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# A Serendipitous Journey

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## LONDON 1928–1951

I was born in London in 1928 and I grew up there. My parents came from Aberdeen in the North of Scotland where I had many relatives. One of my grandfathers owned a mill and the other was a blacksmith. The only academic connection in the family was a great uncle who was Professor of Anatomy at the University of Aberdeen. I was the youngest of five children. I had two sisters, including my twin, and two brothers, one of whom died at a young age and I never knew him. The war was a major disruption and none of them pursued education beyond high school. We lived at first in a suburb called Wood Green before moving, as my father prospered, to the neighboring Winchmore Hill. My father was an executive at an insurance company and we were eventually comfortably middle class.

With my sister I attended the neighborhood primary school whose purpose was preparing children for the 11 plus examination, which was crucial in determining the choice between a future grammar school or technical school education. I passed the examination when I was nine years old and was doomed to repeat it each year until I reached the age of eleven and the system allowed me to move on. This occurred in 1939, the year during which the Second World War began. We happened to be on vacation in Aberdeen as the war loomed and we stayed there through December with my mother. I attended a boys' school, Robert Gordon's College, for one term.

We were all unhappy with the living arrangements and we returned to London before Christmas. We were in London in time to live through the Blitz, which began in earnest in September 1940 and continued at a high level until May 1941, after which there were only sporadic air raids until 1944. It was an interesting time, occasionally frightening. Where we lived in Winchmore Hill went relatively unscathed. There was a mini-blitz in 1944, and much more threatening, the South of England was attacked by V1 and V2 rockets. Fortunately the attacks were of short duration as the launching sites were overrun by allied forces and the war in Europe neared its end. From January 1940 to July 1945 I went to a local school, Southgate Grammar School. During the mini-blitz I served in a team of boys led by a teacher. Our charge was to locate incendiary bombs during nocturnal raids and report to the teacher who was expected to extinguish them with a sandbag before the fuse had time to cause ignition. I remember only one occasion in which we were called into action. We did not call the teacher until we had dealt with it ourselves. He was not happy. Despite the interruptions in my school years—caused by daytime air raids that forced the children into air raid shelters that had been built on the school playing field, and the absence of teachers called into the services—the school managed to provide a broad general education. There were some excellent teachers.

My school days were uneventful. I did well at most subjects without making much effort. I enjoyed mathematical puzzles. I had some modest skills at games, and I played football (soccer) and cricket for my school and for local clubs. I was invited to try out for a London club, Tottenham Hotspur. I also played some tennis and squash and still do. The war was still in progress and I joined the Air Training Corps, which gave me the choice of the Air Force in the event that I was drafted. In 1945 I had completed whatever were the required national examinations. I had no idea as to what I might then do and I decided to postpone the decision by becoming a university student. I applied to University College London (UCL) and was accepted into its Special Honours Mathematics program. This had the advantage that I was able to defer being called up—though the war was over, the draft continued. My father was not enthusiastic but the fees were small and I could live at home and commute to the University. I chose mathematics because I thought I could perform adequately without having to work very hard. After one semester I discovered how wrong I was. I began to work in earnest and I seem never to have stopped. My progress was

disturbed by my contracting scarlet fever. I missed six weeks of classes. I returned to be greeted with a complete set of lecture notes prepared by my fellow students to whom I am ever grateful. I kept in touch with my brilliant fellow student Edwin Power, who became Professor and Head of the Department of Mathematics at UCL.

In June 1947 I passed the final examinations for the B.Sc. degree in mathematics with, to my total surprise, first class honours. I suspect the examiners were sympathetic to my lengthy absence from classes. To complete the requirements for the degree I was obliged to spend another year in a program called Advanced Studies. After the challenge of the previous two years it was a relaxing time and I became involved in student affairs and served as secretary of the UCL football club and played for it. Then came the question of what to do next. I had some vague notion of seeking employment in some financial concern where mathematical skills might be rewarded but by chance I encountered Sir Harrie Massey as I was walking through the corridors of the physics department that I happened to be visiting. He stopped me and after some casual conversation he asked me what plans did I have. I replied, "Nothing that one could call a plan," and he promptly offered to support me with a fellowship to do research toward a Ph.D. in atomic physics. With my narrow concentration in mathematics I had little idea what atomic physics was but I found the prospect of doing research and maybe finding something new very appealing. So after a few days I accepted the offer and transferred to the physics department. With the completion of my degree program, I again requested deferment to continue my studies. This occurred when the United Kingdom had just discovered that despite its contribution to the development of the atom bomb it was not given access to the engineering details of its design. At my interview, I was asked in what area did I expect to do research. My reply, atomic physics, elicited immediate approval of my application for further deferment.

In the Ph.D. program, some courses were offered but none was required, and we were expected to begin research immediately. Professor Massey suggested I look at collisions of metastable helium atoms in helium gas because a program was being initiated to attempt to measure the cross sections for excitation transfer. My immediate advisor was Richard Buckingham, who was to be Professor of Computer Science of the University of London and Director of the Computing Laboratory. He was an expert on interatomic forces. Given the early investigations of Massey and Mohr, the extension of the theory was straightforward and it led to expressions in which the diffusion and excitation transfer cross sections were determined by the gerade and ungerade states of the helium molecule. Rather than construct empirical potentials I decided the time had come for a direct many-electron calculation with some chosen trial molecular wave functions. The calculation turned out to be arduous. There was no easy way to evaluate the so-called molecular exchange integrals. I spent much time without success trying to find a fast method. Computer facilities were minimal, consisting of manually operated mechanical devices. The probability of error was high. It could be minimized by a differencing process but that was very time-consuming and the temptation to neglect it could not always be resisted. When found to be necessary, corrections involved a tedious step-by-step repetition.

Though painful to acquire, the interaction potentials were intrinsically interesting because they had the unexpected feature that they passed through repulsive maxima before turning into the attractive long-range van der Waals force at larger separations. The maxima could not be attributed to avoided crossings, and I was told it must be due to numerical error. It might well have been and I did carry out some limited checking without finding any. We suggested that this kind of overlap of forces might happen more frequently than expected as indeed is the case. The subsequent cross section calculations also demonstrated the importance of the long range interactions.

## BELFAST 1951–1967

With the completion of my Ph.D. requirements in the summer of 1951, there came the question of what to do next. I had applied, without much enthusiasm, for a position with the Atomic Energy Research Establishment at Harwell and I did receive an offer. There was no indication as to how anyone could survive on the proposed salary and I decided to give up science. However David Bates, who occupied the position of Reader at UCL, had just been appointed Professor and Head of the Department of Applied Mathematics at the Queen's University of Belfast and he had at his disposal a position of Assistant Lecturer. He offered it to me. The salary was a slight improvement and the idea of pursuing my own research rather than someone else's was attractive, at least for what I anticipated would be a short duration. I accepted and made my way to Belfast in September 1951. On arriving I discovered there was no draft in Northern Ireland.

It took me some time to accommodate to the culture of Northern Ireland. Issues of no importance to me loomed large, but Queen's was an island, relatively free of the tensions that separated the general community. I did not grasp the depth of the division that existed. There were many positive aspects. I made many friends across the University. The famous poet, Philip Larkin, was one of them. In 1957 I married Barbara Kane and we had four children. Regrettably, ten years later we separated.

In 1951, the Department of Applied Mathematics was barely surviving. That it did was due to John Herivel, who had been carrying the teaching burden almost single-handedly. Initially I taught three undergraduate courses. After one year the University created the position of Lecturer in the Department, which was a tenured position. My position as Assistant Lecturer was for a period of three years. It seemed to me unlikely there would be another position of Lecturer before my appointment expired. After two more years I would be left unemployed, and probably unemployable, given the conditions prevailing in British universities at the time. Rather than give two purposeless years to a losing cause, I decided that there was little point in remaining in Belfast, and with nothing to lose I applied for the Lecturer position with a rather thin record of publications. My situation created a problem for the appointments committee, which knew of my intentions. They resolved it after considerable hesitation by offering me the position of Lecturer. I have spent my entire career in academia, apart from a one-year sabbatical from 1962–1963 at a company in the United States. At the same time as my appointment Brian Bransden took up a similar position in the Physics Department and we collaborated on studies of electron-ion interactions and autoionization and did some simple calculations on two-electron systems. Brian worked on nuclear and atomic physics and he wrote some influential books on scattering theory. To my regret, after two years he departed Belfast for the University of Durham. In the subsequent years additional faculty were appointed to the Department of Applied Mathematics, most with a background in atomic and molecular physics, and the teaching burden eased.

