CHEMICAL HERITAGE FOUNDATION

MICHAEL J. S. DEWAR

Transcript of an Interview Conducted by

James J. Bohning

at

University of Florida, Gainesville

on

22 January 1991

(With Subsequent Corrections and Additions)

THE BECKMAN CENTER FOR THE HISTORY OF CHEMISTRY Oral History Program

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Dr. Michael J. S. Dewar

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MICHAEL J. S. DEWAR

1918 Born in Ahmednagar, India, 24 September

Education

1940	B.A., Oxford University
1942	D.Phil., Oxford University
1943	M.A., Oxford University
1942-1945	Postdoctoral research, Oxford University

Professional Experience

1945	Imperial Chemical Industrial Fellow, Oxford University
1945-1951	Research Chemist in Physical Chemistry, Courtaulds Ltd.
1951-1959	Professor of Chemistry and Head of the Department of Chemistry,
	Queen Mary College, University of London
1959-1963	Professor of Chemistry, University of Chicago
1963-1990	Robert A. Welch Professor of Chemistry, University of Texas at Austin
1990-1993	Graduate Research Professor, University of Florida, Gainesville

<u>Honors</u>

1961	Harrison Howe Award, American Chemical Society
1976	G.W. Wheland Medal, University of Chicago
1977	Evans Award, Ohio State University
1978	American Chemical Society Southwest Regional Award
1982	Davy Medal, Royal Society of London
1984	James Flack Norris Award, American Chemical Society
1986	William H. Nichols Award, American Chemical Society
1988	Auburn-G.M. Kosolapoff Award, American Chemical Society
1989	Tetrahedron Prize for Creativity in Organic Chemistry

ABSTRACT

Michael Dewar begins this interview by recalling his family background and early childhood in India and later at boarding school in England. He describes his public school coursework and texts, and early exposure to science, and explains how financial pressures influenced his decision to attend Oxford University. Next he describes the unique chemistry course offered at Oxford at that time, his professors, lab work, the influence of the war, the graduate degree system at the University, and his early work, which included alkaloids research and theoretical organic chemistry. He discusses his research and colleagues at Courtalds, Ltd., his learning physical chemistry, his work on resonance theory and molecular orbital theory, and his theoretical publications at that time. He also describes his associations with H. Christopher Longuet-Higgins, Charles A. Coulson, and Jack Roberts. Next Dewar recalls the events leading to his appointment as Head of the Chemistry Department at Queen Mary College, as well as the condition of the department when he arrived and his efforts to rebuild it. He also talks about several of his publications before and during the appointment at OMC, including work on resonance theory, molecular orbital theory, liquid crystals, dropwise condensation and heteroaromatics. Next Dewar discusses the factors that influenced his decision to leave England for a professorship at the University of Chicago. He describes the faculty of the department during his appointment, his teaching, and his research at that time. After reviewing his work on hyperconjugation, organomettalic semiconductors, split p orbital method, and the tropylium ion, Dewar recalls his first meeting with Norman Hackerman at the University of Texas. He discusses the effects of political problems within the University administration and the evolution of computing facilities and software there during his tenure. He describes his interest in developing techniques for theoretical calculations, and the resistance of ab initionists to these theories. Next Dewar discusses negative reception to his work on enzymes, and general resistance to new and unorthodox ideas among scientists. He ends the interview with an explanation of how his half-electron model developed and some comments on his students and colleagues over the years.

INTERVIEWER

James J. Bohning is Professor of Chemistry Emeritus at Wilkes University, where he was a faculty member from 1959 to 1990. He served there as chemistry department chair from 1970 to 1986 and environmental science department chair from 1987 to 1990. He was chair of the American Chemical Society's Division of the History of Chemistry in 1986, received the Division's outstanding paper award in 1989, and presented more than twenty-five papers before the Division at national meetings of the Society. He has been on the advisory committee of the Society's National Historic Chemical Landmarks committee since its inception in 1992. He developed the oral history program of the Chemical Heritage Foundation beginning in 1985, and was the Foundation's Director of Oral History from 1990 to 1995. He currently writes for the American Chemical Society News Service.

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INTERVIEWEE:	Michael J. S. Dewar
INTERVIEWER:	James J. Bohning
LOCATION:	University of Florida, Gainesville
DATE:	22 January 1991

BOHNING: Professor Dewar, I know that you were born on September 24, 1918 in Ahmednagar, India. Could you tell me something about your parents and your family background?

DEWAR: Yes, my father was in the Indian Civil Service. I was in India until I was not quite eight. Children at that time had to be sent home to school because there weren't any schools there. It was a curious situation. It took a few weeks by sea, and it was very expensive. There wasn't time for children to come back for the holidays. People in India didn't return until they'd saved up enough leave to make it worthwhile, which was roughly once every ten or twelve years. So the normal thing was for people to send their children home and possibly not see them again until they were eighteen. My father died when I was nine and a half and my mother came back to England, so it didn't apply to me. It did to my sister. She was sent home at the age of eight and they didn't see her again for ten years.

BOHNING: She's older than you?

DEWAR: She's about twelve years older.

BOHNING: Are you the only two in the family?

DEWAR: Yes.

BOHNING: Do you have any early recollections of India?

DEWAR: I remember quite a bit about it. I had a strange upbringing, because there were no other white children in the place at all. My father was a District Commissioner in a fairly remote

area around a place called Chanda. Have you seen the film, "A Passage to India?" The situation was like that except that there were many fewer white people. There were about thirty white people there. I was playing bridge at the club when I was six. In fact, I never met any children at all until I was eight. It was quite a shock, because I was sent home first to stay, not with family, but remote acquaintances. That was a shock, being sent away from my parents for the first time. Then, just when I was getting used to it, I was sent out to boarding school, and boarding schools there were extremely rough and uncivilized places. I had a hell of a time. It was the first time I'd met any children, anyway.

BOHNING: Where was this in England?

DEWAR: A school called Copthorne. It's halfway between London and the English Channel, south of London.

BOHNING: Is there any reason that one was selected to send you to?

DEWAR: I really can't remember. It was quite a good one, particularly because it was one of the standard prep schools for getting to Winchester. I think that my mother hoped I'd get to Winchester, which was a leading public school in Britain scholastically.

BOHNING: How long were you there?

DEWAR: I was there for five years.

BOHNING: What kind of education did you have there?

DEWAR: The standard one for Britain at that time. Mainly mathematics, Latin and Greek. At that time the "classics," Latin and Greek, were very strongly emphasized in all private schools. In fact, I studied classics until I was halfway through my time at Winchester.

BOHNING: I'm just trying to get some dates correct. You went back to England in 1926. Is that correct?

DEWAR: Yes.

BOHNING: And how long were you in the boarding school?

DEWAR: Until 1931, when I got the scholarship to Winchester. I got the first scholarship, which surprised everyone greatly. The reason I got it was quite entertaining. Winchester had a special scholarship examination in which they emphasized originality. One of the questions I was asked was, "What do you think will be the most exciting invention in the next fifty years?" I had taken to reading science fiction, and had just come across a splendid idea which I duly reproduced. Of course, the examiners hadn't read this, so they thought my idea was original. I'm sure that did the trick. [laughter]

BOHNING: What did you tell them?

DEWAR: Well, the idea was that sound waves become weaker with time but never totally disappear, so it should be possible in principle to develop a sound detector which would pick up sounds from anytime in the past. I had several examples of things that would be nice to hear, such as Caesar addressing his army before his battles and so forth. [laughter]

BOHNING: That's very interesting. What can you tell me about Winchester? You said it had the best reputation.

DEWAR: It was the top school scholastically. It's also exceptional in that the Scholars there were segregated in College. This was set up as a charity in about twelve hundred and something by a man called William of Wykeham, to provide education for poor people. The Scholars lived together in College and for them everything was practically free. Since Winchester was the top school scholastically in Britain, scholarships there were the most sought-after in the country. Not surprisingly, the Scholars were extremely bright people. A friend of mine, who was a biology Master there for a time, tried running intelligence tests on them. Over the period he was there, something like ten years, he didn't find a single scholar who was not off the scale. Actually that isn't quite true. There were two who were just marginally on the scale. One of them was a contemporary of mine and everyone thought him extraordinarily unintelligent. There was, however, a bad side to it. Putting a whole lot of exceptionally intelligent people together had the effect of completely destroying their self-confidence. When you are surrounded by geniuses, you don't think of yourself as being particularly intelligent. Most of them indeed ended up in the civil service, which provides nice safe jobs. Few did anything at all dramatic.

BOHNING: You concentrated again on the classics at this point.

DEWAR: I did for the first two and a half years. I had in fact become totally converted to chemistry early on, by accident. There was a library in College to which people sold their old books when they left and new arrivals could buy them very cheaply. This was a big help because many of the Scholars were by no means rich. In my first term I was there buying books I needed when I saw one on chemistry. I had always wondered what chemistry was about, so I bought it and I was hooked from the word go.

BOHNING: Do you remember which book it was?

DEWAR: No, it was just a school textbook. It's vanished, I'm sure.

BOHNING: Had you had any previous exposure to science, chemistry in particular?

DEWAR: The thing I'd been reared on was a wonderful book called the *Children's Encyclopedia* (1). It was a huge work, almost the size of the *Encyclopedia Britannica*. I think there were fourteen volumes, each with over a thousand pages. It was a great big thing. It was moreover edited by an absolute genius called Arthur Mee who clearly knew just what children were like. It was full of information, a lot of it totally useless. It had articles on everything you could imagine, from art to music to science, everything. It was full of pictures and illustrations. I remember reading that almost exclusively for years and years.

BOHNING: Did you have any chemistry sets or any laboratory experience in your education up to that point?

DEWAR: No, I didn't.

BOHNING: So it was just through reading that you acquired that interest.

DEWAR: Yes. In fact, the first national examination I took was a thing called "The School Certificate Examination," which I took at the age of sixteen. I hadn't done any chemistry. I had

special permission to take the exam, which covered both chemistry and physics. I duly passed it, but it was the first time I'd ever carried out any experiments, because they had a lab test.

BOHNING: What kind of experiments?

DEWAR: I remember one involved a Wheatstone Bridge. We had to measure the resistance of something. Now, I'd never seen a Wheatstone Bridge, and I couldn't remember how it functioned. I eventually did get the thing wired correctly by simply connecting the resistances in all possible combinations until I got it to balance. [laughter]

BOHNING: Once you were hooked on chemistry, what changes occurred in terms of the courses you were taking?

DEWAR: I stuck to classics for two and a half years before I finally gave up. I'm really very glad I did, because I hated it. I was never really any good at it, but I think it's a wonderful subject. I have always felt that it should be taught at all schools, because it provides an extremely good logical education right from the word go. Latin is a very complicated language, with hundreds of rules and hundreds of exceptions to the rules. You have to know exactly what rules, and what exceptions to them, to apply in each case. It is also something which most children hate, so they learn early on to work hard at something they don't like. The third advantage is that it's totally useless to most people, so you don't run the risk of turning people off at an early age from something that might be useful to them later on. I think everyone should be taught Latin. I stuck to it for two and a half years, simply because I thought it would do me good, before I finally surrendered and changed over to science.

BOHNING: What did you start doing in science when you changed over?

DEWAR: Just the standard school courses.

BOHNING: Again, I'm trying to get the dates straight. This would have been when?

DEWAR: I went to Winchester in 1931, and I was there for five years until 1936. I went well beyond the school level in chemistry. There was a school science library and I got permission to use it quite early on. I read everything there was in it. That included the standard organic text used in universities.

BOHNING: I was going to ask if there was anything specific in that reading that you remember.

DEWAR: I was totally hooked on organic chemistry by the time I got to Oxford. Two books, one by Schmidt (2) and one by [Paul] Karrer (3) were then the two standard organic textbooks used in universities.

BOHNING: Were you doing any organic experiments along with that reading?

DEWAR: I did in my last year at school, because by that time my teachers realized I was beyond school level, so I spent a lot of time doing experiments in the lab with the chemistry master.

BOHNING: Were you doing synthetic work?

DEWAR: I don't really remember. I remember doing studies of the kinetics of various reactions, for example, formation of urea from ammonium cyanate.

BOHNING: Were you already looking at Oxford University? Was this your goal, to move from Winchester to Oxford?

DEWAR: Yes, and this for purely practical reasons. I went to Oxford—to Balliol College in particular—simply because my mother had very little money. My father had died young, so she had only a small pension from the civil service. It had been a struggle for her getting me through. I don't think she could have supported me through a public school education if I hadn't got the scholarship to Winchester. At Balliol, they not only had an open scholarship, but they had also had a special scholarship for students from Winchester. I was also able to get a School Exhibition. So collectively I was able to support myself at Oxford. So that is why I went to Balliol.

BOHNING: You started at Oxford in 1936 and you had already decided to major in chemistry. What kind of education were those four years at Oxford, in terms of the chemistry?

DEWAR: Oxford was unique in the sense that the undergraduate chemistry course there was nothing but chemistry, not even physics and mathematics.

BOHNING: Really?

DEWAR: Every other university, including Cambridge, did have such courses, but Oxford had nothing but chemistry. England also had a strange system, and they still do, of having everything determined by a single examination at the end of the course. Everything depends on that. If you are sick, it's just bad luck. In the chemistry course you could get a B.A. But you could also stay a fourth year and do research. Then you could get a B.Sc. as well. You had to stay that fourth year to get an honors degree, which was really a four-year course. I finished the first part just before the outbreak of World War II, and I did my year's research during the first year of World War II.

BOHNING: Who were some of your professors?

DEWAR: [Sir Robert] Robinson was the Professor. In Britain at the time, there was only one professor per department, and he was the Professor. The other thing was that at Oxford there were no lectures. Well, there were lectures, but few dimwits went to them. All teaching was done by the so-called tutorial system, in which you had a tutor who each week assigned you a subject to write an essay on. Once a week you'd go and spend an hour going through it with him.

BOHNING: What about laboratory work?

DEWAR: That they did have, yes.

BOHNING: What types? Did you have both organic chemistry and physical chemistry?

DEWAR: Yes, indeed, and also inorganic chemistry.

BOHNING: What about analytical?

DEWAR: Analytical chemistry was not a recognized branch of chemistry in England at that time.

