it up to three hundred, four hundred [degrees Celsius] below the flash point, in the presence of oxygen, and you look at incipient chain reactions that you later see in flames. It was very interesting, introduced me to gas **<T: 10 min>** chromatography, for instance, for the first time.

At Brookhaven, I did radiochemistry both summers with some very good people. [The research here] was much more interesting than the courses. Meanwhile, at Columbia, the world opens up to me in—Columbia has a core curriculum, [. . .] where there are certain survey courses that everyone takes. There's one called Contemporary Civilization, another one called Humanities. Humanities is a selection of great works of literature throughout the ages. Contemporary Civilization is about philosophy and political ideas. So you read everything, from the Greek philosophers to [Georg Wilhelm Friedrich] Hegel and [Immanuel] Kant, a little bit in excerpts. It's actually very nice. And there [were courses in] history, art history, music. The world opened up in literature and the arts, especially in history of art, where I had a wonderful teacher, [Howard McParland Davis]. I took then two more courses. I took a poetry course—that was my first exposure to poetry. I took a Great Books course, seminar where we read a hundred great books in a year. [. . .]

Around the first year, I told my parents I didn't want to be a doctor, so then there was a question, what was I going to be? All this humanities [instruction] was so interesting, really intellectually interesting. I had read some "good" books, quote/unquote, in high school. That was part of being in Stuyvesant. But I don't think they meant that much to me. I think I was just more mature and I was more open to novels and poetry. [. . .]

Often in a European education, if a person did go through a *gymnasium* or a *lycee* in a classical education, they would have been exposed to some good literature, in the old days, at least. And so that has been used as an excuse not to give European science students a liberal arts education equivalent at the university, so they could enter medical school at age eighteen, or chemistry, and take only chemistry courses. I think there is a world of difference between reading *Anna Karenina* at age sixteen and reading it at age twenty. By age twenty, you have fallen in love, and you know what that means. And the maturity, the rise in maturity, is very, very high. So, I really benefited from an American liberal arts education.

And these things stuck with me, the history of art and the poetry. I did not try to write poetry at that point. The man who taught us—there were no writing courses. The man who taught us, Mark Van Doren, a great teacher, taught the Beat poets. [Allen] Ginsberg was one of his students. He could not teach us to write—if you wanted to learn writing, you went to the evening school at Columbia University, the School of General Studies. What a world of difference from your time already and today, where there are writing courses all through college.

CARUSO: Right.

HOFFMANN: Nothing like that in that time. [Van Doren] taught me how to read a poem, and I remember the first poem [I understood], which was Wallace Stevens' "Sunday Morning," and that had a tremendous impact on me at the time.

I think if I did not feel that family responsibility to have a profession I would have gone into history of art. I felt I wanted to get a profession. I told you in high school **<T: 15 min>** I knew I wasn't going to be a mathematician. In college, for the wrong reasons, I decided I couldn't be a physicist, because I had these friends who took physics courses. And I got an A, [while] they got an A plus. To them, it came easy, and I had to struggle. And so I decided I wasn't good enough for physics.

Now I'm doing physics. I'm publishing in *Phys Rev Letters* [*Physical Review Letters*] and *Phys Rev B* [*Physical Review B*]. And of course, I was wrong, because what I mistook was doing well in courses for doing [research in a field. But then] a kid doesn't know what research is like.

CARUSO: So, this before you had gone to the NBS and Brookhaven that you were having—

HOFFMANN: I was going at the same time.

CARUSO: Okay. Because I think you worked with E. [Edwin] S. Newman on thermochemistry and—

HOFFMANN: That's right.

CARUSO: —[Robert E.] Ferguson on the pyrolysis?

HOFFMANN: Yes.

CARUSO: I was wondering what you were learning about the research life and laboratory life from those experiences, since what you learn is college is very different from—

HOFFMANN: [They were] very different. [. . .] The first person I worked with, Newman, did not have a PhD. He was doing calorimetry all his life. He did publish. I remember clearly—how could I forget? I remember a big mistake I made [that summer]. There was a calorimeter, [of the usual kind]. You take the substance, you put it in [an enclosure in a platinum vessel, set it on fire], you measure how much the temperature rises in there very precisely.

Well, you have to know the amount of material, and I forgot in the calculation to subtract the weight of the calorimeter. [laughter] And the platinum was pretty dense, so that I was getting [a value of the heat of the reaction] way off. [Newman] corrected me gently. So, I learned how to do careful experimental work, which I haven't done since. Did I learn to appreciate experiment? [Yes, there] and later.

The second summer project, the pyrolysis of hydrocarbons, that was good physical chemistry of its time, and I learned a little organic [chemistry] then. No publication came from that. Ferguson went on to be a director of the National Bureau of Standards and he was a good person. He had a PhD.

At Brookhaven, I was in the presence of some people who were really good in their fields. There was Julian Miller at Columbia, Jim [James B.] Cumming, who was my supervisor directly, and the head of the group was Gerhart Friedlander, who was a German-trained radiochemist, a very good [scientist]. And I learned [more] about doing good experimental work. I learned also a little mathematics, [. . .] of radioactive decay. [None] of these, did I use later. But the act of publication was enthralling. To see that I could have a paper published. Your first paper means a lot to you. So, those were my first two papers.

[The people who led me to them were] all important to me, but I still would have become a historian of art, I think, [if they let me. Back to what I might do.] The interesting thing was that I didn't even pay any attention to biology. And now [the date is important], '55-'58. Fifty-three is the [James D.] Watson and [Francis H. C.] Crick paper.[11] [. . .] I think, had I been exposed to Watson and Crick, I might have become a molecular biologist. But, first of all, Columbia's biology department—and this was true of every biology department—[did not take up molecular biology immediately. These places] were staffed by] classical biologists. I think I would have taken to natural history type biology, too. **<T: 20 min>** [. . .] I didn't even take a biology course, because I was so against medicine that I didn't even take a biology course.

REINHARDT: When had you heard first of Linus Pauling?[12]

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[11] James D. Watson and Francis H. Crick, "Molecular structure of nucleic acids; a structure for deoxyribose nucleic acid." *Nature*, 1953, 737-8

[12] Linus Pauling, interview by Jeffrey L. Sturchio, Denver, Colorado, on 6 April 1987, (Philadelphia: Chemical Heritage Foundation, Oral History Transcript #0067).

HOFFMANN: At that time, Columbia, in my third year. No, sorry, he wrote the textbook I used in my first year, the general chemistry textbook. It was beautiful drawing by Hayward or someone, beautiful—this is a general chemistry textbook. I still have the book. That's the first I heard.

In my senior year, my third year—so, I got out in three years. My third year, I took a seminar. There were modern organic chemists at Columbia. First, there was Gilbert Stork, though he was very synthetic.[13] Had I been exposed to synthetic organic chemistry—I keep saying these things, "had I been exposed to, I would have become that." I just said it about Watson and Crick—[I might have gone in this direction. But perhaps Gilbert Stork, a great chemist, might not have inspired an undergraduate beginner.]

Incidentally, [the textbook in the good but routine organic chemistry] course, was [Louis F.] Fieser and [Mary P.] Fieser's [classic text].[14] I remember [. . .] to this day, like everyone else who studied from that book, not so much the book or the style but the little historical biographies that are in there. [. . .] Those little biographies, they were three lines, typically, about famous chemists, when he introduced the name. [There is here something about history.]

[Phone ringing]

HOFFMANN: Let's stop for a moment. I'll take that.

[END OF AUDIO, FILE 1.2]

HOFFMANN: Those little historical things were very important for my generation of chemists. And, to me, that's an argument for introducing more history of chemistry into science courses.

REINHARDT: Why have they been important for you?

HOFFMANN: It was just interesting to see how—they were Europeans, and it made me want to find out more about their relationships to each other. [. . .] I'm just looking if I have the book on my shelves here, and we could see what they looked like. But they were really two-, three-, four-line biographies, very brief.

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[13] Gilbert Stork, interview by James J. Bohning and Leonard Fine at Columbia University, 6 August 1991 (Philadelphia: Chemical Heritage Foundation, Oral History Transcript # 0100).
[14] Louis F. Fieser and Mary Fieser. *Organic Chemistry* (New York: Reinhold, 1956).

[Back to the choice of a profession.] Not biology, not physics. [. . .] And I was uninterested in engineering. Engineering, for my parents, would have counted as a profession. [There was chemistry.]

REINHARDT: What did they say about chemistry?

HOFFMANN: I think they sort of accepted it.

CARUSO: I know with my own mother when I told her that I was going to become a historian of science she had a hard time believing that people would actually pay you to do something like that.

HOFFMANN: Yes.

CARUSO: I'm wondering, even if people understood that science exists and that there were chemists, did they have knowledge about what it is a chemist actually did? Did you have knowledge about—

HOFFMANN: [. . .] Yes, I did. I had a little bit from these people at National Bureau of Standards, and a little bit from Brookhaven Laboratory, both special settings, but these were clearly people with jobs [they enjoyed]. I fell in love with professors. We all do. Our professors are role models for us in many ways. I had no idea what an industrial chemist does. I had not been exposed even to the Primo Levi-type description of what industrial chemistry is like. You get a little bit there.

No one in the family was a chemist. There were no scientists in the family. But certainly, there was a lot of respect for science and knowledge, which came with the kind of background that I described for you. This [was a] middle-class European Jewish background; with that came a lot of respect for science.

I don't think that at first they had an idea that chemistry was a profession, even. But somehow they were reassured. I can tell you for my part, I wasn't sure that I was going to be a chemist, until halfway through my PhD, and I'll give you the evidence for that.

So, I was in a straight line. I was going to go to graduate school. This was pre-hippy days. The idea of taking off a year or something, that was not part of my culture. It was not part of the culture of that time. [But a year away, and not in your usual place, was waiting for me.]

CARUSO: Where did you learn about going to graduate school as an option? Were there professors that were counseling you to go in that direction, or was that something you picked up on your own?

HOFFMANN: I picked up on my own. A lot of my friends went to graduate schools, to medical school, so I knew about that [route]. I was also exposed to graduate students. They were my TAs. One was especially important to me, Bob [Robert F.] Schneider, who subsequently was at State University of New York, [Stony Brook]. He was a graduate student. He was my TA in an introductory chemistry course, and then in the organic course, and he was very supportive. Somehow he was sympathetic. [. . .] I remember him very well.

There were graduate students around. I was at a university. In my senior year, I took a senior honors seminar. I mentioned good organic chemists. Two others were there at that time, two good organic chemists. There was one I didn't know. **<T: 05 min>** That was Cheves [T.] Walling.[15] But the two who were younger ones were [Roland C. D.] Breslow and [Thomas] Katz, both [R. B.] Woodward students, so this was my first sort of connection to Woodward.[16] Somehow, they didn't teach the introductory chemistry course that I had. That was taught by an older organic chemist, Charles [R.] Dawson, who is known mainly for some work he did on urushiol, the active chemical in poison ivy. He's also known because he was the PhD advisor of Isaac Asimov, who must have been a special PhD student.

Anyway, Breslow taught the senior honors seminar, and I have somewhere in this office, little cards, sort of index cards, that I kept of papers I read for that senior honors seminar. And they were Pauling, [Robert S.] Mulliken.[17] Aromaticity was in the air. That's when I first learned of Hückel's rule, in that senior honors seminar. By that time, I had already applied to go to graduate school at Harvard.

REINHARDT: Why Harvard?

HOFFMANN: I think I looked at places, and there was, at Harvard at that time, a good theoretical chemist and I had seen some papers by him. I think I first read [Charles A.] Coulson's *Valence* book, which also played an influence on many theoretical chemists.[18] And that person was Bill Moffitt, William [E.] Moffitt. The reason we don't know him so well is he died in my first year at Harvard, and I intended to work with him.

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[15] Cheves Walling, interview by Leon Gortler at Mayflower Hotel, Washington, DC, 12 September 1979 (Philadelphia: Chemical Heritage Foundation, Oral History Transcript # 0009).
[16] Ronald Breslow, interview by Leon Gortler at Columbia University, New York, NY, 19 March and 9 April 1999 (Philadelphia: Chemical Heritage Foundation, Oral History Transcript #0181).
[17] Linus Pauling, Oral History Transcript #0067.
[18] C.A. Coulson, *Valence*, (Oxford: Clarendon Press: Oxford, 1952.

REINHARDT: So, at that time, it was already sort of clear to you that you would like to go into theoretical chemistry?

HOFFMANN: Yes. It somehow was clear. For the physical chemistry course [at Columbia], I actually had a very important, interesting person. [But he was] in his last year of teaching, and he was not functioning well. This was Louis [P.] Hammett of Hammett constants, physical chemistry. But physical chemistry lab was a disaster. I won't even mention the—

CARUSO: I think that holds true for a lot of chemists.

HOFFMANN: And I've just mentioned introductory organic, physical chemistry, and physical chemistry lab. They were all not great courses, and some were terrible. It's a miracle I became a chemist, given those courses. And I think that's where Brookhaven and National Bureau of Standards come in. And then in the last year, finally, some good courses.

CARUSO: Breslow.

HOFFMANN: And introduction to chemical physics. That was wonderful. That's where I first see singlets, triplets. I see, in that course at least, the solutions to the hydrogen atom in quantum mechanics, the differential equation solved. I loved it.

REINHARDT: What did attract you to that kind of thinking?

HOFFMANN: I don't know. I was good at it. I was good at the math. To me, the math was vivified, was brought to life, by its use in this chemical physics course. And the statistical mechanics one was the first time I saw a Maxwell-Boltzmann distribution [law]. I saw the first calculation of the average speed of a molecule in a gas. And all of a sudden, all that calculus I had learned, which I didn't know what it was good for, I saw it used. I saw a differential equation solved. It was wonderful. It was clean. No one gave us an insoluble problem. [Erich] Hückel's theory was presented, but we were given no idea how much calculations was involved [if one wanted to move beyond it]. Somehow, I had mathematical skills which I think were actually underused at that time. I knew I wasn't going to be a mathematician, but I was able to work at a **<T: 10 min>** very high level and learn things very quickly. So, at that time, I learned chemical physics. A little later, with Woodward, I learned organic chemistry. And with [William N.] Lipscomb, to whom we'll come, I learned other things.

But why Harvard? I think because Moffitt was there. It was the top school [in the country]. I didn't get into Yale, into graduate school. Applied there, the second time. The third time was when I applied for a job. Didn't get the job, after graduate school. But then they gave me an honorary degree, and those three previous rejections made a good opening to my honorary degree speech. [laughter]

I began at Harvard, but I still wasn't that sure about chemistry. I began in a program in chemical physics, which meant I didn't have to take so many chemistry courses. I don't know what—

REINHARDT: Was this the program by E. Bright Wilson [Jr.]?[19]

HOFFMANN: Yes. Bright Wilson was there. And then what happened was Moffitt, age thirty-three, dies of a heart attack on the squash court. Leaves behind a small family, and nobody else is doing theory. And so, this is in December [1958]. I arrive in September. Moffitt dies, the person I'm going to work with. And so, one of Moffitt's postdocs is Martin [P.] Gouterman, who came from University of Chicago. He's made an instructor, and the end of the year, he's made an assistant professor.

And on the day he's made an instructor, in February '59, middle of my first year there, [Gouterman] has four graduate students. It's pretty unusual, because there were four people who wanted to do theory. There was nobody else [who would take them on].

Martin Gouterman turned out to be an excellent teacher. He was not promoted at Harvard, and he went on to University of Washington in Seattle and became an expert on something he was interested in from his graduate school days: that is, porphyrin spectra. The four people who went to work with him on that day, all in my class, were Bob [Robert L.] Fulton, who then became professor at Florida State [University], Georg Wanniere , a Swiss physical chemist who was a professor at University of Zürich, and Ron Felton, who was at Georgia Tech [Georgia Institute of Technology].

[The four of us] began to work with [Gouterman]. I take lots of physics courses. I do okay in them. But I'm sitting in on other courses. I sit in on a course [. . .] on science and public policy by someone in the law school. I don't know how I found—I think his name was Price.

REINHARDT: Yes. Don K. Price. Oh, wow.

HOFFMANN: Yes. So, I sit in on a course by Price. [. . .] I sit in on a course on stellar atmospheres with Carl Sagan, who's an [instructor at Harvard at the time]. I'm responsible for [. . .] inviting him to give his first seminar at Cornell when I came here eventually. [. . .] I sit in

[19] E. Bright Wilson, Jr., interview by Raymond C. Ferguson at Harvard University, Cambridge, Massachusetts, 17 and 18 November 1986 (Philadelphia: Chemical Heritage Foundation, Oral History Transcript # 0061).

on that. I decide to go in a summer to an archaeology dig. [. . .] There's a Harvard-Cornell dig in Sardis in Turkey for a long, many years. I apply to that. So does a girlfriend of mine from Columbia. [In the end we do not go to Sardis] because she and I split up. [. . .]

In my second year, **<T: 15 min>** I [. . .] apply for an exchange to go to the Soviet Union, and I'll tell you about that in a moment. And I do go to the Soviet Union in my third year in graduate school. My mother thinks I'm going to get drafted in the Soviet Army, because I was born in the Ukraine. This is only eleven years after we come to America. And I'm born in the Ukraine. But this is an official exchange; her worries were misplaced. I go to the Soviet Union for a year. Harvard doesn't like it because you take a junior year abroad in college. You don't do this in the middle of graduate school, in general, in the United States. [. . .] I'm in the process of switching advisors from Gouterman to Lipscomb. Actually, I did my PhD with both, but I started with Gouterman. [Neither says much].

I think going to Russia, applying for that program and then following through, [constitutes some indirect evidence for the fact that] I wasn't sure about chemistry. I'm doing these other things. But when I come back from Russia, after three years, in 1961, I am sure about chemistry. I switch from Gouterman to Lipscomb. I do my PhD work all in one year, and I get my PhD in '62.

REINHARDT: What ensured you, then? Was it Russia? Was it in—

HOFFMANN: Can't figure it out, [I wish I knew. In Russia] I'm in the physics department at Moscow University. [Culturally a fascinating year, the first year of my marriage too. But I can't point to anything inspiring on the chemistry side but what Lipscomb was doing really did move me].

REINHARDT: That was boron chemistry—

HOFFMANN: Yes. Boron.

REINHARDT: —but in theory?

HOFFMANN: In theory. With Gouterman, I'm already tooling up for the extended Hückel [molecular orbital] method. Gouterman was very interested in porphyrins. I learned something about porphyrins. I actually tried to make some porphyrins. [. . .] I have the first explosion in the new Conant laboratory with stuff scattered all over walls. Lucky I wasn't hurt. Happened at night. I decide I'm not an experimentalist. [laughter]

[To return to theory], I tried to do a calculation on cubane, C_8H_8, which someone at Harvard was trying to synthesize. [As I set up] to do an MO [molecular orbital] calculation, I run into trouble. [. . .] I'm thinking about it in Russia. And on the way back from Russia, during a [stay] in Sweden [I came back to it. Let's go back a little in history]. In 1960, I get married. After the first year of graduate school, I go to a summer school in theoretical chemistry taught by a great teacher, Per-Olov Löwdin. And that's where I meet my wife, is in Sweden [in 1959]. At this point, I learn my eighth language. [Swedish, French was the seventh, in high school]. The ninth one is to come, Russian. [. . .]

Anyway, on the way back from Russia [. . .] I find a solution that I could program to the problem of setting up [an MO] calculation for something like cubane. So, now comes another story which has to do with my professional development, the introduction of computers in chemistry, and their use. My whole life is tied to computers, from those days with Lipscomb till today. My whole life is spent [using computers and] fighting computers and finding ways to extract [understanding out of the] reams of eleven by fourteen accordion-folded paper output, now is on the screen of this device. My whole life is devoted to subjugating those numbers and extracting from them verbal or graphic orbital **<T: 20 min>** explanations. So, I love computers and I hate computers, and I move in a world between them. [. . .]

I learned how to use computers in my first year with Lipscomb, '61-'62, the year I did everything in my thesis. [It seems that at this point] I've got a lot of cooped up energy, because in Russia, there wasn't an opportunity to do many things. [Even] as it was a very productive year. It's also the first year of our married life. It was a very important year for me in a number of ways.

[Even as I wasn't sure about chemistry in 1958-60, as] I'm sitting in on these courses [at Harvard], the ones with Price and Sagan [. . .], exploring an archaeology dig, applying for a program in Russia, [. . .] I'm headed on a straight line for chemistry. [. . .] Somehow, I settle down [in 1961, on returning from Russia], and in [the] Lipscomb [group], not so much in Gouterman's, though Gouterman taught me a lot. [. . .] I'm now becoming a professional theoretical chemist. And at the same time, I'm fortunate [in] that the two people I'm working with, Gouterman and Lipscomb, after I come back from Russia, that they're both interested in chemistry. Deeply interested in chemistry. Gouterman in porphyrins, and Lipscomb in the boron hydrates.

REINHARDT: When you say that, you mean interested in specific classes of compounds? Is that right?

HOFFMANN: Of [compounds of] some complexity, and not a diatomic molecule, which is so boring. Lithium hydride, getting some excited state of lithium hydride, and getting the fourth significant figure in the dipole moment [of the molecule]. These people were interested in real molecules. And that was the beginning [for me, or it hit some resonance with me]. And the interaction with Woodward [kept it going]. I was very fortunate, because also they were introductions to inorganic chemistry with Lipscomb, and perhaps the biochemical side [. . .] with [Lipscomb and] Gouterman. [I never pursued the biochemical link—those are the only kind of molecules I haven't worked on. So] I'm very fortunate that my theorist [mentors] deal with molecules of some complexity. I learned to appreciate the chemistry. [. . .] Gouterman's interest was in spectroscopy of porphyrins, [. . .] very intensely colored.

REINHARDT: So, you used ultraviolet and infrared, or what did you use?

HOFFMANN: [. . .] Gouterman had a theoretical explanation of that very intense line in the porphyrin spectrum, a beautiful symmetry-based [explanation]. So now I get exposed [to symmetry, in the Swedish] summer school between my first and second year. [. . .] Aside from meeting my wife, falling in love, traveling all over Europe, my first trip to Israel that summer. I had a very full three and a half months away from Harvard. I buy a Eurail pass. I go all over Europe. I see for the first time the cathedrals in France that I had studied at Amiens, Rouen, and Chartres [France]. [. . .]

REINHARDT: This is '61?

HOFFMANN: The summer of 1960—

REINHARDT: Sixty?

HOFFMANN: Sixty. Sorry. Summer—no, I'm wrong. Fifty-nine.

REINHARDT: Fifty-nine. So, before the trip to Russia, the time—

HOFFMANN: [I went back in time. In the summer of '59 I go to Sweden, to Löwdin's summer school. In late summer 1960 we go to Moscow, returning in June 1961. To return to '59,] I for the first time have a group theory course. **<T: 25 min>** Group theory is a very elegant part of linear algebra, and when applied to molecules, it's just beautiful. When you can write down the symmetry adapted orbitals for a benzene or for some C2V molecule—in the language of this [formalism of group theory], it was very attractive. Also, the quantum mechanics [I learned that summer] was at a much more advanced level with Löwdin. [. . .] There was no chemistry to speak of there in that school, but the theory was very attractive.

So, why did I go to Russia [in 1960-61]? Because in the fall of 1959, in my second year [at Harvard], there comes to Harvard a very good physical chemist of Ukrainian background, Michael [A.] Kasha, Florida State. He gives a lecture course at Harvard and he talks about the work of two Soviet scientists. One was Terenin in Leningrad, who independently of [Gilbert N.] Lewis came up with the idea of a triplet state for a molecule, [a concept of much importance] photochemistry. And the other was Davydov, Alexander Sergeevich Davydov, a physicist with whom I subsequently worked in Russia, who is responsible [for the idea of an] exciton theory, energy transfer in a molecular crystal. [The idea is that] you have one molecule that's excited, another one in its ground state, and the excitation switches to the second molecule, and then propagates. That's called an exciton.

Kasha talks [at Harvard] very positively of the work of these two Soviet scientists; [. . .] Davydov's work is pretty recent. Somewhere, I read about the [. . .] Soviet-American exchange [International Research & Exchanges Board (IREX)]. It's the [. . .] Khrushchev period, there's a summit meeting, [Nikita S.] Khrushchev and [Dwight D.] Eisenhower [. . .]. Nothing substantive gets agreed on. So, you want to walk away with something that you can show to the press. You arrange an exchange of students; it means nothing.

CARUSO: It means nothing, but it's also a strange thing to have happen at that specific period of time.

HOFFMANN: From 1959 until this exchange died with the end of Communism, there were forty American graduate students in Russia every year, and forty Soviets in the US. The Soviets sent scientists and technologists. The Americans sent Slavicists and historians, which tells you something. And each side sent spies among them. We had an idea who was the CIA person in our group. [. . .] I was interviewed [for the exchange program] at Columbia, by a group of professors. A little later, in 1975, I looked at my CIA and FBI files under the Freedom of Information Act. Of course, the CIA and the FBI both checked up on me, but they didn't do so very well. In that file were interviews with Lipscomb and other people, their names blacked out, but I could tell who was who. But they didn't find something which was in the public record. [No matter], we were cleared. I think most suspicious was the fact that I was marrying a Swede at this point, and this was [strange to the people running the exchange].

[The exchange, viewed from a long-range perspective, was important for Soviet science. Some of the leaders of Soviet science in subsequent years went through that exchange. Coming here was their first exposure to America. You can imagine the impact it had. For instance, one of the leaders of modern Soviet/Russian chemistry], Oleg [M.] Nefedov, went to Penn State [Pennsylvania State University] to work with [Philip S.] Skell. **<T: 30 min>** [. . .] In our year, there were two [American] scientists in that exchange, [myself] and a remarkable fellow, Ole A. Mathisen, who was an expert on salmon, a matter of some interest to both the Russians and to us. He was a Norwegian-American who studied at University of Washington. He had a great time. He got to travel. We didn't get to travel at all.

Anyway, I worked with Davydov, one of the people that was mentioned to me by Kasha. This was 1960-61. I could tell you lots about that year. This was the Khrushchev period. It began inauspiciously. It was the summer of 1960, [right after] the U-2 incident, the American spy plane shot down by a Russia.[20] The world political situation influenced how we were treated. We were not treated well in the beginning, [as a result of the tension around the U-2]. By the end, during the year, [John F.] Kennedy got elected. Khrushchev thought Kennedy was [weak]. We were treated [better]. [. . .]

We had a wonderful year. There were no foreigners in Moscow, except diplomats, a few journalists, no businessmen. It was a very special time. [. . .] Didn't get that much science done, but I did [finish a project] about an intensity of an electronic transition due to intermolecular transfer in a DNA molecule. I published in a Russian journal, by myself, not with my advisor. The relationship with the advisor, [Davydov], was very formal. I would see him once a week for an hour. That's it. There was no other [contact].

Our interaction with Russians in general was complicated. They were very interested, [but they were also] afraid. This was [only] seven years after [Joseph V.] Stalin's [death]. We did not get invited inside a Russian home during our whole year. We were invited into Uzbek and Georgian and Armenian homes, because they were less afraid, those nationalities. But the [. . .] Russians, they were afraid.

CARUSO: What were the facilities like that you were in? Were they comparable to what you were in—

HOFFMANN: Living facilities were good. We lived in Moscow in that big wedding cake building of Moscow University, one of the wings. I worked in the physics department. I had friends in chemistry. [. . .] They had no computers. They had no calculators. The laboratories, they were good in fields in which they had been good. [. . .] They were good in solid-state physics and in theory, because it required no computation.

And the Landau-Kapitsa heritage was very strong, so they could do state-of-the-art work in solid-state theory. But in chemistry, there were a few areas where they were good. Sometimes those areas can be traced back to tsarist times, even. [. . .] In [chemical] theory, there was a controversy about theory of resonance—one of a number of ideological controversies raised by opportunists in Stalin's last days. Loren [R.] Graham, who is a great historian of science, he was in the same exchange, in the same year, has written about [. . .] that resonance controversy. Loren [. . .] knows chemistry very well. He's retired, but you should get him back to talk about that controversy [. . .]. [And he's written about us, the American students in the exchange, in a book called *Moscow Stories*.][21]

REINHARDT: <T: 35 min> So, you were together as a group of expats in a way?

[20] Occurred on May 1, 1960, when a United States U-2 spy plane was shot down while in Soviet airspace while performing photographic aerial reconnaissance.
[21] Loren R. Graham, *Moscow Stories*, (Indiana University Press, 2006).

HOFFMANN: Yes. We [all] lived in this [giant] building. [. . .] There are about thirteen floors in the dormitory wings. All the Americans were in the same rooms, 424, 524, 624 [on different floors]. We figured out there was a cable running of listening devices down through those rooms.