Among the undergraduates were some exceptionally capable students from the local schools, well-trained in mathematics and physics. David Bates immediately established a graduate program and there they were, eager to participate.

I was responsible for the supervision of one or two of these talented graduate students each year. I worked with them on the development of quantum mechanical perturbation theory and variational methods. We explored methods for controlling the accuracy of calculations of atomic and molecular properties by using sum rules. We resolved some conceptual difficulties in existing many-electron theories, and John Lewis and I found a simple sum rule that proved to be a surprisingly powerful technique. I collaborated with my faculty colleague (and close friend), Alan Stewart, on double perturbation theory and on applications ranging from explicit calculations of the Lamb shift of helium to long-range ion-atom interactions and to single-photon double ionization. I

gave considerable attention to the quantitative evaluation of van der Waals coefficients by exploiting the formal connection to the dynamic dipole polarizability at imaginary frequencies. Arthur Kingston, Yoong-Ming Chan, G.M. Stacey, and Donald Davison calculated the coefficients for specific atoms pairs. I returned to this topic forty years later with Mircea Marinescu, Hossein Sadeghpour, Jim Babb, Zong-Chao Yan, Xi Chu, and Gerrit Groenenboom to obtain greater precision and treat complex atoms of experimental interest because of their importance in collisions in ultracold gases and in Bose-Einstein Condensation. I also investigated the theory of atomic and molecular collisions, but realistic calculations beyond the Born and Distorted Wave approximations were impractical except for some special cases. Extending the work of David Bates and Benno Moiseiwitsch, I calculated cross sections for charge exchange collisions of multicharged positive ions with hydrogen atoms, showing why they are rapid processes at low energies. Years later such collisions were recognized as being of astrophysical significance. I had previously obtained the cross sections for charge transfer of  $H^+$  colliding with H atoms at low energies with H.N. Yadav. These cross sections determine the coefficient for ambipolar diffusion. The theoretical cross sections were large, and the calculations stimulated experiments to measure them.

In what was significant to my future research, David Bates had suggested that we collaborate on a calculation of the cross sections for electron capture by fast protons into, not the ground state that Yadav and I had considered, but the excited states of hydrogen. The excited states then radiate. It could be argued that at high energies the cross sections are insensitive to the explicit nature of the target, depending mostly on the ionization potential, which is the same for H and O atoms. The data could then be used to interpret the observations of proton auroras and infer the properties of the bombarding protons from the spectrum of the Doppler-shifted radiation. The research showed me that atomic and molecular physics was a critical component of aeronomy, the processes that determine the response of the upper atmosphere to the action of the Sun. I thought further about atmospheric processes, how one might identify them and, having identified the possibilities, calculate their efficiency in the atmosphere. With the help of David Bates, the world leader in aeronomy, I considered the problem of the sources of the nightglow and dayglow emissions and the altitudes at which they are emitted. We came to the conclusion that, with the possible exception of the red line of atomic oxygen, the altitudes derived from observations were all much too high. Daniel Barbier, a distinguished French observer, commented that with the appearance of our papers and without any change in the observational data the inferred altitudes fell by several hundred kilometers. The low altitudes were confirmed later by instruments carried by V2 rockets that passed through the emission layers. (These were the same rockets I had encountered in 1944.) I very much enjoyed the combination of observations and experiments interpreted by finding the processes responsible for the phenomenon and calculating or measuring the rates of the processes.

In 1954 I was given the opportunity by the Fulbright program to spend the summer at MIT, where they had an electronic digital computer. I learnt enough, with the help of Fernando Corbato, to write a code with which I could evaluate the molecular integrals that had so plagued me in my thesis research. I still remember the joy I felt as those integrals that had taken me hours to calculate streamed out at the rate of one per second. I returned to Belfast determined never to use a mechanical calculator again. It took no time to persuade David Bates that we needed to obtain an electronic computer and he set about to find the funds needed. They were provided by the U.S. Office of Naval Research, which was already supporting David's research. In the negotiations a condition was laid down that I had to agree to administer the Computation Laboratory that was created to operate the computer. We acquired a Digital Electric Universal Computing Engine (DEUCE) in 1961. It was very temperamental as were the two highly skilled engineers who



maintained it. The machine dissipated a lot of heat and the building provided a warm refuge from the Belfast winters. We took pains to encourage its use throughout the University and positioned ourselves for a major upgrade. In a general expansion of computer support for universities we obtained funding from the government of Northern Ireland. I served as Director until 1965 when we were able to appoint a real expert as Director and as Professor of Computer Science. He was Jim Browne, now of the University of Texas at Austin. Jim Browne led us into the new era and established Queens University as a leading institution in the application of large scale electronic computation.

On returning to Queen's after my summer at MIT in 1954, I continued my research in atomic, molecular, and optical (AMO) physics with a succession of talented graduate students exploring an array of atomic and molecular processes. Among those students were Ron McCarroll, Jack Smith, Bill Somerville, Norman Lynn, Tom Patterson, Dennis Parkinson, Ian Morrison, Hugh McIntyre, Kenneth Bell, Donald Allison, and Alan Dickinson, and an able postdoctoral fellow, Mike Pengelly. We considered atomic interactions, range and energy loss of fast particles in gases, transport coefficients, ion mobilities, polarizabilities, multiphoton processes, and selective atomic and molecular collisions. Some happened to be relevant to astrophysics, such as a calculation of hyperfine transitions in hydrogen atoms following a paper by George Field and Ed Purcell. As an example of the usefulness of sum rule techniques, I calculated the two-photon decay probability of metastable  $2^1S$  helium atoms. The result was  $46 \text{ s}^{-1}$ , which is close to the accurate value of  $51.3 \text{ s}^{-1}$ , obtained later. Another example was a calculation with a graduate student, David Williams, of the cross sections for Rayleigh and Raman scattering of Lyman alpha radiation by molecular hydrogen. I like to think this research encouraged David Williams to become an astrophysicist. He is today a leading figure in research in interstellar chemistry and star formation and has served as President of the Royal Astronomical Society.

My calculations at MIT were of the interaction potentials of H and H-. Coulter McDowell was another exceptionally able graduate student. Together we used the potentials to calculate the mobility of H- in a gas of H atoms and the cross sections for charge exchange. My involvement with H- led me into astrophysics. I was attending a meeting in London and there was a discussion of H- in the Sun, and there seemed to be general agreement that H- was destroyed by electron impact. I knew from a study I had made of O- in the ionosphere that Coulomb repulsion would inhibit loss by electron impact and that associative detachment would be much more probable. I estimated the rate coefficient to be of order  $3 \times 10^{-10} \text{ cm}^3 \text{ s}^{-1}$ . I did not publish this result. I was quoted by Bernard Pagel in a published review he wrote in 1959 and by Coulter McDowell, who gave an alternative estimate in 1961. Coulter also drew explicit attention to the process as a source of  $\text{H}_2$  in the interstellar medium. I did not know enough astrophysics to recognize its critical role in the chemistry of the early Universe, which was pointed out in 1968 by Jim Peebles and Bob Dicke. I did know enough to argue that the fine structure excitation of  $\text{C}^+$  and  $\text{Si}^+$  by H would be the major cooling processes in the cool diffuse interstellar gas, and my colleague, Mike Rudge, and I introduced the process in 1964 and published an estimate of the rate coefficients.