BOHNING: In this country at that time, analytical chemistry was certainly a large branch of chemical instruction.

DEWAR: Right, right. But it never had been in Britain. I don't know what the situation is now, but certainly up until the time I left, analytical chemistry was not regarded there as a branch of chemistry.

BOHNING: That's interesting. Tell me something about Robinson. You had associations with him for some time, but what was he like in those early days?

DEWAR: I saw very little of him. The only lectures I went to at Oxford were a series by Robinson. You couldn't get the information otherwise. The series by [Nevil Vincent] Sidgwick fell in the same category because he was writing a book at the time. It was supposed to appear at any moment, but it hadn't appeared. In fact, it didn't appear for another ten years (4). [laughter] Those were the only two I went to. But I got to know Robinson very well later. My year's research for my bachelor's degree I did with [F. E.] King, who was my organic tutor at Balliol College. I had two tutors. The inorganic tutor was Ronnie [R. P.] Bell. Everyone was drafted during the war, and I was told to stay up at Oxford and work on war problems. So I did a D.Phil., which is what Oxford calls the Ph.D. just to be different. I did that with King. Robinson was annoyed at my failure to work with him. I pointed out that he was never in Oxford, and I needed a lot of supervision and teaching in lab work because I was never any good in the lab. I said that I'd stay and work with him later, which I did after I'd finished my D.Phil.

BOHNING: Given the kind of work you were into later on, what was your mathematics background?

DEWAR: I got none at Oxford, but fortunately at that time the levels at school were very much higher than they were here then or are there today. I was good at mathematics, so I was in the sixth form, the top form. I was really doing quite advanced things, like partial differential equations, matrix algebra, and that sort of thing. So I really had a pretty good background in mathematics. But I've always felt the lack of having more; it has always been a disadvantage to me.

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BOHNING: At Oxford was it organic chemistry that attracted you the most, as opposed to physical chemistry?

DEWAR: Oh, absolutely, from the word go. Ronnie Bell made desperate efforts to interest me in physical chemistry by making me study statistical mechanics and quantum theory. I simply rejected the lot. I wish now I hadn't. [laughter]

BOHNING: Yes, considering what happened later on.

DEWAR: I was convinced that physical chemistry was awful. [laughter]

BOHNING: Was your first exposure to quantum mechanics?

DEWAR: Yes.

BOHNING: Did you get any exposure to Hückel theory at that time, or was it still Pauling?

DEWAR: Only basic quantum mechanics. I didn't get on to Hückel theory or molecular orbital theory or anything like that. I was not exposed much to resonance theory. Robinson objected to it, but Robinson's classical electronic theory is in fact equivalent to resonance theory. The two are just different ways of describing the same thing.

BOHNING: I want to look at some of the work that you were doing while you were at Oxford, but before we do that, what about your wartime experiences? What was it like being at Oxford during the war?

DEWAR: Oxford was insulated from the war, because there was a sort of unofficial agreement between Germany and Britain that Germany wouldn't bomb Oxford or Cambridge and Britain wouldn't bomb Göttingen or Heidelberg. There was only one exception. One day a Polish pilot couldn't find his target in Germany. The Poles never brought any bombs back, so he flew around until he saw a city which happened to be Göttingen, and he dropped all his bombs on it. The Germans retaliated by dropping some bombs on Cambridge. The misunderstanding was sorted out through Switzerland or somewhere, and nothing happened again. We had lots of air raid warnings, but nothing ever actually happened. BOHNING: What kind of war-related work were you doing? Is that when you were working on antimalarials?

DEWAR: I started by trying to make new explosives. That wasn't very successful, because at that time, Woolrich Arsenal was the center for explosives in Britain, and they were outraged at anyone infringing on their preserve. The fact that there was a war on didn't seem to them to be any excuse. They retaliated by never testing any of the things I sent them. In fact, one of the compounds I made probably would be quite a good explosive, judging by later calculations at the Piccatinny Arsenal. That was the first thing.

Then I got on to making sulfa drugs. I made several derivatives of pyrazole, but they turned out to be so insoluble that none of them could be tested.

Then I got on to antimalarials. I was given the job of trying to explore new heterocyclic systems. I made a huge number of compounds, none of which turned out to have any toxicity to any microorganism. Then I got on to the penicillin project. I was given the job of making an analog of penicillin. The only trouble was that the accepted structure for penicillin at that time was wrong. So I was actually trying to make an analog of something else, and I didn't succeed in making it anyway. About that time the war came to an end, so all I can say is that I didn't actually hinder the war effort. [laughter] But I nearly did. I used to get directives from some central organization, advertising jobs that I was asked to apply for. I never replied. One day, however, I got a particularly impressive-looking offer. It was a job as chief technical advisor for the erection and operation of factories near London for filling shells and bombs. There was a little note at the bottom saying, "In the event that you do not apply for this position, you will be liable to imprisonment not exceeding two years' penal servitude or a fine not exceeding £10,000 or both!" This I was a bit shaken by, so I took it Robinson. I must admit I was a bit put out, because he just turned white with rage and said, "The fools!" He needn't have put it so bluntly. He literally grabbed it from me, and I was left alone for the rest of the war.

BOHNING: Could you explain a little bit about the D. Phil. degree, because you also list an M.A. degree a year later?

DEWAR: I did. It always confuses people. I always do that deliberately. [laughter] The point is that the M.A. degree is the official senior degree in Oxford which gives a right to vote in Convocation, the body which officially controls Oxford and in which every past graduate has a right to vote in if they have an M.A. degree. To get an M.A. degree, all you have to do is get a bachelor's degree of some kind, and then seven years from the time you entered the university,

you apply for an M.A., which you then get automatically. The M.A. ranks higher than the D.Phil., because the D.Phil. does not give you voting rights in the university.

BOHNING: Were these war-related projects under Robinson's direction?

DEWAR: Yes. They first started off with Freddie King, then later with Robinson.

BOHNING: Your first paper is on yohimbine (5).

DEWAR: That was what I was going to study for my bachelor's degree research. There was a sequel to that, because I thought the established structure was wrong on the basis of a sort of biosynthetic scheme I had for it. I got an ounce of yohimbine hydrochloride with the idea of degrading it, although I never actually did any work on it. The one experiment I did and reported, if I had interpreted it properly, would in fact have established the structure. I got a compound which had been made before and was thought to be yohimbol. Yohimbine is an alcohol carboxylic acid and yohimbol the alcohol. Decarboxylation of yohimbine had been stated to give yohimbol. This is just decarboxylated. The analysis, however, fitted better for the corresponding ketone. I just assumed that the earlier formulation as an alcohol was correct. The fact that the ketone was formed during the reaction showed that the carboxyl group had to be next to the alcohol, which established that the accepted structure wasn't correct.

Yohimbine was supposedly used by the West African natives as an aphrodisiac. Several of us decided we ought to try this one night, so four or five of us organized a yohimbine party. These included a girl in my year who was very attractive and volunteered to come along. We ended up taking three times the maximum recommended dose of yohimbine, and all we could say was that the results were totally negative. I think this girl was rather disappointed. [laughter]

[END OF TAPE, SIDE 1]

BOHNING: Was that the end of your work on yohimbine, then?

DEWAR: That was the end, yes. [laughter]

BOHNING: That's an experiment that wasn't in the literature?

DEWAR: That's not been reported. [laughter]

BOHNING: You also had a paper with [Sir John] Cornforth on the santonin controversy (6).

DEWAR: Yes. I worked with Cornforth in the same lab for years at Oxford, after I finished my D.Phil. It's an amusing story. An Indian had reported the synthesis of santonin in which one of the steps involved the reaction of a ketone with ethyl formate to form a formyl derivative. Although the starting material was inactive, the material he got was said to be optically active. Clearly what happened was that his professor there was not very bright and said, "That's a very interesting result. You must try it on a model compound." So he tried it on cyclohexanone and, sure enough, claimed he got an optically active product. This was obviously nonsense. Cornforth and I repeated this work, and duly showed that the product was totally inactive. That paper is one of the best examples of editorial revision I've come across. We congratulated the author at having achieved a result which could only be expected to occur once in ten to the power of twenty all to the power of twenty trials. The editor didn't like this, so he changed it to say, "This result would violate no laws of physics and would indeed be expected to occur in ten to the power of ten to the power of twenty trials," which if you work it out, is a lot different. He changed our estimate by about one hundred orders of magnitude. [laughter]

BOHNING: I was interested in that because so many of your papers, I don't want to say attack, but certainly go after the establishment and show that things are not what people are saying, that you have a different view. That tends to show throughout many of your papers in later years. Do you have a particular penchant for doing that kind of thing?

DEWAR: No, it's just that I've never had any respect for authority as such. All my work has always been designed to answer specific questions. These usually arose from things in the literature, where I didn't believe the explanation given, and this roused me to do something about it.

BOHNING: You were starting to get into some theoretical work at this point, when the war was over. You looked at the mechanisms of the benzidine and Beckmann rearrangements (7).

DEWAR: Yes.

BOHNING: Up to this point, most of your work was laboratory work.

DEWAR: The point was that during the war I couldn't work on my own problems; this got me interested in theoretical chemistry, because that was something I could do on the side. As a result of that, the first thing I came up with was the structure of stipitatic acid, which I deduced must contain a new kind of aromatic ring (8). That was the start of nonbenzenoid aromatic chemistry; it was the first case of a nonbenzenoid hydrocarbon system. I knew so little about theory then, that I interpreted it wrongly in terms of resonance theory. I didn't realize that this was actually Hückel's C_7 aromatic system. I also pointed out that the same was true for colchicine (9), because alkaloids were the thing I was really passionately interested in and was planning to work on if it hadn't been for the war.

BOHNING: Why did alkaloids attract your attention?

DEWAR: That was the big exciting area of natural product chemistry at the time. All the natural product activity concerned alkaloids. I suppose this was because the methods then available for finding structures worked particularly well for alkaloids. In order to determine the structure of a molecule by degradation, you need a specific point to attack, and nitrogen atoms provide such points. Compounds with only carbon, hydrogen, and oxygen were much harder to deal with.

BOHNING: Where did the theoretical aspect originate?

DEWAR: This happened after the war. At that time, theoretical organic chemistry was a general term which included experimental studies of mechanisms. It included everything except the synthesis. It has now become restricted to applications of quantum theory, but at that time it applied to everything. The other things I'd become interested in were the benzidine rearrangement and pi complexes. When I got to work on my own at the end of the war, the first thing I did was some work on the benzidine arrangement in hope of finding evidence for the pi complex theory (10). What got me interested in theory as such was being asked by the Oxford University Press after the war to write a book on theoretical organic chemistry (11). When I started on it, I realized I didn't know any quantum theory and I didn't really know much physical chemistry.

That was responsible for my move. At that point, I was offered a job as a physical chemist by Courtaulds in a new laboratory they were setting up to do fundamental research. The reason for that was amusing. They had already appointed the heads of the two sections, organic and physical, and they didn't think I would be willing to work under the head of the organic section. But perhaps I might be willing to work under the head of the physical chemical section,

given that I wasn't a physical chemist. So that's how I got onto it. It seemed a wonderful way to learn about physical chemistry; being paid to do it!

BOHNING: Why did Oxford approach you to write that book very early on? You had done some work in the area, but was it enough to warrant a book?

DEWAR: The stipitatic acid paper really created quite a sensation, because it was a problem which every organic chemist in the world at the time had looked at, including Robinson and [Robert B.] Woodward, and none of them had come up with a solution. So my paper really created a big stir. The pi complex theory not so much, but it also aroused a good deal of interest. So I had got quite well known for the work I had done on the side.

BOHNING: You mentioned Woodward. I'm also interested in the whole Ingold and Robinson controversy.

DEWAR: Woodward I didn't get to know until a lot later. There was a great feud between Ingold and Robinson. Quite frankly, I was totally on Robinson's side on this. I never really had much of an opinion of Ingold. I think he's one of the most overrated chemists there have been, and he was also a rather obnoxious person. I had too many bad experiences later on with him, personally. One of the worst was a case where a Fellow at QMC—Queen Mary College—now Queen Mary and Westfield College—Ralph Hudson, had written some papers which were really good and original. He sent them to the *Journal of the Chemical Society*, JCS, and Ingold reviewed them and said they were absolute garbage. Hudson, who was a bit of a nervous type, came to me and said, "What should I do? Should I just forget about it?" I said, "Certainly not." They were badly written, so I helped him rewrite them and I also concocted a letter for him to send with them. This happened when I was in bed with the flu, with a high temperature, which made me angrier. I was really outraged by the whole affair. Since the paper criticized views that Ingold held, he was determined to stop it from being published. I had one or two other cases like that with other people.

The trouble with Ingold was that he got a second class degree at Oxford. An idiosyncracy of the British system, which seems strange to everyone else, is that the Class of the Honors Degree one gets, the Class one gets in one's bachelor's degree, was really vital. It labeled one for life, like a permanent tattoo. When I went to Queen Mary College, I was trying to build the place up, and I would not have dared to hire anyone who hadn't got First Class Honors, however good they were, or people would say, "That can't be much of a place if they're hiring people with Seconds." As I said, Ingold did get a Second, which was probably richly deserved, and he spent the rest of his life trying to persuade himself that he was the greatest chemist in the world, possibly of all time, to make up.

BOHNING: Can you say anymore about the Ingold/Robinson controversy?

DEWAR: It began when Ingold stole a lot of basic ideas from Robinson; I think there's no question about that. Robinson was the type who was easily aroused at such situations and never forgave him.

BOHNING: I'd like to go back to your move from Oxford to Courtaulds. How did they get in touch with you and why did they want you to come there?

DEWAR: Courtaulds was forced to sell all their American holdings during the war. Before lend-lease, America forced Britain to sell absolutely everything they had in America at knockdown prices to pay for arms. It was only after they'd stripped Britain that they started lend-lease. One of the casualties was Courtaulds, which would otherwise now own British Celanese down in Corpus Christi. They got what seemed an awful lot of money at the time; I think it was forty or fifty million pounds. The board of Courtaulds had nothing to do during the war. They would sort of sit around eating large meals and drink wine and decide what they'd do with this nest egg after the war. Remember, it was just after Wallace H. Carothers had come up with nylon, so they decided to set up a vast fundamental research laboratory where things like nylon would appear once a week. The laboratory was not on quite the scale they'd originally planned, because the pot had decreased in value by the time the war was over, but they hired a whole lot of people, turned them loose and said, "Do fundamental research."