REINHARDT: It was more practical. [laughter]

HOFFMANN: [. . .] It was hilarious. Oh, we were treated very well by the American Embassy and by the Swedish Embassy, too, and the Israeli Embassy. I smuggled—I'm not religious, but I smuggled prayer books for the Israelis to the Jewish community, and CDs of music. [. . .] It was a different time, 1960. I'm very glad we did it. We never saw as much ballet and opera as we did in that year, because we could buy the tickets through a special ticket office for diplomats. And at the end of our stay, we had a wonderful trip to Central Asia and to the Caucasus, which is very vivid in our minds, to this day. And we made many Russian friends.

After that, since I could give a lecture in Russian, I traveled very often to the Soviet Union. It remained an interest [of mine]. And it was very important—I've traveled much less in post-Soviet times, because it's not so important now. But before then—imagine how an issue of *Journal of Chemical Physics* [would feel to a Soviet chemist], how carefully it was read, how it was viewed.

And Russian scientists are more interesting people than American scientists. The reason is obvious. [Imagine] you're a [smart] kid age nineteen in the Soviet—you're entering the Soviet university system in 1960, you think you want to study philosophy, God forbid, or history. You're not stupid. You know that you're going to have to follow the party line. And even then, you will have trouble being in contact with the world outside. Whereas if you're a scientist, you're pretty immune from the party line. And you read the same journals [Western scientists do], except you read them more carefully, because they're so precious to you. So, you had a lot of [young bright people] who in our world would have gone into history or art or philosophy, but there became physicists or chemists. They were interesting people. They had interests in art. I made a number of friends. I have them to this day. [. . .]

CARUSO: So, I think [. . .] there are only a few years—

HOFFMANN: There [are] a few years to go still. So, I'm at Harvard. I'm in a program in chemical physics. I take courses mainly in the physics department, [but] I'm in the chemistry department, working with Martin Gouterman. Then Lipscomb comes to Harvard, hired as a crystallographer, [though] he also has theoretical interests. I switched to work with Lipscomb. It was already determined I would switch before I leave [for] Russia. [I'm at this point two years into my PhD study.] At the end of the two years, I'm going to Russia. And I've decided to switch to Lipscomb [. . .]. [On my return] I joined the Lipscomb group. And I begin **<T: 40 min>** theoretical work on boron hydrides. In the Lipscomb group at this point are five or six other theoreticians, plus experimentalists. [. . .] In that year—'61 to '62 —we program a variant of the extended Hückel method. I've told this story of the origins of the method in Eugene Garfield's old *Current Contents*, where he had essays.[22] I wrote [one] on that. [23]

That method is very important, because that allows me then to do organic molecules with Woodward later on. But I program it [initially] for boron hydrides, publish it in a tremendously productive year, '61-'62. I get my PhD at the end, in four years, even though one of them I was away. And I had enough papers; I published [them mostly] in *Journal of Chemical Physics*. [. . .] It was 1962.

I mention [that year because] in 2012, I published a series of four papers in *Journal of Chemical Physics*.[24] I realized that my first publication in *Journal of Chemical Physics* was two back-to-back papers. Then, fifty years later, I publish four.[25] That was a good feeling, that I could publish those papers over a period of fifty years. The whole *Journal of Chemical Physics* [goes back only] seventy-five years, so I was spanning a good part of that.

I [had] a tremendous time [in the Lipscomb group]. There's a lot of [. . .] collaboration among the graduate students. There was one postdoc and three graduate students, aside from myself. [. . .] We program this extended Hückel-type method for the boron hydrides.

REINHARDT: Who did teach you the programming?

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[22] Eugene Garfield, interview by Arnold Thackray and Jeffrey L. Sturchio at the Institute for Scientific Information, Philadelphia, PA (Philadelphia, Chemical Heritage Foundation, Oral History Transcript #0078; Eugene Garfield, interview by Robert V. Williams at Philadelphia, Pennsylvania 29 July 1997 (Philadelphia: Chemical Heritage Foundation, Oral History Transcript # 0165).
[23] Roald Hoffmann, "A simple quantum chemical method," *Current Contents* 29, 1989, 20.
[24] Roald Hoffmann and William N. Lipscomb. "Theory of polyhedral molecules. I. Physical factorizations of the secular equation." *The Journal of Chemical Physics* 36, no. 8 (1962): 2179-2189; Roald Hoffmann and Martin Gouterman. "Theory of Polyhedral Molecules. II. A Crystal Field Model." *The Journal of Chemical Physics* 36, no. 8 (1962): 2189-2195; Roald Hoffmann and William N. Lipscomb. "Theory of polyhedral molecules. III. Population analyses and reactivities for the carboranes." *The Journal of Chemical Physics* 36, no. 12 (1962): 3489-3493; Roald Hoffmann and William N. Lipscomb. "Sequential Substitution Reactions on B10H10-2 and B12H12-2," *The Journal of Chemical Physics* 37, no. 3 (1962): 520-523.
[25] Vanessa Labet, Paulina Gonzalez-Morelos, Roald Hoffmann, and N. W. Ashcroft. "A fresh look at dense hydrogen under pressure. I. An introduction to the problem, and an index probing equalization of H–H distances." *The Journal of Chemical Physics* 136, no. 7 (2012): 581; Vanessa Labet, Roald Hoffmann, and N. W. Ashcroft. "A fresh look at dense hydrogen under pressure. II. Chemical and physical models aiding our understanding of evolving H–H separations." *The Journal of Chemical Physics* 136, no. 7 (2012): 074502; Vanessa Labet, Roald Hoffmann, and N. W. Ashcroft. "A fresh look at dense hydrogen under pressure. III. Two competing effects and the resulting intra-molecular HH separation in solid hydrogen under pressure." *The Journal of Chemical Physics* 136, no. 7 (2012): 074503; Vanessa Labet, Roald Hoffmann, and N. W. Ashcroft. "A fresh look at dense hydrogen under pressure. IV. Two structural models on the road from paired to monatomic hydrogen, via a possible non-crystalline phase." *The Journal of Chemical Physics* 136, no. 7 (2012): 074504.

HOFFMANN: I learned Fortran. The language is still around today. I learned it myself, [with a manual].

CARUSO: So, another language you decided to—

HOFFMANN: [Yes], another language. It was easy. We had to punch cards, as we did for a few years to come. All of us who grew up in that time have the sound of a key punch in our heads. [. . .] And the program had to be recompiled each time—there was this box of cards, which was the program. The input data was just a few cards. But the box of cards had to be carried over to the computer, some other building, and if you dropped it, that was disaster, because the order of the cards mattered. [. . .]

CARUSO: Was it relatively open access to the computer at that time, or were you booking—

HOFFMANN: Yes. [. . .] A computer center [in the chemistry department grew] very quickly, within about two years. [. . .] The Lipscomb group was very computer savvy, because they were doing crystallography, and crystallography depends on computers. So, programming in crystallography was already a going concern in the rest of the Lipscomb group.

Lipscomb became a theoretician. [. . .] But soon he did another transition to becoming a protein crystallographer and a biochemist. **<T: 45 min>** [. . .] At Harvard, I was at the focus of one event there. It was traditional for a graduate student, at the time they got their PhD, to give a physical chemistry seminar, so I did that in 1962 in the summer. And that was attended by the faculty, who usually were critical. At this seminar, I was Lipscomb's first student at Harvard. I was Gouterman's first PhD student at Harvard. When I gave the seminar, it was about the boron hydride calculations. Bright Wilson got up afterwards and gave a scathing critique of the seminar, [of my method], of what I was doing.[26]

A little bit of background. [Edgar Bright] Wilson [Jr.], of course, knew quantum mechanics. There is a wonderful influential book by Pauling and Wilson in the field.[27] Wilson became more and more of an experimentalist. He also was a theorist [of] molecular vibrations, so there is another great textbook, Wilson, [John C.] Decius, and [Paul C.] Cross, *Molecular Vibrations*.[28] I see it on my shelf there. Still useful.

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[26] E. Bright Wilson, Oral History Transcript #0061.
[27] Linus Pauling and E. Bright Wilson, Jr. *Introduction to Quantum Mechanics with Applications to Chemistry*. (New York: McGraw-Hill Book Company, 1935).
[28] Paul C. Cross, J.C. Decius, and E. Bright Wilson, Jr., *Molecular Vibrations: The Theory of Infrared and Raman Vibrational Spectra*, (Dover Publications, 1980).

As far as theory [goes], he took a wrong turn; he became convinced that the way to do calculations was to solve Schrödinger's equation with various approximations, [and] try to get lower and upper bounds on the energy. And [Wilson] was [one of] the powers that be, [. . .] Wilson and Kistiakowsky at that time.

REINHARDT: George [B.] Kistiakowsky?

HOFFMANN: George Kistiakowsky, a great physical chemist, just back not too long before then from being the head of the explosives division at Los Alamos [National Laboratory], [where he] played a crucial part. [One of the few chemists in the Manhattan Project.] He knew about explosions, and that an implosion was necessary [for the bomb operating]. I remember translating a speech [Kistiakowsky] was going to give in Russia into Russian from English. He came from a Russian family, but I knew Russian at this point better than he did. This is why I was involved in that.

Wilson essentially disliked the kind of theory that Lipscomb did. They didn't hire Lipscomb as a theorist. They hired Lipscomb as a crystallographer, a boron hydride chemist. And he did experimental work too. Lipscomb had the characteristic of wanting to say something about anything, and he was very outspoken. [After my seminar], Wilson said, "These are approximate calculations; they can't be right," essentially. The next thing that happened, before I got a chance to answer, Lipscomb [stood] up, and the two of them proceed to have a big public debate about the nature of theory. [I think] I just kept quiet. No, actually, I said something, too. But it was clear to me and to everyone in the room that this [discussion] was not really about my seminar. It was really about Lipscomb and Wilson [and their opposing view of theoretical chemistry]. Interesting.

So, in that year, to draw the timeline, it's now '62, I'm twenty-five years old. I have caught up in the sense that I finished college in three years, and I got my PhD in four. I was really smart then, I could do [anything]. Lying right over there are some of my notebooks from the college days, and there are some problem sets [in them] that I solved, and I couldn't possibly do now. I really drank the stuff in. [. . .]

I applied for jobs. It was post-Sputnik days. **<T: 50 min>** American universities were increasing the number of [available] positions. There were lots of jobs. As a computer-trained theoretician, I was a reasonable commodity. I didn't even think of doing a postdoc. Today you would do a postdoc, but in those days, I didn't. I applied for jobs.

I applied to Yale, where I got rejected another time. I got it in my head to go out west, and the only places in the east I applied were Yale and Cornell.

REINHARDT: So, jobs means academic jobs?

HOFFMANN: Assistant professorships, at age twenty-five, with a Harvard PhD. I got it in my head to go out west, so I applied to University of Washington, [University of California] Berkeley, Stanford [University], Caltech [California Institute of Technology], and University of California, San Diego, which was new then. [. . .] I got a job offer from each of them, except for Yale. Obviously, Lipscomb must have written a good letter. [laughter]

And at the same time, I applied for a Junior Fellowship; I think the advice to do so may have come from Dudley [R.] Herschbach, who was a junior fellow [in his time]. The Junior Fellowships [are] modeled on an English fellowship at a college. It was instituted in the thirties, [they were thought of] as a way to bypass the PhD. It never worked that way. [The position, an independent postdoc], was also used by Harvard to look over good people that it might hire. A number of extremely good people, Harvard faculty members, were Junior Fellows, among them Woodward and Herschbach. And a number of other people whom you've heard of, like McNamara and [Bundy]. Many good people.

[. . .] It paid the equivalent of an assistant professorship [salary], about eleven thousand dollars at that time. It was a reasonable salary. I applied for that and was accepted. It gave you three years to do some research without any responsibilities, without being tied—it was like a super postdoc, and you weren't connected to anyone. [. . .] I don't exactly know why I took that over the [assistant professor] jobs [I was offered].

Let me jump a little bit. Three years later, 1965, I applied to all of the same places that I just mentioned, except Yale. I had given up on Yale. And I got a job [offer] from none of them except Cornell. So, what was the difference? And the difference was that when I applied for those jobs was November, December '64. The orbital symmetry work, first of five communications [was not quite published. It would be two months till those were out. I had spoken about the work only at two meetings]. The first paper doesn't get published till January '65. [A few] organic chemists around the country knew something, that this work was coming, even though the work was not published. [. . .] I will caricature [what I think happened], but in 1962, I was a promising theoretical chemist with [achievements and promise] on state-of-the-art calculations of the electronic structure of molecules. [. . .] And I had clearly an orientation toward computers, which was a very saleable, positive item.

Nineteen sixty-five, I was tainted by organic chemistry. **<T: 55 min>** I was all the same things [that I had been] before, but I had gotten interested in organic molecules. [If] an organic colleague at Berkeley [. . .] said to his physical [colleague], "Hey, I've heard of this great work by Roald Hoffmann and Woodward about the stereochemistry of these reactions," that [might not be viewed so positively—in a discipline-run world it might be seen as just] organic stuff.

Another year later, it would have been totally different. But [in early 1965] Cornell is the only one who held the faith, and that's why I'm here.

CARUSO: So, I mean, why was organic chemistry tainting at this point? [. . .]

HOFFMANN: [At any time, there are standards of quality, what people view as excellent frontier science. It could also be that people didn't understand my commitment to explanations, they saw me as a calculator, perhaps not that "clean" as they wished.] I had developed this method, the extended Hückel theory, which was a semi-empirical molecular orbital method. It involved some parameters. Meanwhile, the theory field had taken off toward what were subsequently called *ab initio* calculations; they were also begun in the Lipscomb group and elsewhere.

[Somehow], by '65, those *ab initio* calculations had a greater cachet than my semi-empirical calculations, and those people who made the evaluations no longer thought I was a state-of-the-art, progressive, [theoretician. Success with organic chemistry did not mean enough to the people who would make decisions on hiring me.]

REINHARDT: So, you were between two stools, in a way.

HOFFMANN: I was.

REINHARDT: And so, I mean, I've read quite a bit about the clashes between *ab initio* and semi-empirical methods. Did this dichotomy, or however you would call it, continue—

HOFFMANN: Yes.

REINHARDT: —in your career? And where would you place yourself in this—

HOFFMANN: [. . .] There's something worth talking about, [. . .] about disciplines, and what's fashionable, what's important, and how a community [reacts to choices individuals make. To answer the question as to why I am at Cornell]: It's the only place that offered me a job in '65.

REINHARDT: The lucky ones?

CARUSO: Yes. [laughter]

HOFFMANN: [. . .] [To get back to the years of a Junior Fellowship.] As a Junior Fellow, I was independent of Lipscomb, with whom I had done my PhD. [. . .] I did not [yet] know Woodward. I had met Woodward [once; I believe] he interviewed all the incoming graduate students as part of a committee. He was a mythical figure at that time. There has been much written about Woodward, including a very good book that [Otto Theodor] Ted Benfey did for the CHF [Chemical Heritage Foundation].[29] Though that book was just before the [Elias J.] Corey claim [of having told RB Woodward the simple frontier orbital explanation which eventually built into a general theory of pericyclic reactions]. Jeff [Jeffrey I.] Seeman is doing a major study of the Corey claim, and [the state of physical organic chemistry in that period, the sixties].[30]

I didn't know any of the organic chemists to begin with. I was an independent theoretician. I had a reasonable salary. I could apply for research grants. And I think I got [in this period] my first NSF [National Science Foundation] grant. **<T: 60 min>** [. . .]

I decided to work on organic molecules. This is without talking to any of the organic chemists. I don't know exactly why [I chose that direction], but I saw that the methodology [I had developed for boron hydrides] could be applied [to organic problems]. I guess the first organic problem that I encountered was during the Lipscomb days. Next to me was Russ [Russell M.] Pitzer—this is the son of Kenneth [S.] Pitzer, a very important American theoretical chemist—and he was doing the first *ab initio* calculation of the barrier to internal rotation in ethane. [. . .]

But he was doing it with *ab initio* methods. I thought I would do that with this extended Hückel method, which we developed in the Lipscomb group. I developed that method a little more and applied it to some simple shapes and geometries of organic molecules. That's the series of three papers in *Journal of Chemical Physics* in 1963, called "Extended Hückel" I, II, III.[31] I wrote those papers [in] my first year as a junior fellow. [After I submitted them], I made an appointment with the leading organic chemists in the department to show them the paper, to tell them what I could do, and to ask them if there were any interesting problems to which this theory could be applied. I went to see Frank [H.] Westheimer.[32] I went to see Woodward, Paul [D.] Bartlett. [I went to see] EJ Corey. That was the second time I met Woodward. He gave me an hour of his time. He listened very carefully. He asked some good questions, but he had no suggestions at that point of anything to work on. Neither did any of the others.

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[29] Otto Theodor Benfey and Peter John Turnbull Morris, eds. *Robert Burns Woodward: Architect and Artist in the World of Molecules*. Chemical Heritage Foundation, 2001.

[30] Jeffrey I. Seeman. "Woodward–Hoffmann's stereochemistry of electrocyclic reactions: From day 1 to the JACS receipt date (May 5, 1964 to November 30, 1964)." *The Journal of Organic Chemistry* 80, no. 23 (2015): 11632-11671.

[31] Roald Hoffmann, "An Extended Hückel Theory. I. Hydrocarbons," *Journal of Chemical Physics* 39, no. 6 (1963): 1397-1412; Roald Hoffmann, "Extended Hückel Theory. II. σ Orbitals in the Azines," *Journal of Chemical Physics* 40, no. 9 (1964): 2745; Roald Hoffmann, "Extended Hückel Theory. III. Compounds of Boron and Nitrogen." *Journal of Chemical Physics* 40, no. 9 (1964): 2474-2480.

[32] Frank H. Westheimer, interview by Leon Gortler, Harvard University, 4 and 5 January 1979, (Philadelphia: Chemical Heritage Foundation, Oral History #0046).

[The first year of my junior fellowship was ’62-’63. We’re now in the second year, I started talking to Corey. He] had an office down the hall [from me in the basement of this old building]. [. . .] And he was very approachable. [I] was younger. So, our ages are now by a factor— we are a decade apart. I am ten years younger than Corey, and twenty years younger than Woodward. Woodward was born 1917, Corey ’27. I’m ’37.

Corey was a full professor, attracted from Illinois. He told me about some problems he was working on, [on carbonium ions and photochemistry]. I think I tried some calculations stimulated by these. There are no papers jointly with Corey, with me, but I thank Corey in several of my papers [of the period]. Also, in the spring of ’64, one of Corey’s buddies from Illinois, Doug [E.] Applequist, an organic chemist, comes [. . .] on a visiting professorship, gives a course of lectures about modern physical organic chemistry.

I had tried before in my first year to sit in on a course by Paul Bartlett, who was the leading physical organic chemist of his time, perhaps, along with [William E. Von Eggers] Doering and [Saul] Winstein.[33] These three people shaped American physical organic chemistry: Winstein, Doering, and Bartlett. Bartlett was a dry American Yankee type, New England. It was not easy to communicate with him. [. . .] I tried to sit in on a course by Bartlett. I have a few **<T: 65 min>** notes from [the course]. But it wasn’t too exciting overall.

But the course that Applequist taught in the spring of ’64—this is the end of the second year of my three-year fellowship—that was all about reactions. [He spoke of] what we would now call two plus two cycloadditions proceeding through di-radicals. He talks about cyclopropane. [. . .] I had started doing calculations on cyclopropanes. He talked about non-classical carbonium ions, which I’d also heard [about] from Corey. I start some calculations, and there’s a paper on non-classical carbonium ions [I write in this period].[34]

Somehow, these people, Applequist and Corey, found a way to get [to] me—they told me about modern organic chemistry. Their subjects were non-classical carbonium ions, organic photochemistry, strained rings. Aromaticity I knew about from my senior seminar at Columbia, with Breslow.[35] But things had advanced. Somehow, these were the hottest topics of physical organic chemistry [of the times, the literature had articles about them every month], and I got excited about them.

[While] I was doing these calculations. I was still very much a computational chemist. So, when on one day in May 1964, my third encounter with Woodward—I told you the first two. One was as [an incoming] graduate student, and the other was [when I told him of my extended Hückel calculations. On both occasions] I didn’t sense any communication.

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[33] William E. Von Eggers Doering, interview by James J. Bohning, Philadelphia, Pennsylvania and Cambridge, Massachusetts, 9 November 1990 and 29 May 1991, (Philadelphia: Chemical Heritage Foundation, Oral History Transcript #0085).
[34] Roald Hoffmann. “Toward an Understanding of Nonclassical Carbonium Ions.” *Journal of the American Chemical Society* 86, no. 6 (1964): 1259-1261.
[35] Ronald Breslow, Oral History Transcript #0181.

Woodward came down with Applequist to my little office, [before or after I had talked with Applequist, and they] told me, essentially, about the electrocyclic reaction [and its simple frontier orbital explanation]. I have it in my notes. I used to keep notebooks then, thank God. These old notebooks, [. . .] these wonderful notebooks that we'd get from this—

REINHARDT: Is this the one of the year? That's later?

HOFFMANN: No, it's another one. This is what they look like. I pasted in things. And Jeff Seeman has been through these [in great detail] I pasted, I wrote. I didn't date them, [not many pages]. I was not an industrial chemist.

REINHARDT: No patents?

HOFFMANN: And [the absence of] dating is a terrible problem in taking apart the Woodward-Corey claim. Here and there, there is a date, but you can see how—

REINHARDT: Not consistent.

HOFFMANN: It's pencil, it's pen, these are wonderful documents. Specifically, the one on the period of the Corey claim is deposited at Cornell in a collection. I have a copy of it. [The ones you see here] are later. But what you can see in these notebooks, and you can see it even here you see numbers. This is where I was in '63, '64. So, there are rows of numbers. I'm doing calculations. There are graphs. I'm beginning to sketch molecules. As this goes on, the molecules get more complex, and I'm beginning to draw orbitals, and the numbers are suppressed. This is part of what I told you about—the struggle with the computer.

REINHARDT: There's one—may I?

HOFFMANN: Yes. Sure.

REINHARDT: Here, Woodward.

HOFFMANN: Yes.

REINHARDT: [. . .] So, you were in touch with William von Eggers Doering as well?

HOFFMANN: He came to give a talk. He wasn't at Harvard then, [still at Yale].

REINHARDT: Oh, I see.

HOFFMANN: We can date these because of some papers I read that have dates in them. So, here is a date. My God, it's later; I'm now at Cornell.

REINHARDT: Sixty-six. Yes.

HOFFMANN: Yes. These are wonderful documents. No one [taught me to] keep good notebooks. I wish I [had] dated them [better, more consistently]. But I did keep them, at least.

Anyway, Woodward **<T: 70 min>** comes and asks me a question about these reactions, and gives me the simple frontier orbital argument, which Corey claims that he told to Woodward. We'll come back to the Corey claim, inevitably. [. . .] Woodward tells me [of two experimental findings]. [One is] abstracted in part from vitamin D [chemistry]. I would never have looked at the literature of vitamin D photochemistry. It's too complicated for me at that stage of life. But he's familiar with it. He knows [it, and he needs the chemistry for a synthesis underway in his lab. The second story he tells me was done by] physical organic chemists like [Emmanuel] Vogel and [Rudolf] Criegee, [two of the superb] physical organic chemists of the time in Germany. Vogel and Criegee's [. . .] experiments I could have understood, but I still didn't read the literature [in sufficient depth].

He brings me those experiments, and he gives me the first simple orbital explanation. And my reaction to that is: "Let me do some calculations." That is, I don't really appreciate Woodward's explanation.

REINHARDT: Have you heard before of frontier orbital theory?

HOFFMANN: Not as such, but I knew [Kenichi] Fukui's work. [I learned of more of it]. What Woodward gives me is a frontier orbital argument, but we didn't call it [that] at that time that. It's an anachronism in the context, even though the word is in the literature before, but it was not used by either Woodward or me.

REINHARDT: What did you use? Do you remember?

HOFFMANN: We just said orbital.

REINHARDT: Just said orbital?

HOFFMANN: Now you need to talk to Jeff Seeman, because he's researched this in some detail, on who knew what when. I go away and do calculations. That is, I put into the computer the coordinates of a [1,3-]butadiene, and I start rotating the outside CH_2's in the two different ways that Woodward told me that they might [be moving to get the observed stereochemistries]. We can trace it in a notebook—I do this with no sense that this is an important problem. You can see that in the notebooks, because [what I do] is interspersed with days and days of stuff on other things [that are of more interest to me. Boring now, but not then].

I come back to [the problem]. Perhaps Woodward asked me about it, I don't know. I come back to it, and the first time I [do the calculations], I get it wrong. [What I mean is that] I don't get a preference for the conrotatory butadiene to cyclobutene closure. They come out about the same [activation energy]. But then I realize that what I'm doing is [calculating] a reaction coordinate, [and that I don't have some essential parts of the atomic motions]. I'm stupid. I just rotate the ends, and I don't do anything else. I realize [at some point that] I must decrease the CCC angle to go from 120 degrees or so in butadiene, to more or less 90 degrees in the cyclobutene. And when I do that, [the calculations] come out the way it "should," [the conrotatory motion favored]. That doesn't happen for three or four months after he tells me that story.

[I was calculating a reaction coordinate. There was no guidance for how to do this—heretofore people had done only simple, simple reactions like D + H2 = HD + H.]

REINHARDT: Was Woodward very impatient?

HOFFMANN: No.

REINHARDT: No?

HOFFMANN: I never remember Woodward impatient about anything. He was sometimes insistent, but not impatient. [. . .] When I do the calculation, I go back [and tell him about it. Jeff Seeman has laid out the time sequence from my notebooks. There are mysteries in it, why I don't tell Woodward of my results earlier.]

Woodward decides to write a paper. We write this paper in October. [Woodward asked me to write a paper, a draft of the theoretical part, and I do. And it's all calculations. There is nothing about the orbital argument. That's all Woodward's.] This is all '64. We submit it in late November. It's published in January.[36] We have various drafts of that first paper. [. . .]

Slowly, with time, and especially [in working] on the next paper on cycloadditions, [and the one after that, on sigmatropic reactions,] I begin to appreciate the value of what we would now call the frontier orbital argument.[37] **<T: 75 min>** That notebook is very interesting to look at—Jeff has made me appreciate what went on then much more by looking at it in such detail, and asking questions. [Roughly] what's happening is that I don't appreciate the simple [frontier orbital] argument, or simple arguments in general. I'm just a calculator, to begin with. But at the same time, I'm drinking in organic chemistry. And I'm learning on my own perturbation theory, which is the natural language behind frontier orbital arguments. I sort of independently discover frontier orbital arguments, without being that much aware [of Fukui's work]—even though I was aware of Fukui's work, I didn't connect it to the [reactions I was studying with Woodward].

And I don't know [of] Michael Dewar's use of perturbation theory [in explaining organic reactions].[38] [. . .] Dewar is [subsequently] so unhappy with us. [For me], it's a wonderful [time], because I'm learning a new field of chemistry, and I'm changing from being a calculator to being an explainer. That was the fundamental transformation that the orbital symmetry story meant for me. I think the seeds [for moving in that direction] were already there in Lipscomb's way.

[. . .] So, I stay one year more at Harvard, '65, '64. I look for jobs. The orbital symmetry papers begin to be published. The first two are published when I'm still at Harvard. The last two at the end of the year, '65. I'm already at Cornell. [. . .] Woodward and I go on working for four years on a long paper. And a lot of interesting things happen. [. . .]

Sixty-three, in the second year, our first child is born, a son [. . .]. [I am working on] the second paper while I'm babysitting for my son. I remember it clearly, my wife was out teaching Swedish, I think. In '65, we come here [to Cornell]. Our daughter was three weeks old. I look at her and I can see how long we've been here [in Ithaca]. Fifty years. And there is more to tell about Cornell and science, but let's stop now. [. . .]

[END OF AUDIO, FILE 1.3]

[END OF INTERVIEW]

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[36] R.B. Woodward and Roald Hoffmann. "Stereochemistry of electrocyclic reactions." *Journal of the American Chemical Society* 87, no. 2 (1965): 395-397

[37] Roald Hoffmann and R. B. Woodward. "Selection rules for concerted cycloaddition reactions." *Journal of the American Chemical Society* 87, no. 9 (1965): 2046-2048; R.B. Woodward and Roald Hoffmann. "Selection rules for sigmatropic reactions." *Journal of the American Chemical Society* 87, no. 11 (1965): 2511-2513.

[38] Michael J. S. Dewar, interview by James J. Bohning at University of Florida, Gainesville, 22 January 1991 (Philadelphia: Chemical Heritage Foundation, Oral History Transcript # 0087).

INTERVIEWEE: **Roald Hoffmann**

INTERVIEWER: **David J. Caruso**
Carsten Reinhardt

LOCATION: **Cornell University**
Ithaca, New York

DATE: **17 October 2014**

HOFFMANN: So, is there anything that comes to your mind from that early period that you would like me to talk about?