It is often said, by theorists, that physics is embodied in its equations, but I think it is to be found in the solutions to the equations. I have spent much time seeking those solutions. In a continuing effort to find simple reliable methods for quantitative predictions of atomic properties, Maurice Cohen, Richard Crossley, Colin Chisholm, Cecil Laughlin, Malcolm Parkinson and I developed an expansion method for isoelectronic sequences, useful for the determination of oscillator strengths. With the advent of electronic computing, the search for simple methods was no longer paramount, and it was realistic to contemplate calculations of higher precision on processes of greater complexity. With me, George Victor developed and Michael Jamieson applied time-dependent Hartree-Fock theory and demonstrated its equivalence to the random

phase approximation, and Arnold Arthurs and I constructed the S-matrix theory of rotational excitation of molecules by particle impact. Arthur Allison and Ronald Henry explored techniques for solving numerically the resulting close-coupled equations. More elaborate versions are in wide use today in theoretical chemistry.

Because of the presence of David Bates, Queen's became recognized as a center of excellence in aeronomy and the associated atomic and molecular physics, and it attracted visiting scientists from the United States and elsewhere. From India came Satya Prakash Khare, and from the United States came George Griffing, Jim Walker, Oakley Crawford, Jim Browne, Paul Hays, Fred Rees, Earl Beaty, and Neal Lane, and I learnt much from all of them. Neal Lane was to become Science Advisor to President Clinton. Together we calculated the probability of free-free transitions in atoms and molecules and studied atmospheric cooling in electron collisions with molecular oxygen.

Increasingly my attention turned to atmospheric science. Michael McElroy, Roy Moffett, and I set up and solved the equations that describe the absorption of solar radiation as it penetrated the terrestrial atmosphere as a function of the solar zenith angle, and we computed the rates of photoionization and photodissociation at different altitudes and latitudes. We used a model of the ion chemistry to determine the ionization distribution and we identified the detailed heating and cooling processes. We confirmed that the electron temperature exceeds the neutral particle temperature in the F region of the ionosphere. Ian Stewart, Jim Walker, and I predicted the intensity and spectrum of the dayglow produced by photoelectron impacts and by chemical reactions. I collaborated with Fred Rees, Satya Prakash Khare, and Jim Walker on studies of auroral precipitation, and using laboratory data of Bill McConkey, Bill and I inferred the energy content of auroras from the measured intensities of the 391.4-nm band of  $N_2^+$ .

Michael McElroy had been studying heavy particle collision processes, but I believe it was his research on the ionosphere that determined the direction of his brilliant career in atmospheric science. He led the development of environmental science at Harvard University, where he is the Gilbert Butler Professor of Environmental Studies.

In 1955 I was asked by David Bates to organize a conference in Belfast on the airglow and the aurorae together with the airglow observer E.B. Armstrong. The conference took place in September 1955, following the IX General Assembly of the International Astronomical Union, which was held in Dublin, Ireland. It may have been the first on the subject. Following a review by Sydney Chapman, the papers discussed observations and theory, instrumentation, laboratory studies, and quantal calculations. Most of the active researchers were present. Another meeting with the title "The Threshold of Space" was held the following year. It was organized by the Geophysics Research Directorate of the Air Force Cambridge Research Center and chaired by Professor Joseph Kaplan, a well-known chemist. The papers pointed to an important development in aeronomy. In addition to presentations on spectroscopy and photochemistry, there was a session on "Rocket Probing of the Upper Atmosphere," in which local measurements were reported and a new era in aeronomy began. Aeronomy was changing from a discipline in which remote passive observations were the source of the data to one in which specific experiments could be designed and in situ measurements could be made. The meeting attracted some famous scientists. Present were Sydney Chapman, David Bates, Marcel Nicolet, Lewis Branscomb, Robert Mulliken, George Kistiakowski, Gerard Kuiper, and George (later Lord) Porter. In 1956 and 1958 rockets carrying ion mass spectrometers were launched by the United States and the Soviet Union, and they revealed that the major ion in the F region of the ionosphere was  $NO^+$ , which immediately established the importance of ion-molecule chemistry in determining the ion composition. Existing models indicated that the reaction sequence was the ionization of O to form  $O^+$  followed by the reaction of  $O^+$  with  $N_2$  to produce  $NO^+$ . The  $NO^+$  was removed by dissociative recombination, the process introduced by David Bates. These early rocket flights heralded the coming of the Space Age.



My travel to attend the meeting was provided by the United States Air Force through an organization called the Military Air Transport Service (MATs). My fellow passengers told me that MATs stood for Maybe After Tomorrow Sometime but I experienced no delays. I was concerned about my return flight, which was due to land at some remote base in England and there were no arrangements for my onward travel to Belfast. Fortunately there was a problem and the aircraft was instructed to land at Prestwick Airport and wait. We landed and the other passengers and crew all went to sleep on the plane. I alighted and walked into the airport to find it deserted. There were no immigration or custom officials and I walked out of the airport and caught a local bus to Glasgow where I took a domestic flight to Belfast. I thought the Air Force might be concerned about their missing passenger but I never heard from them. At the meeting I met Fred Marmo and Murray Zelikoff, who invited me to visit the Air Force Cambridge Research Center and consult with them on questions about possible experiments in the upper atmosphere. I did so for several summers. A group of Air Force scientists left government service to create a private company that would engage in sponsored research. The company was called the Geophysics Corporation of America, changed later to the GCA Corporation. It is no more but I spent a sabbatical year there from 1962 to 1963. During that time I gave talks on aeronomy at several universities and I was struck by the interest and size of the audiences, which were in marked contrast to my experiences in the United Kingdom. I also interacted with members of the Harvard astronomy faculty and in particular David Layzer, who had made important contributions to atomic physics though his main interest lay in galaxy formation and cosmology.

I returned to Queen's with the intent of extending my research to astrophysics, which in my view could be seen as almost entirely applied AMO physics. Setting aside cosmic rays and neutrinos, information about the Universe is brought to us in the form of electromagnetic radiation carried by photons, and the processes that affect them on their journey to Earth belong to the domain of AMO physics.

## **CAMBRIDGE 1967 AND ON**

My knowledge of astronomy was limited and I felt that if I wished to contribute it would best be done in a critical environment where astronomy and astrophysics were actively pursued. Queen's University now has an Astrophysics Center but it did not then. I also felt personally that I had stayed long enough in Belfast and that it was time to move. To my great good fortune Leo Goldberg, the Director of Harvard College Observatory, offered me the position of professor in the Department of Astronomy at Harvard University. It was a joint invitation from Harvard and the Smithsonian Astrophysical Observatory, directed by Fred Whipple.

I accepted and came to Cambridge in July 1967. I brought with me a graduate student, Michael Jamieson, who was completing his Ph.D. thesis. I have enjoyed a productive collaboration with him for the past forty years. Michael is an expert in numerical and computational analysis at the University of Glasgow. My studies were to belong to the disciplines of AMO physics, theoretical chemistry, aeronomy, and astrophysics. There would be considerable overlap. The physical processes were often relevant to aeronomy and astrophysics, and the mode of research I followed in astrophysics was very similar to that in aeronomy.

## **Atomic, Molecular, and Optical Physics**

Astronomers used to think AMO physics consisted of wavelengths and oscillator strengths and not much else, and even from this limited perspective they did not always appreciate that calculating the data to reliable accuracy could be prohibitively difficult. It is recognized now that

the Universe is far from even local thermodynamic equilibrium, and an extensive array of processes must be identified and understood quantitatively if a realistic picture of the evolution and structure of the Universe is to be constructed. Clearly we need electron impact excitation and ionization cross sections, photoionization cross sections, photodetachment cross sections, and radiative and dielectronic recombination and radiative attachment rate coefficients. Heavy particle collisions at low and high energies play a crucial role. Charge exchange modifies the ionization balance in partly ionized plasmas and is a source of emission lines. Excitation of fine structure levels by neutral particle impact controls the thermal balance of diffuse low-temperature gas, and excitation by proton and ion impacts determines the fine structure populations of hot plasmas. Collision-induced absorption and emission contribute to heating and cooling. Molecules can be formed by radiative association and associative detachment and destroyed by photodissociation, photoionization, dissociative recombination and dissociative attachment. If molecules are present, rotational and vibrational excitation leads to emissions that serve as diagnostic probes of the plasma environment. Chemical reactions in the gas phase and on grain surfaces give rise to a chemistry with which molecules of remarkable complexity are created.

