NATIONAL ACADEMY OF SCIENCES

FREDERICK KAUFMAN

1919—1985

A Biographical Memoir by

MICHAEL F. GOLDE

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NATIONAL ACADEMIES PRESS
WASHINGTON D.C.

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September 13, 1919–July 6, 1985

BY MICHAEL F. GOLDE

FREDERICK KAUFMAN WAS a leader in the field of gas-phase chemical kinetics and its application to the understanding of atmospheric and combustion processes. He figured prominently in the national, and later international, debate concerning the possible impact of the chlorofluorocarbon class of compounds on the stratospheric ozone layer. His stance on this issue was typical of his clearsightedness and integrity as a scientist: legislation concerning production and use of these compounds should be based on reliable experimental data and computer models. He urged moderation and caution until the reliability of this information could be established. Subsequent actions, first, to ban the use of freons in aerosol propellants, and second, to control more stringently the production of the potentially most hazardous chlorofluorocarbons, were based on the careful program of chemical kinetic measurements conducted by him and others in laboratories around the world.

Many of these studies were made possible by Kaufman's pioneering work in the 1950s, which adapted the venerable discharge-flow technique of Wood and Bonhoeffer into a modern tool for gaining information on the rates and products of elementary reactions, the simple building blocks of complex reaction mechanisms. Until his death in 1985 he remained at the forefront, exploiting new developments to ensure that the discharge-flow technique remained a highly versatile tool for obtaining bulk kinetic data and of equal importance to the following generation of complementary state-to-state techniques.

Fred Kaufman was born in Vienna and his twin loves of music and chemistry had already emerged by 1938, when, following the annexation of Austria by Hitler, his family emigrated to Panama. Sadly, an accident there to his hands, which required extensive surgery, forced him to abandon hopes of a professional career as a concert pianist. He visited the United States in 1940 for medical treatment and moved to Baltimore the following year. Focusing on a scientific career, he began evening undergraduate courses at Johns Hopkins University while continuing to work full time. In 1944, under a new program, he began graduate work at Johns Hopkins and received his Ph.D. in 1948, bypassing the undergraduate degree. His research advisor was Alsoph Corwin, in the area of chemical kinetics in solution.

He began work in the combustion section of the U.S. Army's Ballistic Research Laboratories at Aberdeen Proving Ground and rose to the position of chief of the Chemical Physics Branch. Although also engaged in pyrolysis and other high-temperature combustion studies, his interest in exploring the underlying elementary gas-phase reactions increased during the early 1950s. With the award of a Rockefeller Public Service Award in 1955, he was able to spend a year in the Department of Physical Chemistry at Cambridge University, which Professor Norrish had established as a center for kinetics studies. There he began his pioneering discharge-flow studies with a survey of reactions of oxygen atoms. Also in this decade he began his long association with the Combustion Institute, and advances in the understanding of elementary gas reactions were regularly reported at the biennial symposia. In 1964 he was invited to move to Pittsburgh, with the establishment of the Space Research Coordination Center at the University of Pittsburgh. The decision was not easy to make, particularly as the Kaufmans' oldest son Roy was already married and settled in Baltimore. However, there were exciting plans afoot in Pittsburgh (unfortunately never realized) for a massive new research center to be built in Panther Hollow, a valley on the edge of Schenley Park and close both to the university and to Carnegie Tech, and Kaufman, enjoying the anticipated challenges, accepted the position of full professor in the Chemistry Department. With his wife Klari and younger son Michael he took up residence in the prosperous community of Squirrel Hill and their house, infused by the warmth of their marvelous personalities, rapidly became and remained an oasis for colleagues, students, and friends.

The Space Research Coordination Center (SRCC) was created with funding from the National Aeronautics and Space Administration (NASA) to promote studies in the natural and social sciences, engineering, and health areas concerned with the aerospace field. Several prominent scientists were immediately attracted to the SRCC, including Thomas Donahue, an aeronomer and the first director of the SRCC, who was already on the faculty of the Pitt Physics Department, and the physicists Wade Fite, Manfred Biondi (moving across town from the Westinghouse Corporation), and Edward Zipf. Kaufman was the sole chemist in the five-story building and, although a new chemistry building became available in 1974 and provided much-needed space for the previously widely scattered department, he chose to keep his office and laboratories in the SRCC building.

The move to Pittsburgh confirmed a shift in the focus of his research from combustion problems to the chemistry of the atmosphere, in particular the stratosphere. His involvement in all scholarly activities rapidly broadened and included advisory service on panels and committees of the National Academy of Sciences, NASA, AFOSR, National Science Foundation, and NRC, and he became director of the SRCC from 1974, chairman of the Chemistry Department between 1977 and 1980, University Professor in 1980, and president of the Combustion Institute in 1982. In 1979, the year in which he was elected to the National Academy of Sciences, he was chosen as the speaker to represent the faculty honored in that year's University of Pittsburgh honors convocation.

He was also fully involved in the teaching program at Pitt, having a preference for the general chemistry courses, while his advanced graduate course in chemical kinetics, presented every second year, provided an excellent introduction to the theory and practice of that field for a succession of physics and chemistry graduate students and postdoctoral fellows. He won Outstanding Educator of America awards in 1971 and 1975.