BOHNING: You had several papers with [C. H.] Bamford (12). Was he the head of the physical chemistry section?

DEWAR: Yes. We worked together nearly all the time I was there.

BOHNING: Who was head of organic?

DEWAR: Percival Moggridge. He died in the first year, or the first few months. He just dropped dead one day in the lab—heart attack, with no warning at all. They didn't replace him, so the whole place never really got off the ground as it was expected to do.

BOHNING: Some of the things you and Bamford did together dealt with polymerization. Was this one of his areas of interest?

DEWAR: No, it wasn't, but we had more or less agreed to work on things which might be of use to Courtaulds. Polymerization was one of them (13). Another was the process to form acetic anhydride by pyrolysis of acetic acid to form ketene, then reacting that with acetic acid. So we had a paper on the thermal decomposition of acetic acid in the gas phase (14). We also did quite a lot of work on the tendering of fabrics. If you dye fabrics with certain dyes and expose them to light, they disintegrate. Nothing really was known about that, except that it was thought to be some kind of oxidation. We worked out the mechanism of that in some detail (15).

BOHNING: How many other people were in your group?

DEWAR: There were about five or six altogether in that group.

BOHNING: Is that where your interest in color came about, when you started working on dyes at that point?

DEWAR: Yes, it was. It also solved my problem about learning physical chemistry. I taught myself quantum mechanics just by reading about it; I've always been a bit unorthodox. I also chose a most unsuitable book, the one by Eyring, Walter, and Kimball (16).

BOHNING: Yes, I know the book.

DEWAR: I found it very hard. I thought it was just a sign of my stupidity. [laughter]

BOHNING: I don't think you're the only one that's found it hard. [laughter]

DEWAR: Yes, it's a rough one.

BOHNING: But that was about all that was available at that time. There wasn't much else available, was there?

DEWAR: No, there wasn't.

BOHNING: In 1947 you had a paper, "An Interpretation of Light and Its Bearing on Cosmology" (17).

DEWAR: Yes.

BOHNING: I have a copy of it here. I was intrigued by it.

DEWAR: Oh, you do? I'd like a reprint; I've lost it.

BOHNING: Well, I can give it to you in a moment.

DEWAR: Thanks very much. Somewhere I've probably got some reprints of it still, but I don't know where they are and I never include it in my list of publications. [laughter]

BOHNING: Why did you write that paper? Here you are working doing fundamental research and you publish something like this.

DEWAR: I have always been interested in astronomy; I got interested in it, among many other things, from articles in the *Children's Encyclopedia*. That, incidentally, was a wonderful work. It's a shame that it hasn't survived, but television would in any case have killed it. Anyway, when I was about twelve, I used a Christmas present to buy a book called *The Splendour of the Heavens* (18). It was an enormous volume, reviewing astronomy as it was at the time, 1925, with chapters written by leading astronomers and full of photographs. It was a very good book. This got me really interested and I've kept an interest in astronomy ever since, up to a sort of semiprofessional level.

One day I had an idea of a possible alternative to general relativity. The idea was to keep special relativity, but regard it as indicating an actual physical change that occurs in things which are moving relative to a local framework, light traveling with velocity c relative to that framework. To work this thing out, I went hunting around the library and found an old paper in which someone had proved that all the experimental phenomena that follow from general relativity can be explained in this way. I even found some evidence for this idea.

I did this for fun. I mentioned it one day to Sir David Ross, who was the provost of Oriel College. He's a cousin of my father's and an Aristotelian philosopher. He was highly delighted, because he had never liked relativity theory anyway. So he got me an introduction to Milne, who was then one of leading theoretical astronomers in the world. I spent a whole afternoon talking to him about this. Milne got more and more agitated. He kept raising new objections, but I was able to meet all of them. Finally he said, "Well, it's obviously nonsense. Anyone can see it's nonsense. But I can't see why it's nonsense. So you must publish it, and let someone else find out what's wrong with it."

So with his help, my paper duly appeared in *Philosophical Magazine* (17). [laughter] I've kept working on it since. The original form was naïve, but there's a version which I think does explain everything, and in fact it fits in nicely with the continuous creation of matter. It also accounts for the background radiation. But I've certainly no intention of trying to publish it.

BOHNING: What kind of reaction did you get when it appeared?

DEWAR: It was totally ignored. I had one request for a reprint. [laughter]

BOHNING: At this point, you also started publishing some papers on resonance energies which were probably more theoretical than anything else you'd done up until that point (19).

DEWAR: Yes, they involved just simple Hückel calculations.

BOHNING: When did you first learn of the Hückel method?

DEWAR: I read about it. Then I started doing calculations myself. At the time, one did everything by hand, which was really quite a business, solving secular equations without calculators.

BOHNING: Yes, I can imagine. Not even mechanical calculators?

DEWAR: No, no.

BOHNING: I remember in the 1950s seeing a room full of theoretical people with mechanical calculators.

DEWAR: Yes. [laughter]

BOHNING: This is about the time that book came out (11), in 1949. What kind of reaction did you have to that book?

DEWAR: The book in fact created quite a sensation. It was late, actually. It took three years to appear, because at that time, after the war, everything was a mess. But it had a whole lot of reviews, each worse than the last, and each time another review appeared the sales went up. It was read by a whole generation of young organic chemists, and it was the thing which really converted organic chemists to molecular orbital theory. It was the first account of organic chemistry in terms of molecular orbital theory.

BOHNING: Had you had any contact with people in the States, such as [Saul] Winstein and other physical organic chemists?

DEWAR: No, none at all. I had not met any of them.

BOHNING: That's interesting.

DEWAR: In fact, I'd hardly met any of the theoreticians in Britain, either. The only one I met was [Charles A.] Coulson.

BOHNING: Later on you had a paper or so with Coulson (20) and also with [H. Christopher] Longuet-Higgins (21).

DEWAR: I knew Christopher well; he's one of my oldest friends. We were in school at Winchester together.

BOHNING: So your association goes back that far?

DEWAR: Yes.

BOHNING: Could you tell me something about Coulson and Longuet-Higgins from a personal standpoint?

DEWAR: The first time I got to know Coulson was when I wrote a rather naïve paper describing calculations for pi complexes using Hückel theory (22). Coulson came up with a paper, which he sent to me before publishing, blasting it and saying it was total nonsense. Being reasonably ingenious, I was able to persuade him that it wasn't nonsense, but at the same time it wasn't sense either; you really couldn't tell. But it certainly wasn't too meaningful. So we published a joint paper pointing out all the potential errors in using Hückel theory for ions, and this appeared next to my paper (20).

There is an amusing sequel to this. I talked about this idea of pi complexes at a meeting in Montpellier in 1950, and Winstein was present. This was just when Saul had come up with his evidence for the norbornyl cation being nonclassical. Saul was outraged. Mary and I knew them, both Saul and his wife Sylvia, well. She told us one day that when Saul proposed to her he had said, "I'm never going to get anywhere. I'm really not good and I'm never going to be more than a second-rate university professor at some minor university." Quite frankly, I think that was a good assessment. Saul really didn't have original ideas. He was extremely painstaking and he got into the area just at the right time and he did extremely good work in it. But he did virtually nothing that was really original. The one exception was discovering this nonclassical ion. So at these lectures he was really outraged. He never did admit that I had any part in it at all. In fact, the climax came when he published a paper with [M.] Simonetta on one of these nonclassical ions (23) without any reference to the calculations I had done (22) and also without reference to my paper with Coulson (20) in which we had shown that such calculations are totally meaningless. I think that was unfortunate. He didn't need to do that. It also did harm because these ions are best regarded as pi complexes. If you look at them that way, a lot of the things about them become immediately obvious.

[END OF TAPE, SIDE 2]

BOHNING: What about Jack Roberts? Didn't he have a little paperback on molecular orbital calculations around that time (24)?

DEWAR: Yes. Jack first visited us after I went to London to Queen Mary College. After that, he used to visit us regularly when he came over and I've known him very well ever since.

BOHNING: What was your reaction to his book, given what you'd been doing?

DEWAR: My memory is that it was fine at that time. You couldn't do a lot, but it's a good account of what sort of things you could do then and how to do them.

BOHNING: While you were at Courtalds, you published a number of theoretical papers. There were still practical papers coming out, but at the same time there were a number of theoretical papers developing.

DEWAR: Not many at the time. There was the original one on pi complexes (22), the one on resonance (25), and I think that was all except for the paper from the Montpellier conference, which appeared in *Bulletin de la Société Chimique de France* in 1951 (26). That's the one where I suggested the pi complex structure for the metal complexes.

BOHNING: In 1950 you had the paper on tropolone (27), and in 1952 you started that series on the molecular orbital theory of organic chemistry (28).

DEWAR: When was tropolone?

BOHNING: In 1950.

DEWAR: I'd forgotten it was so late. Yes, it would be 1950, of course. Yes. I'm getting a bit mixed up with the timing of this, I must confess. The point is that I introduced the tropolone idea when I was at Oxford. What triggered it off was one of the meetings we used to have regularly about penicillin, when people visited from America. This was early on, when no one knew what the structure of penicillin was. It didn't seem to fit any possible formula. One of the people visiting happened to remark that penicillin seemed to be like stipitatic acid, a compound for which you couldn't write a rational structure. So at the end of the meeting I went off to the library and looked at Raistrick's papers and came up with the solution. That was why it happened while I was in Oxford. My paper, however, didn't appear until 1950, and I can't remember what happened in between.

BOHNING: How did you make the connection with QMC, Queen Mary College, when you moved there in 1951?

DEWAR: When I went to Courtaulds I didn't really mean to stay there more than two or three years. But there were absolutely no jobs going in England at the time. The one exception was the chair of color chemistry in Leeds, which I nearly got. I was second. But it was really good fortune for me that I didn't, because it would have been another dead end. [laughter] Then, two things came up at the same time. One was a chair at the Manchester College of Technology— not the University, which is different—while the other was the appointment at QMC. I don't know how QMC got onto me or what happened, because it was really a very extraordinary appointment. I got this offer while I was in America, the first time I'd been there. I had been asked to give the Reilly lectures at Notre Dame. I was there for about two months altogether. I got this offer out of the blue while I was there, not even an interview or anything. I was the youngest person ever to be appointed to a chair in any part of London University, so it was really very odd. I heard later that what had happened at the meeting was that someone said, "It's time that something exciting happened at QMC." QMC was then very much a poor relation of the University of London, in the east end of London, the poor part. They said, "Let's get Dewar. He will stir the place up!" [laughter]

BOHNING: What was QMC like when you went there?

DEWAR: Oh, it was dreadful. The Chemistry Department was a huge, brick building with five floors and no elevator. It looked as though it had been built as an institution for housing poor people. It was in a terrible condition, there was no equipment at all, and there was no money to buy any. It was just a shambles when I went there. The place had been ransacked during the War, when the University was deserted. My predecessor was Partington. Do you know Partington?

BOHNING: Oh, sure! J. R. Partington.

DEWAR: He did nothing about it at all. He made no attempt to get money or do anything with the place. So it really was in an incredible condition.

BOHNING: What kind of students did it attract?

DEWAR: We got very good students, because we only took one in twelve of those who applied and all those who applied were qualified for admission to the University of London. London was next after Oxford and Cambridge on everyone's priority list. There were a huge number of people applying.

BOHNING: What were your goals outside of stirring things up? Were you going to build the Department?

DEWAR: My object was to make it the top Chemistry Department in the University. By the time I left, we had got to the point where people were putting us down as first choice, ahead of Imperial College or University College. We really got the place going. That was in spite of our dreadful building. When I went there I was promised a new building in between five and seven years. They were building a new engineering block, and we were going to be next. But when chemistry started doing so well, they decided to give the new building to physics instead, in hope that it would help physics become better too. That was one of the things that made me leave. It was just the last straw.

But I built the Department up. The first year there wasn't even glassware with ground joints or anything, so I ordered a whole lot of equipment. The laboratory steward who'd been under Partington was horrified. He said, "But, sir, we haven't got the money." I said, "It doesn't matter; we need the stuff." At the end of the year we'd overspent our budget by one hundred percent. The budget was the equivalent of seven thousand dollars for everything—the teaching, the research, all the chemicals and so on. Maybe it was seven thousand pounds. Anyway, whatever it was, it was ridiculous. The College was horrified because nothing like this had ever happened in its whole history.

The laboratory steward was a financial genius. He should really have been on the Stock Exchange. I rapidly corrupted him. I said, "The situation here is ridiculous. We must overspend every year by one hundred percent. No more than that, because that would be unreasonable and we don't want to be unreasonable." He agreed. Every year for five years we overspent our budget by exactly one hundred percent, and each year the college doubled my budget. They did everything they could to stop us from overspending. They had a whole group of people scanning our acounts. However, every time, when the smoke had cleared, we'd overspent the budget by exactly one hundred percent. After five years, when our budget had increased by a factor of two to the fifth, i.e. thirty-two times, it was finally acceptable. So I then used the situation to bring off another coup.

I had been trying to get QMC to appoint a second professor, because one of my problems was that the two senior people in the place hadn't spoken to each other for five years when I went there, and they wouldn't even sit in the same room together. It was just intolerable. I couldn't delegate anything to either of them without the other being up in arms. If I tried to

delegate anything to anyone else, then they both came screaming at me. So I had been trying to get a second professor to insulate myself from them, and the college refused. They said they had no money. After five years, at lunch one day I was talking to the principal of the College. I put the idea into his mind in such a way that he thought it was his. He suddenly turned to me and said, "Why don't we appoint a second professor? You have all these problems with the budget and everything, you could turn it all over to him." I said, "Oh, what a wonderful idea." So we appointed Keble Sykes. I got an invitation to go to Yale for the semester, so I went off to Yale, leaving Keble in charge. The first faculty meeting he had after I left, Jones and [Wilfred John] Hickinbottom came to blows and had to be separated. They were both over sixty. [laughter]

BOHNING: I didn't realize Hickinbottom was there. I remember his book (29).