In the next few years, I was well funded from a variety of sources and I assembled a lively group of postdoctoral fellows, active in theoretical atomic and molecular physics, led by Gordon Drake, who had expected to come to Belfast but found himself in Cambridge instead. Academic positions were not as scarce as they later became and with few exceptions the postdoctoral fellows proceeded to universities. Gordon went to the University of Windsor and has had a distinguished influential career in Canadian Physics. Oakley Crawford was a visiting scientist in Belfast who returned with me to Cambridge on his way to a research position at Oak Ridge National Laboratory. We worked with Arthur Allison on electric dipole scattering of electrons. Robin Reid returned to Queen's, and Cecil Laughlin to the University of Nottingham. Ken Sando, who became an expert on the theory of spectral line broadening, left for the University of Iowa. Merle Riley opted for a research position at Sandia National Laboratories. Jon Weisheit was a graduate student of Neal Lane from Rice University who left for the Lawrence Livermore National Laboratory in 1972. Of the group he was the most interested in astrophysics and he explored the effects in the interstellar medium of inner shell ionization. Arthur Allison, and a year later, Ray Flannery and Hiram (Chip) Levy were appointed to staff positions at the Smithsonian. Ray did research on collisions of atoms produced by ablation of meteoric material and he began his important studies of Rydberg atoms. Ray shared the teaching with me of a graduate course on atomic collision theory before he departed for the Georgia Institute of Technology. Chip investigated atmospheric pollution and examined the role of the OH radical in removing CO near Earth's surface before he moved to the Geophysical Fluid Dynamics Laboratory at Princeton. After several years Arthur Allison returned to the University of Glasgow, where he occupied a high administrative position. While here he was an enormous help to us in guiding our efforts in all matters computational and was involved in a wide range of problems.

Together with George Victor, who later took up a federal position at the Smithsonian, Gordon Drake and I carried out as our initial project a comprehensive study of the radiative properties of the helium isoelectronic sequence based on a variational representation of the Green's function. We evaluated the allowed and forbidden one- and two-photon decay probabilities. We corrected an error in the formulation of the two-photon decay of the  $2^3S$  states and showed the process to be orders of magnitude slower than earlier analyses had indicated, so much so that the metastable state would always be quenched by collisions or other perturbations.

It was believed that the  $2^3S$  states could not decay radiatively by a single-photon transition. However, Alan Gabriel and Carole Jordan drew attention to emission lines in the solar spectrum whose energies matched those of the single-photon  $2^3S-1^1S$  transitions of several helium-like ions. Hans Griem and Gordon Drake soon solved the mystery. The standard theory of quantum

electrodynamics was inadequate. Gordon quickly made the necessary relativistic extension and then applied it to carry out precision calculations of the decay rates. The calculations stimulated extensive experimental tests that confirmed the theory. Similarly precise calculations were done later by Walter Johnson and his collaborators using relativistic many-body perturbation theory.

From the Department of Chemistry at Harvard came Tom Caves. Tom formulated a model potential theory that was further developed and exploited by Jon Weisheit when he arrived in 1970. Tom was appointed to the faculty of North Carolina State University. The unforgettable Chris Bottcher arrived in 1970 and, though he left in 1972 for the University of Manchester, he was a frequent visitor to Cambridge where he was a provocative, stimulating presence. Another frequent visitor who contributed much was Cecil Laughlin. In 1971, Michael Oppenheimer arrived from the Department of Chemistry of the University of Chicago. He initially collaborated with Holly Doyle, who had worked with David Layzer, on developing new methods for determining resonance structures in electron collisions, but his real interests were in interstellar chemistry and atmospheric chemistry. He is well-known today for his research on pollution and his eloquent presentations of the views of the Environmental Defense Fund. Michael is now Albert G. Milbank Professor of Geosciences and International Affairs at Princeton. Also from the Department of Chemistry at Chicago came Kate Kirby as a postdoctoral fellow. It turned out to be an appointment of considerable moment. When Arthur Allison left for Glasgow in 1972, Kate was offered his position as a federal scientist. She accepted. Kate is now Co-Director of the NSF-funded Institute for Theoretical Atomic, Molecular and Optical Physics (ITAMP) and an influential voice for laboratory astrophysics, recognized internationally. In her early research she collaborated with Lewis Ford and Chris Bottcher on dissociative ionization and resonances. Most recently she has studied collision-induced opacity in brown dwarf atmospheres.

We had some visiting scientists who greatly enlivened the atmosphere. Ronald Stewart worked closely with Deborah Watson on a molecular version of the time-dependent Hartree-Fock approximation before returning to England. Deborah was a graduate student in chemistry. The distinguished physicist Walter Johnson spent a sabbatical with us. He collaborated with Chi-Dong Lin, who was a Smithsonian research fellow, and with me on constructing the relativistic random phase approximation and applying it to high  $Z$  systems.

Over the next twenty years I advised eight chemistry students and three physics students. In addition to Deborah, the chemistry students were Steve Wofsy, Shih-I Chu, Charles Cerjan, Jane Fox, Turgay Uzer, Catherine Asaro, and Ron Friedman. With the exceptions of Charles, who took a research position at Lawrence Livermore National Laboratories, and Catherine, who is an award-winning writer of science fiction, all are in professorial positions. Shi-I Chu is the single practitioner of theoretical AMO physics elected to the Academia Sinica in Taiwan. Turgay is exceptionally capable in mathematics and has made major contributions to the theory of the response of atomic and molecular systems to electric and magnetic fields. Steve and Jane are important players in atmospheric chemistry. The physics students were Tim Stephens, Ron Bieniek, and Phillip Shorer. From the beginning Tim had a specific research position in technology in mind. Ron is a professor at the University of Missouri-Rolla. Phillip, who interacted closely with Walter Johnson and Chi-Dong Lin, was an exceptional student who would have become a professor of physics, but he died tragically two years after getting his Ph.D.

### **Harvard-Smithsonian Institute for Theoretical Atomic, Molecular, and Optical Physics**

Despite its obvious value as an enabling science and its direct connection to aeronomy and astrophysics, AMO physics was poorly funded. Partly for that reason but also because of the lack

of recognition of its intellectual promise by other physicists, there was no graduate student in theoretical atomic and molecular physics in any of the departments of physics that have been the principal source of university faculty in the United States with the possible exception of the University of Chicago, where Ugo Fano continued to be active after his formal retirement. The subject was in grave danger of vanishing as an intellectual discipline (and taking fundamental quantum mechanics with it).

Many were concerned. Lloyd Armstrong, Neal Lane, and I organized a gathering of theorists at the annual meeting of the Division of Electron and Atomic Physics (now the Division of Atomic, Molecular and Optical Physics, DAMOP) at the University of Connecticut in May 1984 to discuss the problem and the possible remedies. At the meeting the participants established the Theoretical Atomic, Molecular and Optical Community (TAMOC) as a formal entity. It has met regularly at subsequent DAMOP meetings. The discussions led to a review by the Committee on Atomic, Molecular and Optical Sciences (CAMOS) of the National Research Council (NRC), chaired by Lloyd Armstrong, and a report by the NRC was published in 1987 entitled “The State of Theoretical Atomic, Molecular and Optical Sciences.” The report noted that among the measures that might be taken to strengthen theoretical AMO physics was the formation of an institute that would serve as a focal point to attract talented graduate students into the field and that would facilitate interactions between individual scientists in the AMO community.