REINHARDT: I think at the moment, I don't have a special idea. I think we should go on in the line of events, where we were finishing yesterday. If you don't want to speak about something—

HOFFMANN: [. . .] One thing is what the orbital symmetry story meant to the world of chemistry, and that itself is interesting [. . .]. [The subject] has many dimensions, one is that it was a nexus—a meeting point of two sub-fields of chemistry: theoretical chemistry and organic chemistry. These nexuses—maybe there's a Latin plural—are important in science, and they're interesting. I can point to a few others. But this particular one was prepared for, [. . .] it was in the air. [The solution of the problem of the stereochemistry of electrocyclic reactions] could have been done by any of a number of other people. [. . .]

There was a special confluence [of abilities and interests] in my case, but what I'm talking about is the other precedent for a meeting ground of organic and theoretical chemistry was the rediscovery and fleshing out of Hückel's rules in period 1950-1960, by people like Doering, Breslow, and Katz.[39] I'm thinking of people making cyclopropenium cations, cycloheptatrienyl cations, other two- and ten-electron Hückel systems, and six-electron [ones as well].

In general, European chemistry was behind. I think German chemistry had not yet recovered from World War II, though there was a new generation of physical organic chemists rising. I mentioned Criegee and Vogel were two—and Huisgen, [as well. Stephen Weininger and Jeff Johnson have recently written of this period in the history of German chemistry.] In America, [physical organic chemistry] took root. It was a very exciting period of making aromatic molecules.

[39] Ronald Breslow, Oral History Transcript #0181; William E. Von Eggers Doering, Oral History Transcript #0085.

[The precedent was interest in Hückel's rules]. I think the orbital symmetry work made that very real. After that, there was no way that an organic chemist would not have an introduction to quantum mechanics. That was part of the education, part of the general psyche. It was demonstrated that [molecular orbital theory] was important. [Valence bond theory, up to then the natural language of mesomerism and organic chemistry, sank into the background.] That's interesting.

There were other reasons why the orbital symmetry work was so successful. [. . .] There was a community of physical organic chemists who [were] ready to do the experiments to test the predictions. [. . .] In some ways, the preparation for this [came from the study] of non-classical carbonium ions. Not overall terribly productive, but [the excitement that problem generated] in physical organic chemistry produced students who were able to study these problems. If you make a prediction that takes fifty years to test, it will not generate a dynamic in the field. But if the predictions are testable within a year, [. . .] people test it, publish. Other people notice it, and so on. I think that's part of what went on around the orbital symmetry story in that period, 1965 to '70.

A third thing I would say more generally about what I did [. . .] [on the pericyclic reaction problem, followed up by] **<T: 05 min>** other work [. . .] on reactive organic intermediates, their electronic structure [work] after I came to Cornell, in the ten years before I turned to inorganic problems, the period '65 to'75. [We] created a language for organic chemistry. That language was a mixture of small three-dimensional representations of structures [and of orbitals].

After 1960 or so, with [Derek H.R.] Barton's work, and conformational analysis in organic chemistry, no organic chemist ever drew cyclohexane as a plain six-membered ring. They drew it in a chair form. Nobody typeset norbornane as $(CH_2CH_2)_{2(}CH)_2CH_2$. They showed a three-dimensional drawing. Part of what's going on here is what's allowed typographically by the journals, part [what people felt was essential about the molecule]. What we did was add to an existing stereochemical graphic representation of organic chemistry, a [small] graphic and easy-to-grasp language showing what electrons were doing in molecules. So, people were drawing lone pairs. They drew for the first time the phases of orbitals. That's what became apparent from our work, [that such representations were useful and important to introduce].

So, [. . .] as long as [I and the community] remained with the numbers—where I was in 1964, in sheaves of numbers—there was no way of grafting that information visually [onto the little drawings of molecules] that chemists would communicate to each other on paper, and with paper and pencil, the tools of their time, on a restaurant white paper [napkin or tablecloth]. They couldn't communicate that, [easily or at all], if you had to refer to numbers in a calculation.

But by adding these little orbital pictures, [which] were "commensurate" with the graphic tools already available to organic chemists, [one gained a lot]. And they were not that hard to learn. So, [this mode of representation, mixing structures, quasi-three-dimensional, with orbitals], became tremendously successful. I've written a little bit about it, very little; [. . .] there are many interesting things here related to paper tools and Ursula Klein's ideas about [them].

There are many interesting things here for the history and sociology of science, and the interaction of scientific communities. We were lucky.

[. . .] I want to re-emphasize this, [that one thing is what the complex of orbital symmetry ideas] meant to the world. Another is what it did to me—as I've told you, it transformed me from a calculator to an explainer.

REINHARDT: There are a couple of questions that I would like to ask as a follow up here with that story. The example you mentioned, the non-classical carbonium ion, there is a sort of controversy attached to it, at least a discussion. [Herbert] Brown versus the rest in a way, as I understand it.[40]

HOFFMANN: Yes.

REINHARDT: Was there a similar thing with orbital symmetry?

HOFFMANN: No, [not really].

REINHARDT: Why not?

HOFFMANN: It was immediately accepted. There [were suggestions, e.g. from Michael Dewar that (a) it could have been done in other ways, for instance by invoking aromaticity for the transition states, and that (b) that was said by Evans in the thirties. The claim was forced in several ways and was ignored. Indeed, the analysis could have been done in a number of ways, for instance] with Dewar's papers from 1952, which were incomprehensible to the community.[41] People [came up with alternative ways of doing it very quickly. For instance, in the most credible and teachable way, they **<T: 10 min>** came up with a] competitive way to look at it in terms of aromaticity of transition states. So, there were claims of "precursors," but there was no controversy on the validity of the conclusions. [More than that, in our long paper we added many new reactions that could be analyzed. The people who claimed alternative derivations had four years to come with these. They did nothing new.] It's only now that there is surfacing some controversy, [Corey's claim of having told Woodward the explanation].

The reason [for our success was] this way of thinking [following orbitals through a reaction was portable—others could use it. The theory] made portable, verifiable, sometimes risky predictions which could be, and were, tested within a year or two, and the tests were

[40] Herbert C. Brown, interview by James J. Bohning at Purdue University, 11 November 1994 (Philadelphia: Chemical Heritage Foundation, Oral History Transcript #0117).
[41] Michael J.S. Dewar, Oral History Transcript #0087.

convincing. [. . .] I've written something about why buy that theory, an article in *American Scientist*.[42] Why do people accept theories? In addition to the usual [qualities, that theories explain more of things, and make risky predictions], there are aesthetic elements, and there's storytelling [qualities. Theories] being portable and productive is, I think, important. Productive just means the theory suggests experiments. Theories which don't suggest experiments will languish and eventually fade away, because science is about the interaction of theory and experiment.

Portable just means that [people other] than the person who devised the theory can use it easily, and that's what orbital symmetry was. I remember the day that Jerry Berson called and told us [of his results for] a 1,3 sigmatropic shift, a very specific reaction—he designed a test of it—that it went with inversion of configuration.[43] That was a risky prediction, because a least motion [reaction path], that atoms move least during a reaction, would have predicted the opposite result. But the atoms follow what the electrons tell them to do. [And that's exactly a paraphrase of] our contribution. The point [of the theory being portable] is that Berson didn't have to ask us [what was going to happen]. He could apply the ideas we had [put in his mind to the reaction at hand]. And that kind of power put in the hands of clever experimentalists, had tremendous impact.

REINHARDT: You mentioned already some names, but could you describe [to] us the community of these early adopters, and what their main achievements and their various roles were in that?

HOFFMANN: Well, Jerry Berson was an early supporter. He was a professor at Yale at the time, and a leading physical organic chemist, [and] a student of Bill Doering.[44] Bill Doering was perhaps conflicted [. . .]. There's a complex relationship between Doering and Woodward, which goes back to their early work together in World War II. But Doering also saw the power of this explanation.

Other important actors were the three German physical organic chemists I mentioned, Criegee, Emanuel Vogel, and Rolf Huisgen. A younger chemist, Wolfgang Roth, who was at Bochum, eventually played an important role in [confirmations]. In the United States, there was a [. . .] pretty wide community—[it included Eliot Marvel, Dave Lemal, John Baldwin, many others].

REINHARDT: How did the communication channels work?

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[42] Roald Hoffmann, "Marginalia: Why Buy That Theory?" *American Scientist* 91, no. 1 (2003): 9-11.
[43] Jerome A. Berson, interview by Leon Gortler at New Haven, Connecticut, 21 March 2001 (Philadelphia: Chemical Heritage Foundation, Oral History Transcript #0196).
[44] William E. Von Eggers Doering, Oral History Transcript #0085.

HOFFMANN: They worked through literature and meetings.

REINHARDT: No letters, no correspondence?

HOFFMANN: Yes. [. . .] There was letters and correspondence.

REINHARDT: I'm surprised by the German impact. Because what I remember is that, **<T: 15 min>** what you were also just describing, after World War II, the Germans were behind the Americans, especially with regard to physical organic chemistry, which was, you could argue, then a US specialty, right?

HOFFMANN: That's right. Germany was coming out of a period of pre-war dominance of synthetic organic chemistry. [. . .] The failure [in Germany] to recognize Hückel's idea is another whole story by itself—[Jerry Berson has written about this].[45] There was other important German work, on spectroscopy by Kuhn and also some by Clar [on the aromatic sextet. German chemistry] was coming up fast—[the young people were doing postdocs in US.] Some of these people were trained before World War II, [for instance, Costin Nenitzescu], a German-trained chemist who was in Romania. [. . .]

There's a prescient comment involving orbitals in a recorded comment by Woodward in a 1961 proceedings of a Welch Symposium on chemistry. [. . .] The talk was by Rolf Huisgen about 1, 3 dipolar reactions and [in his comment, Woodward makes] a sketch of orbitals. [. . .] Woodward was a Germanophile in his own way. He also liked England a lot, but he paid a lot of attention to German [and Swiss] chemistry and cultivated his connections there.

REINHARDT: What was the role of Woodward? I mean, he was world famous at that time?

HOFFMANN: He was the leader of world chemistry, I think, taking over from [Sir Robert B.] Robinson and [Sir Christopher K.] Ingold in England.

REINHARDT: What does "leading world chemistry" mean at that time?

HOFFMANN: The work that he did was [. . .] paradigmatic in setting the style of synthetic organic chemistry. At the same time, he had this lifelong interest in the Diels-Alder reaction and its mechanism. [This] goes back to a story he tells in his Cope lecture, which is detailed in the

[45] Jerome Berson, Oral History Transcript #0196.

CHF book, of his writing at age eleven [to the German consul in Boston, and receiving a copy of a journal with the Diels-Alder reaction paper in it].[46] So, Woodward was one of the rare, very rare instances of precocity in chemistry. [Parenthetically], we don't have it much [in our field]. Which I take as a good sign, incidentally. I'm afraid of [precocity], even though I recognize it. It's a sign that there is a talent for something, [. . .] and that there [exists] a natural predisposition [for that. Math and music have precocity in them]. That to me looks in some way as a barrier to my doing well.

REINHARDT: Why?

HOFFMANN: Because I'm not talented. That is, you have to be born with that talent. You have to be Mozart. Okay, so [we know] his father pushes him ahead. That is a—

REINHARDT: Yes. I was just thinking, yes. [laughter]

HOFFMANN: [. . .] I think chemistry and poetry and politics [are fields where talent doesn't matter. I suppose] there are children who are good in their own way in politics. My children, when they wanted an ice cream cone, if they asked for it in English and they didn't get it, they would ask for it in Swedish. That's a primitive exercise of political intuition. **<T: 20 min>**

But in chemistry, in general, there are no children who are great chemists. [Now being serious about it], it takes a balance of judgment and moving in between a logical, intuitive world and a less logical one in chemistry. I think [. . .] it takes maturity to do chemistry.

REINHARDT: [What] was it like to work with a natural-born genius chemist?

HOFFMANN: It was wonderful! He had also mannerisms which enhanced the feeling of genius. [. . .] He created structures around himself, whether it was wearing the color blue, or going to the library and reading the journals in the middle of the night. He limited access to himself, but when you saw him, you had the feeling that all the thought powers of the world converged on you and him at the same time. It was a quality of giving you undivided attention, and a feeling that he was thinking. He liked the Nero Wolfe detective stories; [. . .] I saw a parallel between [Rex Stout's] Nero Wolfe—or my constructed image [. . .] [and Woodward]. It was the reasoning power of a super-rational detective.

He knew the literature [of chemistry intimately]. [. . .] Another interesting story [in my interaction with RBW] is how does a pair of helping hands, which is [how I would describe

[46] Benfey, *Robert Burns Woodward*.

myself] in the beginning of our collaboration, [turn into a collaborator]. He had the first explanation, the simple frontier orbital explanation. He wasn't sure of himself, I think. That was not a characteristic one associated with Woodward, not being sure of oneself. [. . .] But I think he wasn't, and he looked for support from calculations. From what were, at that moment in time, probably the best calculations that one could muster. My luck in this was that I had [command of] these calculations. They didn't remain the best calculations for more than a year, but I had the calculations [at the time].

And so in the beginning, and you can tell that from the drafts which Jeff Seeman is [publishing], that I'm just providing numbers to support Woodward's explanation.[47] How does a pair of helping hands transform into a true collaboration?

The second paper has my name first, which is pretty unusual for Woodward.[48] [Perhaps I put it on first in a draft, but given our roles in science at this time], I wasn't deciding whose name was going to be first. [. . .] How does mentor-apprentice turn into collaboration? [. . .] I think one of the ways this happens is when the young person tells the older person something that the older person didn't know, and when the older person has the charity and the spirit to recognize that he didn't know that. There were such moments around the cyclopropane reaction [at the end of our first paper. And on cycloadditions, I think my clear result that 2+2 was a forbidden reaction] **<T: 25 min>** told Woodward something he didn't know. And then we were in a collaboration.

REINHARDT: Whom did you tell first after Woodward about what you were doing in this crucial first year?

HOFFMANN: In very beginning, the first month or two, I actually told Corey, and Corey gave me, somehow, the feeling that he was involved in the story. And eventually, that bothered me enough that some months later when we wrote the paper, I asked Woodward if Corey had an interest, and Woodward said no.

There was no eureka moment. There was nothing like that. It was a slow evolution over months. And then things went more quickly in '65. [In the beginning], I didn't know this [work] was important. The evidence for that is in the notebooks, as I told you. My wife didn't know it was important. I have talked to her.

I talked to other people, to Lionel Salem, who was a friend. He was an instructor at Harvard at the time. I talked to Lipscomb and Gouterman both, but they were not interested in organic chemistry. The stereochemistry of organic reactions somehow [wasn't of interest to them]. [. . .]

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[47] Woodward and Hoffmann, "Stereochemistry of electrocyclic reactions."
[48] Hoffmann and Woodward. "Selection rules for concerted cycloaddition reactions."

The major interest I got early on, at two national meetings. One [was] an organic symposium in June ’64, where I just mentioned the beginning of the story, [and spoke of my other calculations on organic molecules]. Then in October ’64, the US Army Research Office [. . .] ran an annual symposium at Natick, [. . .] Massachusetts. [. . .] Criegee [gave a major lecture. After it, I made a comment, telling people of the orbital explanation]. And several people in the audience, and Jeff [Seeman] has hunted them down, remember my comments. [. . .] But I think Criegee was puzzled; [. . .] he wasn’t schooled in orbital ways. [. . .]

[Woodward himself was brought up with and used mainly valence bond ideas], resonance structures. Molecular orbital theory comes later for him, I’m convinced [that he learned MO theory through] the influence of Bill Moffitt, that same person that I went to work with at Harvard, who died [in 1958. Moffitt] was a friend of Woodward. [. . .] They were involved in two stories together, the ferrocene structure, and [the theory of] the octant rule. Moffitt provided the theoretical explanation of the empirical deduction of the octant rule, and that is, I think, when Woodward began to think in orbital ideas. This is now around the period of ’55 to ’58. [. . .]

CARUSO: One thing that I’m curious about, **<T: 30 min>** partly because I know what happens in 1981, was there any connection to the science that was happening—you’ve mentioned connections in Europe, but was there any knowledge of what was happening in Japan? Was that a community that really—there was no common language at the time?

HOFFMANN: The Japanese community was rising rapidly, too. Not experimentally in physical organic, there was little tradition there. But the theoretical community was good. I knew of Fukui’s work—[his considerations were at that time all based on Hückel’s theory. Until we devised the extended Hückel method], people were stuck on [. . .] planar molecules with pi systems. [. . .]

A good indicator of the knowledge of the time is Andy [Andrew J.] Streitwieser [Jr.]’s influential book of 1960 on molecular orbital theory, and Jack [D.] Roberts’ much shorter teaching primer.[49] [These introduced] organic chemists [to] molecular orbital theory. There were other important books in Russia and France, but they did not reach the consciousness of the [American and European] organic chemists. Coulson’s *Valence*, a tremendously important book, did not have enough about organic chemistry.[50]

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[49] Andrew Streitwieser. *Molecular Orbital Theory for Organic Chemists.* (New York: Wiley, 1961); John D. Roberts. *Notes on Molecular Orbital Calculations*. (New York: W.A. Benjamin, 1961). See also: Andrew Streitwieser, Jr., interview by Leon Gortler at Latimer Hall at the University of California, 22 January 1981(Philadelphia: Chemical Heritage Foundation, Oral History Transcript # 0007); and John D. Roberts, interview by James J. Bohning, David Caruso and Patrick Shea at Chemical Heritage Foundation, Philadelphia, Pennsylvania, 25 April and 14 June 1987 and 12 April 2012 (Philadelphia: Science History Institute, Oral History Transcript #0069).
[50] C.A. Coulson. *Valence, 2nd ed.* (London, New York: Oxford University Press, 1961).

There was a lot of discussion about reactivity indices from Hückel calculations, [indices] which would tell you where nucleophilic or electrophilic [. . .] reactions would go on organic pi systems. [Fukui] devised his frontier orbital ideas in the context of a reactivity index, and because his background was also from polymer chemistry, he was one of the few who talked about radical reactions. [His work] was known to the community of theoretical chemists. [. . .]

I meet Fukui [for the] first time in February '64. There is a Sanibel conference run by Löwdin, and Fukui [and I go to] it. He comes to visit Harvard—[Fukui is very interested in the extended Hückel method]. I was his host [in that visit. But it is a few months short of my hearing about the electrocyclic reaction problem.] We talk, but [not] about these reactions. Our work [on electrocyclic reactions, and then cycloadditions] was developed independently. But it could have been done with his methodology. He could have done it. He didn't, until after. Jeff Seeman has a catalogue of maybe about fifteen people who [were intellectually in a position to do] what we did.

REINHARDT: You were describing the reaction by physical organic chemists, but of course, there's also the other important community for you, which is the theoretical chemists.

HOFFMANN: Yes.

REINHARDT: What was their reaction?

HOFFMANN: For the first [few months] or so, there was [little] reaction. [. . .] Which is why I didn't get those jobs that I told you about. Then what happens is [Hugh] Christopher Longuet-Higgins and Abrahamson, who was a very good physical chemist, a postdoc of Longuet-Higgins, submit in December a more symmetry-based explanation of the stereochemistry **<T: 35 min>** of electrocyclic reactions and draw some of the first [. . .] published correlation diagrams, which show how levels behave in the course of reaction.[51] We get that paper as a preprint. We [may have gotten] it to review. We approve it. That paper gave me the idea of using the correlation diagrams, which I had drawn previously for some [transformations, such as that of tetrahedrane and cyclobutadiene], but didn't realize how important [a tool] they were. The [correlation diagrams] gave me another way, [perhaps simpler], to analyze [. . .] cycloadditions. [Meanwhile I am doing calculations, following orbitals through a reaction.] So, we use [correlation diagrams] in our second paper.

Somehow, Longuet-Higgins, using [his] formal symmetry-based approach, legitimizes in the eyes of theoretical community, of which he was a prime member, our [approach].

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[51] H.C. Longuet-Higgins and E. W. Abrahamson. "The electronic mechanism of electrocyclic reactions." *Journal of the American Chemical Society* 87, no. 9 (1965): 2045-2046.

REINHARDT: Did he know about your first paper?

HOFFMANN: Yes. First of all, he knew about the problem, because Woodward posed it as a problem to him [earlier in 1964]. Did he know of our first paper when he published his? No, [. . .] he didn't know [of our first paper] at the time he [with Abrahamson] . . . [Once we got his preprint, in December 1964 or January 1965], Woodward sent him a preprint of our paper. [. . .] In our third important paper on sigmatropic reactions, we didn't use the [correlation diagrams—though they fill my notebooks of the time].[52] We used symmetry [of orbitals in the transition state of the reactions], but we didn't use correlation diagrams [in the third paper].

Those correlation diagrams were imprisoning, in a way, even as they were very useful. But [they] connected me again to the theoretical community. The theoretical community, though, was moving beyond the extended Hückel calculations that came out from the Lipscomb work, [the extended Hückel calculations] that I used on the orbital symmetry story in the beginning, and that I continued to use from then on for thirty years to do a lot of good chemistry.

Those semi-empirical calculations, which were at the forefront of theoretical chemistry in 1964, within two or three years were viewed as too simple. They were surpassed by the so-called *ab initio* calculations. And so as a joke, later on, I would say that, "We do the kind of calculations—extended Hückel calculations—to which all other methods are superior. And you can be sure that the authors of those methods tell us so."

What I [was] reflecting on, [slightly bitterly], was typical referees' comments that we got. They would say, "This can't be right, [it's done with an unreliable method]." And of course, what kept us going is [that]—first of all, the [method wasn't] so bad: it captured the [electronic] essence of the process. Second, I knew the chemistry, which the other theoreticians didn't. So, what [those nasty critics] didn't realize is [that] they were saying that [chemistry] is not a matter of solving the equations exactly. It's a matter of getting an approximate theory and it making chemical sense. Somehow, I stayed ahead, because I knew the chemistry.

REINHARDT: So, what you are saying, if I understand right, is that this was application driven, chemistry driven, organic chemistry driven at that time?

HOFFMANN: Inorganic chemistry very soon [thereafter]—

REINHARDT: Very soon, also.

[52] R.B. Woodward and Roald Hoffmann. "Selection rules for sigmatropic reactions."

HOFFMANN: Seventy-five on.

REINHARDT: But it was problem driven and not method driven, **<T: 40 min>** in a way.

HOFFMANN: Absolutely. I was interested in explaining chemistry. I loved chemistry.

REINHARDT: But if I understand what you say, you encountered problems in your own community as a theoretician?

HOFFMANN: Yes.

REINHARDT: How did you solve that part? Did you solve—

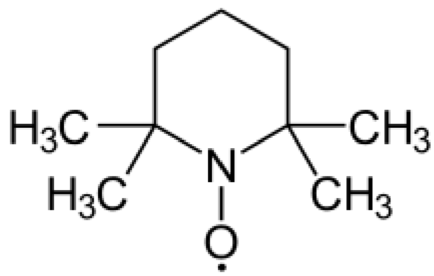
HOFFMANN: By keeping on doing more chemistry [of use to the community. It was not easy]—at one point, [true] much later on, I lost all my funding. The bad referees' comments, you can overcome, you can answer [them]. The bad reviewers' comments on a grant proposal you don't get a chance to answer. [. . .] In early 2000, I lost all my NSF funding—[NSF was the only agency that would support the fundamental chemistry I was doing]—on [the basis of reviews] which mixed some skepticism about the science we were doing with some nasty comments about the outreach. I was beginning [to run] this *Entertaining Science* cabaret, and I put [my experience with the cabaret] into the outreach section. [53] And some people didn't like it—[it hurt that NSF did not "protect" me, taking its outreach criteria for funding seriously].

[I came back, NSF came back]. I regained the funding in two years, so it was not a problem. But [all these years] there was a continuing criticism of [my] methodology. And, at the same time, an appreciation [of the work] by the chemical community in each [subfield of chemistry that I entered. Still,] I think many, many theoreticians did not understand why our work was so successful. And the answer was simply that I was [fundamentally] a chemist. [. . .] And that's [. . .] what the Woodward story—[the collaboration with RBW]—taught me.

Later, I went into inorganic chemistry largely on my own—[with some guidance from Earl Muetterties]—and I learned that field. And now, in the last twenty, thirty years, I'm in solid-state chemistry, mostly inorganic, and close to condensed metal physics, [more specifically] materials under high pressure. It's always been the greatest fun to learn the knowledge base, the experimental knowledge base, in each of these communities. [I continue to enjoy this] to this day. Just yesterday, we're doing something on nitroxyl free radicals. Back to

[53] See http://www.roaldhoffmann.com/entertaining-science.

organic chemistry. [I just did not know much stable free radicals. Then I found a group of papers that showed me that] nitroxyls [R_2NO] are a class of stable free radicals. Stable [here] meaning kinetically persistent. [And for that matter, also thermodynamically stable.] The molecules are simple, a nitrogen bonded to an oxygen, and two substituents, methyl groups, [on the N. How stable these are is demonstrated by TEMPO, a lovely red compound]—you can buy a bottle of one of them, and [when you do, you have in your hand a mole of unpaired electrons. They] don't dimerize.



The usual fate of free radicals, [molecules] with an odd number of electrons, [is that they dimerize readily]. So, hydrogen is a free radical—a hydrogen atom, [so is] a methyl group, CH_3, [or phenyl] C_6H_5. [. . .] You [can] generate them, you can study them in a matrix at liquid helium temperatures. You can study them flying down a molecular beam. But if you try to isolate them, they dimerize, because their reaction, [say of] two hydrogens to give H_2, has no barrier and is exothermic by 104 kilocalories. So, [free radicals] dimerize like a shot. [But the] nitroxyls [I am talking about, that Peng Xu in my group has studied,] don't dimerize.

We were just looking at why they don't dimerize. [. . .] It turns out [first of all that the dimers, with NN, NO, or OO bonds are relatively unstable, those bonds weakened by the lone pairs next to them. The nitroxyls instead form weak complexes, dimers with an NO parallel to another molecules ON, sort of side by side. There is a bonding interaction between the two radicals, but it is barely stronger than a Van der Waals contact. The ON…ON distance is a long] 2.8 angstroms. We have [. . .] a molecular orbital analysis of this.

There I am, looking at the **<T: 45 min>** literature, and it's still fun, fifty-four years down the road, [to learn that you can have a bottle of unpaired spins].

REINHARDT: How do you see molecules?

HOFFMANN: I see them the way they are represented on the page. I think our imagination is geometric, rather than algebraic. I even think that's true of mathematicians; [. . .] though algebra has by and large won the day in mathematics. But I think the inner representations that are in [mathematician's minds] are geometrical, though sometimes I think lines of an algebraic proof acquire geometric form in the mind. A friend of mind in philosophy of mathematics has written a little about this, Emily [R.] Grosholz at Penn State. She'd be interesting to have at [the Science

History Institute]. She and I have written two articles about iconic and symbolic representations in chemistry.[54]

Chemistry is a curious mixture of the two. It's obvious from the beginning. You write a formula, C_2H_6, the C and the H are symbolic, and the 2 and the 6 are iconic, right in there—[representing real ratios of atoms in the compound. I spoke about my] adding those orbitals to the geometric stereochemical formulas [that chemists were used to. Well, in doing so] we are walking in some land between symbolic and iconic, semiotic representations. Emily and I have written a little about that. And I like case studies. We took a paper by Andy [D.] Hamilton and took it apart in terms of the semiotic representations [used in the paper]. [. . .]

How do I [see] molecules? So, I see them at various levels, and I can move between [those levels. In the beginning,] I see a structural formula, like I see it on a page. I sketch it, as a quasi two-dimensional representation of a three-dimensional object. [That's the next level.] I do not think [easily] of the atoms vibrating, [though I know they are]. [. . .] I turn on some switch [in my mind, and I begin to think of the atoms in the molecule] vibrating. [. . .] But in the first instance, I see it just like you see it on a page. This is why [the evolving] story about paper tools, typographic conventions, [and the various ways we have of] representing molecules is important.

So, as long as [printers] insisted that they could not set [lines at an angle in chemical formulas], and could only set straight lines, [then such "rectilinear" formulas] were imprinted in the minds of chemists. [I think this is why it took] seventy years between Sachs' representation of the six-membered ring in cyclohexane and Barton's stereochemical analysis. Why [so long]? After we thought that [Jacobus H.] Van't Hoff and [Joseph A.] Le Bel gave us a way to see [. . .] "chemistry in space"—that's [the title of Van't Hoff's book] in Dutch, and in the French edition of the 1874 book.[55] [. . .]

[One has to have a] stereochemical imagination [for chemistry]. [. . .] We now have computer drawings of the molecules as they emerge from a crystal structure. [But they] are not portable; they are not sketchable by a chemist **<T: 50 min>** on a piece of paper. There will come a day when, [as] in the movie *Matrix*, all of us have plugs in the back of our head. Those crystal structures will come [into our mind via] some implant, and those crystal structures will be immediately turned into virtual reality. [. . .] [A stereo image will flash into our mind]. And then the [chemist's] imagination may change. And then these two-dimensional media [that] have served the community for hundreds of years— the chalkboard, this piece of paper here—they will be obsolete.