DEWAR: It was a very original book. It was excellent; very good indeed.

BOHNING: It's a very unusual approach, but I used it many times in graduate school. I still have my copy.

DEWAR: I have too; it's around somewhere.

BOHNING: You produced an awful lot of work during that period at QMC.

DEWAR: We did. We got a lot done.

BOHNING: It's really quite amazing.

DEWAR: It was basically controlled by what we could do, because we had so little equipment. I'd been there six years before we got even an infrared spectrometer. We were really lucky.

BOHNING: Shortly before you went there, you gave the Reilly lectures at Notre Dame in 1951. Did that series of papers that began the molecular orbital theory of organic chemistry come out of those Reilly lectures (30)? DEWAR: Oh, yes. What happened was that Christopher Longuet-Higgins and Charles Coulson had developed the idea of using perturbation theory in organic chemistry on the grounds that this should be the best way to calculate the small differences in energy on which chemical reactivity depends. However, they missed the essential point that made the whole thing work. I hit on this when I was preparing my lectures for Notre Dame, so that's what set the whole thing off.

BOHNING: What kind of reaction did you get to that initial series that all occurred together in the *Journal* (30)?

DEWAR: I'd been told that you had to keep papers very short in JACS [*Journal of the American Chemical Society*], so I wrote them very concisely. The referees agreed that the material in them was all nonsense and that the author must be mentally defective. At the same time, they said the papers should be published, but should be shortened by twenty-five percent. So by the time they were shortened, they were totally unreadable. [laughter] I discovered later that JACS at that time had a policy of not publishing any theoretical papers whatsoever. This had started a few years before, for some reason or other. They not only published my papers, but also rescinded the ban because of them.

BOHNING: That's interesting. I think later on when you had the second book, twenty-five years after the first one (31), you commented in the introduction that that set of papers was indigestible.

DEWAR: They were. They were terribly difficult. [laughter] That was because they were already very condensed and then I had to shorten them.

BOHNING: Was that your first time in the United States?

DEWAR: Yes, it was.

BOHNING: Were you in touch with other people in the States at this point? Earlier you said you had no contact with physical organic chemists in the United States.

DEWAR: Hardly at all. There were just one or two who visited in London, but very, very few. No, that visit was when I got to know American chemists. I traveled around a lot and saw a lot of them.

BOHNING: Anyone in particular?

DEWAR: One of them in particular was [Norman] Kharasch. We corresponded regularly after that.

BOHNING: What was his reaction to those lectures?

DEWAR: Oh, he didn't know anything about it.

BOHNING: I see. He was from a different era.

DEWAR: Yes.

BOHNING: But did he encourage you to continue this approach?

DEWAR: No, because it really wasn't anything to do with him at all. He was interested in polymers and free radical reactions. He was one of the people who reviewed my book. He was very conservative and rather meticulous. When I first met him, he apologized for his review. I said, "No need for apologies; your review it increased the sales greatly!" [laughter]

BOHNING: Around that time, you also had another paper on the correspondence between resonance and molecular orbital theories.

DEWAR: With Longuet-Higgins.

BOHNING: You really criticized the old Resonance Theory (32).

DEWAR: Resonance Theory doesn't follow from Valence Bond Theory as is usually assumed. In fact it has no real basis. The only reason why it works is the almost accidental correspondence which Christopher and I pointed out. BOHNING: Yes, I found that very intriguing.

DEWAR: It's my own fault, you know. It's a shame, because that theory is still by far the best qualitative approach there is to organic chemistry, and it's never been picked up. It has remained totally unknown because I never wrote a book about it. One of the bad things I inherited from Robinson was the feeling that one shouldn't publish papers unless one has to. Having put all this in print, I thought it would be wrong to do anything more. But I should have written a book about it, and that was very foolish. I probably would have, but this was when I moved to QMC, and as I've already said, I had a hell of a time there, struggling to start research in a place with no money or equipment or anything, and with Jones and Hickinbottom to contend with as well. I nearly had a nervous breakdown the first year I was there. After that I pulled myself together and didn't let it get me down again. But it was very rough. I really hadn't time to even think about writing a book. But it's a shame, because if I had, the book I produced with Ralph Dougherty (33) would have provided me with a flying start.

BOHNING: But you made the comment in the second book—the molecular orbital book—that organic chemists in general were still quite ignorant of molecular orbital theory, and that those who didn't pay attention to it were doomed to solving minor problems.

DEWAR: I'd forgotten that. [laughter] Yes, they were.

BOHNING: I don't know if you used the word doomed, but it was similar to that. You were really quite a disciple of molecular orbital theory and its approach to organic chemistry.

DEWAR: Yes. I got devoted to it early on. It goes back to developing what I christened the PMO theory in my lectures at Notre Dame.

BOHNING: I'm still curious as to the resistance you may have met in introducing extensive theoretical work in what was traditionally organic synthesis, a lot of basic organic chemistry. Was there much there much resistance to that, or could you convert people?

DEWAR: In what sense?

BOHNING: In terms of their using MO theory. Perhaps I'm putting too many things together. You did a lot of theoretical work, but later you also did a significant amount of experimental work, which brings the two together.

DEWAR: All my work, or nearly all of it, was experimental until quite late on. It was only relatively recently that I took to theory in such a big way. Twenty years ago, most of my published work was still experimental.

BOHNING: We haven't even touched on the heterocycles and a lot of other areas yet, but I guess what I'm after is the change that was occurring in this time period in the early 1950s. Physical organic chemistry was really becoming one of the biggest things. How were people reacting to the kinds of things you were doing? You said Kharasch didn't know anything about it.

DEWAR: No, he didn't, nor did anyone else. If I'd written a book about it, I think I could have converted them. The book I wrote got people interested in molecular orbital theory, but it remained very qualitative.

BOHNING: Do you think things were different here in the States than they were in England in that respect?

DEWAR: I don't think so. I think they were very much the same. Teaching was still done entirely in terms of Resonance Theory. For a long time there were no textbooks dealing with molecular orbital theory.

BOHNING: Unless you wanted to wade through Eyring, Walter and Kimball as a start!

DEWAR: I wasn't thinking so much of quantum theory in the technical sense, but just introducing students to the idea of orbitals.

BOHNING: How did you do this at QMC?

DEWAR: I just taught one course there which appeared in the form of a paperback book. At that time in Britain, the school courses went up to quite a high level and were taught in the same

sort of way that they would have been in a university. However, there was nothing in them about modern atomic theory. What I did in my course was to fill in this gap. In this one term I gave a complete account of modern ideas in chemistry, starting with atomic structure, wave mechanics, orbital theory, thermodynamics, statistical mechanics, reaction kinetics, the whole lot. It was great fun and my people enjoyed it. It also acted as an intelligence test, because people who did well in my course always did well in their final degrees, while the ones who failed, failed.

BOHNING: It certainly takes a more rigorous intellectual approach to things, by going through quantum theory.

DEWAR: Yes, but I don't think you need to go through it mathematically. You really don't need that. You can teach orbital theory very well in qualitative terms. Then you can go on to perturbation theory without having to solve equations or anything. I think this is really the way to go. That's why I think it's such a shame that this approach—and it's my fault entirely—has never been adopted. It took about twenty-five years for a book to appear on it, the one I wrote with Ralph Dougherty (33). Hardly anything needed to be added to bring it totally up to date. The only really new idea was the concept of anti-Hückel aromatic systems, which is needed to treat pericyclic reactions. So an almost identical book could have been written back in the 1950s. I think if it had been, the results would have been very dramatic. When it did appear, most of the references in it were to papers published more than twenty years previously, so people assumed it couldn't be any good. What I should have done was call it something different, presenting the ideas in it as something entirely new, with no references to the literature at all. A lot of people have done that to my published papers, so I should have done it to my own. [laughter]

BOHNING: Very early on at QMC, you had a symposium on molecular rearrangements. Winstein was there, and others. There's a review of that in the literature (34).

DEWAR: At QMC?

BOHNING: In 1954.

DEWAR: Did I? I don't recall that at all.

[END OF TAPE, SIDE 3]

BOHNING: This paper summarizes the conference.

DEWAR: Oh, it comes back now. I'd quite forgotten it.

BOHNING: You had a pretty good lineup of people, and I was wondering what brought this about and what the results were.

DEWAR: My memory is totally blank on that. I really can't remember anything about it now.

BOHNING: Winstein was the only one that was from the States, from what I can see.

DEWAR: Yes.

BOHNING: Even Hickinbottom was there.

DEWAR: He was a local, yes.

BOHNING: I just wondered, because holding that symposium would be part of your building up the department.

DEWAR: I really am upset at forgetting about it.

BOHNING: You also did some work on liquid crystals at that time (35). How did you get into that area?

DEWAR: When I went to Courtaulds, I started thinking up things to do with polymers, which I knew absolutely nothing about at all. It occurred to me that if you use a liquid crystal as a solvent, it might speed up polymerization by lining the molecules up so that they join up end to end more easily. We tried this, but the results were negative. However, the idea of using liquid crystals as solvents remained in my mind and at QMC it occurred to me one day that molecules
dissolved in a liquid crystal might be aligned, something that could be checked by spectroscopy, using polarized light.

Since I had an Indian who wanted to be given a problem, I put him onto studying binary systems of pairs of liquid crystals, to see under what conditions one could get a mixed liquid crystal as a first step to studying solutions in liquid crystals. We published two papers reporting our results (35). However, I never did any more because I couldn't get any students interested in the problem. Being the Professor, I could, of course, tell anyone to do anything, having total power; but I never liked doing that. I've always liked giving students a choice of projects. The trouble with liquid crystals was that the students would ask me where they could go and read up about the problem. I'd say, "Well, no one's done any work on this at all; it's entirely new." When I said that, they'd immediately conclude that something must be wrong with it. So it was a long time before I could get anyone to do any work with liquid crystals again.

BOHNING: What level were the students at Queen Mary who were doing research with you? Would that be the B.A. level?

DEWAR: They were all working for D.Phil.s, the Ph.D. level. I only had one postdoctoral fellow, and that was Roland—Roly—Pettit. That was because he got an 1851 Exhibition. These came from the big World Fair in Britain in 1851, which made a profit unlike any similar function since. Those in charge used the money to found a scholarship scheme to bring people back to England to study. Pettit already had a Ph.D. in Australia, but he was sent over officially to study for a Ph.D. with me. Apart from him, I never had any postdocs.

BOHNING: During that time you were at Queen Mary, about how many students did you have? You were there for eight years, something like that.

DEWAR: I've got this all on record, but I think it must have been about twenty.

BOHNING: Twenty in eight years—given the conditions under which you were working, that's amazing.

DEWAR: Yes. They were all in one great big lab. It was all I had.

BOHNING: Were the students working with other people?

DEWAR: Yes. I think the total number in the department was about fifty.

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BOHNING: That's a very good number. Also during this period you had a series of papers that seems out of place. It was something called "Promoters for the Dropwise Condensation of Steam" (36).

DEWAR: Right. The faculty at QMC used to have lunch together in the college dining room, so one met people from other departments. One day at lunch, one of the engineers got talking to me about the problem of dropwise condensation. The trouble with condensers is that the water normally condenses in a film. Now water is a very bad conductor of heat, so the rate at which steam condenses is limited by the rate at which heat is conducted through the film of water. If the surface were water-repellent, so that the water condensed in drops, it would condense up to twenty times faster. My colleague asked me if I thought there was any way one could coat the surface of a condenser to make steam condense in drops. I said I thought that could be done quite easily. Then he asked if I would work on it. I said, "Only if you find me money to do it." So he rushed off and duly found a source of money from somewhere or other.

In the meantime, I had a student who needed some source of support because he should have had a First class degree and only got a Second. It was almost impossible for people who didn't get Firsts to get any support in Britain from the government. So I put him onto this, and this was how it started. I assumed that a lot must be known about it already, and people must have tried the obvious thing, which was to attach water-repellent molecules to the surfaces. It turned out that no sensible work had been done on it because it had all been done by engineers who knew no chemistry. Our original idea was to try a number of simple molecules and find which was the best. Since condensers are made of copper, which has a high affinity for sulfur and selenium, and since hydrocarbons are water repellant, what one needed was a long chain hydrocarbon with an anchoring group containing sulfur or selenium. The student made about eighty such compounds, with various groups containing sulfur or selenium. Anytime one of them got on the surface, it never came off again. So in that sense, the project was a total failure. Everything was one hundred percent efficient!

We tried one of them in the condenser of a ferry boat going across the English Channel. We drove down to Southampton. The first time we went there, the engineer was obviously horrified at having his ship and engines played around with by ignorant amatuers. The student would climb inside a condenser while the engineer stood there wringing his hands and saying, "Take care, take care." [laughter] After that, we used to go down once a month, and the student would climb inside the condenser with the portable steam generator. When he came out saying steam was still condensing in drops, everyone cheered. At the end, everyone was quite pleased and realized that their ship was being used for an important experiment. [laughter] BOHNING: You also started the heteroaromatic work at this time. How did you get into that area?

DEWAR: That happened because I had an Indian student who arrived to do a Ph.D. When he arrived, he already had an M.A., and he said, "For my M.A. I worked with compounds which were liquid. I would like, if possible, to continue working on liquid compounds, because I have no experience with handling crystalline materials." I was obviously in an inventive mood that day, as I said, "Oh, in that case you will make these boron compounds!" [laughter] This was an idea I'd thought about vaguely before. He said to me, "But will they be liquid?" I said, "Who can tell? No one has ever made any of them." So the official purpose of his work was to synthesize new liquid heteroaromatic compounds. One of the compounds he made did in fact turn out to be liquid! But that's how it all started (37).

BOHNING: Did you have theoretical interests in those compounds at that time as well?

DEWAR: Not specifically, but obviously they were interesting in the sense that they were isoelectronic with aromatic hydrocarbons. It was interesting to see how stable they would be.

BOHNING: That work went on for a long time.

DEWAR: Yes it did. I got fed up with it in the end. It's surprising, actually, that it hasn't been taken up by other people, given the interest aroused by any new aromatic system. Here we have a whole new class of aromatic systems, and one could do similar things with elements other than boron and nitrogen.