After consulting with Kate Kirby and George Victor and with their help, I wrote a proposal to the NSF for an Institute for Theoretical Atomic and Molecular Physics (ITAMP), extended later to Theoretical Atomic, Molecular and Optical Physics (but still ITAMP). It included a request for funds to support graduate students, visiting scientists, postdoctoral fellows, and science workshops. The proposal was successful. The Institute came into existence on November 1, 1988. I was the first Director, Kate was the Deputy Director, George Victor organized the Visitor Program, Brendan McLaughlin was appointed a research physicist and member of staff, and Jim Babb accepted our offer to become the first ITAMP postdoctoral fellow. George Victor retired in 1994 and Brendan left for a position in Belfast that same year. Hossein Sadeghpour was an NSF-supported postdoctoral fellow. He accepted a Smithsonian position as a research scientist and took over the Visiting Scientist program. Jim Babb was appointed to a similar position and took charge of computing initiatives for the Institute. In the proposal was a commitment to create a position of Professor of Physics in the Department of Physics at Harvard to be filled by a distinguished theoretical atomic and molecular physicist. Rick Heller was appointed to that position in 1993 and replaced me as Director. Rick remained Director until 1998 when he also became Professor of Chemistry. Kate Kirby served as Acting Director for three years and then became Director in 2001. Recently, in recognition of the increasing participation of the Physics Department, it was decided to share the Directorship between Kate Kirby and Mikhail Lukin. Mikhail is Professor of Physics at Harvard. Earlier, he was an ITAMP postdoctoral fellow. The proposal contained a commitment by the Smithsonian to consider creating another senior position for a theorist in AMO physics. That has not happened yet.

The Institute has been in my view very successful. It is now in its nineteenth year. Its workshops have identified and stimulated the leading areas of new AMO physics. Its postdoctoral fellows have been remarkably successful in obtaining academic positions and the future of theoretical AMO physics seems secure. I recognize that this is due in part to the extraordinary resurgence in experimental AMO physics that has occurred in the past two decades.

In addition to the support for AMO physics provided by the Institute, the Smithsonian Astrophysical Observatory funded for a limited time a predoctoral program designed for graduate students from other universities who wished to spend some time at the observatory. To do so they required the approval of their advisors. Through it we attracted some outstanding students.

Mircea Marinescu and Ionel Simbotin came from the University of Bucharest, Phillip Stancil from Old Dominion University, Atul Pradhan and Robin Cote from MIT, Weihong Liu from New York University, Jathindas Tharamel from the University of New Hampshire, Robert Forrey from the University of Delaware, Roland Gredel from the University of Heidelberg, Moncef Bouledroua from the Badji Mokhtar University in Algeria, and Roman Krems from the University of Göteborg.

I set aside for special mention Ewine van Dishoeck from the University of Leiden. She had acquired a strong background in theoretical chemistry working with Marc van Hemert and she had decided that her further research should have significance in astronomy. There was an IAU symposium on Interstellar Molecules in 1979 in Mont Tremblant in Canada that I attended. Ewine was not a participant. She emerged from the surrounding countryside where she had been camping with her future husband Tim de Zeeuw. Camping in remote locations is a favorite pastime of theirs. She found me and introduced herself, telling me that Teije de Jong had advised her that I might be a suitable advisor. A brief conversation was sufficient for me to invite her to Harvard for a few months to learn some astronomy and begin applying chemistry to astronomical phenomena. And so it happened. She obtained a grant to work on her Ph.D. degree at Leiden and Marc, Harm Habing, and I shared the responsibility for advising her. She divided her time between Cambridge and Leiden. She wrote an impressive thesis on the properties of the OH radical and molecular clouds. After earning her Ph.D. degree from the University of Leiden, Ewine was appointed a Junior Fellow at Harvard from 1984 to 1987. She is Professor of Molecular Astrophysics at Leiden and is a major figure in star formation, leading a large group of theorists and observers. She has won many awards, including the Maria Goeppert-Mayer Award of the American Physical Society and the Bourke Medal of the Royal Society of Chemistry, and has been elected a Foreign Member of the National Academy of Sciences.

The Institute does not support postdoctoral fellows to work with individual members, but I had some funding from the NSF and the Department of Energy that I could use. Investigating heavy particle collisions were Bernard Zygelman, Tim Heil, Sergio Bienstock, Yan Sun, Mengli Du, Roman Krems, and David Cooper, a CFA-supported postdoctoral fellow. Bernard and I, together with Piotr Froelich, and others, investigated collisions of hydrogen and antihydrogen atoms. Mineo Kimura and Piotr Froelich were visiting professors from, respectively, Japan and Sweden, who made valuable continuing contributions to the research programs. Bernard and Roman worked out the elaborate formalism needed to describe the collisions of complex atoms, and Roman explored their behavior at ultracold temperatures. Recently Bernard has carried out a comprehensive study of hyperfine transitions in collisions of hydrogen atoms. Andrei Derevianko extended many-body perturbation theory and carried out high-precision calculations of atomic properties. Tim, Sergio, and David studied heavy particle collisions in charge exchange and mutual neutralization processes. Mengli Du discovered a new way of evaluating complex summations in quantum mechanics and Yan Sun developed innovative methods for evaluating the response of molecules to radiation, which we applied to atmospheric and astrophysical phenomena.

Remarkable experiments are in progress on ultracold gases and I played and continue to play a small part in the work of the NSF-supported Harvard-MIT Center for Ultracold Atoms (CUA). I worked with Roman Krems (now a member of the chemistry faculty of the University of British Columbia), who made important contributions to our understanding of the effects of magnetic fields on collisions of atoms and molecules at ultracold collisions, and with Naduvalath Balakrishnan, who explored the behavior of chemical reactivity in the limit of zero temperature. Enrico Bodo, a visiting scientist from the University of Rome, Sapienza, working with Franco Gianturco, also participated. Recently with Enrico and postdoctoral fellow, Peng Zhang, we have studied low-temperature near-resonance charge exchange.

In connection with the role of energetic atoms in the chemistry of weakly ionized plasmas, Vasili Kharchenko, Peng Zhang, and I have studied the transport of hot atoms through a neutral gas by numerically solving the linear Boltzmann equation, and we have found that the conventional distinction between Rayleigh and Lorenz gases does not hold in practice for actual gases.

## Aeronomy

I continued my activities in aeronomy as a leading participant in the Atmospheric Explorer mission in which three satellites were launched, though only satellites AE-C and AE-D provided useful data. It was a team effort. Michael McElroy, Jim Walker, and I were the three supporting theorists. The spacecraft had a propulsion capability that enabled measurements to be made at altitudes between 100 km and 250 km. Simultaneous measurements could be carried out on the neutral and ion compositions, the electron and ion temperatures, the photoelectron energy distribution, and the intensities of the solar UV emission. We used the measurement data in an interactive process with the intent of determining the distribution of the solar energy absorbed by the atmosphere into ionization, luminosity, and heat. Engaged in the theoretical studies were Arthur Allison, George Victor, Michael Oppenheimer, and Kate Kirby. Michael McElroy commented that in five short years the nature of upper atmosphere research was transformed by the AE program.

The same theoretical approach could be applied to the other planets. Michael McElroy, Tom Degges, Ian Stewart, and I reported preliminary investigations of the sources of the dayglow observed on Mars during the Mariner 6, 7, and 9 missions. A more comprehensive study of the upper atmosphere of Mars was made with Jane Fox based on the Viking 1 measurements, and the escape of nitrogen from the atmosphere was explored. Jane is a Fellow of the American Geophysical Union. She was a Harvard graduate student in chemistry. We also considered the ionization, luminosity, and heating of Venus based on the data from the Pioneer Venus space probe. The calculations for Mars are now being employed in discussions of the data from the Mars Express.