CARUSO: And just to follow up on this, one question I have then is, what is the value in being able to see molecules? Thinking about it both as the two-dimensional sense, the drawings that

[54] Emily Grosholz and Roald Hoffmann. "How Symbolic and Iconic Languages Bridge the Two Worlds of the Chemist," in *Of Minds and Molecules: New Philosophical Perspectives on Chemistry*, ed. Nalini Bhushan and Stuart Rosenfeld (Oxford, New York: Oxford University Press, 2000), 230-247.
[55] J.H. Van't Hoff. *Lagerung der Atome im Raume*, tr. And ed. By Arnold Eiloart (London: Green and Co., 1898).

you've just done, but also the three-dimensional sense. What value does that add to or what knowledge does that help us understand in terms of chemistry and . . .

HOFFMANN: [. . .] First of all, there is the macro to micro motion. [. . .] From the substances in compounds made in a laboratory [to a microscopic understanding, on the scale of atoms] in molecules. That was the greatest conceptual transformation in chemistry [toward] the end of the nineteenth century, and [into] then the twentieth. The growing conviction that [there existed a] microscopic structure of molecules, even before we knew that structure, before we had any idea of the metrics. You have to remember, the crystal structure of diamond was done just about [one] hundred years ago, for the first time, during World War I. It was the first time we had [experimentally] the length of a CC bond.

The conception that inside [of matter] there were molecules, and that their shape affected reactions, [that reactions were to be seen as] transformations of molecules, was a slowly growing construct of the late nineteenth century, I think. [The model took hold, in more ways than one]—that those molecules are quasi-classical objects, so they are like balls connected with springs, maybe, if not sticks. And that [. . .] the transformations were of value—and I mean [. . .] commercial value—[was very important. In what we can loosely speak of as a] billiard ball imagination, [we could conceive of] these little microscopic objects changing in a course of reaction. We could imagine an S_N2 substitution, or we could imagine [a reaction of] an aromatic [molecule. It was amazing that you could turn such reactions], making let us say nitrobenzene from benzene, [. . .] that you could turn this to practical value. [. . .] I think steroid transformations are a crucial point in the twentieth century, [for this class of molecules are] so central to many biological functions. [Think of] cortisone, the birth control pills, bile acids—all these are **<T: 55 min>** steroids.

And, obviously, [interest and value arise from] function, [as exemplified by] amphetamine, serotonin, neurotransmitters, rather simple molecules. That you could affect a small change—amphetamine there—and that you could plan a synthesis of an interesting steroid, [those are incredible achievements from a molecular model]. Woodward plays a role in [the way forward], and so does [Carl] Djerassi, in the mid-twentieth century.[56] [They] convinced the community that they could make almost anything in the [organic world], and that's where we are right now.

That that way of thinking—[an atom is a ball—is] a classical quasi-mechanical, quasi-Newtonian way of [imagining and manipulating] the molecular world. [To act on it] you had to establish that [actions] on a microscopic level could affect properties at a macroscopic level. That was at the nineteenth century [and into the first half of the twentieth]. In scope and structure, vibrations don't matter much, though, [carefully thought about], they actually enable the reactions. Organic chemists thought about [their world pretty] mechanically. So did inorganic chemists.

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[56] Carl Djerassi, interview by Jeffrey L. Sturchio and Arnold Thackray at Stanford University on 31 July 1985 (Philadelphia: Chemical Heritage Foundation, Oral History Transcript #0017).

CARUSO: Well, one other thing that I was going to ask, I know you mentioned having spoken to Woodward about whether or not Corey played a role prior to publication, and also that you had spoken to Corey. In the wake of the publication—

HOFFMANN: I didn't speak to [Corey and Woodward] as clearly as [now I wish I had]. But you have to put this in a context of our different status in life, and the power relationships, [in 1964]. I mentioned I was twenty-seven at the time. Corey was thirty-seven. Woodward was forty-seven. Woodward was at the top [of his profession, Corey moving to leadership]. I was a very bright postdoc.

CARUSO: I was just wondering if in the wake of the publications, Corey made any contact about the—I mean, I know that he writes something in 2004. I was just wondering—

HOFFMANN: One sentence. [laughter]

CARUSO: One sentence.

HOFFMANN: Is what he writes in 2004.

CARUSO: Okay. So, there was nothing in the interim that was expressed to you? [. . .]

HOFFMANN: [Yes, there were scattered comments to me] in the interim—which Jeff will detail. He never talks to Woodward about it. [Corey] apparently talked about [the matter] to other people in the Harvard department who advised him to do nothing. In the period [in 1964 that] we're doing the work, he obliquely talks to me. It's as if he is trying to talk to Woodward through me. [Ultimately, I think this was the wrong thing for Corey to do, to effectively try to communicate to one of his colleagues through a younger student. At the time, EJ gives me in the conversations we had] the sense that he, [EJ], has a stake in the work, but [. . .] he doesn't say so explicitly. My memory is not too good. Maybe that has to do with the [wartime], too. [I am not looking for excuses]. My memory in general is not—except for chemistry—is not that good.

Corey [makes] a comment to me that I don't understand at first, in the seventies, when he visits [Cornell]. He says, "I really made your career when I told Woodward the story," [as best as I remember it, or something like that]. **<T: 60 min>**. At this point, Woodward's still alive. [This feeling of a great injustice done to him, an idea stolen, has eaten away at Corey all his life, it seems. And it bursts out from time to time].

[I was told that he once spoke of the matter] in a course he teaches. [. . .] Some of Woodward's students are in a course; they go to Woodward and [ask] him, and he tells them that there's nothing to this story. [At another time he puts it in a small biography on his webpage at Harvard, I was told. But he doesn't speak to Woodward, nor publishes anything staking out his claim in Woodward's lifetime.]

[. . .] In 1981, when Nobel Prize is announced to me and Fukui, Corey writes to me, and those letters are detailed in my article, and those letters are [. . .] on deposit in the Cornell [University] Library.[57] In [these letters he] accuses Woodward and me of dishonesty and conspiring to keep his, [EJ's,] contributions quiet. At this point, Woodward is dead two years, 1981. He dies in '79, aged sixty-two.

[There is a pervasive sense of honesty in Corey's statements. He has been hurt, deeply so. I do not doubt that there was an important conversation with RBW prior to my getting involved in the story. But because of Corey's reluctance to speak to RBW or in public during the fifteen years when he could have done so, we only have his account of what happened in that conversation. Corey] has assembled a dossier on the case, [with] what he sees as evidence of what happened. [And recently he has sent to me a paper he has written on the matter. At other times, he has said that something will be published after he passes away.] I hope that he tells his side of the story [now, because waiting would put] a great burden on his family [to decide whether to publish Corey's account]. [. . .]

CARUSO: Right.

HOFFMANN: [. . .] I still have hope [Corey] will talk to Jeff Seeman, [who is a superb and fair historian, with special competence in the state of physical organic chemistry in 1960s. Perhaps,] when the reality of Jeff's publication on [the Corey claim and the discovery of the orbital symmetry control of reactions is published—I estimate it will be two books' worth—maybe EJ] will talk to Jeff. [I wish he would.]

CARUSO: [. . .] Okay. Did you have—

REINHARDT: Are you okay with that?

CARUSO: Yes.

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[57] Roald Hoffmann. "A Claim on the Development of the Frontier Orbital Explanation of Electrocyclic Reactions," *Angewandte Chemie* 116, no. 48 (2004): 6748-6752.

REINHARDT: My proposal would be actually to go into a bit different territory now.

HOFFMANN: Yes.

REINHARDT: And you mentioned yesterday the importance of this love-hate relationship with computers.

HOFFMANN: Yes.

REINHARDT: And I think that that's a good point.

CARUSO: Right. And I was going to ask that also in the context of—I mean, you start at Cornell in 1965. So, you're transitioning to a faculty position. I'm also wondering what Cornell has in terms of computer systems at that time, because I'm not sure how they compared to Harvard.

HOFFMANN: Yes. Harvard was the place of **<T: 65 min>** one of the first [electromechanical computers, the MARK-I -IV. By the time I came to graduate school in 1955 we had at our disposal early IBM computers, with programs on cards, made using keypunches].

Cornell's facilities in computing were comparable to those of Harvard. Computing was important to me. [. . .] The appointment I was offered [at Cornell was that of] an associate professor without tenure, a rather unusual appointment. It recognized the Junior Fellowship years [at Harvard] as important. I did not receive tenure till '68, and a year later was promoted to full professor, probably as a result of an offer, one of two offers that I considered seriously in my life, which was from the ETH [Swiss Federal Institute of Technology] in Zürich in organic chemistry, in '68. [The ETH] was the top department in the world [. . .]. [It had faculty such as Vladimir] Prelog, [Albert J.] Eschenmoser, Duilio Arigoni and [Jack D.] Dunitz, those are pretty incredible people.[58] I and my wife were Europeans initially, so the cultural shock would not be that great, but for various reasons, we decided not to go. I don't think the ETH people knew how to [run a modern search—for instance,] they didn't invite my wife to come along on the interview. [. . .]

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[58] Vladimir Prelog, interview by Tonja Koeppel at the Swiss Federal Institute of Technology, Zürich, Switzerland, 17 January 1984 (Philadelphia: Chemical Heritage Foundation, Oral History Transcript # 0038); Albert Eschenmoser, interview by Tonja A. Koeppel at the Swiss Federal Institute of Technology on 7 October 1985 (Philadelphia: Chemical Heritage Foundation, Oral History Transcript #0019).

We stayed [at Cornell]. I could tell you some of the reasons. But they have to do with Ithaca more than [the ETH]—with a very collegial department here. The second offer [I contemplated was in 1974], from Harvard [. . .]. Woodward still very much alive. Corey certainly an ascending power. There were two poles in the organic department.

What was interesting was [that] at the end of the Junior Fellowship, Lipscomb apparently suggested to the department that they offer me a job at Harvard. Somehow, I think the physical chemists didn't think I was [good enough; I described earlier] this Wilson-Lipscomb tension [in 1962]. I wasn't offered a job. In 1965, I'm working with Woodward, and I'm a student of Lipscomb, two great chemists in that department. But [their opinions] weren't strong enough to convince the physical chemists to hire me. It would be interesting to [read of the discussion, among them].

The Harvard offer [was] in '74, I turned that down. [What] I got out of it was the bathroom in back of that wall. I call it the Harvard bathroom. Cornell said, "What can we do for you?" I said, "You can match the salary." I wasn't going to go, in the end, for, again [as for the ETH offer], a variety of reasons. A lot had to do [with my perception of] Harvard. I [thought of the department] there as a bunch of primadonnas, rather than a collegial department. [. . .]

REINHARDT: What was the job you were offered? Was it in physical chemistry, or—

HOFFMANN: Yes. [. . .] Well, there's no great divisional structure in American universities. But yes, [theoretical chemistry. The same people were there in 1974 at Harvard], but the dynamic had changed, and [my] work was seen as valuable. I wasn't going to go, [Cornell asked what I wanted], so I said I wanted a bathroom. So I got a bathroom.

Anyway, at Cornell, I was quickly promoted to tenure. There was a little episode with one negative letter from, [apparently], **<T: 70 min>** Michael Dewar.[59] But they overcame it. Things went very well here [at Cornell], and I've been very happy here. The department is collegial. I've been chairman; we all take turns at being chairman. [. . .] Teaching is [valued], which is important to me. I taught introductory chemistry half the time, by choice. [Other people active in research teach introductory chemistry—I like that]. Slowly, I developed an interaction with people in the humanities. It was much easier to do this here than it would have been at Columbia or Harvard.

What happens there is [that] people don't live near the university. They disperse [after work]. And if I want to meet someone who is, [say], a well-known poet, [to meet them informally] would be harder to do it. You don't just go over to somebody and say, "Can you look at my poems?" You have to meet them socially first, and then maybe you feel comfortable saying that, "I also write, and could you take a look at these?"

[59] Michael J.S. Dewar, Oral History Transcript #0087.

And here, Archie [R.] Ammons, who was a wonderful poet and became a friend and my guru in poetry, he went to the [same] farmer's market where I went every weekend, and we went to the same coffee shop. I could meet him, [I could talk to him. Ithaca] also was a good place to bring up children. Here, you could hope to buy three acres of land, one hectare. Imagine buying a hectare of land in Zürich around your house. We got used to living in nature. [. . .]

CARUSO: And what is it like establishing yourself as a theoretical chemist at a university? A lot of the people I've interviewed, they talk about, you know, setting up a lab, and getting graduate students. What was it like for you, establishing yourself? Is there a similar process?

HOFFMANN: [. . .] At a major American university, part of your world is the department, another part is the world outside. [. . .] The world outside means publishing and getting grants for support of research, and those are evaluated by people not at your university at all. [. . .] It's an interesting balance—[the world at the university, the world outside]. The two worlds influence each other. How your colleagues treat you in terms of a promotion or a salary depends on your reputation outside as well.

In terms of physically starting up, it is very much [the same as it was]—you get graduate students, and then if you have research grants, you can have postdocs. These days, we supply [even] a theoretical chemist with about a half a million dollars, [a "start-up" package]. [. . .] And an experimentalist with a million. [The money ultimately comes from the university. Part of the start-up funds could be used] for a postdoc for a year or two. I didn't [get] anything like that, but there was a little money for computing, which was charged at that time. There was no secretarial help. Later, I had some [money to hire a secretary or assistant] from a research grant. [. . .]

In the beginning, we could buy books on our research grants. [I bought lots of books.] Later, we were not allowed to do that by the government [regulations]. There was travel money from the research grants. [. . .]

I had my first graduate student within a year, but in the first five years, I published more with **<T: 75 min>** undergraduates than I did with graduate students. [Cornell undergraduates were—and are—so good! When I was] teaching introductory chemistry. I would pick the best student in the class and offer them a summer job. And I then I had a coworker for three years. [. . .] There were some very good people in that group, [including Warren Hehre, who went on to found a quantum chemistry software company].

I don't think I published a paper with a graduate student until four years [at Cornell]—it just takes time for a graduate student to tool up. There were postdocs [that I worked with in those beginning years]. Among the first of [many German coworkers—in the end I had] twenty-two German ones—was Rolf Gleiter, who then became a professor at [University of] Heidelberg, [Germany]. [Another Heidelberg professor, Peter Hofmann, was a postdoc here, a third, Lorenz [S.] Cederbaum, was a senior visitor.]

We developed the beginnings of a research group, I would say, within about three years or so. [Over the years,] the group varied in size from nothing in the beginning to about ten people [at its highest]. Ten people counts the postdocs, graduate students, and one or two undergraduates at all times. Right now, after retirement, my group has gone down (by choice), and it's now at four people or so—postdocs all.

REINHARDT: How was the division of labor, if there was any? Did you have to cover certain specialties, certain methodologies in your group? Or was everybody doing almost the same thing, but just at different levels of expertise? Could you describe that a bit?

HOFFMANN: [. . .] That's an interesting question; [could this be] the secret of success of American graduate education in chemistry, or in science in general? The background [is this, as I see it]: at the end of high school, the typical European *gymnasium* graduate is two years ahead of the American one. At the end of the university, [age twenty-two or twenty-three he or she is] still two years ahead. The reason [. . .] is that we have a liberal arts education, [while] in Germany, they're studying all chemistry, or in Japan.

So, at the beginning of a PhD in chemistry, at age, [typically], twenty-two, twenty-three, the American is two years behind, I would say. By the end of the PhD, they've caught up. [Yes, part of the story] is that the PhD [study period] here is longer. It takes typically five years. In Europe, it is often three years. In part, [a key to catching up] is that we have very well-structured courses, actually as part of the PhD, [at least] at the beginning. Not too many [courses, but good ones]. The second part, I think the hidden part, is the [American] structure of group meetings, and [the structure of a cohesive] scientific group. [In my case], we have two [meetings] a week, lasting for typically two to three hours each. We didn't have one [. . .] yesterday, but we had an extra one the day before.

Every group is different. Some group [meetings] are very structured, so that people are assigned to report on their work at regular intervals, or they have assigned certain journals [from which] to bring an article from literature. My group [meetings] were not structured. I just asked, "Has somebody seen anything in the literature?" If they don't bring something in for six weeks, I go and talk to them and say, you should bring it in. They listen.

[Or] we talk about some research [at these group meetings]. I bring some things from the literature. Later this afternoon, one of the people has got an interview for a job in Canada for an **<T: 80 min>** assistant professor [position]. He's going to practice his talk on us. We do that—everything. It's in those group meetings [that] I will make comments, that this work is a piece of crap, even though that work is supported by the National Science Foundation and published in *JACS* [*Journal of American Chemical Society*]. At other times, [I'll say, "this is really nice."] The students[/postdocs/visitors] get an idea of informal evaluation of quality in science. I give sharp criticism of their presentations, [they know I have listened to them, seen their slides, every slide]. It's actually a wonderful structure, [this group meeting].

[. . .] You asked a little different question, and that is how the work apportioned. I've always operated on the principle that everybody in the group knows what everybody else is doing. And they help each other. So, I give them grief if they tell me that, "I couldn't get this program to work," or "I couldn't get it to give this particular indicator out of the computer software," and I find out that they didn't ask somebody in the group about how to do it. Usually, they do ask, and they learn.

[. . .] The papers [we publish] often involve two people in the groups. [. . .] I like to have each person working on more than one problem at a time. I just think it's more efficient [that way]; if they run into a problem on one [project], then they shift to the other. [When they join the group], I ask them [. . .], "Is there something you want to work on?" If they give me something reasonable, I will [generally] say yes, because by now, we essentially [can] work on anything except biochemical molecules. Organic, inorganic, solid state. [All of them present problems that interest me. And I love it when the postdocs through their interests take me into another field, something I could not have imagined I would be working on.]

If they don't have anything [from their side], then I give them a choice of two or three projects. [. . .] Those colored folders up there [pointing to a stack of folders] are projects. [They may be a] group of papers about something that I think is worth working on. Other [potential problems] come up from visitors coming by, from letters, from the literature.

We are often in a mode of solving bonding puzzles, something weird in the geometry of a molecule or a reaction. My general feeling is that everything in the world is connected to everything else. That's something I try to teach [my coworkers]. So that it doesn't matter what we begin to work on, it's going to be connected to something else [we've done, or that they are interested in, or that the community finds exciting].

I have a lot of trouble with mission-oriented research, like working on hydrogen storage, or [. . .] on better batteries. [I know these are important]. I have occasionally tried to get some [financial support] for those things. But I've been fortunate most of [my] life to get support from the NSF to work on any molecule under the sun. This is a great luxury. We [do] have a track record for [making] connections [between different areas of chemistry] and for getting something interesting—[understanding, suggestions of new molecules]—out of it.

REINHARDT: How do you establish these connections? I mean, I understand that you start with very specific molecules, maybe with unusual geometry.

HOFFMANN: Maybe.

REINHARDT: And I understand also that you need quite a bit of expertise in a certain class of compounds. I mean, some groups just work as you told us about Gouterman's, right, about porphyrins.

HOFFMANN: Yes. **<T: 85 min>**

REINHARDT: [All] their life. Obviously, you do almost the opposite, any molecule under the sun.

HOFFMANN: Yes. Any molecule under the sun.

REINHARDT: What is the common denominator? How do you build these bridges in the group?

HOFFMANN: [. . .] I think the common denominator is that I'm building a world view [constructed] of little pieces of theory that explain structure and reactivity. Though recently, I've been interested in [. . .] superconductivity, [a desired] property. [The worldview, put together from little pieces of theory, is] an orbital view. I believe that it's the electrons in the molecules [that are responsible for their shapes and properties]. And I want to see how that is played out. [. . .]

[Let me] give you two case studies. [. . .] One that we're involved in [just] now [has to do] with these nitroxide radicals. It started from a very physical chemistry problem. A new postdoc in the group, [Tao Zeng], came from Canada. [. . .] He came with his own [support] and is working together with me and a new [younger colleague], Nandini Ananth. Tao and Nandini decided we would work on singlet fission. Singlet fission is a very hot phenomenon now, driven by solar energy conversion. The normal way that solar energy conversion operates is you excite a molecule with the sunlight. That molecule passes on the excitation in a crystal or in a liquid to an interface. [. . .] One molecule [is] excited, the next molecule [is in its] ground state, and then the [excitation migrates, a so-called] exciton forms. [. . .] I worked on [exciton theory] in Russia in [1960. The excitation moves] to an interface, where the excited state transfers an electron to an acceptor molecule, typically a fullerene, and the electron goes off with the fullerene as a negative charge, and what's left behind is a positive charge on the molecule.

So, essentially, an excited state is split into an electron and a hole. The two propagate. They generate the current. [This is the] principle of solar cell construction, a chromophore to capture the energy, migration of the energy to an interface, the creation of an ion pair, and that's the current.

There is a natural limit on the efficiency of this [scheme, of 33] percent, for thermodynamic reasons. A way to surpass that limit is what singlet fission is. In singlet fission, you make an excited singlet state of a molecule, a normal thing, by absorption of light, visible light. And then that singlet state generates [not one excitation, but two independent one, two triplet states. Normally the excited state, a singlet, would go down a triplet state, which then might emit light, phosphoresce. But in singlet fission, the product from that singlet is two triplet state molecules. There is] **<T: 90 min>** a thermodynamic condition that the energy of the singlet [be] twice the energy of the triplet. Otherwise, this won't work. The two triplets then migrate, and so this is a way of getting two photons [out of] one.

REINHARDT: Do you double the efficient, then, for that?

HOFFMANN: Not quite, but—

REINHARDT: Not quite.

HOFFMANN: Not quite, but you surpass the previous limit. This has been shown experimentally. So, what molecule would do this? [One has been] probed experimentally, [pentacene], which is the workhorse right now of the solar cells that are being designed, [. . .] five benzene rings in a row. We wanted to see how pentacene works, how [singlet] fission works first, and then in a second paper, [. . .] we design alternatives to pentacene [for] singlet fission.[60] In the first paper, I had a minor part. That problem was brought to me by the postdoc; [. . .] I clarified some things, helped them along. I would say of the three authors, I deserved less than one-third of the credit.

In the second paper, in the design of new small molecules, we identified [that] property of the pentacene molecule that makes it meet the singlet fission criterion, that the singlet should be twice the energy of the triplet. This identification was not original to me; it was due to Joseph Michl and to a Japanese group—they made a tentative connection between the diradical character of the molecule and the singlet fission.

[. . .] A diradical means two unpaired electrons. What a diradical guarantees is a low-lying triplet, because [in] a diradical, the triplet and the singlet, the two ways of coupling the spins, are about the same energy. [In a "complete" diradical, the triplet would actually be too low. So, we want] some diradical character, but not [too much]. [. . .] I thought that we could induce this [partial but significant] diradical character by substituting two carbons by boron and nitrogen. I love this BN [boron nitride] substitution. I had [first worked on it in my] boron hydride days with Lipscomb. [The substitution pattern worked in this paper with Tao Zeng. We came up with] three candidates, small molecule candidates for singlet fission. We know of two groups around the world that are trying to make it. What I can bring to this is the realism of fifty years' experience. I can predict which molecules might be actually persistent, stable. [. . .]

[60] Tao Zeng, Roald Hoffmann, and Nandini Ananth. "The low-lying electronic states of pentacene and their roles in singlet fission." *Journal of the American Chemical Society* 136, no. 15 (2014): 5755-5764; Tao Zeng, Nandini Ananth, and Roald Hoffmann. "Seeking small molecules for singlet fission: a heteroatom substitution strategy." *Journal of the American Chemical Society* 136, no. 36 (2014): 12638-12647.

So then [. . .] **<T: 95 min>** I've got a new way of thinking about molecules, [specifically those with] substantial diradical character, meaning that a triplet is close to a singlet. [. . .] I pick up a paper which talks about stable free radicals, and that paper talks about these radicals stabilized by [. . .] "captodative" stabilization.[61] There's a word [for you]: "capto" is acceptor, "dative" is donor. So, it's a pi [electron] system [with a] radical site. [It's substituted by a pi-electron] donor, [say an amine], and an acceptor, so that this could be BH2. [That's the pattern we used] in that second paper.

I began to think about stabilizing radicals by donors and acceptors. Then I started reading about what stabilizes radicals in general. I find these nitroxyl—[the official name is aminoxyl]—radicals, which are RR'NO. [TEMPO is the poster child, that stands for 2,2,6,6-tetramethylpiperidin-1-yloxyl—stable free radical. We're] trying to figure out why they are stable. [. . .]

I have a new postdoc [in my group, Peng Xu]. Her [. . .] PhD is from Iowa State, [but on more complicated] theoretical problems. So, to get her going, I ask her to do some calculations on two nitroxyls, a diradical formed from two of these hooked together. I thought maybe it would be interesting [. . .] to put them in a five-membered ring. [Here], I'm thinking like an organic chemist, and then I'm thinking of coupling the two: [. . .] I'm trying to generate a diradical. [Back to diradicals—everything in the world is connected to everything else.]

I think of this as just as an exercise, mainly, for [Peng] to get some chemical experience. [Why are monoradicals] so stable? [It could be that] the dimerization product of the two has a very weak bond. So I say [to Peng], "Study the dimerization of the nitroxyls." She does that, and gets that instead of forming a full bond, they are sitting close to each other, [forming] a partial bond. I think we'll have a paper out of this. The problem has [certainly evolved], from singlet fission [in] pentacene through [stabilizing a nitroxyl, to a new kind of aggregation of diradicals]. We have something on the dimerization of nitroxyls, which I never would have worked on before. But this is part of the dynamic, [the beautiful dynamic of connections, of working with different skills, who bring their own interests to our group].

In this case, part of the dynamic is also [in linking up] chemical physics, solar energy cells, to organic chemistry, [and the persistence of] stable free radicals. These nitroxyls [are used as] spin labels. People build them into a biological molecule in one place, and then they can study **<T: 100 min>** [the geometry of the biomolecule by the interaction of its nuclei with the odd electron in the spin label]. I know that I could write an NIH proposal around those [radicals], but I'm not going to do it. [. . .]

CARUSO: So, I'm not sure if you want to speak more about your transition from organic to inorganic around '75. If you do, I'd love to hear more about that.

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[61] Heinz G. Viehe, Zdenek Janousek, Robert Merenyi, and Lucien Stella. "The captodative effect." *Accounts of Chemical Research* 18, no. 5 (1985): 148-154.

HOFFMANN: Well, it's not that I was tired of organic chemistry. After the orbital symmetry story, I [looked in some detail, and learning all the way], into [. . .] the electronic structure of most of intermediates in organic reactions. This meant [. . .] carbenes, carbonium ions, benzines. That work went very well. I very quickly got [. . .] into thinking about molecules that don't exist. That is, making predictions of molecules that [might possibly be made]. One of the early, interesting, success stories was a 1970 paper.[62] I don't know what got into me, but I asked [myself (and then a student and a colleague)], "What can we do to make methane planar, instead of tetrahedral?" [This is described in] an article [entitled], "Square Planar Carbon." [The paper is] an example of the utility of MO [molecular orbital] theory. One of the very, very, very few advantages of theory over experiment is that you can do calculations on molecules that are unhappy in some way energetically, just as easily (really, just as badly) as you can do on [a molecule that is] happy.

Of course, [. . .] it's not to judge how unhappy planar methane is relative to tetrahedral. The answer is 100 kilocalories, which is greater than the strength of a CH bond, or about equal. And it's not even a minimum on a potential energy surface. It actually [optimizes to a pyramidal] structure. The purpose [of the calculation], of course, is to alleviate the [molecule's] unhappiness. It's to devise [. . .] a strategy for making [that molecule "happier,"] and still retain that unusual feature [of being square-planar].

[That way of thinking] became a kind of leitmotiv for other things [we did]. We stumbled into it, but [the general strategy] is right there in the beginning. We calculate methane square planar, we look at its orbitals, [those that make it lie at high energy]. And we design then a strategy [for stabilization, which in the case at hand] involves attaching pi acceptors and sigma donors as substituents. [. . .] No one has made such a molecule, [yet]. There are a few molecules, organometallics, [that approach the design]. Nothing very stable.

But [the idea, the strategy, it certainly has] generated food for theoreticians. There've been a few hundred papers [implementing and extending the idea]. That [project—square-planar carbon]—was lots of fun, and I've done that again in some other things. But the first time I stumbled into it. Even right now, we are thinking about something else which is equally **<T: 105 min>** unlikely, and that is what can we do to a methane to keep it tetrahedral, but to make it a triplet ground state? [It appears that having] two very electronegative substituents, two very electropositive, gets very near. [Like] a carbon with two lithiums and two fluorines on it. [. . .] These are not your normal molecules. They're not going to be made in grand quantities. [But perhaps they can be studied] in a matrix isolation experiment. [. . .]