BOHNING: The one thing that strikes me, even up to this point in the late 1950s, is the diversity of the work that you did. I don't want to say you were jumping around a lot, but there were always new areas that you were developing.

DEWAR: I've always had very wide interests. There are two other things about this, too. I've always thought that graduate students should be given individual problems, and not just bits of a major problem. One of the things I learned early on, after coming in contact with Collingwood, was his principle that the purpose of any experiment should be to answer a specific question. That's how I've always operated. The boron nitrogen work was an exception, where we were studying just the specific properties of a whole class of compounds. So, a lot of them were made

for specific reasons. Otherwise, all my research has been directly aimed at answering specific questions. So I usually published only one or two papers on each topic because the work they reported was enough to answer the question I wanted to know the answer to.

BOHNING: What kind of contact did you have with the Oxford and Cambridge people while you were at Queen Mary?

DEWAR: None at all.

BOHNING: None at all. That's interesting.

DEWAR: No, none at all. I'd occasionally go back and visit people at Balliol, but chemically, not at all.

BOHNING: You had this molecular rearrangement symposium that we just saw. Did you bring in other people? Did you have a seminar program in which students were exposed to outside speakers?

DEWAR: No, we didn't. The only thing we had was an annual lecture for the students, where we had someone visiting who gave a lecture.

BOHNING: Then we get to hyperconjugation. I'm not sure whether that was still developing in England or when you got to Chicago.

DEWAR: That was in England. I'm trying to think about the timing. I was dubious about the whole concept of hyperconjugation. My idea was that one could account for everything in terms of changes in bonding with hybridization. Howard Schmeising and I produced two papers (38). He did some calculations with a very primitive computer, which were perhaps not too meaningful, but we also came up with a very strong qualitative argument supporting the idea. So that's what really got me going on it.

BOHNING: I noticed that in that one paper you acknowledged General Electric [GE] for computational facilities.

DEWAR: Yes. This was a primitive computer using relays rather than vacuum tubes. [laughter]

BOHNING: Was this the first time you got into any kind of computer work?

DEWAR: Absolutely, yes.

BOHNING: I'm assuming you didn't have a computer at QMC, or did GE give you something?

DEWAR: No, we didn't have anything. The student went over there to use it. I can't remember how we first got in contact with them. I think he had in fact been working there for the summer before he came to QMC.

BOHNING: You still didn't have any mechanical calculators at this point?

DEWAR: We did get a mechanical calculator.

BOHNING: So you were really working in some isolation. You had no contact with Oxford and Cambridge, and you didn't have much contact with people in the States.

DEWAR: I was almost completely isolated.

BOHNING: That's interesting.

DEWAR: I was really working entirely on my own on things I was interested in.

BOHNING: You've already said, in a number of cases up to this point, referees said that it was nonsense, but it was still published. What kind of problems did you have getting these papers published?

DEWAR: That wasn't a problem in those days. The JACS case was exceptional and, as I said, this was at a time when JACS officially had a policy of not publishing any theoretical papers at all. I didn't publish anything else there for many years; all my work was published in Britain. Things were very different then. Referees were really conscientious and didn't come up with hysterical attacks on authors. In fact, the Chemical Society had a rule. Their instructions to referees were quite simple. They said the referees should confine themselves to pointing out errors of fact or logic in a paper and that their opinions were of no interest.

BOHNING: Ingold notwithstanding. Did he referee on any of your papers?

DEWAR: No, he never refereed any of my papers. At that time, you see, I was doing very little kinetic work or anything like that. It was nearly all synthetic.

BOHNING: Then you moved to Chicago in 1959. You had met Kharasch earlier, but how did that move come about? I've read that it was somewhat difficult in a way to leave England.

DEWAR: We thought an awful lot about it. It was Kharasch's chair that I was offered there. It was a hard thing to decide, because my boys at that time were fourteen and twelve, and we'd bankrupted ourselves sending them to private schools in Britain, which were very expensive. We were really concerned about them. We just wondered how it would affect them. We wanted to go because things got really difficult in England in the sense that I still had this really terrible building at QMC.

I should, in fact, have got the chair at Oxford when Robinson left. Robinson was a real autocrat in the place, partly because there was no one else there who was any good. He had no way of bringing good people in, because the appointments were all College appointments; there were virtually no university lectureships or anything. The people teaching the university laboratories were Fellows of colleges over which Robinson had no control. In fact, he only appointed one person who was a physical organic chemist. He was very well known in the 1950s and did lots of early work in radical reactions. I can't remember his name right now. It'll come back in a minute. But when he left, everyone in the department wanted to have a nice quiet period with someone who wouldn't chase them around. What they wanted was someone to stabilize the position that Robinson had achieved in the department. I should have got that chair. Looking back, I'm glad I didn't, because if I had I would have stayed in England. I don't think I would have been too happy.

BOHNING: What swayed you, then, to finally accept the offer at Chicago?

DEWAR: We talked about it for months. I remember one time in Madrid we turned our kids out on a boat on the lake in El Retiro, the big park there, and they rowed around for two or three hours while we just sat talking about it. But the thing that finally settled things for us was the discovery that Chicago had a wonderful school, the so-called Laboratory School, which at the time was really quite unique. In it people could go at whatever pace they liked with no age limits. You could be at different grades for each different subject. If you got beyond the school level, you could even take courses at the university. That was what really convinced us to go.

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From my own point of view, I was anxious to go. I couldn't get any work done in London. For one thing, I was on six University Committees. To be on even one was considered a great honor, but I've always hated committees. My feeling about committees is that either the other members think the same way I do, in which case it is a waste of my time attending meetings, or they disagree, in which case it's a waste of my time arguing with a bunch of obstinate fools. I'm really not a committee man. Furthermore, these Committees met at the Senate House, the administrative center of the University of London, which was right in the middle of London, and it was a hell of a job getting to and fro by car from QMC. I was spending half my time just traveling around London by car, wrestling with traffic jams.

The climax came when I was elected one of the Honorary Secretaries of the Chemical Society. There were two, and it was a very prestigious appointment. But as far as I was concerned this was the last straw, because the Chemical Society was in yet a third place. I just couldn't get any work done at all. The only way I could deal with the situation was by leaving the country. We had also got a bit disenchanted with Britain. The class system disgusted us and the British Labor government had made a shambles of the place. We didn't like it. The other thing was that whenever we had British guests at our home in London for dinner parties, we'd have a terribly sticky time with our guests, wondering what we should say and wondering if we had done anything wrong. Things were quite different when we had American friends visiting. Then we had a really good time. So we decided we were on the wrong side of the Atlantic.

BOHNING: But you hadn't really looked outside the country. They came to you, is that correct?

DEWAR: Yes. I hadn't looked at all.

BOHNING: Once Robinson's chair at Oxford wasn't available, did you have any other options in England, or did it look like until Chicago came through you were going to stay at QMC?

DEWAR: I was offered the chair at Glasgow, which was a big one, but I didn't have the slightest inclination to go from London to Glasgow. That wasn't any help.

BOHNING: What did you find when you came to Chicago? What was it like in the department?

DEWAR: Oh, we had a wonderful time. We enjoyed Chicago very, very much.

BOHNING: Who was there in the department at the time?

DEWAR: [H. C.] Brown was the main organic chemist there. Henry Taube.

[END OF TAPE, SIDE 4]

DEWAR: We became very close friends with the Taubes. It's terrible, you know, I've always been hopeless with names. I get worse with time.

BOHNING: Was [Harold] Urey there?

DEWAR: Harold had left. He'd gone to La Jolla. Bill [Wilbert H.] Urry was there-the organic chemist. Gerhard Klaus. [pause] It will come back, gradually. Stewart Rice.

BOHNING: How would you compare your position in Chicago to the one you had just left?

DEWAR: Chicago was a joy; London had become a misery.

BOHNING: When you were in Chicago, you didn't have any more administrative responsibilities.

DEWAR: None.

BOHNING: What were your teaching responsibilities?

DEWAR: Hardly any. Indeed, one of the few faults of Chicago was that there were so many faculty that it was quite difficult to get any teaching at all. You had to fight. They were quite concerned at my coming at the thought of having someone else competing for courses. So they invented one for me, which was an introductory course in organic chemistry for nonmajors, which was full of premeds.

BOHNING: How did you find doing something like that?

DEWAR: I really enjoyed it.

BOHNING: That's interesting.

DEWAR: I have always enjoyed teaching very much, and I think elementary courses are the most fun to teach, because there you don't have to put effort into preparing them. It's just a challenge to get the stuff across to people. I always have enjoyed that. It's one of the things I really missed in Austin, that I didn't teach there. The reason I didn't teach was that when I got there, I found that all the teaching was so circumscribed by state laws that I didn't want to get involved in it. Also, I knew that if I started teaching courses, people then would expect me to go on doing so. So I kept out.

BOHNING: There are a number of things you did when you were in Chicago. The book on hyperconjugation came out then in 1962 (39). I remember that book. In fact, I have a copy with me here.

DEWAR: That was fun, because I had given a notorious lecture on hyperconjugation, proving that it didn't exist. [laughter]

BOHNING: I also wanted to ask you about George Wheland, because you refer to his work in a number of your papers. He was an early figure in much of the early quantum mechanics in organic chemistry. Did you meet him at all?

DEWAR: Oh, yes. I knew him very well in Chicago. By that time, he was coming down with multiple sclerosis. He was already very under the weather with it. He hardly came into the building at all. I met him on my visit to the U.S. in 1957.

BOHNING: I was just curious how he viewed your approach to things.

DEWAR: We got on very well. I don't think we ever had any real arguments.

BOHNING: What about the book on hyperconjugation? How was that received when that came out?

DEWAR: I don't really remember.

BOHNING: That was the Ronald Press. They put out some good books in those days.

DEWAR: They did, yes. That was one of the early ones.

BOHNING: You also got into organometallic semiconductors in Chicago. How did that come about?

DEWAR: This was just an idea I had, a new class of semiconductors that I had predicted on theoretical grounds. We decided to make one example of a polymer just to provide an excuse for publishing the idea (40). I never did any more work in the area, because I was unlucky. First, the student I had studying the problem became interested in theory and took to doing theoretical calculations instead of experimental work. Then I assigned the problem to a postdoc who was totally incompetent. He was nice, but really hopeless. So I never did any more work on the problem. I still think it's a good idea.

BOHNING: Did you have any computer facilities available?

DEWAR: No. Chicago had a computer, but I hadn't taken to computation when I went there. It was also very expensive. You had to pay for every second at the full commercial rate. The thing which got me started on computing was an invitation from Bell Telephone Labs. After I'd been in Chicago for about a year, 1960, I think it was, they asked me if I'd like to go there for a month in the summer and just do anything I liked and give them two or three seminars. This became an annual event. I went there every year. They let me use their computer, so that got me going. I also got to know Larry Snyder very well and I managed to get him to write a program for the pi-SCF method.

BOHNING: I think while you were still in Chicago there was a conference, and you had one paper on resonance and conjugation in which you said that resonance effects are very generally less important than has commonly been supposed (41). This came out of the 1958 conference on hyperconjugation.

DEWAR: No, that was earlier. I published two papers on this. The first was one with Howard Schmeising. The hyperconjugation conference was later (38). I'm trying to think when the conference on hyperconjugation was.

BOHNING: The date I have here is 1958, which would have been before you came.

DEWAR: I was over in the summer for visits in 1958 and 1959. So that would be right, because it took quite a time then for the papers to appear in print. The paper appeared in 1959, so the work was done earlier. Then there was the split p orbital method.

BOHNING: Yes. The SPO method. Split p orbital.

DEWAR: I was dabbling around at that time with calculations. The name was suggested by an Argentinian chemist, Nora Hojvat. She's now Nora Sabelli; she married another Argentinian and is at the University of Illinois in Chicago. She's quite well known in the theoretical area. She had been doing calculations on very small molecules of interest in astronomy. I put her on to this work. My idea was that electron correlation should tend to make two electrons in a p orbital stay in opposite lobes and that the way to allow for this was to treat the lobes as individual orbital functions. Nora's English was very good, but not perfect, so she described the halves of p orbitals as split p orbitals (42). I said, "That's a marvelous term!" [laughter] It upset people terribly. Everyone came up with arguments showing that the whole treatment was a lot of nonsense. In fact, it's quite sophisticated. I was able to meet all the obvious criticisms without difficulty. The only valid objection which someone finally came up with after about six months, was that the orbital lobes are not orthogonal to the core orbitals, and this upsets things.

BOHNING: At this point there was a lot of work on pi complexes and the tropylium ion.

DEWAR: Yes.

BOHNING: How did the tropylium ion follow from what [William von Eggers] Doering had done?

DEWAR: It was when Roly Pettit was with me in London. We set out to make tropylium. Our original idea was to make it from the appropriate cycloheptatriene carboxylic acid, which [Eduard] Büchner had reported. One other way was the halogenation and dehalogenation of cycloheptatriene, but we kept off that because we knew Bill Doering was working on it. We lost out on the carboxylic acid route because we believed Büchner's formulae for the isomeric cycloheptatriene carboxylic acids. He had reacted benzene with ethyl diazoacetate and depicted the product as having a norcaradiene structure with a three-membered ring. Isomerization of this was claimed to lead to a cycloheptatriene carboxylic acid with the carboxyl attached to the saturated carbon in the ring. We tried about a dozen ways of turning this into tropylium, none of which worked. Also, we did not try the obvious one, i.e., Curtius degradation to a chlorocycloheptatriene, because we knew that Alan Johnson was trying that, so we left it to him. When we failed to get tropylium by the fourteenth method we tried, I heard from Johnson that he had abandoned work in the area. He found that Curtius degradation led to a urethane which hydrolyzed extremely easily to form just urethane itself. He assumed this was because the tropylium ion was so stable.

This seemed to us nonsense. As soon as we heard that he was doing no more work on it, I told Roly, and within a day, he had got this urethane, hydrolyzed it, and found cycloheptadienone as the other product. So it was obvious that the urethane was in fact an enone. Buchneil acid was in fact the one we wanted, a cycloheptatriene with carboxylic attached to the saturated carbon. Every single synthesis we had tried gave tropylium when we repeated them with the "right" acid. So for about a year we'd been isomerizing the acid we wanted to something else!