Jeng-Hwa (Sam) Yee was a research assistant here for two years. Sam is an expert instrumentalist who wished to give some time to the practice of quantum mechanics. He set up the theory and calculated the cross sections for collisions of ground and metastable oxygen atoms with which we investigated the influence of atmospheric winds on the profile of the oxygen red line. In other applications I enjoyed a long collaboration with Steve Guberman and Arthur Allison on the transmission of UV radiation through the atmosphere. I also studied the dayglow and the auroras of Jupiter with Weihong Liu, a very able graduate student from New York University. We did detailed analyses of the UV spectra. We were able to reproduce the observations of the dayglow by combining the contributions from photoelectron impact excitation and fluorescent scattering and did not require an additional energy source. We also argued for the existence of a significant temperature gradient. Jupiter is a source of X-rays. Vasili Kharchenko and I have shown that the X-ray spectra can be explained by energetic positive ions  $O^+$  and  $S^+$  deposited in the atmosphere and undergoing impact ionization, stripping, and charge exchange collisions. Vasili is a member of ITAMP and now Professor of Physics at the University of Connecticut, with whom I have collaborated extensively.

The remarkable discoveries of extrasolar planets will lead to new challenges and an exciting future in aeronomy.

## Laboratory Astrophysics

A large part of my research in AMO physics is directly relevant to and stimulated by aeronomy or astrophysics. I label it laboratory astrophysics, which in my case means theoretical studies. I



present three examples. Molecular hydrogen has unique radiative and collisional properties and is a powerful diagnostic probe of its environment. It plays a crucial role in controlling the evolution of the astronomical objects in which it exists. Tim Stephens, a Harvard physics graduate student, and I decided to calculate accurately the response of  $\text{H}_2$  to UV radiation. Phil Solomon and Chandra Wickramasinghe had pointed out that  $\text{H}_2$  was destroyed in the interstellar medium by the absorption of interstellar radiation shorter than 110 nm into excited electronic states, which then spontaneously radiated into the vibrational continuum of the ground state, and Ted Stecker and David Williams had made an estimate of its efficiency in the interstellar radiation field. All the basic molecular data were available and Tim and I thought it would be interesting to follow through with an accurate prediction if only to demonstrate that such calculations were possible. We wrote down the quantum mechanical formulation of the process of spontaneous emission into a continuum and evaluated the probabilities of dissociation for every vibrational level of the two accessible excited states. With Arthur Allison I had previously evaluated the absorption oscillator strengths so we were in a position to determine the photodestruction rate for any specified radiation field. We could also calculate the fluorescent spectrum. Using the Sun as the source we did this calculation also for Jupiter. The destruction process yields energetic hydrogen atoms and is an important heating source.

It happened that laboratory measurements of the fluorescent spectra for both  $\text{H}_2$  and  $\text{D}_2$  had been made by Gerhard Herzberg some years earlier, but because of the absence of any clear relationship between the spectra of the different isotopes their origin had not been identified. He thought it might be  $\text{H}_2^-$ . Gerhard was visiting Harvard in 1973 carrying a microphotometer tracing with him, which he showed to me. The calculations exactly matched the experiment. The process was mentioned by Ed Condon in 1928 but this was the first clear demonstration of it. The fluorescence process populates the discrete vibrational levels as well as the continuum, and the discrete levels can decay with the emission of electric quadrupole photons, mostly in the infrared. With the help of Kate Kirby, the individual quadrupole transition probabilities were calculated by Jean Turner, who was an undergraduate at Harvard at the time. They were employed later by John Black, who was a brilliant graduate student in astronomy, to obtain the resulting infrared and visible spectrum.

Another source of excited vibrational levels is the  $\text{H}_2$  formation by associative detachment of H and  $\text{H}^-$ . Ron Bieniek and I extended a theory of the reaction to determine the rovibrational distribution. An attempt to find the spectrum in the planetary nebula NGC 7027 by an undergraduate, Alain Porter, John Black, and myself was unsuccessful.

An example from aeronomy had to do with the formation of nitric oxide (NO). It had been suggested that energetic nitrogen atoms produced by dissociative recombination of  $\text{NO}^+$  might survive long enough to react with molecular oxygen. A postdoctoral fellow, N. Balakrishnan, now professor at the University of Nevada, Las Vegas, calculated the energy loss processes and, with Vasili Kharchenko, solved the Boltzman equation for the nonequilibrium energy distribution in the atmosphere and determined the reaction rate coefficients.

The strength in theoretical AMO physics does not mean the future of laboratory astrophysics is secure. The title of the first issue of the *Astrophysical Journal* published in 1895 was “An International Review of Spectroscopy and Astronomical Physics,” and astrophysics used to be one of the frontiers of AMO physics. It is no longer. If laboratory astrophysics is to survive, let alone prosper and meet the increasing needs of astrophysicists, it requires their long-term support.

One problem facing laboratory astrophysics, and indeed many areas of physics, is the acquisition, verification, and dissemination of atomic and molecular data. ITAMP conducted a workshop to discuss what might be done.

The workshop “Atomic and Molecular Data for Science and Technology” took place in June 1996. Emerging from the workshop was the recommendation that a conference series be initiated at which the many issues confronting the providers and users of data could be addressed on a regular basis. The series is called “The International Conference on Atomic and Molecular Data and Their Applications (ICAMDATA).” I was the first chair, followed by Ratko Janev, and then by Graeme Lister. The conference is international. It has been held in the United States, the United Kingdom, Japan, and France, and the meeting in 2008 will be in China.

## Astrophysics

In the Department of Astronomy I first interacted with graduate students Edward (Ned) Wright, Michael Jura, and Paul Kalaghan. Ned and I calculated the cooling that could arise from the presence of the molecule HD. I cannot resist quoting from our article, published in 1972. In it we asserted that “in the prestellar era the relatively large primordial abundance of deuterium will cool a molecular gas to temperatures less than about 20 °K [sic] even in the absence of heavy elements and an unusually massive first generation of stars may not have occurred.” We may not have been the first to make this point but certainly we were not the last. For his Ph.D., Ned went on to work with Giovanni Fazio on far-infrared observations of HII regions with a large balloon-borne telescope. Mike Jura and I wrote a short paper on the influence of radiative charge transfer on the  $\text{He}^+/\text{H}^+$  ratio, after which Mike constructed a time-dependent model of the ionization and thermal structure of the interstellar gas by a method not unlike that I had used in determining the structure of the ionosphere. Paul Kalaghan was unusual in that he was an experienced radio astronomer who wished for his thesis to involve himself in quantum mechanics, which he did by working out the theory of the hyperfine structure of the molecular ion  $\text{H}_2^+$  and calculating the hyperfine parameters, a nontrivial problem. Having determined the transition frequencies, I joined Paul in a search for the lines using the Haystack Observatory. We found a strong signal immediately. My excitement steadily diminished as the night wore on and the signal weakened to eventually disappear. This was my one and only observing experience.

Joe Onello was another astronomy graduate student interested in quantum mechanics. He applied the Z-expansion method to the determination of oscillator strengths. Joe continued research as a professor of radio astronomy.

I had anticipated that learning astronomy would be accelerated by interacting with observers and that was true, but the presence of a theorist, Dick McCray, contributed still more to my education. Dick and I wrote a review article, “Heating and Ionization of HII regions,” for the *Annual Review of Astronomy and Astrophysics* that combined Dick’s understanding of the large scale properties of the interstellar medium with my knowledge of the atomic and molecular processes. We pointed out that much of the cooling arises from collisional excitation of the excited fine structure level of  $\text{C}^+$ , which emits radiation at 156  $\mu\text{m}$ . The line intensity is a measure of the total energy input into the medium. Dick and I also briefly explored the role of negative ions in the formation of interstellar molecules. Dick left for the University of Colorado in 1971. We carried out a joint study later with Stephen Lepp on the chemistry of the ejecta of SN 1987a.

In plasmas produced by high frequency radiation of cosmic gas, multicharged ions coexist with neutral hydrogen and helium atoms and charge exchange reactions occur and modify the ionization structure. They populate excited states that may radiate. Scott Butler, in collaboration with a postdoctoral fellow, Tim Heil, developed the theory of such processes and determined the rate coefficients for astrophysically relevant processes and explored their consequences for his thesis. Scott and Sally Baliunas pointed out that for some ions the reverse process of charge transfer

ionization would be rapid and must be included in ionization models. Graduate students David Neufeld and Amiel Sternberg (Amiel was a student at Columbia University) and postdoctoral fellow Sergio Bienstock also contributed to understanding the influence of charge transfer. Tim Heil left for the University of Georgia. Sergio departed for a financial institution, as did Scott Butler by way of the Sloan School at MIT.