I went from organic [chemistry] to inorganic, in part, because I came from inorganic [chemistry], from the boron hydrides. [It seemed at the time like] there are light years between

[62] Roald Hoffmann, Roger W. Alder, and Charles F. Wilcox Jr. "Planar tetracoordinate carbon." *Journal of the American Chemical Society* 92, no. 16 (1970): 4992-4993.

boron hydrides and transition metal complexes. [But that gap has been bridged, experimentally and theoretically].

[. . .] There is another interesting story [that I am involved in right now], in which symmetry considerations in orbitals [matter. And that story developed before our considerations on orbital symmetry control of organic reactions. This is the story of crystal field theory equals ligand field theory, a theoretical understanding of prime importance in transition metal chemistry and physics. That the d orbitals of a transition metal split three below two in the field of six ligands goes back to 1929. And the orbitals were drawn out then]. [. . .] The crystal field theory was invented by Hans [A.] Bethe, actually, a Cornell connection, in a PhD thesis in 1929.[63] [This was in the] early days of quantum mechanics. A very important [set of papers followed by John H.] Van Vleck, [. . .] a physicist in the United States.

REINHARDT: At Harvard.

HOFFMANN: [For a long time, physicists were most interested in the theory, even as it somehow was very "chemical." World War II intervened. The molecular orbital version of the theory was revived in the 1950s], by [Carl J.] Ballhausen in Denmark, [and by C. K.] Jørgensen, another Dane working elsewhere. [. . .] Leslie [E.] Orgel [wrote] a very influential textbook; [he] went on to be a [prominent] molecular biologist, just died recently.[64] Christopher Longuet-Higgins played some part in [this, as did] Harry [B.] Gray.[65]

[The rediscovery of crystal field theory] coincided also with the [revolution in] organometallics and the ferrocene synthesis. [. . .] But that's another story.

I had the inorganic influence [of the] boron hydrides [early on in my career]. There came [then] to Cornell Earl [L.] Muetterties, who is no longer alive, who then went on to Berkeley. [He really inspired me]. For ten years we worked together: first, on mainly main group [compounds, the archetype being] PF5, pentacoordinate phosphorus. [This introduced me to the] stereochemistry [of inorganic compounds, eventually] organometallics.

I then started on transition metals; [. . .] our first paper was '74. I think by 1980, we were fully into the electronic structure of organometallics, [led by some] very talented postdocs. [You may have noticed] that I did something unconventional in the Nobel lecture. I did not talk about the orbital symmetry work, [spoke of the] isolobal analogy, as a bridge between organometallic and inorganics. I thought that [this choice] was in the spirit of Woodward.

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[63] Hans A. Bethe. "Splitting of terms in crystals." *Ann. Physik* 3, no. 5 (1929): 133

[64] Leslie E. Orgel. *An Introduction to Transition-Metal Chemistry: Ligand-Field Theory*. (London: Wiley, 1960).

[65] Harry B. Gray, interview by Arnold Thackray, Arthur Daemmrich, and David Brock at California Institute of Technology, Pasadena, California, and Chemical Heritage Foundation, Philadelphia, Pennsylvania, on 22 July 2002, 23 August 2006, and 9 September 2012 (Philadelphia: Science History Institute, Oral History Transcript #0256).

By that time, [and simultaneously with the inorganic work], we developed around 1980 the facility to do electronic structure [calculations] of extended systems, meaning minerals, metals, and [in general extended] **<T: 110 min>** solid-state compounds. I worked on that, I would say, desultorily [at first], in the next twenty years. [But then the fascination of these compounds] took over.

REINHARDT: What does facility mean in this regard? You mentioned the facility to deal with these extended structures.

HOFFMANN: Yes.

REINHARDT: Can you describe—

HOFFMANN: [. . .] On one hand, it meant programs to do this. [But] really, what it meant was learning the language of solid-state physics. One of the few books, science books I've written, is called *Solids and Surfaces*, and it's about that.[66] [It's] the language of Brillouin zones, of reciprocal space, of band structures, [and] of Fermi levels. It's the language of solid-state physics.

We came into it from orbitals, and I could see [so clearly] how one moved from orbitals of individual molecules to chains of molecules to the infinite solid. And the physicists didn't see it that way. They [began] instead [with] an infinite solid, [the motion of] free electrons [in it. Then they turned on] the perturbation of the [specifically located atomic cores] on the free electrons. [My way] was putting it together from the [orbitals of the] pieces.

[Aided by some very talented graduate students and postdocs,] I slowly rediscovered all of solid-state physics. [I had at this point] a bridge then between solid-state physics [and solid-state chemistry. When I was] to write something for [*Distillations*]. I wrote about this—"Passerelles."[67] [The small essay is] about building bridges between organic and inorganic, and between chemistry and physics. In another way, maybe there is another bridge to the humanities [that I am treading]. [. . .]

REINHARDT: How did you do that with solid-state physics? I mean, we are now around 1980, I guess?

HOFFMANN: Yes. That's when I began.

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[66] Roald Hoffmann, *Solids and Surfaces: A Chemist's View of Bonding in Extended Surfaces*, (New York: VCH Publishers, 1988).
[67] Roald Hoffmann. "Passerelles." *Distillations* 30 no. 2 (2012), 37.

REINHARDT: Solid-state physics, of course, at that time was a very established field.

HOFFMANN: I know.

REINHARDT: Hard to penetrate, in a way and how did you deal with that? Whom did you talk to, if you talked to someone? How did that happen?

HOFFMANN: I talked to a few people. More recently, I've been talking much more seriously with a leading physicist who had written one of the great textbooks of solid-state physics, Neil [W.] Ashcroft—together with [Nathaniel David] Mermin.[68] Neil and I have joined research groups around the high-pressure area, which is one of my recent interests.

In the beginning, I talked to a few chemists who already were working on that frontier. They were [Michael] Mike [J.] Sienko, here [at Cornell], my colleague, who died in '81. And there was Arndt Simon, who has just retired from the Max Planck Institut for Solid State Research in Stuttgart, [Germany]. [As I described above, I built up] a molecular orbital way of doing solid-state physics, and I learned it just by examples, [by constructing the band structure of first one extended system, then another] of molecules and classes of molecules that we did, just as I learned perturbation theory in the orbital symmetry days. Knowing the formulas [involved], not understanding [exactly what was going on, but wanting to understand things from what I knew, being certain that the connection was there to be found—I found a way to understand, a way I could teach to others]. It's just the way it works for me. It's just lots of fun to penetrate a field that way.

So, then I combined two articles. The only two scientific books I've written. This is **<T: 115 min>** a certain regret, that I haven't written more. Both come from articles, the one with Woodward, the long article in *Angewandte Chemie*, is reprinted in book form.[69] I similarly took two articles, and now not just reprinting, combined them, one from *Angewandte Chemie*, one from *Reviews of Modern Physics*.[70] I was able to publish our chemical view of surfaces in this orbital way eventually in *Reviews of Modern Physics*. Even that publication is prefaced by a comment by the editor saying, "Here is something interesting from a well-known chemist, and he has not quite the usual way of looking at this physics stuff, but we'll let him publish it." Not exactly, but there is a little of that tone [in John Wilkins' comments on the paper].

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[68]Neil W. Ashcroft and N. David Mermin. *Solid State Physics*. New York: Holt, Rinehart and Winston, 1976.
[69] R. B. Woodward and R. Hoffmann. *The Conservation of Orbital Symmetry* (Weinheim/Bergstr: Verlag Chemie, 1970.)
[70] Roald Hoffmann, "A chemical and theoretical way to look at bonding on surfaces." *Reviews of Modern Physics* 60, no. 3 (1988): 601-628. ; Roald Hoffmann, "How chemistry and physics meet in the solid state, *Angewandte Chemie International Edition in English*, 26, no. 9 (1987), pp.846-878.

I took these articles. I put them in a book. [. . .] The book has about two equations in it, and the rest are pictures of orbitals and lots of graphs. [In writing it], I had a twofold idea. One was to teach chemists not to be afraid of the language of solid-state physics, and second was to show to physicists that chemical ideas of bonds and orbitals have significance for doing solid-state physics.

What I can say now, and what I do say in some talks, is in [part of my agenda] I have succeeded. There are now two generations of solid-state chemists working on high temperature superconductors, on magnetic materials, on all these things, who have learned that language from my books. Who've learned not to be afraid of solid-state physics.

In the second aim, convincing physicists that there's something of value in a chemical way of looking at bonding for [understanding] extended materials, nothing. No reaction whatsoever. So, that tells you something about physics and chemistry. In part, we are dealing here with the effects of reductionism in practice—[that it is too hard for physicists to accept that chemists understand something better than they do. Yet] the solid-state physics community is the one closest to chemistry, and the one least susceptible to reductionism, compared to elementary particle physics or [other subfields].

It's been lots of fun, interacting with physics, and the high-pressure community has given me a new playground, the behavior of matter under high pressure. It's not just graphite going into diamond, but also that you get entirely new phases of matter. So, lithium and beryllium form no compounds at one atmosphere. There is no one to one compound, LiBe. There is no alloy. [All we have is] solutions of one in the other. But under pressure, you get four phases that are thermodynamically stable. [There is some sign of one of these that we have predicted.]

Recently, we had a little bit of luck [with] a prediction we made on benzene under pressure. [. . .] The pressures I'm talking about are not the routine pressures of an industrial Haber-Bosch process, which are 300 to 500 atmospheres. The chemical industry can sell you a reactor operating at 500 atmospheres today. We are talking about pressures at the center of the earth, which is 3.5 million atmospheres. You can study those [conditions experimentally], between polished flat faces of gem quality diamonds, and a little cell that [can be held in one hand] **<T: 120 min>** Just two diamonds, a hard metal gasket—a [plate] with a hole drilled in it, [. . .] the sample with diamonds above and below. The whole thing put in a hydrostatic mechanical press, which [perhaps is a meter or two high]. You can reach 3.5 million atmospheres in a reaction space of about a tenth of a millimeter cubed. Still microscopic.

REINHARDT: How do you study the stuff in there?

HOFFMANN: We are lucky. It's diamonds that you have to use, because they're transparent.

REINHARDT: So, you use spectroscopy?

HOFFMANN: [. . .] You can do x-ray diffraction in the limited angle range, because the [geometry of the] diamond is a cone, roughly. [. . .] You can do Raman and some infrared. UV [(ultraviolet light) spectroscopy is not informative, overall. In a few cases NMR (nuclear magnetic resonance) has been measured, but not in the usual analytical organic mode—you can do solid-state NMR, and that has given us some information]. You can attach electrodes, so you can study conductivity. [But most] of the evidence comes from x-ray diffraction [and scattering] and Raman [spectroscopy].

[. . .] How do you know what pressure is in there? You throw in some tiny ruby crystals into the reaction chamber. Ruby is an impurity of chromium in alumina. [. . .] The [Cr^{3+}] is [. . .] a chemical gauge of the pressure. There is a three below two splitting of the [Cr d] orbitals, going back to Hans Bethe again, a crystal field splitting of the levels in an octahedral field. [And three valence electrons in that d level. The color of ruby comes from] the electron jumping [between the 3d orbitals available to it]. The pressure changes the spacing between these two levels, and thus the color of the ruby changes. [. . .] I think it's amusing that the crystal field of chromium is used to measure pressure at 3.5 million atmospheres.

[Remarkable things happen under pressure, not just the formation of Li/Be compounds. For instance], xenon can be made metallic. [. . .] Just imagine that. It doesn't surprise you that xenon can be made a solid. [Under pressure, atoms have to get closer together. So it is no surprise that gases become liquid under pressure—think nitrogen, oxygen, natural gas, which is mostly methane. Apply more pressure and you get a solid—think of dry ice, solid CO_2. Graphite goes to diamond when compressed—deep underground, or in the laboratory]—because the density of diamond is bigger than the density of graphite. [. . .]

Anyway, any gas [will condense under pressure to a solid]. But then you compress [solid xenon] still further for xenon, the energy levels of the xenon begin to overlap, and you get a metal. [Some ionic sats become metallic—that's pretty incredible. You can see the great fun in this.]

REINHARDT: Now you are talking almost like an experimentalist.

HOFFMANN: I know. So, part of the secret of my success is I am, underneath, a chemist who is hiding as a theorist. Just joking, but I can say it another way. [. . .] Had someone exposed me to an inspiring organic course when I was an undergraduate, I'm sure I would have become a synthetic organic chemist. I just like the complexity [of molecules, the millions of combinations that one can make from a limited number of building blocks].

I just told you a story about nitroxyls, [stable free radicals]. It involves a journey from pentacene to diradicals to nitroxyls. Many theoreticians [will undertake that journey if there's a reason. Ideally a reason supported by funding. The reason is to craft a workable solar energy harvesting system. But I am interested in the sequence in another way, coming from the sheer variety of matter and tracing what is possible.] **<T: 125 min>**

[. . .] I take the organic chemist's point of view that the world out there is made out of tunable [molecules that are synthesizable]. So if the molecule isn't quite right, we change it. I got that confidence from talking to Woodward [in those wonderful days in my youth]. I got the confidence that organic chemists can make anything in the world by a Lego construction technique, [that there was no barrier to testing whether a theory was right or wrong—the molecules to do the testing could all be made. With a lot of effort, to be sure. There's more to organic chemistry—for instance, the logic and art of organic synthesis]—but I think that's the true beauty of organic chemistry, the infinite tuneability of properties that we can get.

I mentioned steroids. I mentioned amphetamine. [. . .] What a difference in [the biological effects of] a steroid [is made] by putting a methyl group there. That's the difference between testosterone and one of the female sex hormones, is just a methyl group. And [another] of those female sex hormones is a precursor of testosterone, and another one follows from the [biosynthetic] processing of testosterone. So, nature has made all of these—[or to put it another way, the workings of] evolution [have created these] processes. [. . .] So interesting.

The real joy is that fifty-four years down the line, if we count from [. . .] 1960, when I came back from Russia, the next molecule down the line in the journal still remains a lot of fun. I [am fortunate, to] find new things as I go along.

CARUSO: How did you find out about Woodward's death?

HOFFMANN: Let's see. I believe a colleague, a friend of his, Elkan [R.] Blout called me.[71] He was a close friend. He may have lived in the same apartment building. [RBW] was sixty-two [when he died]. He had stopped smoking, finally, about two years before, so there must have been [. . .] some medical episode where a doctor told him [to do so]. [. . .] He had smoked two, three packs of cigarettes a day all of his life.

We had a close relationship [in the course of the orbital symmetry work, then an interruption in the beginning seventies—perhaps I needed to establish my own research directions. Then] a period near the end of his life where we worked on [the electronic structure of some hypothetical two-dimensional materials. A paper came from that, in the last year of his life. Some of those systems were in time made]. [. . .]

We did those five communications in 1965, the first submitted in '64. Sixty-five was the year I came [to Cornell]. The last of these communications [. . .] were submitted when I was

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[71] Elkan R. Blout, interviews by James J. Bohning and Arnold Thackray at Harvard Medical School, Harvard School of Public Health, and Cambridge, Massachusetts, 30 May 1991, 13 September and 22 November 2002 (Philadelphia: Chemical Heritage Foundation, Oral History Transcript # 0263).

already here. We worked for another **<T: 130 min>** four years on the long paper in *Angewandte*.[72] [In that paper] we have original things. [. . .] Thus, even though every [theoretician] jumped into the field [. . .] —and this is something which Seeman will detail—they [seemed] obsessed with showing that the same results [that we obtained] could be gotten in another way. [Dewar is a good example, and Zimmerman too—I mention the theoreticians who also had excellent organic credentials—they could have gone on to explaining new chemistry and in this way established credibility that their approach was superior. But they didn't].

One of the [subjects that we introduced in the long paper was that of] antarafacial cycloadditions, where you added to an ethylene [or polyene] component on opposite sides in a cycloaddition. [. . .] We published [our long] paper [in late] '69. We did not [. . .] work together for eight years [after that]. I went off into these organic intermediates and inorganic [chemistry]. Woodward [and Eschenmoser finished the B12 synthesis].

[RBW and I] ran into a little bit of trouble on a personal [matter] around 1970, when we were at a meeting in [Karlsruhe, I think]. Aside from smoking, [RBW] was a drinker. [. . .] He made a fetish out of this, drinking a bottle of scotch while he was giving a lecture. [. . .] I don't think he was an alcoholic, but he drank a lot. At this meeting, [. . .] he gave [a lecture]—[traditionally these] lasted four or five hours. [. . .] Someone put out a bottle of scotch on the desk, and he drank from it, and made a big show of [it], [. . .] a kind of teenage bravado. [. . .] At some point, I wanted to say to the person who was pouring, "Don't do that, please," but [. . .] I didn't have the courage. The talk lasted maybe an hour longer than it should have, because [of] the effects of the alcohol. [. . .]

Afterwards, I said to [RBW], "Let me drive you home." And he said, "No, no," and he insisted on driving me. He had his car there. [. . .] I felt so bad about myself not being strong enough to tell him to stop the drinking and to not drive. [Perhaps] that was a [small] breaking point [in my relationship with RBW]. Maybe just as well, because I needed to establish my reputation in some way, [to be] independent. And I did, through the [organic intermediate and the inorganic work we did].

Then around '77, RBW called me up and told me about [his ideas on the] design of organic conductors. We worked on that; [it] was one of the first papers where we [applied] a program for [calculating] extended structures. **<T: 135 min>** We had an early calculation of graphene in there, [one of the first—I'm proud of that]. We wrote a paper, which was published in the *Proceedings of the Royal Society,* together with a very brilliant postdoc [Myung-Hwan Whangbo], who wrote the [underlying computer] program [. . .].[73]

There was much more, [in our] conversations [on the design of organic conductors and superconductors]. There were hundreds of pages of writings and drawings by [RBW]. Let me

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[72] R.B. Woodward, and R. Hoffmann. "The conservation of orbital symmetry." *Angewandte Chemie International Edition in English* 8, no. 11 (1969): 781-853.
[73] M. H. Whangbo, R. Hoffmann and R. B. Woodward, "Conjugated one-and-two dimensional polymers." *Proceedings of the Royal Society of London. A. Mathematical and Physical Sciences* 366, no. 1724 (1979): 23-46.

show you [the images], because they're quite incredible documents. Those drawings and papers were on [RBW's] desk in 1979 when he died. [. . .]

Woodward's family took away those papers [after he died]. [. . .] They thought there was something of commercial value there, the usual thing that drives families. To exploit [the ideas commercially would be] difficult. In the end, the [family conserved the drawings, digitized them]. [. . .] And they gave the papers to Michael [P.] Cava, an organic chemist working on organic conductors, to edit them.

[Cava] started to write [the work up], together with a postdoc. [Both of them then died—no, there's no Egyptian curse on this work. The papers came] to Bob Williams, [a student with [Woodward] and family friend. They asked me to join in finishing a paper Cava had begun. So we did], in *Tetrahedron*.[74] "RB Woodward's Unfinished Symphony." So, it has Cava and a postdoc and me and Bob Williams on this. [. . .] It's illustrated by reproductions of—

REINHARDT: Oh, he did these by himself, these drawings?

HOFFMANN: Yes. This is Woodward's drawings, hand drawings. Wait till you see this.

REINHARDT: Oh, wow.

HOFFMANN: So, we actually did some history of science here. [Look at this—RBW is drawing] these polymers, and he's counting electrons. Here's more. [The drawings, hundreds of them, are on RBW's] classical yellow paper—this is acid-full, and decaying rapidly. [A second type of paper he used is] marginally better, turning yellow. Sorry. Here's more.

REINHARDT: They are beautiful.

HOFFMANN: They are. Here are some of the polymers he designed. Where we could, we illustrated [the *Tetrahedron*] paper with his drawings, because they are so attractive.

CARUSO: Yes.

[74] M. P. Cava, M. V. Lakshmikantham, R. Hoffmann, and R. M. Williams, "R. B. Woodward's unfinished symphony: designing organic superconductors (1975-1979)," *Tetrahedron* 36, no. 67 (2011): 6771-6797.

HOFFMANN: [You see] numerology. The paper [is] decaying here. It's so sad. Look at that. He did this by hand, little—

REINHARDT: He was an artist, right?

HOFFMANN: Yes. His daughter has written a thesis about [RBW] being an artist.[75] **<T: 140 min>** He thought of architecture [as a profession], certainly, and he was very good at drawing. [I'm so happy that we have preserved] these papers; in an appendix, [many are reproduced]. Look at these. The meticulous nature of [the drawings], how he carefully sketches the [molecules]. Look at that, [even] orbitals! He [used] a compass to [draw] these.

You know, he didn't use a template. You can see the hexagons are not perfect. He had *Angewandte Chemi*e's old template—he and I used it extensively. [But these orbitals he sketched freehand]. He's doing a calculation of the total space filled by the atoms of ion. [RBW] loved algebra. [. . .] There are six hundred pages like this.

REINHARDT: So, he had this on his desk when he died?

HOFFMANN: Yes.

REINHARDT: So, you were in close contact again?

HOFFMANN: Yes, we were. I came during that period and we worked on [the *Proc*. *Roy*. *Soc.* paper]. Among the six hundred pages [left on his desk—the ones the family kept]—are two or three pages of mine, [recognizably so]. This here, notice the difference. This is mine.

REINHARDT: Calculations there.

HOFFMANN: Well, there's some calculation there, some sketching, some—

REINHARDT: Yes. Sure.

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[75] See C.E. Woodward. "Art and elegance in the synthesis of organic compounds." In: *Creative People at Work: Twelve Cognitive Case Studies.* New York: Oxford University Press,(1989): 227-254.

HOFFMANN: But it's not as neat as his [wonderful, precise writing and drawing]. But that was the last thing. [. . .]

REINHARDT: I see. So, that's *Tetrahedron* published in 2011.

HOFFMANN: Yes, 2011, *Tetrahedron*.

REINHARDT: We'll certainly look that up.

HOFFMANN: So that period—[1977-79]—was a period of renewed work between Woodward and me on organic conductors, connected to my growing interest in extended materials, and his. He came to me again [to seek expert help on calculations], essentially. We got one lone paper out of it. There could have been more. Since then, people have made some of these nets, [the ones that Woodward designed in 1977-79]. But [people are] not aware that Woodward suggested [the networks]. Many have not been made.

So, he died in '79. The Nobel Prize was '81. There is no question that [RBW] would have shared in the Nobel Prize, because our names were [inextricably intertwined]—it was collaborative work. We knew we had been nominated for it, because . . . there's an amusing story, two stories.

[The Nobel Prize in science is a surprise only to journalists. We know very well who has done Nobel Prize-caliber work in our profession—I could name ten groups with whom my colleagues would be happy if they received the Nobel Prize. One reason you know you have been nominated is that] the people who nominate you [. . .] cannot resist telling you about this. The reason, [I think, is that] they think that some of it rubs off on them, [so to speak].

The second [reason is that some countries—Japan and France among them]—have well-oiled institutions to nominate every possible person from that country who has a chance for the Nobel Prize. There are only about one thousand people each year who can do the nominations. They are the members of the [Royal] Swedish Academy of Sciences, the Scandinavian Academies of Science, former Nobel laureates, and about three, four hundred people who are chosen on a rotating basis from the full professors of departments [of chemistry] around the world. They are the nominators.

Anyway, the Japanese committee entrusted with this [task, instead of just going ahead to nominate Kenichi Fukui], in typical Japanese fashion, [sent] to Woodward—[not me, of course]—one day, [a committee of] three Japanese scientists. [. . .] An appointment was made. They [wished] to ask for his permission to nominate us together with Fukui.

REINHARDT: That's kind.

HOFFMANN: Very Japanese. Woodward received them, gave them a drink, all [most] formal. He called me afterwards, and we both **<T: 145 min>** agreed it was very Japanese. They had decided that Fukui had a chance, and they were [absolutely] right.

CARUSO: How did you find out officially? I mean, you knew that you were being nominated. How did you find out?

HOFFMANN: We knew we were nominated for a number of years. In the beginning, it's exciting, and you begin to listen on the day of the announcements. [When nothing happens, your reaction depends on your psychology. Some people become obsessed by it. The more rational reaction, the realization that at the top, in the actual choice, it's a chance event, would lead you to relax and let things come as they may. But it's hard to be rational].

[Why do I say it's a chance event? You know that you have done Nobel-caliber work. But so have ten other groups. Or twenty. In the end it's a group of Swedish scientists, with a research staff, but also with their education and prejudices—good ones—who choose three people max out of what I imagine is a field of about fifty deserving nominees. Five Swedes, or seven—the Nobel committee, makes the recommendation to the chemistry section of the Nobel Academy, which then makes a recommendation to the full membership. As far as I know, once in the last one hundred years has the full membership of the Royal Swedish Academy of Sciences rejected a recommendation by this committee. So, it's essentially five Swedes who decide.]

Let me put it another way [to make the point]. The Nobel Prize was just given for a single molecule photochemistry [and physics]. Of course, [in] the days before, people asked me, journalists and others, "Who do you think is going to get the Nobel Prize?" [I answer all questions, so] I made up a list of eight groups or areas. [If you watch the process, it becomes clear that the Prize recognizes fields more than individuals. Eight groups I wrote down. The actual choice, with which I was happy, except for a person who was omitted, was not among them.] After you realize [the chance nature of the process], you let go of it. [At least, I was able to do so].

On the day it happened, I was at home. [. . .] The decision is [usually] leaked by the Swedish Academy to a Swedish newspaper or two so that they can call first. In the old days, they would send a telegram. I think [. . .] that newspaper had trouble getting me, perhaps called the wrong Hoffmann. [Laughter]

My wife said that she had some inkling, because a friend of ours, a Swedish scientist—[I forgot to tell you that my wife is from Sweden]; I speak Swedish **<T: 150 min>—**[called her and asked for my photograph]. [. . .] She was a member of the Nobel committee; [my wife didn't tell me about the call], which is just as well.

I was at home; it was nine in the morning. No, it must have been earlier, because usually the committee—the decision is at noon [Swedish time], but I don't know. Anyway, I heard it on the radio! I was fixing my bicycle in the garage and I had the radio on to listen to the news. I didn't know it was the day, [I just wanted to hear the news]. I immediately ran in and called my mother. You heard about my mother before, why [she was so] important [in my life. I wanted to reach her] before the calls would start coming in, and they did. [. . .] Unfortunately, my stepfather had died two months before, so it was a sad time in the family. But of course, my mother was very happy.

REINHARDT: What did she say? Do you remember?

HOFFMANN: [. . .] There is a Yiddish word for it, "*naches*", comes from a Hebrew word, not from a German one. It means the joy your children bring you. [. . .] In most languages, you would need a few words for that, but there is a single Yiddish word for that, to bring *naches*. She was very happy.

REINHARDT: Who came with you to Stockholm?

HOFFMANN: We spent some money bringing some family there. The closest living relative on my father's side, his brother, Yehuda [Safran], from Israel, and his wife, [Yehudit Safran]. The only one living of the people who were in the attic was my Uncle Frank [Rosen]. He came. My sister, Elinor [Hoffmann], and [our] children, [Ingrid and Hillel Hoffmann,] of course. My stepfather was not alive, [as I said]. His sister, Giza [Kornreich], came. So, it was a rather small family group. Close family from three families: my mother's, my father's and [stepfather's]. Then we had a very large Swedish local contingent. We hired a boat and had a party two days after [the Nobel ceremony] on a boat. This is now December. Eva's—[my wife's]—family lives on an island outside of Stockholm, [but] we couldn't quite get into the bay where they live. [. . .] We took this [old-fashioned] boat out [on the water] with a big band on it. It cost ten thousand dollars to hire the boat, but it [was worth it]. We had a good party for the Swedish relatives and the other ones who came, with some music. The setting was [winter spectacular]—an icebreaker to open up a channel in this bay, the passage frozen over. [. . .] We had a good time.

The Nobel Prize winner in literature that year was Elias Canetti. [His] is a complicated history, **<T: 155 min>** Bulgarian, Austrian, lived in London, a novelist, writing in German. Turns out Elias Canetti has a PhD in analytical chemistry. [He tells the story] in his autobiography —he did it to please his mother. [. . .] He tells the story well. But even while he was getting the PhD, he was sitting in a café in Vienna in the twenties and writing his great novel, *Auto da Fé*.[76] [And I did not please my mother by failing to become a real doctor. (I'm smiling).]

I asked [Canetti], "What did chemistry mean to you? Did it contribute anything to your writing?" And he said, "It gave me a sense of structure." I don't think he meant chemical structure in the sense that we have talked about. [I think] he meant that things were related to each other, that there was an order. That was an interesting comment.

That was 1981. I was forty-four, which was young for a Nobel laureate, very young. Fukui was older; he's no longer alive, [as we speak]. That's his picture there [on the wall]. He came from an old Japanese aristocratic family. [Fukui] had much more difficulty with the Nobel Prize than I, because he was the first Japanese Nobel Prize winner. He was shy, retiring by nature, and he was pushed into positions of making [public pronouncements]; [. . .] they just made more of a fuss about it, for natural reasons, [and for cultural ones]. The first Nobel laureate in chemistry from Japan. There have been a number since.