In the meantime, Bill Doering played a dirty trick on us. He just read the literature. He found that [Jacob] Meisenheimer had a compound in about 1890 which he described as being a chlorocycloheptatriene, but with properties which obviously were wrong. He said it was a crystalline solid. Doering repeated Meisenheimer's work and showed that the compound was in fact tropylium chloride.

BOHNING: You did an awful lot of work on boron nitrogen compounds during the period in Chicago.

DEWAR: Yes. That was a sort of stable diet which we carried on for quite some time.

BOHNING: How many graduate students and postdocs did you have in Chicago?

DEWAR: I really don't know offhand. I know the total number I've had is getting on to about two hundred fifty or something like that. We've kept in touch with them, or did for many years, in official annual newsletters, but lately these have become a bit spasmodic. Did I send you a copy of the latest newsletter?

BOHNING: No.

DEWAR: I must look around and see if I have one. I'm sure I have.

BOHNING: That would be nice.

DEWAR: You might find it interesting, because we tracked down all except two or three of the people in my group and kept touch with them. This has all their addresses.

BOHNING: There was another paper on electrophilic addition to olefins (43). You looked at the sterochemistry of adding deuterium halides to acenaphthylene in which everybody had said it was <u>trans</u> and you found that it was mostly <u>cis</u>.

That's interesting. Why did you try this experiment?

DEWAR: I really wanted to know what happens. We were looking for evidence for pi complex intermediates. The question here was whether when you attach a proton to a another bond it forms a carbonium ion or a pi complex. There really was no information about that.

BOHNING: During those four or five years in Chicago, were you developing more of a relationship with American physical organic chemists?

DEWAR: Oh, yes. In 1957, I spent nearly six months over here and traveled all over the country and saw practically everyone, and I kept up close contacts with all those I met. I visited again in 1958 and 1959 before we moved to Chicago, traveling around a lot each time. Those times I was just on my own.

BOHNING: You mentioned something earlier about Texas. You were only in Chicago four years. Were you thinking of leaving Chicago? Were you specifically thinking of looking somewhere else?

DEWAR: Oh, no, not at all.

BOHNING: It was just that Texas came along?

DEWAR: Yes, Texas came along. It was one of these really wild things.

BOHNING: When did you first meet Hackerman?

DEWAR: In 1957, on my big trip to America. That was when Roly Pettit's first wife developed schizophrenia and her family, who were wealthy land owners in Australia, came over and carried her off back to Australia. Roly was very broken up, because he was very much attached to her. They wanted him to go back to Australia because they were buying her a farm. She had been told she had to live a totally quiet life. Roly refused to do that, because he said that only thing he had left was chemistry. He wrote to her every day for eighteen months and she never replied, so eventually he divorced her. He really wanted to get away to somewhere entirely different. Just at this point Bill Doering had heard that they were looking for chemists at Austin. He knew Roly because he had visited me often in London, starting in 1951. He used to visit us regularly. So he told Texas about Roly. When we went in 1957, it was just when they were considering him. When we left Yale, we drove all around the country in an ancient car we had bought. We made a trip to Austin specifically so I could tell Norman Hackerman, who was then the chairman of the chemistry department, about Roly. So that's how we first got there.

BOHNING: What was the state of the department in Austin when you went there? Was it still building, or were you in on the ground floor of his new regime?

DEWAR: The Chemistry Department had some quite good people in it. However, they had very little equipment.

BOHNING: Was the Welch Foundation money available?

DEWAR: That had been going for quite a long time.

BOHNING: Did you go there as a Robert Welch professor?

DEWAR: Yes. I wouldn't have considered going otherwise. This was a research chair, so I didn't need to do any teaching. I certainly wouldn't have been prepared to go to a State University otherwise.

BOHNING: But you said they were still short on equipment.

DEWAR: The department was, but I managed to get a small NMR spectrometer. It took me quite a time to build up my own group.

BOHNING: How was Hackerman as a Chairman? Was he supportive?

DEWAR: By the time I went he was Vice President and Provost, and after that he became the President. [William] Shive was the Chairman. He was a biochemist. The thing about the place was that Billy was indirectly related to Norman and knew him very well. Billy was terrified of causing Norman any problems, so he never spent any money because he didn't want to cause Norman budgeting difficulties. Norman also was unwilling to do anything for the Chemistry Department because he was afraid of being accused of partiality.

BOHNING: That's not the best combination.

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DEWAR: It's a very bad combination. Texas A&M, which had no inhibitions of that kind, ended up with far more equipment than Austin had.

BOHNING: Texas A&M attracted some pretty good names in chemistry too. Derek Barton went there, and [F. Albert] Al Cotton.

DEWAR: Al Cotton, yes. Al Cotton was the one who really put the place on the map. It was hardly known before. His going there was a great shock to everyone, but the truth of the matter was that he had always had right wing views, and the situation at MIT with the war in Vietnam made him move somewhere to the right of Hitler. The second thing was that he enjoyed horses and had never been able to do anything about it. There, he was able to get a ranch.

BOHNING: Who else was at Austin at the time?

DEWAR: There really wasn't anyone much. In organic chemistry there was Phil [Philip S.] Bailey, who was there because of his life work with ozone. But otherwise, the other people were practically very little known. In physical chemistry there were quite a number, like Stuart Rice. But it was lacking in people with any real standing.

BOHNING: When did that department really start to grow?

DEWAR: The sad thing is that having got me, they should have gone all out to bring in more top people, and they never did. This is the combination which I just mentioned of Billy not wanting to spend money and Norman not wanting to do anything special for the Chemistry Department. My going there suddenly put the place on the map, and the place did have money for hiring young people. We were getting extremely good young chemists but were unable to keep them, and we did not make a single high level appointment. It was about twelve years before they even tried to get anyone else at a high level. The best they got was Dick [Richard B.] Bernstein, who only stayed two or three years. When Norman left, the whole place fell apart.

[END OF TAPE, SIDE 5]

DEWAR: His successor was a totally incompetent person called Spurr. Norman had always kept the whole place running superbly, the only problem being his desire to spend as little as possible. Norman's attitude was that the purpose of the administration was to serve the faculty, and his duty as the chief administrative officer was to see that they bloody well did, which was an unusual attitude. But it was wonderful for us. Everyone in the administration wanted to help one if they could. If you had any sort of hassle with any of them, you could always bring it to an end by saying, "I'll have to take the matter to Norman Hackerman." They knew that you would,

and they knew that Norman would listen. And they knew that if Norman thought they were being stupid and bureaucratic, he'd have the shirts off their backs. With Spurr, the whole place fell just apart and totally disintegrated. In the end I just got fed up with the situation and left. I can't remember who was appointed in my place. I go blank with people; it's awful.

It's probably a sign of Alzheimer's disease, except that, as Mary says, if it were I'd have been suffering from it from the age of twenty. Oh, yes, it was Josef Michl. I was largely responsible for his going there. But it's a sad business, because he wasn't treated at all sensibly. He also got fed up with the place and left and so did his successor.

BOHNING: While we're on that subject, why did you make the move here from Texas?

DEWAR: At the end I got totally fed up with the place. Spurr was bad enough, and his successor, a woman whose name I forget, was even worse. She was put in as a stopgap because at the time, they weren't able to get anyone else to take the Presidency. The Regents fired Spurr after four years. They put her in as a stopgap on the grounds that she only had four years to go until retiring age. If they'd known how bad she was going to be, I doubt if they would have. Finally, when she left they got a really good president, Peter Flawn, who was excellent. He did a tremendous job in cleaning the place up. At this point, the trouble with the university was that the State Legislature got their fingers into the place and, even worse, so did the State Board of Control. The next thing that had to be done was to get them out. I think that at this point the Regents refused to go along with Flawn. It's pure guesswork on my part, but I think that's what happened. When he took the Presidency he said he would only accept it on the condition that he had total support from the Regents to make the University a top-level university. He would leave immediately if he felt he was not getting full support from them.

His successor was from the business school. A youngish man. I think he got his degree in advertising. He was a total disaster. Every promise that had been made to get me to go to Texas was broken by these creeps. One of these was that I would be able to remain indefinitely after retirement on a half-time basis as long as I wanted and the University wanted. Furthermore, the Department voted unanimously that I should be allowed to keep my chair full-time because there were only two or three years until the thing would become moot anyway. I went to this President asking what he intended to do, and I couldn't get him to reply for two and a half years. Finally, I got a note from him while I was in Gainesville, terminating my appointment. I was incensed. We went out and looked at houses, saw one we liked, and bought it. Why Gainesville? Because we had already decided to come here when I retired. We knew the place well, having visited here a lot, and knew a lot of the people here.

However, at this point the Texas Legislature rushed through an emergency bill abolishing retirement age at universities in Texas. The story is that the President first heard about it when he read about it in the student newspaper! They hadn't even bothered to tell him! Why they

didn't, I don't know. Everyone thought this action was because of me, but I don't think it was. [laughter] But anyway, I stayed on a year because I had people in my group finishing whom I wanted to see through, and I also rather enjoyed rubbing the President's nose in the dirt.

I really meant to retire when we came here because there are lots of things I have always wanted to do and never had time for. I had really looked forward to giving up chemistry, but when the Department here heard I was coming, they immediately rushed around and offered me a professorship, so here I am for a bit longer. There is still one piece of research I really want to finish; I think I'll stay until I do that.

BOHNING: Here you certainly have a group of people interested in the same area you're in.

DEWAR: Oh, yes. That of course is how we got to know Gainesville.

BOHNING: They have been here for some time. I've forgotten what it's called, but there's an institute here in quantum chemistry.

DEWAR: Quantum Chemistry Project, I think it is. It has never affected me in my work much. I've always worked entirely on my own. I never interacted with people to any great extent, maybe because I never was able to do so early on. But I think that's just the way I operate. I like to think of things on my own.

BOHNING: I've heard people say that there is an advantage to that in the sense that their thinking is not cluttered by input from other people.

DEWAR: This is absolutely true. When I went to Courtaulds to work with Bamford, we began work on polymerization without either of us knowing any of the literature about it. We only read it up later. I think that was a good thing. We did it quite deliberately. We said, "If we read the literature, we won't do anything new. If we set off to do things that seem to us interesting, we probably will." That's true. If you read too much about an area before starting work in it, it's very difficult to think of anything new in it.

BOHNING: What were the computing facilities like in Texas? Did they develop there at all for you?

DEWAR: Oh, yes. Furthermore, they never charged for use of the computer. Now, of course, that is quite normal, but at that time it was very unusual. The computer they had was a CDC-1604, which was similar to the IBM-7090, one of the better computers at the time. But after I'd been there just two or three years, Norman Hackerman decided that if they were going to make the university one of the top ones in the country, there should be some area where it was absolutely on top. So Texas was the first university to buy a functioning CDC-6600. There were two earlier ones, but ours was the first which really functioned properly from the word go. At that point, we had the best computing facilities in the world. No one else had a 6600 which worked. Unfortunately, it wasn't kept up when Norman left. UT let things slip. So we didn't keep up that position. It was actually a great pity; they should have done it and they would have if Norman hadn't left.

However, there still was a problem. Since anyone could use the computer, everyone wanted to, to show their intellectual superiority. So most of the time available was taken up with pointless calculations while those who really needed the computer were kept waiting. In the end I solved the problem by getting a grant, with matching funds from UT, to buy a computer of my own. It was, if I remember rightly, VAX 1178. While the VAX was of course slower than the 6600, having it all to ourselves for 24 hours a day meant that we could get far more done. Now, of course, the introduction of work stations and PCs has transformed the situation. The computer I now have at home is a lot faster than the 6600 and cost several hundred times less.

BOHNING: Let me follow up on something you said earlier. You said you still had something you wanted to finish here, and I wanted to ask you what that was.

DEWAR: Oh, yes. For the last fifteen years my real goal has been to get an effective theoretical treatment of transition metals. We tried very hard, and we finally came to the conclusion that it simply cannot be done using the formalism we had in MNDO or AM1. So we are now calculating integrals theoretically and then scaling them by a function of distance, to allow for correlation. This is something we tried years ago in Austin, but at that time the extra computing time needed was so great that we couldn't even try it. In fact, the whole of my work on theoretical chemistry has been limited simply by the current state of computers. My purpose has always been purely practical, to get methods which can be applied to real chemical problems. That means doing calculations for quite big molecules, and for reactions of quite big molecules. The treatment we used at each stage in the work was limited to the least awful approximation that allowed one to do calculations at all. Now computers are faster, so we can do things better. We have got going on this quite well, and I'm sure we can produce something useful in a year or at the most two years. I have lots of ex-members of my group who can carry on once we do it. The difficult part in developing a new method is always the first step. Once the basic method has been developed for one element, it's easy to extend it to additional elements. In this case there shall be no big problem in extending it to transition metals.

BOHNING: Where have the two hundred and fifty students or so that you mentioned before gone? Are they mostly in academic positions?

DEWAR: No. Many are in academic positions, but I think the majority went into industry, national laboratories and things like that. I've always impressed on my students that they shouldn't go into teaching unless they enjoy teaching for its own sake. I think one of the troubles is that people go into teaching thinking it's a nice soft option and one that will let them do research. I've always pointed out to my students that the research done in industry is just as intellectually interesting and in some ways a lot more challenging. A lot of my best people have gone into industry and done very well in it.

BOHNING: How did you find getting support? I see that you had a lot of support from the Air Force. You talked earlier about the problems in England, but once you got to Chicago and into Texas, how did you find getting support?

DEWAR: In Chicago there were no problems at all. I had seven grants from different agencies. After I left Chicago, quite early on at Austin, most of these grants continued. I hadn't run into problems starting up at Texas because of the Welch Foundation. The amount of money I got from it was only about a quarter of what I had had, but I got it right away. However, everyone thought that because of the Welch Foundation people at UT didn't need money at all. I'd never had a research proposal turned down in my life until I went to Texas. I didn't even in England. But now I did. I was in real trouble 'till one day I had a telephone call from Amos Horney, who was head of the AFOSR [Air Force Office of Scientific Research], or the chemistry branch of it. He said, "Are you going to be in Washington soon?" I said, "No." He said, "Well, I want to see you. Could I come and see you in Austin?" I said, "Fine." He said, "What about tomorrow?" I said, "Well, that's fine." So he arrived and said that he had decided that, instead of spending all his money on small grants to lots of people, he was going to spend a good chunk of it taking up the whole research support of four people, and he asked me if I would be one of them. After giving this due thought, I graciously agreed, and AFOSR has in fact been my main source of support ever since. I couldn't have done the work I've done without it, because it gave me total freedom. It let me work on absolutely anything I wanted. As time went on, the dollar decreased in value and a point came when AFOSR could no longer support all of my research, but they still went on being my major source of support.