Tom Cravens graduated with his Ph.D. in 1974. He collaborated with Chris Bottcher and Kate Kirby on line broadening and with me on the energy deposition of cosmic rays in a gas of molecular hydrogen. His subsequent research has focused largely on the Solar System. It was Tom who first identified the source of the X-rays seen from comets. He has been elected a Fellow of the American Geophysical Union. Vasili Kharchenko and I used his model of the X-rays to calculate the actual spectrum. The process also occurs in the heliosphere and contributes to the diffuse soft X-ray background. These calculations involved two undergraduates, Matthew Rigazio and Ronald Pepino. In collaboration with the *Chandra* observation team, we employed our X-ray spectrum to infer the solar wind oxygen ion composition. My last graduate student, Cheng Zhu of the Physics Department, studied a number of astrophysically significant processes, including with Jim Babb, line broadening of alkali metal resonance lines. Cheng joined a financial concern.

## Astrochemistry

In the early 1970s, there was an explosion of activity in the discovery of interstellar molecules and the discipline of astrochemistry was born. David Bates and Lyman Spitzer had earlier put forward a model of the composition of diffuse interstellar clouds, and John Black and I moved to extend it by including molecular hydrogen in the chemistry. We used the photodissociation rates of Tim Stephens to compute the distribution of hydrogen in atomic and molecular form as a function of optical depth, in effect adding UV photons to the dense cloud chemistry of Bill Klemperer, Eric Herbst, and Bill Watson. As the reaction initiating the carbon chemistry we adopted the radiative association of  $C^+$  with  $H_2$  to form  $CH_2^+$ . We were able to reproduce the abundance of CH measured toward Zeta Ophiuchi by postulating a rate coefficient for radiative association of the order  $5 \times 10^{-16} \text{ cm}^3 \text{ s}^{-1}$ . We chose the intensity of the radiation field to match the populations of the rotational levels of  $H_2$  and the cosmic ray flux to match the abundance of OH. The same arguments were applied to the Copernicus data on rotational populations of several clouds by Mike Jura. Given the cosmic-ray flux we derived the cosmic abundance ratio of D/H from the HD/ $H_2$  ratio with the assumption that the source of HD was the reaction of  $D^+$  with  $H_2$ . Similar calculations for the clouds in front of zeta Persei and omicron Persei were done by Tom Hartquist. Because the rate coefficient adopted for the dissociative recombination of  $H_3^+$  was too small, the inferred ionization rates were too.

We explored various aspects of the chemistry with postdoctoral fellows and graduate and undergraduate students. With Teije de Jong from Amsterdam, Shih-I Chu calculated the cooling due to CO in a collapsing cloud, and with Michael Oppenheimer I studied the effects of an evolving increase in the abundance of CO on the temperature. With varying combinations of Michael, John Black, Tom Hartquist, Teije de Jong, Jean Turner, Tom Cravens, and Shih-I Chu we examined the chemistry of sulfur, silicon, hydrogen chloride, and formaldehyde. With Steve Berry we investigated the ionization due to the process of associative ionization. Michael and I drew attention to the important role of charge exchange with metals in providing a lower limit to the fractional ionization in dense regions and its sensitivity to depletion. Tom Hartquist, Holly Doyle, and I considered the possibility that the ionization rate in the galaxy might not be a constant. With a group that included an undergraduate, Dylan Jones, we evaluated the photodissociation

and photoionization rates in dense clouds resulting from the excitation of  $\text{H}_2$  by the secondary electrons generated by cosmic-ray ionization, a mechanism introduced by Sheo Prasad and Shankar Tarafdar.

The chemical composition is a powerful diagnostic of shocked conditions where enhanced temperatures and densities exist. Following an initial study by Tom Hartquist and Michael Oppenheimer, David Neufeld carried out a comprehensive analysis of dissociative shocks that took account of the precursor radiation and the temperature structure. Wayne Roberge was a graduate student with whom I looked into the mechanism of collision-induced dissociation and its dependence on density. Later Wayne and I collaborated with Bruce Draine on the influence of magnetic fields and chemistry on shock waves. Margaret Graff was a CfA postdoctoral fellow who knew a lot of chemistry, and she and I considered the effects of nonequilibrium reactions.

Stephen Lepp arrived as a postdoctoral fellow in 1984. We explored the influence of deuterium atoms on the fractionation mechanisms introduced by Bill Watson, and with Jeng-Hwa Yee we investigated the possible changes to the nitrogen chemistry that might result from hot atoms. Stephen and I discussed the changes to the chemistry that would occur if polycyclic aromatic hydrocarbons (PAHs) or large molecules turned out to be a major component of the interstellar gas. We pointed out that radiative attachment of electrons to them would be a significant source of negative molecular ions. In a review published in 1999 I commented, "For carbon chains a substantial fraction may exist as anions." Such anions have now been detected by Patrick Thaddeus and his group. Stephen Lepp, Ewine van Dishoeck, John Black, and I constructed a model of the Zeta Oph cloud that included PAH molecules, and we found that negative PAH ions exceeded PAH neutral molecules in density at the center of our model cloud.

Stephen Lepp arrived with a background in the chemistry of the early Universe. The Recombination Era saw the dawn of chemistry as the first molecules were formed in the Universe. The abundance of  $\text{LiH}$  was a crucial issue because if enough of the lithium could be converted to the molecule  $\text{LiH}$  it might be detectable during the Dark Ages. We pointed out that the early discussions of  $\text{LiH}$  did not take into consideration that the formation of  $\text{LiH}$  had to await the transformation of the lithium to neutral lithium atoms. Phillip Stancil was a predoctoral fellow from Old Dominion University, interested in astrophysics and an expert in atomic and molecular physics. He joined Kate Kirby and me in a calculation of the rate coefficients for the formation of  $\text{LiH}^+$  and  $\text{LiH}$  by radiative association, which he, Stephen, and I then applied to the early Universe. We found that the abundances of  $\text{LiH}^+$  and  $\text{LiH}$  would be comparable but negligible. We also presented models of the evolution of the other constituents.

Dave Hollenbach and Xander Tielens explored the behavior of interstellar gas under the action of intense radiation fields in what they called photodissociation regions (PDRs). Because in such regions molecular formation is driven by photoionization and molecular destruction is driven by photodissociation, I suggested the alternative, photon-dominated regions (still PDRs). Earlier Ewine van Dishoeck and John Black had constructed an array of diffuse cloud models, extending John's thesis, and they now included more intense radiation fields in interpreting measurements of the infrared spectrum arising from vibrationally excited molecular hydrogen. Amiel Sternberg and I examined the effects of collisions on the spectrum and obtained models at higher densities. We demonstrated that the differences between the infrared spectra of PDRs and shocked regions diminished as the gas density increased. Many of the needed collision data were obtained from Stephen Lepp, Victoria Buch, Roland Gredel and Stefano Tine. We reviewed the chemistry of the dense gas, and graduate student Vladimir Escalante examined nitrogen recombination and carbon emission lines in specific PDRs.

Infrared emissions were detected from carbon monoxide and silicon monoxide in the ejecta of SN 1987a. Stephen Lepp, Phillip Stancil, Dick McCray, Weihong Liu, and I put together a

chemistry that reproduced the observations. The initiating step was radiative association. Weihong and I were able to explain the unusual temperature distribution.

Cesare Cecchi-Pestellini was a regular visitor and we worked together on the calculation of rotational excitation rate coefficients and, with Sylvia Casu, proposed time-dependent and density-dependent models of diffuse clouds.

X-ray dominated regions (XDRs) were investigated briefly by Stephen Lepp and Roland Gredel and more comprehensively by Min Yan, who was a Harvard graduate student in astronomy. He also investigated the changing chemistry with the increase in the heavy metal content.