[Fukui] and I got along very well from the beginning. We have not published anything together, but four of his students came as postdocs with me over the years.

REINHARDT: Before the Nobel or after?

HOFFMANN: Before and after. [. . .] They have become some of the leaders of Japanese science, all theoreticians. [They were Akira Imamura, Hiroshi Fujimoto, Kazuyuki Tatsumi, and Kazunaru Yoshizawa.] And we have visited there. I would say [we have had] very good connections. I think the reality is that our work shed light and gave importance to what Fukui did. [I and Woodward used] Fukui's frontier orbital ideas intuitively early on. [And frontier orbital ideas] grew into prominence in my own work later on.

[I suspect that] being Japanese did not hurt, in the deliberations of the Nobel committee. [The quasi-political realities of awards that have been received by too many Americans in the past are that as many non-Americans in a nomination today as possible is a plus.]

REINHARDT: **<T: 160 min>** What did it mean to you?

HOFFMANN: Of course, it was very nice. It was very nice for my mother. I wish my stepfather had lived, for the family. So, I wasn't the only Jewish émigré scientist to get the Nobel Prize. So many [of us] were Hitler's gifts to America, [that's] one way to say it. An amazing flowering of talent [in the US and in the UK, the countries that welcomed us. Not that

[76] Elias Canetti, *Auto da Fé*: *A Novel*, (Farrar, Straus and Giroux: Reissue edition, 1984).

everyone succeeded—there were many who could not reestablish themselves at the level they deserved]. You find some of [their stories] in the histories of German biochemists.

REINHARDT: Ute Deichmann?

HOFFMANN: [I'm thinking of the essays and books of] Lothar Jaenicke, connected to Ute Deichmann—[Ute was for a time in Jaenicke's department—Jaenicke] has written these remarkable [two volume collections of biographies of German Jewish biochemists and biologists]. [. . .]

[But let's return to what the Nobel Prize meant for me.] Overall, the Nobel Prize is an absolute plus to only two people or institutions—your parents and your university—for different reasons. Parents get some of that *naches* that I mentioned. Your university uses you shamelessly in advertising. It's okay, it's okay. Cornell has done [much] for me. They can use [our connection].

For everyone else, it's not necessarily a plus. [. . .] Yes, I can get more money for a certain kind of lecture as an honorarium than I [could have otherwise. Though my lectures are in demand for another reason. It's because they bridge art and science]. I can, if I want to, advance into administration. [It's not a path I have chosen]. [. . .]

Maybe I should have established an institute [somewhere]. Europeans and Japanese do that, [and Salk and Edelman did it.] **<T: 165 min>** [On the negative side], the press offers you infinitely more opportunities to make a fool of yourself. That's the best way to say it. An example is [William B.] Shockley [Jr.] and his views on race. [You can see that being repeated with Jim Watson. Any contrary idea will be exaggerated and taken advantage of by the press.]

Will I get better students [after a Nobel Prize]? More students? [On the latter, not many new ones—because some might be afraid or unsure of their abilities.] Maybe some postdocs, came with their own money. Most of [the many] German postdocs [who worked with me] came with their own money, thanks to the DAAD [. . .] or the Volkswagen Foundation. [. . .] So did French and Japanese. That was a great contribution to my research.

Some distance is generated between me and students, undergraduates, as a result [of the Nobel award]. This is fortunately easily overcome, either by me or by the students, if they're Americans. But in China or Japan or India, I have never had such quiet audiences, attentive audiences, and it's because of [the Nobel Prize. But why are they there? The modern twist is that the answer is] the incredible pressure to take selfies with me. [. . .] It got out of hand— at two places, once in South America, once in India. I was talking to an audience of undergraduates, which I like to do, and then there was such a crowd wanting to take pictures that it was dangerous. [The crowd] pressed me against the balcony railing. I thought I was going to fall over. There was no crowd control there. And [the images] were obviously not to send to their teacher, but to put on Facebook. So, [here we see] modern mass culture integrating with some presumed mystique of the Nobel Prize.

You're asked to sign lots of petitions. You have a chance to do some good, but in a number of those, you get a feeling that they really don't care [how I think], whether I support nuclear disarmament [or another cause]. They just care that they have my name on a petition. This induces an alienation of the individual from [their name].

Research grants and papers are a real problem, and I've written a little about that. Where does the id come out? It comes out in the dark, when you think you can't be seen. That's the refereeing process on papers and the grant process. If there are going to be some jealousies or envy, that's where it's going to surface. And I can tell you, it does. I get comments like [. . .], "One would not expect a Nobel laureate to do this." Now why are they saying that? [They are venting, that's clear. And] **<T: 170 min>** the editors know this. [. . .] But on proposals, it's deadly, because these days, to get support, you need all 'excellent' reviews. Just 'good's will not do.

So, I have seen really nasty things said about my papers by reviewers, and I think they're driven by this. So, that's a minus [of getting a Nobel Prize]. [. . .] A paper was rejected from three journals, and we eventually got it into *New Journal of Chemistry*.[77] [My experience here] is different from Woodward's. [Because] Woodward did not publish much, like I do. In his lifetime, [. . .] there are one hundred twenty-five papers.

So, when Woodward sent in five communications in one year, those communications were accepted without review, and the editor said so. But that's the luxury you buy when you get yourself in a position of not publishing—he published too little, so people knew there was great work in the theses that should have been published of his students. [Woodward] took infinite pains in writing his papers in a certain high style.

[. . .] The most difficult [consequence of an early Nobel Prize is psychological. You've heard me say that] I've had the luxury to work on the next molecule down the line, just because I thought it was interesting. Well, that's the way I worked from the beginning, but then a natural question, not only for journalists, but also for even other people to ask you after you get the Nobel Prize is [. . .], "What will you do next?"

So, Toni Morrison's or Norman Mailer's next novel is looked at in a different light because of the Nobel Prize. [What's wrong with that question is that in it is an expectation that you will do more, or do it better]. [. . .] If you are going along, not thinking about what you're going to do next, but letting the molecules and the circumstances guide you, in the way that I've just explained around that pentacene story [and the postdoc guiding me to a new field, you may just] begin to ask yourself, **<T: 175 min>** "What am I going to do next?" [That question

[77] M. M. Balakrishnaraajan, P. D. Pancharatna, and R. Hoffmann, "Structure and bonding in boron carbide: the invincibility of imperfections," *New Journal of Chemistry* 31, no.4 (2007): 473-485.

changes things, it makes you self-conscious about your work. And that is a feeling that in some way runs counter to creativity]. [. . .]

[I overcame that.] I worked my way through that [question], and I feel good about what I've done, that I've kept that freedom to do the next [interesting] thing. [. . .] But it bothered me for a while, that question of what are you going to do next.

And it was very nice after the Nobel Prize to get an ACS [American Chemical Society] award in inorganic chemistry, and then one in chemical education, because those represented somehow [recognition of other things I've done]. After the Nobel Prize, in general, you don't get awards. It's okay. And it's part of [the] mystique [of the prize]. What you get is honorary degrees, [which] you stop accepting them after a while, because you realize that they're serving the people [who give them] more than you.

Overall, [the Nobel Prize] is a mixture of pluses and minuses. When [. . .] some of the negative things that I've just told you, [occurred], I would say, "It's good I've survived that." What I mean by that is that I'm still able to do good science, to publish fifty years in *JChem Phys* [*Journal of Chemical Physics*] after I first published [an article in that journal. It's good, I can still get] excited about the nitroxyl radicals. That I have been able to do science, good science, and keep an enthusiasm for the chemistry, meanwhile doing these other things, too. For it is now thirty-three years since that Nobel Prize. That's a long time.

REINHARDT: Was this excitement about molecules the reason that you resisted the move into management of science? You mentioned the MIT presidency and things like that.

HOFFMANN: Yes. I have a natural impatience with [social interactions. I realize they lubricate the wheels, and we have such generous donors in the American university system. I wish that there would be a way to penetrate to the passions or expertise of a person. Everyone has something interesting about them.] But part of the job, it was clear to me, of being a university president, was you have to go to interminable dinners with people who [may] give you money.

REINHARDT: You bet.

HOFFMANN: [You've had to do this in your job]. Some of the [people we meet indeed] are interesting, and I now know how to [learn from them] those passions [that make them human]. But the thought of being a university president, doing that all the time, is just too much. I knew you could do good things, but it was not what I wanted to do. [. . .]

CARUSO: Yes.

[END OF AUDIO, FILE 2.1]

[END OF INTERVIEW]

INTERVIEWEE: **Roald Hoffmann**

INTERVIEWER: **David J. Caruso**
Carsten Reinhardt

LOCATION: **Chemical Heritage Foundation**
Philadelphia, Pennsylvania

DATE: **21 March 2015**

CARUSO: So, today is March 21, 2015. This is another oral history interview session with Dr. Roald Hoffmann. We're recording it here at the Chemical Heritage Foundation. I'm David Caruso. I'm here with Carsten Reinhardt. As I mentioned before we began, we're going to pick up where we left off, and at the end of the last session, we were talking about how you received the Nobel.

CARUSO: And the significance that it played for you as an individual, and the role that it played for the institution as well. Some of the things that you had mentioned were that, you know, Cornell was very excited about it. Very happy to celebrate that. That you enjoyed bringing family members to receive the award. But on an individual level, mostly what the award did for you was it gave you a chance to maybe receive grants a little more easily.

HOFFMANN: No, I didn't say that.

CARUSO: No? Okay.

HOFFMANN: It made me get more money for the same lecture I would have given before for less money. [Getting] grants it didn't make easier. [Nor did it help in publishing papers.] If anything, it made things marginally harder. [Yes], it would make it easier to publish a book which was science popularization [. . .], but I somehow didn't seem to write those books, with the exception of one, *The Same and Not the Same*.[78]

I don't mean to accent the negative [in my describing the consequences of the Nobel Prize]. But I'm interested in destroying the journalistic myth of what the Nobel Prize is. First, that [being awarded] it is a surprise is bizarre, especially in science. It is a surprise in literature and in peace, but [often so] for [. . .] the wrong reasons. Because [in literature] it's only given to

[78] Roald Hoffmann, *The Same and Not the Same*, (New York: Columbia University Press, 1997).

one person, and because [that person] represents the peculiarities of the eighteen-member Swedish Academy, who have each their own favorite writer, and who also prefer to recognize people from less well-known countries if they can. [Of course, nothing's wrong with this; we need to be educated on good writing.] And the Peace Prize is a matter of other politics. I love President Obama, but to give the Peace Prize to President Obama [was strange, and I suspect] made his life harder.

But in science, of course we know who is good. We know what work is good. We get invitations to lectures. We get invitations to [meetings, our] work is recognized [in a variety of ways], and it never is a surprise in science. [. . .] Journalists want it to be a surprise. [. . .]

[I am also] interested in deconstructing a mystique of chemists or of scientists as being superior to other human beings. [Superior in some way]—being smarter, more ethical, more logical. [And I know that I am not superior to others. In science, as in] any field, there are contentions, there are personalities, there are typical human qualities [at work. I am] not falling into a social construction of science. [There is real knowledge that is gained, and its advance is more than a power struggle. It is just that scientists] are human beings, and the miracle of science is that something gets done about advancing reliable knowledge when it's done by fallible people such as scientists are. And it's the system that works overall, which is quite remarkable.

Part of [good scientists] being fallible human beings [and not angels] is they're jealous **<T: 05 min>** or envious. [. . .] And a Nobel Prize engenders, because of the mystique attached to it, [those human weaknesses to come out]. You could see this in, for instance, after the prize came on MRI [magnetic resonance imaging], some people [felt they] were slighted. There were advertisements, there were campaigns out there, for [the people who were] not recognized. [I suspect that the Nobel Committees, made up of very good people, spends much of their time agonizing over not leaving anyone out. Especially graduate students and women.]

[To return to myself, you can sense that I am personally upset by the way my papers or proposals have at times been received]. [. . .] I lost all my NSF funding at some point, [. . .] on the basis of two such negative comments. One comment was about "outreach." [. . .] I was taking the NSF criterion of a broader interest literally, and I devoted a [small] part of my proposal to the *Entertaining Science* cabaret in New York City. And one of the reviewers said that, "[for] Dr. Hoffmann [to think] that this is of any relevance to his doing science is beyond understanding." [That was] nasty.

CARUSO: Yes.

HOFFMANN: [. . .] I lost the funding for two years. I regained it.

The effect of a Nobel Prize [was harder on] Fukui, my co-winner of the Nobel Prize. [He had a myriad of public commitments, and it was, I know difficult for him. In the end people constructed] an institute for him, a private institute from private donations. [. . .] There are analogues in the United States with an institute that [Gerald M.] Edelman has on memory and the brain. [Perhaps I should have worked to create such an institute.]

Another direction to go is into university administration or other public [service]. [. . .] But I wasn't interested. As for publishing outside of science, except for popular science, [the Nobel Prize] makes no difference. The world of poetry and theatre is totally immune to the Nobel Prize in chemistry, except that [once you get a poem or play accepted, then they may use that in] advertising or marketing, [. . .] mention the Nobel Prize on the back cover of the book. [. . .] But it doesn't help getting it published, getting it accepted.

CARUSO: Yes.

HOFFMANN: When I submit a poem for publication, [one writes a short] cover letter. [. . .] **<T: 10 min>** I do write it on chemistry department stationery—[or used to]—electronic submissions have [obviated the letter]. The reason [I do this is that I know the process]. The typical [poetry] journal is put out by an English department at some university, say University of Mississippi. [. . .] The work is really [done] by graduate students in English [or creative writing] who each read every day. [. . .]

[More people think they write good poems than are willing to buy poetry magazines]. So, lots of people submit. These poor graduate students read fifty poems a day, and they select two or three for the editor to read. And so one thousand poems get filtered into fifteen, twenty. [My first audience] is that poor graduate student. I will do anything reasonable to at least make them read the poem. If I write this cover letter on chemistry department stationery, [perhaps, just perhaps] they'll wonder, "Why is that coming from the chemistry department? That's not where we usually get poems from."

CARUSO: Yes.

HOFFMANN: So, that's all I'm working on.

CARUSO: Well, I'm curious to know a couple of things. When did you start to invest more time into things like poetry? I know you have books coming out in the nineties and thereafter.

HOFFMANN: That's right.

CARUSO: But I'm curious to know when that was an exploration that you become—

HOFFMANN: I began to write poetry before the Nobel Prize, not too long before, in mid-life. It was around 1976 or so. I had been exposed at college, [at Columbia], to poetry and loved it, by a great teacher, Mark Van Doren. And I knew a poet I had mentioned, Archie Ammons, a little bit, socially, at Cornell. [. . .]

The line [I followed] is not the Carl Sagan line—[who could have served as a model]—which is from science, [. . .] to popularizing science, to [. . .] a television program, and then wrote a novel. A two million dollars advance didn't hurt, on *Contact*, the only novel [Sagan] wrote.[79] [. . .]

In my case, the line was poetry, then popular science, or writing for general audience and lecturing, and then the theatre. [. . .] I sort of filled in the popular science, the ground in between the science and creative writing [in time]. I started writing [poetry] around [. . .] 1977, when I was forty years old. I don't know why I hadn't written [for the general audience before]. First of all, I thought that I was good at scientific writing. I was also good at teaching introductory chemistry. [. . .] In my mind [the latter two] are connected with each other, and I've written a little bit about the [inversion of the] usual equation of good research makes good teaching. [. . .] I think good teaching makes good research. [. . .]

<T: 15 min> I think the key to good teaching is twofold, and connected to the key to good scientific research writing. The two elements are empathy to the audience, so that you feel the level of understanding of the audience. In a class of one thousand, which is the largest class that we [have at Cornell in chemistry—actually], the lecture room would only hold four hundred, so the lecture had to be repeated three times. [. . .]

The magic of the teaching act is [that] you can talk [simultaneously] to several audiences at once. [. . .] These several audiences are the people who understand everything you say, the people who are asleep, [the ones who hear] but don't understand. And [. . .] everything in between. [Meanwhile], you're one person. The words come out of your mouth, what [Jacques E.] Derrida would call, "The message that abandons."[80] [. . .] I think the reason [teaching] works is because not everyone is listening to every word. [People] hear what they want to hear. [. . .]

So, there is empathy. The other [important factor] is related to the poetry. There [also] has to be some action on the part of the teacher that communicates an emotional involvement in the teaching process. That the student feels that the teacher cares that he or she understand, without making [the student] feel bad about not understanding. [. . .] That it's a human being talking, and not just reading from a book.

[79] Carl Sagan, *Contact*, (New York: Simon and Schuster, 1985).
[80] J. Derrida, "Signature Event Context" in *Limited Inc*, translated by Samuel Weber, Jeffrey Mehlman, (Evanston: Northwestern University Press, 1981).

That emotional contact is [something] good teachers learn how to establish. You don't do it by looking at the same student all the time while you're talking. All you succeed [in then] is making [that student] feel uncomfortable. [You certainly don't look at no one, at the ceiling or blackboard.] But you shift your gaze, but you look at faces. [. . .] There are also various [ways you can signal] your humanity—[admitting things you do not know, pointing to matters of interest in media].

[. . .] To get back to the poetry, I felt I was good at this establishing an emotional tie with a student. I felt that I could do that in a poem, where the emotional tie is more important, perhaps, than anything else that you establish. Many poems fail because they are too hermetic. The experience of the poet does not communicate to the experience of the reader.

[In a recent talk about the relationship between art and chemistry, I spoke about science and abstract art, their relationship. And finished with a Rainer M. Rilke quotation, some lines from a poem, about angels. I can't do that in a scientific paper I write, and it would be hard to work it into an introductory chemistry lecture. But I did learn from poetry the art of introducing some emotional context into teaching.]

REINHARDT: What was the first language you used in writing poetry?

HOFFMANN: English. [. . .] I could only write in English. By that time, the other languages had faded. Polish and Yiddish **<T: 20 min>** were my native languages, but English took over. I let it take over, and I'm not too proud about losing those two languages. I've kept a little of them. Then [came] other languages. Russian and Swedish came in, and German. I can talk in those, but I can't write in those.

REINHARDT: You mentioned two poets as teachers, and some influence.

HOFFMANN: Yes.

REINHARDT: Have you had others?

HOFFMANN: The poet I read who was a major influence was the mid-twentieth century great poet Wallace Stevens, and it was in Mark Van Doren's course that a Wallace Stevens' poem, "Sunday Morning," made [a great] impact.[81] That was the first poem that really meant something to me.

[81] Wallace Stevens, "Sunday Morning," *Harmonium*, first published in *Poetry*, 1915.

REINHARDT: Why?

HOFFMANN: Just the [high] tone, [and the small things he spoke of, coffee and oranges. The poem spoke of a] woman on a Sunday morning, looking at some oranges, and feeling the world in there. It somehow meant something to me, [perhaps it was the implicit paganism in the poem]. There is [also] a weird set of poems which had an influence on me in the first year of college—[poems used as the text of a musical setting]. The poems are in *Carmina Burana* by Carl [H. M.] Orff.[82] I went back and learned some Latin in order to read the original; they're written in a mixture of [Old High German and Latin]. The poems were found at a secularized Benedictine monastery in Bavaria, [Germany], Benediktbeuern. [There were these] ribald poems circulating between the monks, found in the library there. Well-handled, circulating for five hundred years, and then published.

Carl Orff used some of those poems in his work *Carmina Burana*, which must have been written in the late thirties, 1930s. Orff is a problematic person, because he worked with the Nazis. He was also a great music educator. He specialized in sound patterns, rhythmic patterns, instruments for children. He wrote three [major works] based on [. . .] Latin lyrics. They [. . .] celebrate love, gambling, all the things that monks were not supposed to do.

[The poems have been] translated. There's a book by Helen [J.] Waddell called *The Wandering Scholars*, and it's about [the culture of the] troubadours and the monks.[83] A story of counterculture in medieval and Renaissance times. Somehow, that [poetry and music appealed] romantically to this nineteen-year-old. [. . .]

I remember clearly when I first heard *Carmina Burana*. It was at age eighteen; [the performance] by students at the High School of Music and Art in New York. I had a friend who was at that high school, and took me along. I was bowled over, as they say, by the music. [. . .] But given my scholarly, academic nature, I actually [went on to learn] some of the language [of the Latin poems] in order to understand the poems around beginning of college. [. . .] Wallace Stevens was more intellectual, and very trimmed down. [In his work] are very precise shifts of meanings of words and expressions, and a [special] use of syntax, [which is also] what Archie Ammons' poetry [has]. **<T: 25 min>**

I began to write poetry. I sent it out [to small magazines at] that time, '76, '77. I got rejection slips. [. . .] Eventually, I struck up a social relationship with Archie Ammons, and a group of us [. . .] began to meet at a coffee house, the Temple of Zeus, that was on campus. There I was and Phyllis Janowitz, who was a professor of poetry in the English department. [Phyllis] was an inspiration [in another way], too, because she became an assistant professor at age forty-five. [. . .] And Archie, and [Carl] David Burak. David Burak was a campus radical who was an SDS [Students for a Democratic Society] leader in terrible times, ten years before

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[82] *Carmina Burana*, composed by Carl Orff in 1935 and 1936, based on twenty-four poems from the medieval collection of the same name.
[83] Helen Waddell, *The Wandering Scholars*, (London: Constable, 1927).

this time, in the late sixties. [Then] he became a poet. David and I were the non-professionals in poetry, and Janowitz and Ammons were the poets.

In part, this was an Ammons admiration society. [Archie] Ammons was one of these people who needed a lot of stroking, [even as he was very generous with his attention]. In time, we began each to bring a poem to this [meeting] and read it. It took me a while to understand the criticism, and Archie and Phyllis were quite gentle. And they were good teachers. We never revised a poem and brought it back—we just brought another poem. [. . .]

Eventually, I got a poem published. It was [. . .] after the Nobel Prize, around ’83, about seven years after I started writing. Then things went better. [In the mid-eighties, I also] spent three summers, a month each summer, at the [Carl] Djerassi Resident Artists Program [Woodside, California]. That concentrated time [devoted to writing] helped me.

[So, the poetry began]. The popular science writing started with *Chemistry Imagined*, and [*The Same and Not The Same]*.[84] From Helen [J.] Waddell’s *Wandering Scholars* and *Carmina Burana*, I learned about emblem books of the Renaissance. There is [in these] an image, mysterious, often very much like chemical drawings, a verse, and a motto. [Their origins are part of the revolution of] secular publishing. The first was written by Andrea Alciato in [1530]. They’re tied up with the beginnings of printing, [connected to medieval] bestiaries, with maps. [The emblem books] were tremendously popular.

I had an image of [creating] an emblem book of chemistry, and that’s what [led to] *Chemistry Imagined*. [. . .] In the eighties, [. . .] I got that NSF grant to support the artist who collaborated with me [in the book, whom I had] met at the Djerassi Foundation. All of these things are [connected] with each other. [It’s wonderful to have a life of connections.]

CARUSO: And that was Vivian Torrence?

HOFFMANN: Vivian Torrence, [yes]. *The Same and Not the Same* came out of some general [audience] lectures. [So, there’s a lesson there—ask scientists to give general lectures, they will rise to the occasion, so to speak.] The first time I was asked to give a general lecture [was the thing] called the Silliman [Memorial] Lectures, [. . .] at Yale. That was before the Nobel Prize, 1980. As part of the lectures, you are required to give one lecture for a general audience; I think that was the first lecture I constructed of this type. [. . .] **<T: 30 min>** It came off well, and then I somehow accepted more invitations of that type.

The Same and Not the Same came out of lectures I gave at Brookhaven. I didn’t think much about it being a book, but I had some luck [here]—I came into contact with Columbia University Press, who prints the texts of these lectures. [And at the CU Press,] I came upon a

[84] Roald Hoffmann and Vivian Torrence, *Chemistry Imagined: Reflections on Science* (Washington, DC: Smithsonian, 1995).

[design director, Teresa Bonner], who shared my feelings about having lots of art in the book, and who convinced her bosses of Columbia University Press [. . .] to print the book on paper that could take a color illustration on every page. That was non-trivial in those days. It had to be glossy paper. Today, the technology is different. [. . .] She came up with suggestions for illustrations [. . .] and got me back to thinking about art history, [which had attracted me so much in college]. I always had been looking at things.

The Same and Not the Same has turned out to be a very successful book, [with use in general science courses]. It's one of the best-selling books of Columbia University Press. [. . .] It has sold about fifteen thousand copies since it was printed, which is a respectable number for a science book.

[. . .] Then I began to work on the book about science and Jewish religious tradition, *Old Wine, New Flasks*.[85] Each of these [books] has [an origin story; taken together] somehow I was filling in the ground [between science and the humanities. I had the chance, or made the chance, to write about] the relationship of chemistry and philosophy, religion, history. Everything is connected to everything else. [In the case of] the book with Vivian Torrence, *Chemistry Imagined*, I [had] another stroke of luck, and that is [finding a receptive editor], Madeleine Jacobs. Before she became the CEO of the ACS, [she] worked for the Smithsonian. I submitted [the book] there, she liked it, and helped me get it published. [. . .] The Smithsonian Institution Press [was a prestigious publisher. We had an art exhibition, too, that went to several places.]

[The book went out of print, but Vivian and I would buy up copies from booksellers, often discarded library copies. I love the idea of this recirculation. One amusing story is that in 2018 a blogger mentioned the book, reproduced some images (without asking permission), and the used copies of the book all of a sudden went up in price to thousands of dollars for a few weeks, then to sink back to normalcy.]

[In *Chemistry Imagined*] there was a pairing of collages and essays. [For one of them,] I read the story of the discovery of oxygen. I [. . .] then became aware that Cornell had a Lavoisier collection. And the curator of that collection, David [W.] Corson, showed it to me. [In the collection were not only books, but also] Madame Lavoisier's *necessaire*, [. . .] a travel chest she had. It's illustrated in the *Oxygen* play.[86]

I looked at it, and it was a magical object. [. . .] There is a power of objects. [And books. And] **<T: 35 min>** old [musical] instruments. [And] chemical kits. [. . .] Madame Lavoisier's *necessaire*, handled with white gloves on in the Cornell Rare Books Collection, is not a book. Actually, on the outside, it [pretends] to be a book. [. . .] It was made by an English company selling in Paris, [France], in the first decade of the nineteenth century, during the Napoleonic wars. [. . .] The etiquette from the manufacturer is in there; that's how we know who made it.

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[85] Roald Hoffmann, *Old Wine, New Flasks: Reflections on Science and Jewish Tradition*, (W H Freeman & Co, 1997).
[86] Carl Djerassi and Roald Hoffmann, *Oxygen: A Play in Two Acts*, (University of California: Wiley, 2001).

On the outside, the *necessaire* is made to look like a book, folds up into a book. [It says on the spine "Histoire des Theatres."] The article, "des," is plural. That's a mistake in French, but it's okay, I suppose—it was done by the English. [. . .]

Handling that object made me want to write more about [it], and eventually, that turned into the play. But before the play, I learned [more of the history of the discovery of oxygen, about Joseph Priestley. And Scheele, as well as Lavoisier. That is] a two-page essay, which was one of the thirty collage/essay pairs in *Chemistry Imagined*. The essay was called "The Air of Revolution." [. . .] That planted the seed of the play. All these connections.

CARUSO: Yes. One thing that I'm curious to know a bit more about is how did—I mean, you talked about having this poetry group. You're at Cornell. It's a large university in a small town. How did the initial connections come about to these other individuals? Were you just calling professors up and saying, "Hey, I'm writing some poetry, I want—"

HOFFMANN: The first thing to say is it was much easier for this to happen at Cornell than it is at Columbia or Harvard. The reason is that we are in a small town, so you see the same people in the social [setting], and you can [more easily] overcome the [first barriers to meeting, talking]. You see them at the farmer's market. You see them at the gym. You see them in the coffee shops. Whereas at Harvard and Columbia, the professors would disappear to the wilds of New Jersey or Lexington or Arlington, and you'd never see them socially, except during the day. So, it was easier [at Cornell, in Ithaca].

I remember [how I first met Archie] socially. I went on a Saturday morning to an art gallery, which was run by the wife of an English professor, a colleague of Archie's [at Cornell]. It was called Ithaca House. [. . .] She invited me to have a coffee, and Archie was there, sipping coffee [as well]. So, it was a typical Ithaca [moment].

And I then kept bumping into [Ammons, at our] farmer's market, [at a Cornell coffee house]. **<T: 40 min>** We started talking. And at one point, I worked up the courage to show him a poem, before [our small group started meeting]. So much easier in a small-town setting, [this interaction].

[. . .] I [also] sat in on some literature courses to keep up with the languages [. . .] I knew, [. . .] Russian and German. [The professors actually liked to have a faculty member sitting in]. In German, there was Eric [A.] Blackall, a great scholar of German literature. [. . .] I remember two courses in German. [. . .] One was a course by a nervous assistant professor on Austrian writers [and critics] in the early twentieth century, [. . .] like [Karl] Kraus., [Robert] Musil, who wrote *Der Mann ohne Eigenschaften* [*The Man Without Qualities*]. And [Rainer M.] Rilke and [Franz Kafka. That was fascinating]. [. . .]