BOHNING: Did you give the Welch money up altogether when you got this, or did you keep Welch support?

DEWAR: No, the Welch I kept. It was, as I said, about a fourth or a fifth of the total. Because of silly restrictions, it was in fact far less useful per dollar than any of my other sources of funds. This goes back to the origin of the Welch Foundation. Welch was a bachelor who had no family at all, and he made a huge amount of money out of oil. His only friend was a young chemist called William Milligan. When Welch died, he left all his money to set up the foundation to support chemistry in Texas, making Milligan director of research at the Foundation for life. It's an indication of his ability that shortly after the Welch Foundation was founded, Milligan came up for tenure at Rice and in spite of the Welch Foundation, they turned him down. [laughter] Not suprisingly, he ran the Welch Foundation in a rather strange way.

BOHNING: They certainly have sufficient funds, because the amount of support they give out is quite large.

DEWAR: It started out with thirty million dollars, and when I was there in Texas it got up to between forty and fifty million. I think now it's over two hundred million.

BOHNING: Where do you think physical organic chemistry is today? You've seen it develop over a long period of time now.

DEWAR: I've been unhappy about it for a long time. I think it's getting better in the sense that traditional physical organic chemistry, which consisted of studying kinetics and mechanisms of reactions, became totally sterile many years ago. I found I'd been nominated about twenty years ago for the ACS Award in Physical Organic Chemistry. I was the third person to be nominated. The first two were Winstein and Ingold. I asked for my name to be taken off the list on the grounds that I would consider it an insult to get the award and so be labeled a "physical organic chemist." [laughter] I did in fact eventually get it. Mary Anne Fox in Austin didn't know about this and nominated me and I didn't want to let her down, so I said, "Yes."

I think it's got to be a real mess for most of the people in it. They're just floundering around doing experiments without really proving anything. The good part is obvious. For example, the development of new techniques like NMR that have now been taken over by organic and inorganic chemists. As for reaction mechanisms, I have always thought they can be studied effectively only by combining experiment with theory. You have to have experiments, but they should be combined with theoretical calculations. This of course is now becoming generally accepted.

BOHNING: With respect to the kinds of calculations you've been doing for a while now, are other people working in the same area using the techniques you've developed?

DEWAR: Oh, yes. An increasing number of people. Very much so, in fact. We have of course had total hostility from the word go from most of those in the ab initio area. This isn't true for the people at the top. I'm on very good terms with them. But the rank and file still regard me as a menace. This is really not surprising. The area first developed around about 1960 when computers first became available, and [Robert S.] Mulliken was going around saying how all the problems of chemistry would soon be solved by quantum mechanical calculations. Everyone was pouring out money in the 1960s to support work in the area. At that time, the only calculations you could do were for diatomic molecules, and these were so bad that they didn't really mean anything. There were in fact only two or three second rate people doing such calculations. All the good theoreticians were in other areas. Mulliken himself never did any calculations. Neither did [John S.] Slater and all the other top people. The people doing work in that area were, to say the least, mediocre and they were moreover physicists with no knowledge of chemistry. The students they got were therefore not only the dregs but the dregs of those in the physics departments, with absolutely no knowledge of chemistry. So when Chemistry Departments were hiring faculty in the new area of Theoretical Chemistry, these were the people who got the early faculty positions. Later, when the area began to become interesting, and chemistry students wanted to learn about it, these were the people they studied under.

The methods being used now were developed, I think, by [John] Pople in the 1950s. He abandoned the whole approach in 1958 on the grounds that it could never give really accurate results. His conclusion was that you have to include interelectronic distances in the wave function. People had found this already early on in the case of the helium atom and the hydrogen molecule. There was nothing new about it. There must be a way for doing this. [C. C. J.] Roothaan published one approach and he was working on two others when he died, but nothing has been done since. When I first came across this, people were doing calculations using very primitive ab initio methods which didn't mean anything. The energies they calculated were terrible, so the only way they could get sensible results was by introducing adjustable parameters. But they weren't testing their methods to see if this was true, because they didn't want to waste computing time on it. As I have often said, this is the first time in the history of science that people have been allowed to carry out and publish calculations using untested empirical methods.

I became interested in the area by pure accident. In Chicago, I had a student who wanted to carry out MO calculations. So I put her on to doing some semi-empirical ones using Pople's pi-SCF method. To my amazement, this worked incredibly well. In fact, the final form of that treatment is probably the most accurate quantum mechanical treatment that's been developed. It gives heats of formation in aromatic hydrocarbons at least as accurately as they can be measured. This convinced me that, following this approach, one could end up with a general treatment of molecules which would be really accurate. So I tried including all of the electrons. When we started work on this area we were very restricted by the limited capabilities of the computers then available, but we kept going and we started getting results. We've had total hostility from the beginning from the so-called ab initioists, because what I was claiming was that we were able

to do things at least as well as you could by ab initio methods that needed a thousand times more computing time. This naturally upset people in the ab initio area.

[END OF TAPE, SIDE 6]

DEWAR: Most of the ab initioists were moreover doing calculations using programs other people had written. Most of them couldn't possibly have written the programs themselves. There are still a lot of very second-rate people in the area. The good ones I'm on good terms with; I have no trouble with them. But unfortunately, places like NSF and editors of journals have lists of theoreticians to send things to as referees, and half of these "official" theoreticians are people who really are no damn good and have very strong feelings about what I'm doing. It's been very frustrating. Until I got into this area, I never had problems with referees. I had always welcomed referees' comments. Even when they were offensive, they were always helpful. If they were offensive, it was usually for good reasons. I was glad to have been prevented from doing something wrong. But in the theoretical area, from the word go I had nothing but obstruction and personal insults. It's been very distasteful.

BOHNING: I won't ask you who the players are on the negative side, but who are the players on the positive side, the ones who are in the top rank?

DEWAR: The good ones? Well, Fritz Schaefer is obviously doing very good work. There are two or three others. Mike [Michael C.] Zerner. He's one of the few people in the semiempirical area. John Pople, of course, is very good. I've never had trouble with him. I'm on very good terms with [Per-Olov] Lowdin.

BOHNING: At one point there was something that came out of Indiana University, involving an exchange of computer programs.

DEWAR: Oh, yes, the Quantum Chemistry Program Exchange.

BOHNING: But that's no longer in existence, is it?

DEWAR: Oh, no, it's still going strong.

BOHNING: It is? I used to get something from them and then it sort of disappeared. I thought it folded.

DEWAR: Oh, no. But now you have got to pay for most of their literature and ask for it specifically. It's going from strength to strength. It's in terrific shape. It's a very good thing.

BOHNING: Who started it?

DEWAR: I don't know. It was one of the quantum chemists at Indiana.

BOHNING: Jerome Karle once told me that for a lot of the work he was doing, they had written a lot of their own programs (44). At one point, somebody came in trying to sell him a commercial program. He insisted that he wanted to see the code. Not the results; he wanted to see the code. When he looked at it, it was a program <u>he</u> had written, and someone was trying to sell it to him.

DEWAR: [laughter] Life is like that.

BOHNING: Are there any problems like that now?

DEWAR: Oh, yes. There are a lot of similar problems in that area. One of the things that I think unfortunate is that people in the area now have settled on this as a way of making money. John Pople and several other people have set up companies to exploit their work. I've never done this. I've always made all of our programs freely available. Also, one advantage of being treated as a sort of pariah is that no one else has tried to get into the same area. Young people who might want to wouldn't be able to get research support to do it. Another thing, too, is that developing semiempirical procedures is a hellish business. It's extremely laborious and it needs an enormous amount of computation and people with the patience of saints. It also really needs someone with some curious kind of special ability.

The advances we've made have always been when I've got someone who just happened to be good. The effect of this is that I've been able to prevent these methods from proliferating. In my group, I always had a fixed rule that people could make changes in our procedures, and they could do calculations using them if they wanted, but I would not publish the results. Anything to be published had to be done with the official procedures, so you didn't get all sorts of different bits and pieces. As a result, our "official" methods are unique. In actual fact, all methods now are essentially empirical. Even in the best ab initio methods, the errors in the absolute energies of molecules are gigantic. So the only way they can work is by a cancellation of errors, and the only way to tell whether or not they do cancel is by trial. In the ab initio area, there must be four or five hundred different methods to choose from and hardly any of them have been properly tested, or indeed tested at all. No one knows how well they work.

In our case, because there are so few procedures, each has been thoroughly tested. Apart from the fact that we've done a lot of calculations ourselves, other people have used them too, so it's a huge body of knowledge as to how well they work, and you know where you are. The only exception to that came recently with the one personal problem I've had with someone in my group. The only lemon I've ever had in it. This was Jimmy [James P.] Stewart, who came to me as a postdoc on a leave of absence from a faculty position in Scotland to write programs. When he arrived, I gave him the job of taking our programs, which were then all in bits and pieces, and putting them all together in one big package, which he did very nicely. I called this MOPAC, Molecular Orbital Package. However, when he was leaving, he claimed that this was his program and he was going to take it with him and take full charge of it. I didn't want bloodshed and I didn't want to wreck his carreer, so I just let him take it and we set up our own program called AMPAC. That's why there are two different programs, unfortunately. AMPAC is in fact much better, because it was written from scratch by Daniel Liotard who came to me from France, and was a much better programmer than Jimmy.

The other thing was that Jimmy got on to trying to find a successor to MNDO. We had in the end decided that we couldn't get d orbitals into MNDO, and there were also various things wrong with it which we were unable to correct. In MNDO, there was far too much repulsion between non-bonded atoms. One way to deal with this was just to put additional terms into the core repulsion function. We had tried this earlier, but it hadn't worked because it increased the computing time too much, and we couldn't handle it. Jimmy also tried this and wrote a program for it. Unfortunately, he wouldn't listen to any advice. He had his own ideas on how to do it and went ahead. I told him he was going the wrong way, but he wouldn't believe me. After eighteen months, he came up with what he said was the final version. I discovered it had charges of half a unit on hydrogen atoms in paraffins in addition to other failings. It just gave the right numbers and he was going to tally by these. His view was that all you had to do was to get the numbers right by state optimization, and if anything was wrong, then you just put in more molecules and went on in a sort of brute force method. It doesn't work.

At this point, I took the project away from him and gave it to a graduate student, [Eve G.] Zoebisch, who started again from the beginning. The resulting treatment, AM1, was entirely due to her (45). One other member of my group helped, but she really did all the work. I duly gave them both credit for it. Jimmy was outraged. He's a very arrogant person. I'd never had problems of this kind with anyone else before. He went off to the Air Force Academy and proceeded to come up with a new version of AM1 which he called PM3. There are things about this which are grossly wrong, and people are coming up with more and more things wrong about it. In any case, it certainly isn't a big advance on AM1. This was done just to show that his

approach worked. The whole affair was very irritating, because in the first place, it would have been much better for him if he'd been at all reasonable. He could have got a great deal out of working here with me. As I have already said, he was good at programming. He just wasn't very good at deciding what to program.

BOHNING: Are there any other areas that you think we should cover? Is there anything else that you'd like to add?

DEWAR: I don't really think so. We've covered most of them. There are lots and lots of things we've done, of course.

However, there are two recent things we've done which could be really important. One was to show that activation barriers to reactions can be due entirely to desolvation. You do it quite slowly. In the hydrolysis of esters, for example, in the gas phase there isn't any barrier at all. The barrier in solution arises entirely from the need to desolvate an ionic reagent, in this case hydroxide ion, before it can attach a neutral ester. As I have pointed out, this idea provides a very nice explanation for the way enzymes function. They function simply by getting rid of the solvent in between the reagent and the grouping of the substrate which is going to react with it. This in fact is now becoming generally recognized. You can speed up ester hydrolysis by some twenty-five orders of magnitude by going to the gas phase. There is therefore no difficulty in explaining the high rates of enzyme reactions.

BOHNING: I noticed that several of your recent papers dealt with enzymes.

DEWAR: Yes, two (46). In fact, if it weren't for the PNAS [*Proceedings of the National Academy of Sciences*], I couldn't have published the work, because the papers I sent to biochemical journals were sent to enzyme chemists to referee, who thought my idea nonsense. I probably wouldn't have been able to publish it at all. So I sent it to PNAS, which doesn't referee papers submitted by members of the Academy. Enzyme chemists all around were absolutely outraged, not so much by the theory I put forward, but by the fact that somebody who wasn't an enzyme chemist had the effrontery to come up with a new idea in this area! [laughter]

This is really one of the worst things about American science. I think many people in it tend to treat it as a religion. Everyone has their own fixed beliefs, and they defend them to the death. They regard any attack as a personal affront. It's just like denying some basic principle of Christianity. The worst thing, of course, is that science is now being divided into smaller and smaller compartments, and the people in each compartment resent any intrusion from the outside. In a lot of compartments the people aren't even that good. There's a general agreement that "experts" in any area are the sole reliable authorities. But of course, "experts" in some areas are

more expert than those in others, so in many areas the only way you can get new ideas is from outside. It really is a bad business. I've had this more often than most people because I do wander around a lot; I have come up with a lot of new ideas, and they frequently have been ones which were unorthodox by the standards of the day. The enzyme one is the most intriguing.

BOHNING: And yet the general public has the feeling that scientists are these marvelous, openminded, unprejudiced, unbiased people.

DEWAR: Oh, it's totally untrue. They're the most prejudiced and biased people around. I think it's worse in this country than most, because this is a very religious country. It has a tradition of religion. Even if people aren't religious in the ordinary sense, they absorb this sort of general religious attitude at an early age. So they really get upset by their beliefs being challenged.