## Working Group on Astrochemistry

The essential subject matter of astrochemistry is the formation, destruction, and excitation of molecules in astronomical environments and their influence on the structure, dynamics, and evolution of astronomical objects. The molecules provide powerful diagnostic probes of the ambient physical conditions in which they are found. Progress in astrochemistry rests upon a diversity of observational, experimental, and theoretical skills and a broad knowledge of chemistry and astronomy. Along with many others, I felt that the common focus provided by a permanent working group would advance the subject. With the strong support and enthusiasm of Shankar Tarafdar of the Tata Institute in Bombay (Mumbai), I proposed to the IAU that a Working Group in Astrochemistry be established. The proposal had the support of Commission 34 and the group was cosponsored by Commissions 14, 15, 16, 28, and 40. The proposal was approved and in 1984 the Working Group in Astrochemistry came into existence. It has been a great success and it has seen astrochemistry come of age as a uniquely significant component of astronomy. I was the first chair of the Working Group. In 1992 I was succeeded by David Williams, who gave way to Ewine van Dishoeck in 1999. The Working Group has organized a series of IAU symposia based on the example of IAU symposium 87 held in Mont Tremblant in Canada in 1979, with the title "Interstellar Molecules." The first was IAU symposium 120 in 1985 in Goa in India, the second was IAU symposium 150 in Brazil, and the third was IAU symposium 178 in the Netherlands. The fourth, symposium 197, was in South Korea and the fifth, symposium 231, was in the United States. Eric Herbst was the secretary of the scientific organizing committee of the most recent symposium. He published in the proceedings a very instructive overview of the state of astrochemistry today and David Williams gave his vision of what it might be tomorrow.

## Administration

I came to Cambridge in 1967 expecting and intending to spend my working life in research and teaching. All my discussions about my joining Harvard had taken place with David Layzer and Leo Goldberg. I had little interaction with Fred Whipple before I arrived, but he was very welcoming when I did and provided support for my initial wave of postdoctoral fellows. However there were problems in the relationship of the directors of the two observatories, Harvard College Observatory (HCO) and the Smithsonian Astrophysical Observatory (SAO), which soon became apparent. They were probably inevitable, arising, I believe, from the distribution of resources available to Leo and to Fred. The relative freedom Fred had in making appointments and the support SAO could provide (from which I benefited) was in marked contrast to the strict limits on the number of professorial positions imposed by Harvard. Fred was able to appoint senior scientists, more or less at will for a time, that could greatly impact Harvard, and he seemed determined to do so. After some turmoil, Leo resigned in 1971 to take up the position of Director of Kitt Peak National Observatory. I was invited to serve in his place as Director of HCO and

Chair of the Department of Astronomy by Dean John Dunlop, a famous labor negotiator and an unusually persuasive individual. He told me that I was a unanimous choice but he did not say who he had consulted nor how many. I agreed to become Department Chair and to serve as Acting Director of HCO but I insisted that the primary charge be to find a permanent Director. In an unusual departure from the normal procedures in response to the divisions among the astronomy faculty, the University created a search committee consisting of Professor Ed Purcell of the Department of Physics and Professor Bill Klemperer of the Department of Chemistry and myself. After a careful search we recommended that George Field be offered the position. The University approved our recommendation and George accepted the invitation. George took a leave of absence in his first year so I had to continue acting as Acting Director for another year. There had been many discussions about the structure of the two observatories and a committee of distinguished astronomers had been formed to advise the University. I, along with several others, had recommended that there be a single director of the two observatories.

The dissension between the two directors would disappear (though the issues that divided them would persist in a new probably unrecognized form). In any event the Secretary of the Smithsonian Institution settled the question by inviting George Field to be Director of SAO. George soon took steps that created the Center for Astrophysics.

I continued as Chair of the Department until 1976, doing what I could to repair the fissures that had developed and to clarify another issue, which was the distribution of responsibilities between the Chair and the Director. During this time I served on the AURA board and I briefly chaired the Advisory Panel for Astronomy of the NSF. Of more importance to me Helmut Abt asked me to succeed Don Osterbrock as Editor of *Astrophysical Journal Letters*.

## ***ASTROPHYSICAL JOURNAL LETTERS***

Don Osterbrock had taken over the editorship of the *Letters* in 1971 but retired when he was appointed as Director of Lick Observatory. John Mathis then served as interim Editor. I was offered the position effective in 1973 by Helmut Abt, who was the Managing Editor of the *Astrophysical Journal* and oversaw publication of both the main *Journal* and the *Letters*. I was intrigued by the thought of editing what was or could be the leading journal in the world in astrophysics where the latest and most exciting discoveries would be published. Instead of setting papers aside in the hope I would get to them later, I would be compelled to read them promptly and carefully and be obliged to consult other papers as I chose the appropriate referees. It seemed a very good way to learn astrophysics and so it turned out, though I learned still more about people. I accepted the invitation to become Editor, expecting to serve for a few short years. I stepped down 29 years later.

With the hope that if they were short enough, the papers might actually be read by a diverse audience, I imposed a strict limit on the number of pages. The page length was a point of friction on occasion. The problem stemmed from the space occupied by the figures. The decision on the space they required was made not by me but by the printer who was motivated solely by considerations of legibility with the consequence that the papers might exceed the four page limit. It was more provoking still to the authors if the paper turned out be significantly shorter than four pages after I had insisted it be abbreviated. They could always point, and they usually did, to examples of published papers that exceeded the limit. I was encouraged to insist on the limit by the result of a change by the publisher to a larger page size that increased the space by 50%. The fraction of papers that were submitted over the new limit was unchanged.

I established four positions of Associate Editors who agreed to be available on an occasional basis to provide advice on specific issues that might arise and generally to represent the views of



the astronomical community. The appointments were nominally for three years except for that of Gene Avrett, who functioned as a permanent Deputy Director and was so named in 1987. Gene had as a particular responsibility the oversight of the development of the computer-based processing of manuscripts in the editorial office and the introduction of the electronic version of the *Letters*.

We began to encourage authors to submit papers to us electronically in 1986, when the software was designed and written electronic document management was in its technological infancy. The system that we created with the expert help of Robert Hewett was in advance of its time and it greatly accelerated our transition to full electronic handling. The referees were extraordinarily responsive to electronic transmission of manuscripts and reports and the refereeing times were substantially diminished. With the encouragement of Gene and myself and officers of the American Astronomical Society, Peter Boyce and Bob Milkey in particular, the University of Chicago Press eventually took over the processing of manuscripts from submission to publication and is largely responsible for the system that is in place today, leaving more time for the Editors to function as Editors.

During our years in office Gene and I were supported by a group of remarkable assistants who were devoted to the well-being of the journal.

## CONCLUSION

I have been fortunate that my journey enabled me to be present to see extraordinary and remarkable advances in our understanding of the Universe and to participate with many collaborators in the contributions that have been made by applications of AMO physics. I have witnessed the growth of atomic and molecular astrophysics as it responded to the discoveries arising from the arrival of new telescopes with enhanced spatial and spectral resolution and the extension of observations from the optical to X-rays, extreme UV, near and far infrared, millimeter and radio regions of the electromagnetic spectrum. Perhaps AMO physics may yet play a significant role in determining the nature of dark matter and dark energy. Certainly it does in establishing the state of the early Universe and the formation of the first identifiable cosmological objects. ITAMP will run a Workshop on Atomic and Molecular Physics in the Early Universe in March 2008.

Finally I have been involved in helping the emergence of astrochemistry into what it is today—a powerful unifying discipline, reaching into all areas of astronomy and answering deeply significant questions of star and planet formation and evolution. To this end I have written several reviews, delivered at the IAU and other symposia. The discovery of extrasolar planets has opened an exciting new chapter of astrochemistry in which aeronomy and astronomy are intimately linked.

## DISCLOSURE STATEMENT

The author is not aware of any biases that might be perceived as affecting the objectivity of this review.