And then Eric Blackall taught a course on [Johann W.] Goethe's poetry. [He pulled me into participating]. He asked, "Why don't you—could you talk about Goethe's science?" So, I read [Goethe's] *Theory of Color*, and [his] particular dislike of Newton.[87] [. . .]

In Russian, [I sat in on a course]. Alex [Alexander K.] Zholkovsky taught a course on [Boris L.] Pasternak's poetry, Pasternak's poetry. [Zholkovsky, now] at University of Southern California, [was a great teacher]. He came from a structuralist school, [that of] Roman [O.] Jakobson. [. . .] These were people who applied to the literature a [. . .] quasi-scientific [way of thinking. But] Alex Zholkovsky was also one of these people, like a number of Russians, who could recite Pasternak and Mandelstam and Tsvetaeva. [. . .]

It was easier at Cornell. This is one of the good things about Cornell and Ithaca. That it allowed me to make contact with people in the humanities.

CARUSO: Were you an anomaly, as far as you knew, in terms of that connection? Or were there other science professors that were involving themselves in the humanities?

HOFFMANN: I was not the only one, but I was an anomaly; there were just not that many. There were other poets who were not [faculty, but in the] community. [For instance, Fred Muratori, who works in our library, is an excellent poet]. There are people all around [us who write. For instance, Rick Mullin, who is a senior editor for] *C&E News*, [and also a very good painter]. **<T: 45 min>**

[. . .] I was somewhat of an anomaly sitting in on courses. [. . .] The languages were an entrée. So, being a European [was important].

CARUSO: And what about becoming more known or people finding out about your interests outside of Cornell University? I mean, you mentioned the Djerassi [Resident Artists Program]. I assume that was something you had to apply to?

HOFFMANN: I had to apply for [these artists' colonies]. But I think [the connection with] Carl made it easier. [I had an easy time interacting with the artists; I felt open to] collaborations with the artists. [And from their side], they liked those collaborations.

CARUSO: Yes.

HOFFMANN: And to me, it was exciting. It was a different group of people.

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[87] Goethe, Johann Wolfgang von, *Theory of Colours* (Ger. *Zur Farbenlehre*), published by John Murray, 1810.

REINHARDT: What was the reaction of your chemist colleagues?

HOFFMANN: [The] overall [reaction] is a mixed one. [Certainly,] colleagues were musicians. [If I were a typical] middle-class German kid, German-Jewish kid, [headed for science, I bet] there would be no way that kid could escape violin or piano lessons in the mid-twentieth century. It was part of being part of the bourgeoisie [cum intelligentsia].

I escaped music lessons because of the war. [Maybe that wasn't so good; maybe I wish I had that musical education.] When chemists write a memoir, you are likely to find poems as epigraphs. They know at some level [. . .] poetry's power and its value. [There is Fritz Haber], writing this doggerel verse, [as he did]. He loved it, but he didn't write serious poetry.

But then you see [Humphry] Davy. In a different world, a different time, [he] could have been a real poet, if he had not been a scientist. [Davy's] poetry does not travel well, [but] I think in his time, he was taken seriously.

[My] colleagues value the poetry. Scientists [. . .] sometimes have a slightly negative valuation of the humanities. [It comes up in small ways. For instance they have no patience for problems that still bother us, problems that may have non-unique] resolutions, [but no] solution. [Take] free will and determinism. If you can't decide which [we have], and if freshmen students can have an opinion about that, maybe it's not worth studying. [Never mind that twenty-five hundred years of intelligent discussion has not resulted in an answer]. **<T: 50 min>** Of course, [those are just the problems worth talking about.]

[Scientists are also intolerant where apportionment of money is involved]. God forbid the university should give a free computer to the humanities professors but not to the chemistry professors. They just forget that the scientists have four hundred million dollars in [government] research funds coming in, but the humanists have half a million. [Those are actual Cornell figures].

Of course, the social construction of science movement did not help in general, because it was viewed as some weird incursion from the humanities—[confusing social sciences with humanities]—with their strange ideas about what constitutes reality

[To return to poetry,] I think overall [that colleagues] are glad somebody is doing it. [. . .] They [do] value it in some way.

The next set of reactions are [along the lines of], "You have the luxury of doing this. I'm an assistant professor. How is this going [to affect my promotion?" They're right]. We have no system of valuing external activities of this type for a science professor. That is not only true for me. Emily Grosholz at Penn State [Pennsylvania State University], is a professor of philosophy.

[. . .] She and I have written one article together.[88] She's also an established poet, an associate editor at *Hudson Review*. One time, she put in her annual report to the chairman of her department in philosophy [a list of] the poems that she published that year. The chairman said, "Remove those poems." So, professionalism is rampant, [and not just in science]. The assistant professor is not going to be [evaluated on what he or she does outside of science].

[. . .] When [a reaction by colleagues] shades over to, "I could do it if I only had the time," now that is something else. They don't realize, because they haven't tried it, how difficult it is to write poetry. [. . .] I go through more drafts on [my poems] than I go through on [writing] a scientific paper. [That was also true of] the essays that I wrote for *American Scientist*. [. . .]

Now maybe it's because I've gotten better at the scientific paper, six hundred of them down the line. [But it's not that.] Every [paper gets my undivided attention; the collaborators know it. But poetry, or plays, or popularizing science ones are not easy to write. All I can say is "try it."]

[. . .] A number of people who come **<T: 55 min>** from especially European backgrounds have perhaps more of a valuation of culture, *kultur* with a capital K, than most Americans. [It's interesting to] look, for instance, in Feynman's books, a kind of aspirational bible to young scientists. [I see a divided outlook in those books. On one hand], he did take off a year to do music in Brazil. At [another] point, he reports his attempts to find value in poetry. [And he doesn't get it, he doesn't find the value for human beings in it].

CARUSO: Given some of what we've been talking about, I now have a better sense of how you met other professors in the humanities and things like that. Were similar things happening—so I guess this is a two-part question. Were similar things happening with meeting professors in other departments, science departments, like in physics, in biology, and things along those lines? And I'm also curious to know what is going on outside of your science? I don't know if I really want to use the word outside. How is all this other stuff—what role is it playing with the science that you're conducting in the post-Nobel period?

HOFFMANN: My outreach in science has been more towards physics, and none toward biology. [. . .] When chemistry wasn't inspiring in college, why I didn't get interested in biology? Because this [time—I was at Columbia 1955-58—]was two years after Watson and Crick. [. . .] Well, no one was teaching about Watson and Crick in the biology department at Columbia [at the time]. [. . .] I would have had to know much more to realize that there was a revolution forming.

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[88] Emily Grosholz, and Roald Hoffmann, "How Symbolic and Iconic Language Bridge the Two Worlds of the Chemist," in Nalini Bhushan and Stuart Rosenfeld (eds.), *Of Minds and Molecules: New Philosophical Perspectives on Chemistry*, (New York: Oxford University Press, 2000).

[Later there was another chance; and I did do a paper with Harold A. Scheraga on peptide conformations.[89]] I was working with a methodology, the extended Hückel method for calculating electronic structure, which [. . .] was not good in detail on energetics. I could have parameterized [the method] to death, [so to speak], to get energetics right. Energetics of what? For instance, [. . .] the conformational energies of amino acids, or [the energetics] of hydrolysis of phosphate esters, something important in biology.

I realized in reading a little biology that control in biology, due to the workings of evolution, was [exercised] by accumulating small differences of energy. It wasn't that all of a sudden a new active site was created by having totally different functional groups on the amino acids surrounding the [reacting molecules]. Rather, there were some little motions, adjustments. [. . .] And I couldn't get small energies right with my method. [It was pretty] obvious that evolution works this way, by [putting together] small [differences] to create a big effect. It is true that there are some places [in biology] **<T: 60 min>** where there is a large input or change in energy. For instance, in photosynthesis, there comes in a photon or two photons with a total energy of several hundred kilocalories per mole. But [that energy] very quickly gets degraded, [taken up by] many ATP molecules that then [carry on] the commerce of the cell, as far as the energy is concerned. [I just didn't see that my method would get right small amounts of energy. I did not like parametrization, either.]

I [have a done a little work on] metalloenzymes, but somehow, every attempt I've made to get interested in biology, except culturally, has not been successful. [It's very exciting to know these things, how they work.] Somehow my [mindset] and the way biology or biochemistry works did not come together.

On the physics side, it's been different. I'm conflicted, because I'm interested in fighting the reductionism that is rampant in physics vis-à-vis chemistry, especially. I believe that chemists [actually] understand things better than physicists as far as bonding [goes]. But that's not what the physicists think, and it's not what many chemists think. I could go into why I think we understand better, but that's another story.

I have reached out to physics; [it was natural to do so, in electronic structure of extended systems—metals, minerals, the like]. I've seen that in dealing with that community—[solid-state physics]—there is value to the chemical ways of thinking. [. . .]

So, how did I reach out? [. . .] The interactions with these other communities in part were made feasible by structures that existed at Cornell. In particular, a center for materials research, which is the oldest one of these umbrella grants originally from DARPA [Defense Advanced Research Projects Agency], now from NSF. [It's called the Materials Research Center.]

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[89] J.F. Yan, F.A. Momany, R. Hoffmann, and H.A. Scheraga. "Energy parameters in polypeptides. II. Semiempirical molecular orbital calculations for model peptides." *Journal of Physical Chemistry* 74, no. 2 (1970): 420-433. Also, see Harold A. Scheraga, interview by James J. Bohning at Cornell University, Ithaca, New York, 10 February 1987 (Philadelphia: Chemical Heritage Foundation, Oral History Transcript # 0064).

[. . .] Second, there is a tradition of [such interaction]n at Cornell. [It] is worth a PhD thesis, and has to do with the fact that three people came over from Europe in the thirties or forties [to Cornell]. They were Peter [J. W.] Debye, Hans Bethe, who came in '33, and the third one is less well-known, Henri [S.] Sack. Sack became a department chair in engineering. Bethe became a valued [faculty] member in physics. Debye, who could have been in the chemistry of physics department, was in the chemistry department. [He] was chair of the chemistry department [in the 1940s].

[These three scientists] knew each other from Europe, and they each moved across physics and [other fields—chemistry, engineering disciplines]. And they somehow created a culture [of interaction—it was before my time, but I felt it]. Hans Bethe is remarkable, because we think of him in terms of the mechanism of solar energy generation and of the work on hydrogen and atomic bombs. [. . .] But he also consistently pushed for the valuation of solid-state physics in a time after the Manhattan Project when nuclear physics was dominant. **<T: 65 min>** [Bethe] created a structure at Cornell called the Laboratory of Atomic and Solid State Physics [that allowed this subfield of physics to flourish]. I did not know him well; there was too much of an age difference. [. . .]

The [interaction between chemistry and physics at Cornell was also enhanced by Michael Fisher, Ben Widom, and Ken Wilson, all working on phase transitions. And eventually I was drawn to the interface. So, the last fifteen] years, I've been working on materials under high pressure. This is a collaboration with Neil Ashcroft, who is a leading solid-state physicist. [You may know him as the coauthor of a classic] textbook of solid-state physics, [together with David Mermin].

Neil Ashcroft, originally from New Zealand and England, then came to the United States and to Cornell the same year I did, '65. But we didn't publish a paper [together] until 2006. That's forty-one years. We knew each other; we respected each other. But it took a Polish postdoc of mine, [. . .] an outgoing postdoc, Wojciech Grochala, who is now back in Poland, [. . .] went over and talked to Neil. I didn't tell him to go and talk to Neil—he went over and talked to Neil. He was [and is] that way, [quite wonderful and enterprising]. [. . .]

Neil [told him about an idea about superconductivity], and Wojciech said, "Let's do this—study these things under high pressure." [I agreed]; so I had a part in giving the postdoc some freedom. And eventually, [with a talented graduate student, Ji Feng], we looked at the structure of silane, SiH_4, under pressure.[90] [From that point, our research groups joined, quite spontaneously. In time we got] a joint research grant. We're both seven years retired, we're both active in research, and we're working. We have published [over] twenty papers together in the last years. I wish all postdocs were like [Wojtek, that's what he is called.]

[90] Ji Feng,, Wojciech Grochala, Tomasz Jaroń, Roald Hoffmann, Aitor Bergara, and N. W. Ashcroft. "Structures and potential superconductivity in SiH_4 at high pressure: En route to "metallic hydrogen"." *Physical review letters* 96, no. 1 (2006): 017006-1–017006-4.

REINHARDT: You described once how important experimental science is for your theoretical work.

HOFFMANN: Yes.

REINHARDT: Could you go into the perspective of what we are just talking about? Go into a bit more detail, what the important points for you are, and who the important people over your career that imprinted something on you and your work?

HOFFMANN: Yes. I am a theoretician. I have always been [one], though the first two papers I published were experimental ones. One was when I was eighteen, on thermochemistry of some compounds in Portland cement.[91] [. . .] The next paper was on a low level [radioactivity] counting system for the carbon-11 isotope, which has a twenty-minute half-life.[92] [It's] made from a reaction of carbon-12 with a proton [in, and proton and neutron out of the nucleus. Both publications came from summer jobs.]

Experiment was imprinted on me by the fortune of work with two important people, Lipscomb and Woodward. [. . .] Lipscomb was many things, a crystallographer, a boron hydride chemist, a theoretician also, and eventually a [structural] biochemist. I worked with Lipscomb on boron hydrides, which were a very active field of research at that **<T: 70 min>** time, around 1960. My PhD was in 1962. It is on the theory of polyhedral molecules, with Lipscomb and with Martin Gouterman. Martin Gouterman [was my first PhD advisor, also a brilliant theoretician, a world expert on spectra of] porphyrins.

I even tried to make a porphyrin in my first year in graduate school! [Well, I] had an explosion, making a mess of a brand-new laboratory in a new building. There was no group to work with, so I improvised [the synthesis myself]. I didn't seal the glass bomb very well, and it exploded, thank God hurting nobody. [. . .] That was the last experiment I did, first year of graduate school.

Gouterman was very interested in spectra of porphyrins, [as I've mentioned. The colors of these molecules] are very intense. [They are also related to] phthalocyanines, [another class of intensely colored molecules. We all know the red of the heme group in blood platelets; a porphyrin is there.]

I was sensitized to experimental work. Lipscomb consistently made connection to experiment in the boron hydrides. Coming to visit us, for instance, was Fred [Marion Frederick] Hawthorne, bringing us news of the first synthesis of icosahedral $B_{12}H_{12}$ [as its potassium salt]. We immediately did a calculation on that. Hawthorne told of the carboranes, compounds which

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[91] Newman and Hoffmann. "Heats of Formation of Hexacalcium Dialumino Ferrite."
[92] Cumming and Hoffmann, "Efficient Low-Level Counting System."

two BH groups were replaced by CH groups of that ion to make a neutral $C_2B_{10}H_{12}$. We did calculations of various isomers, comparisons with stabilities [were available]. Experiment was there, emphasized by Lipscomb at every point. [In another part of the lab,] crystal structures [were done, and synthetic boron chemistry, too].

Then [there was this long, intense period of work] with Woodward. [. . .] Jeff Seeman [has begun to] tell the story of our interaction.[93] Jeff has also looked carefully at my notebooks. [. . .] The miracle is I kept notebooks in those times, [even if I didn't date them well]. They're not like [industrial company notebooks], where you date every day and you witness it. [In mine], every few weeks there is a mention of a seminar and there is a date. [In my notebooks are described] the calculations I did. [. . .] They're a record of my development in organic chemistry. [. . .]

I was just drinking in organic chemistry. I was sitting in on an important course [taught] by Doug Applequist. I kept the lecture notes from that course, [which] introduced me to physical organic chemistry.

With Woodward, I was dealing with someone with an encyclopedic knowledge of the literature. That comes through in everything that people write about Woodward. [I have this] image of Woodward in the library, looking through *Chemische Berichte*, in his blue suit.[94] He knew so much; of course, one of the reasons the orbital symmetry story made an impact [was that] it dealt with new experiments, that [in turn] were related to old experiments. The new experiments were from physical organic chemists in the US and in Germany, especially Vogel and Criegee, [who noted] certain [striking] specificities in some reactions. The old chemistry was **<T: 75 min> [**not that old, but] the very complicated natural product chemistry of vitamin D and its transformations with heat and light. The Vogel and Criegee [work] was accessible to me. The vitamin D stereochemistry, dealing with complicated natural products, looked too complicated to me, a theoretician. It's Woodward who had to pull out the essence, because he [needed it for] a synthesis of his own. He had to pull out the stereochemical essence [of the old and new reactions], and simplify it to the point where I could do calculations on it.

But of course, what made the orbital symmetry story successful, aside from the nexus between molecular orbital theory and organic chemistry that it formed, was that it -- accounted for things. [The theory] rationalized reactions, but it also made predictions of stereochemistry of certain reactions. The predictions were readily verifiable on the timescale of one year [of work], and there was a community out there of physical organic chemists [who could test the predictions. That community was formed elsewhere, in the then fashionable work on] non-classical carbonium ions, with [tests of] the utility of the Hückel model. [. . .] There was a community there [ready] to do experiments, which didn't take fifty years to do. It could be done in a year.

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[93] Seeman. "Woodward–Hoffmann's stereochemistry."

[94] *Chemische Berichte* was a German-language scientific journal of all disciplines of chemistry from 1868 to 1945, published by Deutsche Chemische Gesellschaft.

There was a tremendous flurry of activity testing our predictions in various ways. [These communities of people ready to experiment once a direction comes into focus are very important]. There is such a community [now in physics], on superconductivity. Any time somebody comes up with a new material, immediately there are one hundred papers [on that material. One could say that] there are a lot of underemployed solid-state physicists [out there], waiting for the next molecule, for the next [material]. I was very lucky [in the orbital symmetry control story, blessed by such a community. It generated a dynamic of experiments].

[. . .] In terms of instruments and techniques, there is another story [here, that of] computers and quantum chemistry calculations. [. . .] My whole career is tied up with computers, but the peculiar success of what [. . .] evolved [with time—approximate calculations on organic and, in time, inorganic, molecules—] was that I somehow grew more interested in chemistry. [And importantly], I learned how to construct explanations. I did that from the work with Woodward, more than [with] Lipscomb. With Lipscomb, I'm still in a calculator mode.

I think what I learned from Woodward was the power of a simple explanation, [and that it was available from the frontier orbitals of a molecule]. I rediscovered a language of quantum mechanics. [I say rediscovered because I knew that language and theory, but didn't really understand how it worked, what its implications were. This was perturbation theory, which allowed me to draw interaction diagrams, construct the course of individual levels as a reaction proceeded.]

[. . .] So, the story of me and computers is a long story. [I could not have had a career without them, but] much of what [I did and still] **<T: 80 min>** do is fighting the computer. [I've learned how to extract explanations from reams of date, millions of numbers on a monitor.]

REINHARDT: How do you do that?

HOFFMANN: Well, [. . .] it didn't come overnight. It evolved. [. . .] Woodward came to me with a simple orbital explanation [of the stereochemical course of what came to be called electrocyclic reactions] in terms of the symmetry properties of highest occupied molecular orbital. I began as a calculator, and [while] not disbelieving his explanation, I [felt more comfortable, I think, with actually carrying out a calculation. Boy, I was well-prepared. The extended Hückel method gave me the ability to study simple organic reaction. I said— to Woodward, to myself]—"Let me do a calculation on butadiene closing to cyclobutene." And [when] I did a calculation with the ends of the butadiene molecule rotating this way, and the other way, the first time they didn't come out supporting [Woodward's] simple argument.

I then realized that what I had done was [that I had chosen an unrealistic reaction path. There was no guidance. It's a long way from H+D2 reactions—which was in the literature—to butadiene closing. I had] kept [the carbon skeleton] of butadiene molecules [. . .] frozen [as the reaction proceeded. This couldn't be right—what had to happen] was that the CCC bond angle had to go down as it formed a ring from the chain.

When I put that [into the calculation], I recovered the orbital argument that [Woodward] had. [It took me a while to realize] that [his] simple orbital argument had power, more than the calculations. [At this point, we saw that Longuet-Higgins and Abrahamson had a way of following the orbitals through a reaction more completely than the simple frontier MO argument did]. I had drawn [correlation diagrams before], but I hadn't realized their power. [. . .] I knew symmetry and correlation diagrams, and I applied that [approach] quickly.

I saw the explanatory power [of simple MO arguments]. [. . .] The numbers were not [teachable]; this simple explanation was. And somehow, I began to use more and more of these [orbital arguments]. And [in] the language of perturbation theory, a certain way to deal with small changes in geometry or in some other aspect, a [technique common in] quantum mechanics, I worked out [over time] a mixed verbal-visual language of explaining orbital interactions. [It's less mysterious, less magical, than it sounds.]

The [components of] the visual language were, first of all, the orbital level, those little drawings of the two p orbitals. [Then they were allowed to mix with each other, through overlap. In this way we generated] orbital interaction diagrams. [The levels mixed, they] repelled each other. This result comes from perturbation theory, that when two levels interact, one goes down, the other one goes up. [. . .]

It wasn't just me, but others, [as well. The components of that language, of orbital interaction, were already in place, already in the toolkit of theoretical chemists. You can see how some people, like Lionel Salem, just could run with it.] **<T: 85 min>** We constructed a visual language, mixed symbolic and iconic, to use semiotic terms here. Iconic, [in that] these little drawings represented where a lone pair, [or a level with two electrons], was [in energy]. The symbolic [part was in the algebraic description of the energy levels mixing with each other]. [. . .]

[You know], chemists will do anything to get an explanation. [. . .] All the categories you devise, inductive, deductive, symbolic, iconic, natural, unnatural, they're going to violate all of those. They're going to make a DNA molecule that takes the shape of a cube—[why not? Scientists] are anxious to understand, and my current metaphor is they're scrabblers, that they'll do anything to get up to the top of the hill.

REINHARDT: Isn't that what you just described for chemists that make them better understand than maybe physicists do, one of the things?

HOFFMANN: [. . .] One of the reasons. The other part is that they know less mathematics. [Some do know a lot.] Therefore, they deal more in verbal constructions. [Here's the difference:] if you take an average experimental physicist, they know more mathematics [than a corresponding chemist] because of their education [in] mathematical physics. [. . .] The average experimental chemist will learn just enough to understand and not much more. [Take] NMR:

you get a certain number of [chemical shifts], but let's not worry too much about the physics of the actual coupling constant that makes for the splitting of the lines. [. . .]

Faced with the complexity of chemical bonding, I think there are two reasons why chemists understand things better. One is because they [are less familiar with] mathematics, [they seek] to get qualitative explanations, based on these kinds of pictures that I have drawn. [They have to try harder, not relying on the crutch of mathematics. So, paradoxically they understand the chemical bond more physically than physicists].

The other [reason is in] the poetics of particularity in chemistry. That is, given that there are [100] million molecules, they present many, [many] situations of bonding. [Some are repeats, like CC single bonds]. But there are enough other [kinds of bonding situations that one is forced by the richness of molecules to come up with different ways of bonding: covalent, ionic, electron-deficient, and so on. A new problem surfaces: how to see the relationship between all these bonding types. I think I'm good at that. I know the art of constructing connections.]

[. . .] Solid-state physicists [. . .] are close to chemistry. The superconductors [may be] cuprates, and then tomorrow they're iron selenides, and then [LaH_{10}. That diversity brings condensed matter theorists close] to us. By and large, physicists construct a reality that they deal with, **<T: 90 min>** which is not as rich in examples as the chemical reality that we are confronted with. I should write about that sometime. [. . .]

CARUSO: We've been speaking a bit about the science and how you were pursuing it. The interactions you had somewhat with physicists. One thing that you had made reference to, but I wanted to—

HOFFMANN: I'm interested in interactions in general. I entitled the Nobel lecture, "Building Bridges Between Inorganic and Organic Chemistry." The building bridges metaphor [is a theme for me]. My father was a civil engineer, so maybe there is something there. And he did build, if not bridges, culverts and small bridges, [and roads around that small Polish town where we lived]. In the brief life that he had—he [died at] thirty-two. [. . .]

The inorganic/organic [link] was very important to me, and now I have [built] a bridge to solid-state physics. In some sense, my activities in the humanities can be viewed as another kind of [bridge-building] behavior. [The classes I sat in that I told you about, my coffees with Archie]. [. . .] I find it interesting to build connections. [. . .] It feels important to me, and I'm willing to risk some things [to make the connections]. Writing poetry is risking a number of things. [. . .]

CARUSO: Earlier today, you made mention of the fact that with your NSF funding you were criticized for the outreach component, and it had to do with the—I think you were referencing the science cabarets.

HOFFMANN: Yes.

CARUSO: So, I was wondering if you could tell us a little bit about how those science cabarets came about, and what it is that you wanted to achieve with such things. Especially since we're talking about bridges and—

HOFFMANN: [We have the Entertaining Science Cabaret at] the Cornelia Street Café, [a classic West Village restaurant and performance space]. Cabaret is not the right word exactly. [. . .] The origin story [begins with me, when] I'm on a sabbatical at Columbia for a half-year in 2002, and K. C. Cole, a science writer who writes mainly about physics, **<T: 95 min>** who by that time is based in California. She has written a book, *The Universe in a Teacup,* about how physicists searching for nothing found the theory of everything. [. . .] The nothing is the ether, and the theory of everything [is] quantum mechanics.[95] [. . .] In the book, she cites some things by me, maybe a poem, and she cites Oliver Sacks. His book *A Leg to Stand On,* is about how he loses the sensation of a leg in an accident, the nerve gets damaged, and he talks about that feeling [of no feeling].[96]

[KC, who goes by her initials K.C. has] a book. She wants to publicize the book. [She writes] to the owner of this Cornelia Street Café, Robin Hirsch, an entertainer and the restaurant owner, [. . .] says she wants to do a reading to publicize her book. Robin is running something every day of the year at the entertainment space [of the Cornelia Street Café]. This is a sixties jazz club setting with sixty seats in a narrow room, and a little eight-by-eight-foot stage in front. Upstairs is a restaurant. [Every day of the year, twice an evening, there's a show there: spoken word, music, art].

[KC] writes to [Robin], she wants to do a talk about her book. He says, "You're not famous enough." She doesn't give up. She comes to me, and she says, "Would you do it with me?" And I say yes. She goes back to Robin. He says, "Neither of you are famous enough." [KC] doesn't give up. She and I talk. We decide to invite Oliver. Oliver is a friend of mine; [sadly he is close to death now]. We ask Oliver, because he's quoted in the book. [. . .] All of a sudden, we're famous enough.

So, [Robin] puts us on the schedule. Oliver has a friend, Ren [Lawrence] Weschler, who is now a director of [an Institute for the Humanities] at NYU. [. . .] He was a writer for *The New Yorker* at that time. [Ren wrote a] *New Yorker* [column about our show, in which he cites a

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[95] K.C. Cole, *The Universe and the Teacup: The Mathematics of Truth and Beauty*, (Harcourt, Inc.: 1999).

[96] Oliver Sacks, *A Leg to Stand On*, (New York: Touchstone, 1984).

poet] at the café. He asks him, “What are these people going to talk about?” And the poet, Angelo Verga, answers something [along the lines], “Well, they claim they’re going to talk about nothing, and isn’t that a great subject?” [laughter]

Three hundred people show up on the street for this show. There is room for sixty. The police are called [in] to disperse the unhappy people who couldn’t get in. The café owner is overjoyed. [laughter] And we have a good evening. I’m the entertainment, in a way, [as I read some of my poems related to KC’s theme]. The others are more serious. Interesting, that I would say the poetry’s not serious, Anyway, I’m the entertainment here.

[. . .] I realize we have something. [Three parts, science and art. We didn’t have music yet, but we had poetry.] It came together entirely by chance, [with] KC who was the driving force. I then write to Robin and ask him, “Hey, can we do this on a regular basis, once a month?” And he says yes on the basis of that big crowd.

I schedule a [second] program. **<T: 100 min>** [. . .] I asked Lynn Margulis, whom I knew. I knew she came to New York [regularly, as] she had a son living in New York, one of her children with [Carl] Sagan. Lynn was [. . .] an iconoclastic biologist. I invited her; her son [Dorion] talked. And they had a grandson who played rock music. [. . .] Anyway, they were the second show. And we got a good crowd. We filled the place. So, at that point, we had it, [the basic formula of science and entertainment. We have been on] for twelve, thirteen years. I now have somebody running it with me, [Dave Sulzer, who goes in the music business as Dave Soldier. Dave is] a neurophysiologist at Columbia, and a [talented composer and] musician himself. [We’re on] once a month, [every first Sunday of a month, ranging far afield in both the science and the entertainment]. For instance, the next program will be on Easter Sunday, two weeks from tomorrow. [Yes, we run] into Super Bowl Sunday, [and Labor Day. We beat them all, fill the joint].