I have a lovely example of that in the controversy over the norbornyl cation. I was the one who originally suggested the interpretation which made it reasonable for ions of this type to be stable, because the resonance description doesn't explain that at all. In terms of resonance theory, radicals and anions should be just as stable as cations, because you can write exactly similar resonance structures for them. In terms of MO theory, only cations can be "nonclassical," because in the case of radicals or enions, one or two electrons have to go into anti-bonding orbitals. So I had a vested interest from the beginning in the norbornyl cation being non-classical. In fact, I'm the only person involved in the controversy who ever changed sides. I changed sides partly because of new experimental evidence and partly because our theoretical calculations indicated that norbornyl cations should not in fact be symmetrical. I remember I got a letter from George Olah, who's a very old friend of mine, but is one of the main protagonists for the non-classical structure. He begins, "Dear Michael, how can you do this to me after all these years?" [laughter] JACS sent my paper to Herbert C. Brown at Purdue to referee, and he said it was "the most important contribution to theoretical chemistry in the last fifty years."

BOHNING: What about Paul Bartlett? Didn't he at least oppose the idea of a non-classical ion, at least the name?

DEWAR: I don't recall. I have always had a very high opinion of Paul. Not at all liable to get stuffy ideas. Things have got much worse lately. One particularly sad thing is that journals have changed too. In the old days, when you had a single editor of JACS, the editor developed a sort of megalomania and basically didn't give a damn about hurting people's feelings or what they thought. He did what he thought was right. I have a wonderful example of that, relating to a past editor of JACS, Marshall Gates.

This concerned my infamous "half-electron model." Let me tell you how this developed.

In MO theory, each MO represents the motion of an electron under attraction by the nuclei and repulsion by the other electrons. Since each MO can hold only two electrons, the ground state of a normal "closed shell" molecule is one where the 2n electrons occupy in pairs the n MOs of lowest energy. The occupation number of each MO is therefore zero or two.

The repulsion between two electrons occupying different MOs depends on their spins. Other things being equal, the repulsion between electrons of similar spin is less than that between electrons of opposite spin. This is because according to the Pauli Principle, two electrons with similar spins cannot be at the same place at the same time, and if the probability of them being at the same place is zero, then the probability of them even being close together is also reduced. So the repulsion between the alpha spin electron (x) in an a MO (A), and the two electrons occupying some other MO (B), are not the same. The repulsion between x and the alpha spin electron in B is less than that between x and the beta spin electron in B. This, however, is balanced by a similar difference in repulsion between the beta spin electron (y) in A and the electrons in B. So since all the MOs are empty or doubly occupied, all the electrons are moving in similar potential fields, in accordance with the MO picture in which they occupy similar MOs.

Consider now a radical. Here there is an electron (z) with no partner. If z has alpha spin, the repulsion between it and the alpha spin electron in B is less than that between z and the beta spin electron in B. So now it is no longer correct to assume that the "paired" electrons occupy similar orbitals. The MOs occupied by the alpha and beta spin electrons are different. One cannot therefore treat a radical by standard MO theory simply by specifying an occupation number of one for the singly occupied MO. This leads to major complications.

It occurred to me to wonder what would happen if one could replace z by a pair of "halfelectrons," imaginary particles with half a unit of charge and half a unit of spin. In this case the symmetry between alpha and beta sin electron would be preserved so one could still use standard MO theory. The only difference would be a spurious energy term representing the repulsion between the "half-electrons." This, however, can be easily calculated, being just one-quarter of the term in the standard treatment that represents the repulsion between two whole electrons in the corresponding AO. So we tried this out by carrying out calculations for a number of radicals and found that our simple approach gave results in good agreement with sophisticated methods that needed far more computing time.

I then discovered that there was in fact a good mathematical justification for our procedure. Indeed, I discovered later that this had been published years before by Leslie Orgel in a paper (47) which everyone had forgotten. However, I wrote up our work in terms of our picture of "half-electrons" just for fun, to see what would happpen, and sent the paper off to Marshall Gates. It came back with violent reviews from two referees, one of whom indeed clearly nearly had a heart attack. He wrote three pages, saying, inter alia, "After the split p orbital monster, here is something even worse, the half electron." [laughter] However, Marshall included a friendly letter, saying that while my idea was clearly wholly heretical, he was quite prepared to publish it, but had I any changes I would like to make in view of the referees' comments. I had in fact a second "respectable" version of the paper in which we developed the mathematical treatment of the approximation and then pointed out the amusing physical picture that corresponded to it, and that is what actually appeared in print (48). But if I had stuck to the original version, Marshall would clearly have published it, regardless of the referees' comments.

Beech

This couldn't possibly happen nowadays because editors have to accept the opinions of referees. I once wrote to one of the present Editors of JACS about a paper I had submitted, pointing out the stupidity of the comments of one of his referees. He wrote back, "How can I possibly send this to him or publish your paper? If I did, it would hurt his feelings, and I can't afford to upset our referees because then they wouldn't referee papers." Very curious and very unfortunate.

I might add that I would hate to have papers published without their being refereed. I have too often been saved by referees' comments. Indeed, in my time I have withdrawn a number of papers because referees pointed out omissions or errors that I had overlooked. It also doesn't worry me in the least if referees choose to be personally offensive. I just want the editor to act as a fair judge if I point out errors in their comments and not to reject my papers out of hand because of comments by self opinionated people, hiding behind a cloak of anonymity.

BOHNING: What do you think of the quality of the students today at the graduate level, compared to over the years that people have been working for you?

DEWAR: Oh, I think they're very good. I have no complaints. Things have become harder and harder for them, because chemistry is becoming such a huge subject, but I think they're okay.

BOHNING: In that respect, then, do you see more and more specialization in chemistry education as people focus in on narrower areas?

DEWAR: It's very difficult. I think the problem with education really goes back earlier, that far more should be taught in grade school. The level reached in grade school here is really appalling, far behind Europe. That's where things get so backward, and it continues to a large extent in high school. High school is the place where people should get their general education. When they get to the university, they should specialize far more than they do here, and things should be taught at a much higher level.

BOHNING: But does that narrower focus stifle creativity? In your own example, your ideas moved around quite a bit, and yet I know people who, if it's not in their one area, they don't want to hear anything about it.

DEWAR: Very true. It's a different attitude. Some people just like staying completely in one area and some don't. I don't; I have always wandered about, not just in chemistry but also elsewhere.

BOHNING: Have you done any writing outside of chemistry, given your classics background and everything else?

DEWAR: No, I never have. I have a book I'd like to write, but I don't know if I'll ever get time to write it. I think the only thing I've done outside was a paper which I was persuaded to send to *Science*, which rejected it. It was on the fifty-five mile speed limit. If you look at the evidence, published in full by the National Research Council as a little paperback, it fails to show that the fifty-five mile speed limit has saved a single life at all. The arguments NRC give are total nonsense. As I said earlier, the experts in different areas differ in expertise, and after all, the study of traffic isn't something which attracts high-grade minds, so you wouldn't expect great intelligence there or people who had been properly trained in scientific principles.

[END OF TAPE, SIDE 7]

DEWAR: My contribution related to statistics in Texas. Just before we went to Texas, the state raised the speed limit on all roads—two-lane as well as divided highways—from sixty to seventy. I thought that a very nice gesture, recognizing that I was coming. According to present ideas, this should have led to absolute mayhem because cars on the roads were far more dangerous then than they are today. If decreasing the speed limit to fifty-five saved lives, then raising it from sixty to seventy should have led to a massacre. But in fact, if one analyzes the statistics properly, one finds there was a decrease of six percent in the death rate on Texas roads that year.

My argument was really quite simple. The majority of deaths on the road occur in collisions between cars. Such collisions are analogous to the collisions between molecules involved in a bimolecular reaction in the gas phase and their number should likewise depend on the square of the particle (car) density. Why the square? If cars travel twice as fast, they will get to their destinations in half the time so there will, on average, be half as many on the road at any given time. The chance that a given car will be involved in a collision in a given length (x) of road is then halved. Since there are half as many cars on the road, the chance of a collision in x is therefore reduced by one half times one half equals one quarter. However, since the cars will

be travelling twice as fast in a given period, the net reduction in collisions is one quarter times two equals one half. Doubling the speed should therefore halve the death rate. This of course doesn't take account of accidents not involving collisions. Nor does it allow for the limited abilities of drivers, which means that higher speeds make them more likely to lose control of their vehicles. However, the statistics in Texas showed quite unambiguously that the death rate on roads did in fact fall the year the speed limit was raised from 60 to 70. So the safe limit at that time, in Texas at least, was certainly not less than 70 miles per hour, and now that cars are safer, it would probably be higher. In any case, the 55 miles per hour limit must certainly have killed at least four or five thousand people in Texas alone.

BOHNING: Is there anything else you'd like to add at this point?

DEWAR: I can't think of anything specific.

BOHNING: I'm curious about your interactions with a number of people.

DEWAR: Ask any questions you like.

BOHNING: You mentioned Carl Djerassi earlier. You made some comments that I was intrigued by and wondered why you felt the way you did about him.

DEWAR: I think he's a show-off. He's extremely conceited and I think he thinks everything revolves around him. I have nothing against him other than that. I've only met him a few times and haven't talked to him a great deal.

BOHNING: That's one of the reasons I asked you that question, because Djerassi is writing novels (49) and Roald Hoffman is writing poetry (50). I wondered whether you might be involved in doing some things like that.

DEWAR: Well, I have tried to do some writing, but neither poetry nor novels. I don't think Carl's novels are a going to be a contribution to literature.

BOHNING: They haven't had very good reviews.

DEWAR: They certainly haven't, have they? [laughter] I must admit, I have similar feelings about Roald's poetry too.

BOHNING: I just found one of his books and I was reading it before I came down. There's a lot of chemistry in his poetry, anyway.

DEWAR: Yes.

BOHNING: At least in terms of chemical terms. Since most of your work's been theoretical-

DEWAR: In volume, though, it hasn't. I think more than half is experimental.

BOHNING: I know your heterocyclic work goes on and on and on, but I guess-

DEWAR: At one time I had a group of about twenty-five people; I thought that was too many, and it shrank. As it shrank, my theoretical work was becoming more and more interesting. I also found that it's very difficult to do both. I would get people whom I would put onto an experimental project, and then, being in my group, they would decide they would like to find out how to do calculations. The next thing I knew, they were doing calculations and I couldn't get them back into the lab. I had three or four really good experimental projects that were never finished because of that.

BOHNING: What do you think comes first, the experiment or the theory, in your own approach? You get a new idea and you know it has both theoretical and experimental implications. Which would you approach first?

DEWAR: One would obviously carry out calculations first, because they're so easy to do. The thing about experimental work is that it's very time consuming and very expensive. You should get any help that you can from theory. This has been my point. The methods we've developed have been really intended for organic chemists to use themselves. We developed them because as an organic chemist I wanted them for my own use.

[interruption]

That person is my postdoc. He's Chinese and extremely good, one of the best people I've ever had. He's a senior faculty member at the University of China. He was with me for about two years in Austin and went back just before the Tiananmen Square affair. I got a message from him saying he thought he could get out if he got an invitation to a conference. So I got him an invitation to a conference in Austin, the Southwest Theoretical Conference. Then I got another message. He couldn't write to me but he wrote to a Chinese member of our group, saying that he thought if he got an invitation, he might be able to get his wife and child out too. So I wrote him saying that I'd be delighted if he could stay on longer and would support him as long as he could stay, and that if he did manage to come I hoped he would bring his wife and daughter with him, because we would so much enjoy meeting them. To my surprise, he managed to get all of them out. Now, of course, he can't go back. So he's the one who's working on this new thing. I have another Chinese friend of his who's coming next month, but I'm not having more than that. [I need] two just to work on this project.

BOHNING: That's what you have going now, just these two?

DEWAR: That's what I'm planning to have. I don't want more. I'm really going on very largely from a sense of duty. If I don't do this, no one may, and I think it's something that needs to be done. As I have maintained all along, there is no use having a theoretical treatment if it is useless. A treatment which you can't do calculations with is useless even if it's one hundred percent accurate in principle. So my object all along has been to get treatments which are good enough to be useful and at the same time can be applied by people to problems arising from their own experimental work. More and more people are using our methods now, very rapidly. For example, someone who's at Eastman Kodak in Rochester about eighteen months ago did a survey of chemical pharmaceutical industry. He found that of the money spent on computing, forty percent was being spent on calculations using our procedures and less than one percent on ab initio methods.

BOHNING: That's certainly a good test of your methods.

DEWAR: [laughing] Well, industry doesn't spend money without some good reason. We ourselves have come up with quite a number of things. Our calculations have led to a complete revision of ideas about pericyclic reactions, and I think now we've got the situation concerning them on very firm ground. Relatively few of them are genuinely synchronous. There's a simple reason for this. In the Evans-Polyani picture, the transition state is a structure where the bond(s) that break are partly broken and the bond(s) that form are partly formed. If a reaction involves synchronous breaking of two bonds instead of one, the energy of the transition state should be

double that of one for an analogous reaction in which just one bond is broken. So an alternative path involving breaking of the two bonds in two separate steps should be correspondinglyfavored.

A pericyclic reaction is a two-bond reaction, so it should tend to take place nonsynchronously. However, the Synchronous Transition state [TS] can be written as a hybrid of reactant-like and product-like structures, and if the resonance between them leads to sufficient stabilization, the synchronous process may be preferred. This is the reason why M. G. Evans originally came up with the idea of aromatic transition states back in 1938. It occurred to him that the transition states or a synchronous Diels-Alder reaction is like benzene, with six orbitals overlapping, and should therefore be aromatic. So that's really how he got the idea originally.

But it's obviously touch and go whether specific pericyclic reactions are or are not synchronous; the Cope rearrangement certainly isn't synchronous. The Diels-Alder reaction, I think, is in most cases not. That's another thing we've come up with. The other I've mentioned already is the possibility for desolvation to be the whole factor in determining a rearrangement reaction.

BOHNING: I don't have any more questions at this point, and I've enjoyed spending the last four hours with you.

DEWAR: [laughing] Yes, you must be worn out!

BOHNING: No, I've enjoyed it very much, and I want to thank you for taking the time.

DEWAR: You're very welcome.

[END OF TAPE, SIDE 8]

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