In 1984 his sixty-fifth birthday was honored by special symposia at Harvard University and at the University of Pittsburgh. However, it was an anxious time for his family and friends, because of illness that struck the previous year. The intensity and commitment of his research effort did not abate, however, and it was at a conference that his last illness started, leading to his death in July 1985.

Kaufman's major research contributions were in the areas of combustion and atmospheric science. By the 1950s it had become clear that combustion, for instance in flames, comprised a complex array of simpler reaction steps involving atoms and radicals. Rather than attempting to characterize these reaction steps, and thus the complete mechanism, from observation of flames, Kaufman was among those who realized the importance of determining quantitative data for each elementary reaction in isolation from competing reactions. To form the relevant atoms and radicals he revived the discharge-flow technique dating from the 1920s and developed techniques to allow quantitative detection of these species, thus allowing rate constants for their reactions to be measured. Initially at the Ballistic Research Laboratories and then at Cambridge University in 1955-56, he characterized gas phase titration reactions of N and O atoms, in particular that of oxygen atoms with nitrogen dioxide, and monitored their progress by chemiluminescence (i.e., ultra-violet and visible light emitted during the reactions). In a major publication arising from his work at Cambridge, Kaufman showed very clearly the broad range of elementary reactions. Thus the reaction of oxygen atoms with NO was found to be termolecular, requiring a third-body or chaperon to stabilize the nascent hot nitrogen dioxide molecule. In contrast to several fast oxygen-atom reactions, those with nitrous oxide and carbon dioxide occurred far below the collision rate. In addition, each chlorine molecule was able to consume several oxygen atoms by way of a chain reaction, which much later was recognized as a key sequence in the removal of stratospheric ozone by chlorofluorocarbons.

The discharge-flow technique was rapidly and ingeniously exploited by Kaufman and others, such as Schiff, using mass-spectrometric detection, and Westenberg, who succeeded in measuring absolute concentrations of radicals using electron spin resonance. However, a more sensitive general detection technique was needed and Kaufman in 1961 applied resonance ultra-violet absorption to the detection of the hydroxyl radical OH formed by the important titration reaction of hydrogen atoms with nitrogen dioxide. The key was the use of a source lamp that emitted OH radiation, thus optimizing overlap of the emission and absorption line profiles. The use of OH in this pioneering experiment was prophetic, because it became established later as the most important radical in neutral combustion and atmospheric chemistry.

This detection technique evolved during the next decade to the more sensitive resonance fluorescence, in which the fluorescence following the photon absorption event was monitored, and then to laser-excited fluorescence, in which the resonance lamp was replaced by a much more intense tunable laser light source. With these improvements a powerful technique was in place to allow a vast range of elementary reactions to be studied.

The heart of combustion and atmospheric processes, as with biological processes, is the chemistry of carbon, hydrogen, oxygen, and nitrogen. Kaufman's work was focussed remarkably tightly on key reactions of small molecular fragments containing just these atoms, with only a few excursions into studies involving chlorine, hydrogen chloride, and hydrogen fluoride. A partial listing of the reactions that he and his coworkers studied includes most of the fundamental reactions of combustion and atmospheric chemistry:

- Recombination of hydrogen, oxygen, and nitrogen atoms;
- Combination of oxygen with nitrogen atoms;
- Reactions of hydrogen atoms with O_2 and HO_2—of oxygen atoms with O_2, NO, NO_2, O_3 and HO_2—of nitrogen atoms with NO—of electronically excited nitrogen atoms and molecules with O and O_2—of hydroxyl radicals with OH, HO_2, O_3, CH_4 and several Cl-substituted methanes—and of the charged species O_2^+, NO^+ and H_2O^+.

The primary goal of these studies was the rate constant, which is closely related to the probability that an encounter of the reagent molecules would lead to reaction. Kaufman consistently sought to achieve direct measurements, in which the concentrations of the reagent species were known from measurement rather than inferred from modeling calculations, and in which interfering secondary reactions were avoided or rendered unimportant. This required a constant search for new titration reactions to generate the radicals of interest. In addition, ultra-sensitive detection techniques were required, because in some cases secondary reactions could be controlled only by using extremely low radical concentrations. A particularly challenging example concerned the reaction of OH with HO_2, which is a major sink for HO_x species in the atmosphere and which engrossed the chemical kinetics community for much of the 1970s and 1980s. Both reagents are unstable radicals and susceptible to self-reaction and other competing reactions. Initial rate investigations were indirect and produced widely scattered values of the rate constant. In his first publication on this reaction, in 1978, Kaufman carefully discussed the criteria for successful modeling of the reaction system and was characteristically cautious about the validity of the derived rate constant. Three years later his laboratory established a much more direct route for the investigation of this important reaction.