We charge twenty dollars. You get a free drink for that. [Let me] give you an idea of how far afield we go, [how we think about planning an evening]. For Sunday, Easter Sunday, I thought, Easter. Eggs. We’ve got to do something on eggs. In Sweden, there is a tradition. The children put [an egg-shaped container] under their bed, and there’s some sweets put into it. [You have] Ukrainian eggs that are colored [artistically, and] eggs baked into Greek pies. [Anyway, we have to have eggs].

I went to the café chef, Dan Latham, who’s a laid-back Southerner, and I said, “We got to do something on eggs.” He had done one program before, where he had participated, on snails. Where I had Mandë Holford, who is [a chemist at Hunter, who studies] the venoms from beautiful [and poisonous] snails. I combined that with the café chef cooking edible snails.

So, this time, the café chef is going to make some things from eggs. Then I had to think, what science can I pair with that? If I were at Cornell, we have a poultry department or sub-department somewhere in the ag school, and I would turn there. A long time ago, I knew [Alexei] Romanoff who was a world expert on eggs. But I’m in New York. There aren’t too many poultry [science] departments in New York City.

So, what am I going to do? I don't know. Turns out there are people raising chickens in Brooklyn and Queens. There's a whole association of them. But then I remembered I had seen a book by a science writer called [Andrew Lawler]. [Andrew has] been writing steadily for *Science* and for *Discover*. He [had just come out with] a book called *The Chicken that Crossed the World* -- and it's a cultural history of the chicken, about biology, too.[97] About making of vaccines, [as well. Lawler wrote] about how the use of poultry **<T: 105 min>** has gone up in the United States as a meat, as a source of protein, relative to beef. [Lawler is based] in North Carolina, [but perhaps by chance he will b]e in New York. We don't have a budget [for the show, but I liked the idea so much that] I'm paying [from my own pocket] for a hotel room [for him] in New York for one day. Usually, we don't pay anything; [the performers just get some] free dinners.

So, that's the program. It [will be] called "Eggstravaganza." The science part [will be done this time not by] a scientist, but a science writer. But they're often better at doing the science than the scientists! And the entertainment part is the chef making some egg dishes.

CARUSO: What sort of responses have you gotten to—

HOFFMANN: Very positive responses from people. I've been asked to move this uptown or to [. . .] some other place, [but I like it where we are]. A competing show, [perhaps originally based on what we did, but really original, is the] Secret Science [Club, now at the Bell House in Brooklyn]. I envy what they do. Dorian Devins, who organizes that, fell into a relationship with a café in Brooklyn that bought a rock club, and they moved [into that. No entertainment, loud music around the science.] Imagine a hall, a [large] hall, [several] hundred young people. Raucous [music], and then a scientist talking for thirty minutes. What I envy is they have a young audience, where we don't, we have a generally aging audience. But it's okay. [. . .]

[In our show,] the scientist [also] talks for half an hour. [But we do have the entertainment, and that's important to me, for I want to normalize the science, make it part of the cultural scene.] After five years' work, I could convince the café to put in a projector. [. . .] Until then, I would bring down a projector from Cornell and we'd [project on a sheet]. The scientists in general—one or two exceptions in twelve years—are unwilling to talk without showing slides.

CARUSO: There are a couple of other things I want to talk about, which, I mean, in some ways, this is going to backtrack us a little bit. But I wanted to have some more information about—for example, I'd like to start with the *World of Chemistry*, PBS [Public Broadcasting Service], and hear a little bit about how that came about and why it came about.[98]

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[97] Andrew Lawler, *Why did the Chicken Cross the World?: The Epic Saga of the Bird that Powers Civilization*, (New York City: Simon and Schuster, 2014).
[98] *The World of Chemistry*, directed by Isidore Adler and Nava Ben-Zvi, presented by Roald Hoffmann, PBS, 1990.

HOFFMANN: Yes. That took two years of my life, from about '87-'89. And I'm glad I did it. I didn't get paid for it. I got leave from Cornell for about a year, to do it. [The project was conceived] in the mind of a person who's no longer alive, Isidore Adler—Izzy Adler—who was a professor of nuclear chemistry at University of Maryland and was interested in education. He pitched the idea [to the Annenberg Foundation], was encouraged, and [then] wrote a [better] proposal. [Adler put together] a committee of [five] other people. **<T: 110 min>** One of them was an enterprising [and ingenious] Israeli science educator, Nava Ben-Zvi. She has just retired in Israel. She and Izzy were the directors of the project. [. . .]

I was brought on as a presenter; [. . .] the Nobel Prize [and my relative youth] played some role in that. In the end, [. . .] I wound up not just a presenter, but I worked with the other five people in writing the scripts for the shows. The project was of some magnitude, twenty-six half hour shows, directed for PBS. [It was conceived with what might have been] a misplaced ideal of a remote learner situation. [. . .] The idea was it would be shown on public access TV or PBS, and then people could register at a community college [to do a laboratory, and] get credit for that as a course. It was ahead of its time, [and the remote learning course was impractical. But until today it is shown on PBS stations at strange hours, and people write to me about it.]

The funding [came primarily] from the Corporation for Public Broadcasting, which [. . .] had in the previous year sponsored a physics course out of Caltech, [produced by a leading] physicist educator, David [Goodstein. Perhaps that course was difficult for the audience. Some funding was raised from additional sources, American Chemical Society, Eastman Kodak, Dow. Not too much. The main funding, the total budget approached three million dollars, and that was to make twenty-six episodes. On our project the producer was] Richard Thomas, a leading science [director], who had played an important part in a previous series on PBS [which] was very successful called *The Brain*, around the eighties.[99] He was the executive producer. [There was an] academic team of six people, and production company [based in the] Washington area. [. . .]

The average budget sort of per episode, half hour episodes, was fifty [. . .] to seventy-five thousand dollars. It would be more today, in today's money. To put that in focus, it was one half to one third the price [per minute] of a [then contemporary] *NOVA* program.[100] [We had] less money than a *NOVA* program, but still, this was professional TV, [and as such] very expensive. [. . .]

To this day, I get telephone calls or [an] email message a week from high school students who are seeing those. This is twenty-five years after [the initial airing of the show]. Occasionally, it's shown on some PBS stations as a filler in the middle of the night. [. . .] It's funny—one time I got a call from a student, a former student of mine, and he said, "Dr. Hoffmann, I have to tell you this. I went home to my parents' and I fell asleep on the couch with

[99] *The Brain*, produced by Richard Thomas, PBS, 1984.
[100] *NOVA*, created by Michael Ambrosino, PBS, 1974.

the TV on. And I woke up in the middle of the night and there you were on the TV!" He said, "I thought I was having a nightmare." [laughter]

[*The World of Chemistry*] **<T: 115 min>** was difficult to make, for a variety of reasons. I was on for three minutes in each show, the beginning, the end, and sometimes in a bridge [segment] in the very middle. There was another live component [to the show. This] was a lecture demonstrator, [Donald L.] Don Showalter, who was [at the] University of Wisconsin at Stevens Point. We were the only two live people [on the show, aside from people being interviewed]. The most expensive element [in the programs] was the rather primitive animation, the kind of animation which a high school student could make on a home computer today in five minutes. [Then it] cost much more [per minute] than any other [piece in the program].

[One of the strengths of] the programs [. . .] came out of an improvisation, [when we couldn't afford a live scene]. I'll give you an example. There is a program on electrochemistry. [In the subject and the program, a prime example of this aspect of chemistry is the] process for making aluminum, by [running a current through] a molten alumina salt. [. . .] We [wanted to set the equipment up in a lab] and film the [process. But] we didn't have money. So, we used Alcoa footage, so-called stock footage. It's an advertisement for Alcoa, which shows [off], of course, their grandiose plant. [But in this way our audience got to see a more realistic industrial process than we could have showed them].

[I learned a lot about making films. The montage editor, who would take free footage from NASA, from other government or industrial sources—these were important, creative people. A knowledgeable person could have looked at some of that montage, could have said, this comes from this company, this comes from that company. We didn't know that. We thought nobody would know.]

The program was successful. We went back a few years later to make more programs. We couldn't get the funding. [Perhaps we had hit] some economic downturn. [But] there is nothing better out there, [in the way of chemistry programs at the high school/college level. So, somewhat dated as it is—forget about all the hair I've lost since then]—there are teachers still using this. It's dated a little, but teachers are still finding it useful. [. . .]

We also made a mistake. We didn't write a textbook to go with [the program. There was one, but it was not carefully enough coordinated with the video series. It's okay; on balance we made something valuable to the community. And learned much in the production. There is one program out there] that's better than what we [had made]—idiosyncratic but better. [These] are the periodic table videos by Martyn Poliakoff and made with a BBC [British Broadcasting Corporation] producer, [Brady Haran]. They are—[by design]—offbeat little videos, five minutes or so, about different elements, different scientific discoveries. [They're great!]

CARUSO: In 1996, you became the Rhodes Professor of Human Letters.

HOFFMANN: Ah, yes. Frank H. T. Rhodes was eighteen years president of Cornell. [. . .] And he became a figure on the national [educational] scene. I'm **<T: 120 min>** very glad to have that association with him. [Frank] is still alive, a very important person for Cornell. [. . .] This professorship, [which has only small] resources [attached to it]. It was a recognition by the university of my interest in the humanities. What exactly humane letters means is unclear, and people have trouble translating it. [Perhaps] it just means that the [holder] is interested in [humanity, and in letters. And that certainly am. And in everything else]. [. . .]

CARUSO: Did you know that you were going to receive it? I mean, is this like the Nobel, where—

HOFFMANN: Oh, no. [. . .] Usually, named professorships are a [relatively modest] way for a donor to leave an impact on the university. It takes two to five million dollars to endow a named professorship, something like that. [It costs far more to have] a building [named after you]. To name [a professorship] after Frank Rhodes [is a tribute as much to Frank as it is the donor and the holder of that chair]. But it [carries with it minimal] resources; [it is primarily an honorific designation].

CARUSO: Okay. I was in part curious about it, in part, knowing that *Old Wine, New Flasks* came out in 1997.

HOFFMANN: [There] was no relation.

CARUSO: Okay. Can you tell us a little bit more about why it is that you undertook that book? I mean, in our interviews, you haven't spoken too much—I mean, you've spoken about, you know, growing up, being Jewish. But, you know, Judaism hasn't necessarily framed a lot of our discussion. So, I'm wondering where—

HOFFMANN: And [Judaism] doesn't frame much of my life, though I feel very Jewish. And having lived through the Holocaust, it leaves a trace. [More recently], I've written [a] play about my mother and me and our survival. [. . .] Jewish identity is constructed in many different ways. As I told you at the beginning, the name Roald [itself came out of my parents thinking in 1937 in Poland of how to name a Jewish child]—that you would give your child a secular name and not a Jewish name.

CARUSO: Yes.

HOFFMANN: [. . .] It was easier to be a Jew in America, of course, but I wasn't very Jewish, [somehow. Perhaps I was, in an unconscious way, going to a high school for science where most students were Jewish, going to leftist summer camps. But then] I married somebody who wasn't Jewish, and that got me in trouble with the family. They got over it when they had grandchildren. But it made life uncomfortable for my wife for some time.

I named my son Hillel [J. Hoffmann], a very Jewish name, but our daughter is called Ingrid [H. H. Zabel, with some family roots, but] in my mind, it's after Ingrid Bergman. [laughter] So, we're constructing our identity in some complex way. Just before I came here on Wednesday morning, I spoke to a high school class [. . .] in Ithaca about being a child during the Holocaust—a tenth-grade class. I do a lot of these talks.

More recently, I've written some poems about that time, [in them perhaps] trying to unearth some memories. I've not written a biography, [as such], but I've written little [biographical] pieces here and there. And [then] I wrote this book [about science and Jewish religious tradition]. The book came about by accident, like everything else [in my life, it seems]. What happened was **<T: 125 min>** that I was getting an honorary degree [in] Beer Sheva, where Ute Deichmann is now, Ben-Gurion University of the Negev [Beersheba, Israel].

They wanted me to give a general talk; I had [one] at that time called, "Natural/Unnatural," about the dichotomy between natural things and synthetic things. It's a chapter in *The Same and Not the Same*. [After] I gave that talk, [. . .] Shira Leibowitz, [a woman working in the Rector's Office, told me she was] translating the talk into Hebrew, [for eventual publication]. And she said, "You know, there is a discussion in the Rabbinical literature [about natural/unnatural]." [. . .] She was clearly an observant woman, [wearing] a scarf, and modest clothing. [. . .] Anyway, we started talking, and [in the end] decided to write an article about it [together, which was published in an American literary magazine]. [. . .]

I found out that she was married to [Elhanan Leibowits, whose father], Yeshayahu Leibowitz, [I knew from the literature. The latter] was a biochemist, and a maverick religious [thinker]. He's no longer alive. And his sister was Nechama Leibowitz, [a great Biblical scholar]. Both Yeshayahu and Nechama were people of the Buber-Scholem generation. They were German [in origin], trained in philosophy, in the case of Yeshayahu and Nechama. And then went to Israel. Nechama is the author of some psychologically perceptive commentaries on the Bible, [which] many people know.

Shira was an American who married into that family. [. . .] She had an engineering degree, never practiced, but she loved science. At the same time, she was very aggressively religious, but in a rather special [leftist] religious family, if you can imagine that. [This is the Leibowitz family, people of a] totally different mentality from the settlers in the West Bank. [In time Shira and I] planned a book, [which] we wrote [in the] nineties. Meanwhile, Shira's husband died. She remarried, [an American Jew of a very conservative political and religious orientation. I worried if] we could finish the book, because it wasn't obvious within the tradition that [Shira] moved in that wives write books.

[There were constraints in working with an Orthodox, observant person.] We worked all the time with the door open, so to maintain proper modesty in the environment. [. . .] When we went looking for the snails that produce indigo [in a bay on the Mediterranean], I went in the water with her sons, but [Shira could not go in with us. Here's an amusing story.] When we came out [of the water], someone took a photograph of [the two of us] holding some of the snails that produce the snail indigo, which is Tyrian purple. [The] picture is of Shira in her modest dress and of me, and we're both smiling. **<T: 130 min>** [Such photos, of both authors smiling, are rare, since collaboration on a book is not an act that induces smiling. Seeing that photo], I said, "We've got to use this on the back cover of the book." And she said, "I have to ask my rabbi." I said, "Shira, what is it? Is it my nipples showing through [the wet T-shirt]?" And she said, "Well, I don't know. You just don't look presentable." [. . .] I wasn't wearing a risqué bathing suit or anything. It turns out it was my naked knees showing. So, we cut off the picture at the waist, and then we could [use] it. So, that's part of the story. [laughter]

[*Old Wine, New Flasks* is a rare book in several ways.] A testimony to the divisiveness of the religious situation in Israel was that book was not translated into Hebrew. No publisher would touch it. [Because the division between the secular and the religious in Israel is great, there is no middle ground]. It's been translated into Spanish and Italian. [. . .]

Shira's two eldest sons served in the military. There [are] more and more Orthodox in the military. But they refused to serve on the West Bank. And one of them was imprisoned for disobeying orders. [. . .]

I learned a tremendous amount [in writing the book]. I knew Hebrew, but the Talmud is written part in Hebrew and part in Aramaic, and the Aramaic was too much, and [. . .] I didn't feel that comfortable with Hebrew, either. So, I read it in translation. [. . .] There have been good translations for one hundred fifty years. [. . .]

Basically, I seem to be able to think the way that the religious think; in particular, the way the Talmudic scholars think. [. . .] I feel the same way, incidentally, about other religious traditions with a scholarly tradition. [I have] the Catholic tradition [in] mind—it has two millennia of scholarship and commentary on everything.

[Let me digress for a while.] I had to give a talk to Yeshiva University, a place where people study to be rabbis, but also secular studies. They [had all the first-year students] read Bertolt Brecht's *The Life of Galileo* [. . .] to stimulate a discussion—at this Jewish religious university!—about science and religion.[101]

I read the Brecht, [I told them the circumstances of the play, how Brecht] exploited women to write those plays. [How] that particular play was changed several times in response to his shifting politics, and in response to Soviet propaganda. [. . .]

[101] Bertolt Brecht, *Life of Galileo*, (1938).

I also looked back in the Galileo's life, [and the story I first found through, I think, Santayana, of a Jesuit priest asking Roberto Cardinal Bellarmine] what shall we believe about the Copernican tradition? [Bellarmine] **<T: 135 min>** answers in this remarkable letter, which essentially says that if the proofs were in that Copernicus and Galileo were right, the church would adjust. But the proofs are not in, he says. He was wrong. [But more importantly, Bellarmine voices a rational position, which comes out of a tradition of respecting] scholarship.

[Back to my attitudes toward religion. Even if I am an atheist] I can empathize with the religious ways of thinking. I also like ritual. [. . .] When I wrote the book from Shira, people, in fact, Jewish friends of mine who were religious, interpreted my sympathy [as an opening to] attempt to convert me back to observance. [. . .] What they didn't realize was [. . .] that I have the same feeling when I go to Afro-Brazilian possession rites [or a Pentecostal service, or in a synagogue. I realize I'm in touch with something, and I respect it.]

[. . .] I learned a lot about my own tradition, a tremendous amount. [Perhaps I have become] more Jewish [from writing the book, even as I am atheist. I've gained] respect for that tradition which I come from.

CARUSO: I have two other topics that I just wanted to touch on, and I think we should have enough time—

HOFFMANN: Yes, then we'll have to stop. [. . .]

CARUSO: Yes. You did start to tell us a little bit about the origins of the play *Oxygen*.

HOFFMANN: Yes.

CARUSO: I'd just like to hear a little bit more about that, working with Carl Djerassi, especially in light of his passing recently.

HOFFMANN: So, [. . .] in *Chemistry Imagined* you can see an essay called "The Air of Revolution," which traces the [history of the discovery. I thought it was fascinating that] Lavoisier, the [banker, the political] conservative, [. . .] is the chemical revolutionary. While Priestley, the political and religious radical, though a discoverer, turns out to be [a believer in the old theory], of phlogiston. [. . .]

The makings of the play were there [in the story. But] to me, the dramatic situation, which I mentioned to Carl, and which was behind our first attempts to write the play, was [the choice facing] Lavoisier in 1774, in September. [I imagine him sitting at home, thinking]. The week before, Priestley has come to have dinner with him, and he hears that Priestley has made this new air in which a splint flares up and mice live longer. Lavoisier needed [such a substance, for] he knew that things burned in air **<T: 140 min>** up to a certain point [. . .] and then stopped burning. But he hadn't quite pushed himself through to [the idea of the homogeneous air being made of two gases. Nor had he found a way of making just oxygen].

The same week, according to our best estimates, within a week of that dinner with Priestley, Lavoisier gets the letter from Scheele that says that Scheele has made [just] this air. And [Scheele] asks Lavoisier to do the [confirming] experiment. It's a pretty aggressive letter, [as I read it]. He's asking [. . .] Lavoisier to prove that he, Scheele, was right.

[Here's] Lavoisier at home, the only [person] who understands [the essence of burning and respiration. And along come two] other guys [who discover the gas Lavoisier needs, who tell him how to make it. How does Lavoisier deal with this dramatic situation?] So, the answer is he doesn't deal with it very well. He tries to take the discovery away from Priestley by recreating the experiment. [. . .] Priestley objects. Priestley's not going to be kept quiet in this. Eventually, [Lavoisier] gives him grudging credit.

And Scheele's letter he doesn't answer. [Lavoisier] doesn't answer. I believe [that], unlike what we have in the play, I think he saw [that letter—we postulate he didn't]. Why didn't he answer? I don't know. Lavoisier is an imperfect person. [In the end, we decided that] Lavoisier weighing what to do doesn't translate immediately into drama. So, that scene never found its way in the play, though it was initially so [in my mind].

[But let us go back before the writing of the play. That Lavoisier's dilemma] might be a dramatic situation [was with me from the beginning]. It flits through my mind it could be a play. I do nothing about it until one day I meet Carl Djerassi [. . .] around '97 or something like that, and I tell him this story. Carl [by then] had written his first play, *An Immaculate Misconception*.[102] [. . .] He says, "Let's write a play about it. "And I say, "Sure."

And from then on, [Carl, who is a most energetic person,] is pushing to write the play. [. . .] We meet one more time, actually, in a New York hotel, and we start out. He drafts a prenuptial agreement. [. . .] We agree his name will go first. [And that all receipts from the play] will go into a certain joint account. [. . .] If there is a dispute about something that we will mutually agree on some theatrical expert who will resolve the dispute. We actually invoke that mechanism once or twice later on. But most of the time—as I just said it at the Djerassi memorial, and it evoked a laugh—most of the time when there was a serious disagreement, and there were some, I asked him to have his wife decide. Because I knew his wife, [Diane Middlebrook], was strong enough to tell him off, [. . .] and I was right.

CARUSO: What were some of the things that you disagreed about?

[102] Carl Djerassi, *An Immaculate Misconception*, (World Scientific, 2000).

HOFFMANN: [. . .] In writing any sort of creative fiction or a play, poem, what two people are going to disagree [about is] humor and pathos. So, what one person thinks is funny, another person is not going to think funny. [By] pathos, I mean evoking emotion. What one person thinks pulls on the heartstrings, [another] person thinks is maudlin, is too much. We had some such disagreements. But we worked together, [mostly apart. We did have] one prolonged period together of ten days in London, where [we worked in Carl's] apartment. [We divided up scenes, [wrote them, then read for each, revised. It was not easy.]

Having Djerassi as a **<T: 145 min>** theatrical agent helps a lot, because he applied to the task the same skills that made him a good businessman. He [pushed] people incessantly to produce [our play. There were artistic disagreements. But we got over them. What also helped was that Carl had money.] It's not that he necessarily agreed to pay for the production.

CARUSO: Yes.

HOFFMANN: There are other ways. He would agree to [invest in or] sponsor the production of [another play] in order that this [one] be produced. It's like companies avoid taxes. [The skills that made him a good businessman served our play. After *Oxygen*,] we went our own ways. [Carl] was single-mindedly devoted to the plays, but also, to fiction and nonfiction. I decided to keep on with the science, [as I do to this day, while at the same time doing writing outside of science. Perhaps this was an unwise decision, but it is the road I took.] I've written two plays since. [And] I have had much less success in having these staged. Because I have not had Carl as a business manager]/coauthor]. He was phenomenal.

[Carl Djerassi a great scientist. And] he was ego incarnate. Though he complained about having to push himself forward all the time [to get his plays produced], he loved it. At the same time, [he] was brutally honest about pushing himself forward, [his advocacy of his theatre]. He was very, very honest. [Carl] was not easy to work with, because we're [such] different personalities on this, on the ego side. That pushing, [all the self-advertising one seemed to have to do] was very difficult for me. [. . .] He believed that it didn't matter who the publisher [of a book] was. You got the book published. That helped the next book, helped the production of the play, and so on. And I just didn't have that kind of feeling about [publicity/advertising life around a work of theatre or poetry. I think Carl was actually right, about what had to be done. But I could not be like him]

[Carl did many good things in this world. He founded that artists' colony, DRAP, in honor of his daughter. And that provided again and again a good place for me to write.] One of his great [unsung] achievements is [advancing chemistry and biology] in Latin and in South America. He trained generations of Brazilian chemists. And in Mexico, just the idea of having a major company doing research in Mexico, did wonders for Mexican chemists and for the chemical industry. So many South American chemists were postdocs with Djerassi, and he had a great influence. There was also a very important National Academy of Sciences report that he did in the mid-sixties on science in South America. [Carl was a] remarkable person.

CARUSO: So, the last thing I wanted to talk about and I fully realize that Carsten and I got to hear an hour-long talk about this last night, so—

HOFFMANN: Yes. You can use that as part of the interview. Just incorporate that.

CARUSO: But you also did mention when we spoke during the first part of the interview a few months back, the consequences or—I'm framing this as, you know, the art of science. You were talking a bit about the consequences of paper drawings in relation to 3D crystal structures and new ways of visualizing things. And I was just wondering if there was something you can say in the short amount of time that we have **<T: 150 min>** left about that very broad issue.

HOFFMANN: As I made it clear, drawing molecules, and in my case, adding to [those drawings] of orbitals, has been essential to chemistry. [Together with] measurements, spectra, [the new] methods of structure determination and of separation are what's made modern chemistry, organic and inorganic, [be productive, inventive, useful].

[Our representational techniques—drawing molecules— are critical. There was this wonderful period of fifteen years in mid-nineteenth century when the practice was formed.] Alan Rocke traces the stages—Kekule in five years, drawing benzene in [three or four] different ways. He's playing. [. . .] Kekule is very much a man after my own heart. He's playing with these [paper] representations, trying [out different ones. It's] so interesting.

Drawing molecules is very important. You find chemists sketching molecules all the time, during seminars, [waiting for airplanes]. I was joking [in my lecture] that we're not talented at [drawing, yet we have to do it. So, we learn], we learn how to use this particular method of representation. [Or actually several different methods—a Newman projection, a poor attempt at a perspective drawing.] I mentioned ChemDraw and the revolution that [this program has] made in representing molecules.

I've written elsewhere about the relationship of our small orbital pictures to caricature, which is another medium where essence of motional gestures is captured in a few strokes of a pen. There's a relationship to "primitive drawings," [from Inuit or aboriginal cultures. There's a relationship to cubist paintings—you emphasize the form of the molecule, and in the same drawing you look at its side. Pierre Laszlo and I have written about representation in chemistry.[103]]

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[103] Roald Hoffmann and Pierre Laszlo. "Representation in chemistry." *Angewandte Chemie International Edition in English* 30, no. 1 (1991): 1-16.

CARUSO: [. . .] Sure.

HOFFMANN: It's very important, [this matter of representation. And] it's changing. Computers have changed it, [the ChemDraw program] I describe. India ink on tracing paper is gone. [. . .] I demand more of my students, [in the way of] pictures of molecules [as they discuss them with me. There are also some remarkable software packages for representing extended, repeating structures]. [. . .]

[Further change is afoot.] We recently had our first 3D printed model of a benzene crystal, [as we try to figure out] how benzene [polymerizes] under pressure. [. . .] If 3D printing becomes cheaper, which it will, people will make models again in substantial volume. And I think the virtual reality [is going to influence chemistry in time]. [. . .]

[The tactile-visual link] interests me. I've sometimes talked to some psychologists, trying to get them interested [in the role of that link in chemical representation], but I haven't found [the right person to join me] to write something about that.

[With respect to virtual reality in model building, no measure] of simulation of reality is going to replace the real thing. [One can say the same thing] about pornography. Is pornography spoiling sexual experience for our young people? They're exposed to much more of it. [Yet] the actual **<T: 155 min>** act of making love is so much more [psychologically convoluted, across the senses], than any simulation you can imagine. [So, exploring love is] going to remain both a source of tension and concern [and discovery and wonder] for our teenagers. [. . .]

REINHARDT: What is the real thing in chemistry for a theoretician?

HOFFMANN: For me, it is still the molecule, and the orbitals. I see those orbitals as little [. . .] two-dimensional [iconic symbols]. I can put them into three dimensions, but I see them largely in two dimensions.

[The output of a wave function on the screen of a monitor is] a list of component [atomic functions], maybe fifty to one hundred terms long. [Mathematically, algebraically, they are coefficient of polynomials multiplied by an exponential. I see them, I have learned to see them, as little lobes with phases. Oh, do the phases matter! Others see little plastically isosurfaces from a contour diagram. I think I see them better.]

[Why do I think I see them better? My facility with these orbitals was honed during a time where I had to look at piles of these eleven by fourteen accordion sheets of printed numbers which were spewed out for the computer. From my beginnings] in the extended Hückel method, I learned to truncate [that expression of hundreds of coefficients], to throw away the small parts, don't sweat the small stuff. [I then looked at the biggest coefficient, and drew] it out as a symbol, [that lobed (and loved) orbital. [We did not have the contour drawing software, I had to reduce the information by looking only at the largest coefficient. That was such good training.]

So, there in that process, I was [not only reducing the information content but also] moving toward the explanation. I was [. . .] throwing away most of it, [the parts that mattered least. I was] keeping the essential part, and translating it into a picture. Those are the keys to my forming the explanation.

[It did not hurt that] I had a facility with words [too. (Shall I thank my college writing teacher for that?)] So, what I wrote about [those orbitals, even if it was still science, was simplified to be understandable. And] convincing in some way. Somehow I learned how to make people feel it, that [the orbital explanation] mattered to me, so it should matter to them.

How to make people feel [that the action of sharing with them what I finally understood was] an act of sharing and giving, rather than an act of reaffirming ego? [I think I have taught the art of doing this, the art of teaching, to my students and collaborators.] [. . .]

CARUSO: All right. Thank you.

REINHARDT: Thank you very much.

[END OF AUDIO, FILE 3.1]

[END OF INTERVIEW]