Through the succession of reliable measurements from his laboratory and his outspoken criticism of less direct approaches to rate determination, Fred achieved a unique position within the chemical kinetics community. He represented the highest of standards and helped instill in his younger colleagues a similar spirit. He rapidly became involved in the debate concerning possible ozone depletion through artificial introduction of chemicals into the atmosphere. The relevant chemistry was believed at the time to be dominated by gas-phase reactions involving ozone and oxygen atoms with hydrogen-, nitrogen-, and halogen-containing molecules and radicals, and could be modeled by combining the results of investigations of individual elementary reactions with independent information on species abundances in the atmosphere and gas transport. Kaufman was one of the scientists called on to testify before congressional committees concerning the possible impact of supersonic transport engine exhaust gases on the ozone layer. Later he served on several panels, such as the National Academy of Sciences' Committee on Impacts of Stratospheric Change, which were particularly concerned with the long-term effects on the ozone layer of the release of chlorofluorocarbons. His contributions were recognized by the dedication of the massive 1985 atmospheric ozone report to his memory. His special role in the chemical kinetics community was likewise recognized with the posthumous award in 1987 of the Polanyi Medal by the gas kinetics group of the Royal Society of Chemistry.

Kaufman's role in the area of combustion chemistry was somewhat different. Because of the very large number of elementary reactions involved and the high temperatures of flames, the input rate data were less precise than in the atmospheric chemistry models. Kaufman served in part as a unique resource to the modeling community. His advice was invaluable in assessing the likely reliability of rate data, but he was also adamant in demanding proper sensitivity analysis and assessment of uncertainties in the conclusions drawn from the analysis of the data. Many were the times when his eagle eye caught a suspicious-looking rate constant in a speaker's presentation slide; there followed an incisive and pointed question. His purpose was never to belittle the author, but rather to instill the same critical approach to the analysis of data as he insisted on in his own laboratory.

Fred participated in the biennial symposia of the Combustion Institute for over two decades. He rose over the years to be a member of the executive committee, vice-president from 1978 to 1982, and president from 1982 until his death. He was the plenary lecturer at the 19th Symposium in 1982. Interestingly, in the 1980s his research turned again to fundamental kinetics problems in combustion chemistry, with a major study of the reaction of hydrogen atoms with oxygen molecules (which controls the second explosion limit of the hydrogen-oxygen reaction) and a survey of reactions of the methoxy radical, CH_3O.

Collaboration with his SRCC colleagues, especially Wade Fite and Fred Biondi, helped to spur his involvement in two related areas of reaction rate measurements, namely ion-molecule reactions and reactions of electronically excited species. In the first of these areas, his group undertook a major study of reactions of ions with water and of water ions, H_2O^+, with several neutral molecules. Equally important to understanding of the upper atmosphere were investigations of the rates and products of reactions of excited nitrogen atoms and nitrogen molecules, especially with oxygen atoms and molecules.

As mentioned already, one of Kaufman's innovations in these studies was the use of resonance radiation absorption to monitor the concentration of the reactive atom or radical. These applications were complemented by more fundamental measurements of the radiative transition probabilities for species such as hydrogen, nitrogen, and oxygen atoms and hydroxyl radicals. This work and the special nature of the SRCC led to one of the most unusual and interesting projects of his career. The catalyst was James Anderson, who came to Pitt as a postdoctoral associate of Tom

Donahue. Anderson's doctoral research involved use of resonance radiation to measure the hydroxyl radical in the atmosphere and he was intrigued by Kaufman's applications of the technique. From the resulting collaboration of Anderson, Donahue, and Kaufman was born the plan to measure by resonance absorption the oxygen and nitrogen atom densities in the upper atmosphere. The experiment, which also involved graduate student Terry Rawlins and Bob Hudson of the Goddard Space Flight Center, was implemented on the Apollo-Soyuz space mission of 1975, the light sources and detectors being mounted on Apollo and reflectors on Soyuz, both flying at an altitude of 225 kilometers. In the time-honored way of experiments, the first attempt, with a spacecraft separation of 150 meters, yielded no signal except for possible weak resonance fluorescence; however, on the following orbit with the craft now 500 meters apart, excellent absorption and fluorescence data were obtained.

How did Fred Kaufman conduct his research? From the late 1960s he rarely was active in the laboratory, but he was nevertheless in control of each project. He was always accessible to his group and would listen carefully to each student's tale of success or woe. He was invariably courteous but one sensed his irritation when the experiment failed to cooperate for whatever reason. He met at least once a week with his entire group and a lively discussion would inevitably ensue. This intense involvement in science extended outside the laboratory; whether at conferences, dining a visitor, or sitting hunched over the telephone, he always had the goal of a full understanding of the problem at hand. Under his tutelage, his students blossomed—some would take longer than others but usually he had the intense satisfaction of seeing yet another mature scientist leave the laboratory and move on to make his or her mark elsewhere, normally still in gas kinetics or related areas. Of his forty or so pre- and postdoctoral associates, some seven are currently in academic posts, nine involved in government research laboratories, and most of the remainder in other high-technology research positions.

Kaufman's immersion in chemistry made him sensitive to the major questions in the field. A significant portion of his research was devoted primarily to improving fundamental understanding of how reactions occur and how molecules gain and lose energy. If he could be said to have been fascinated by a single chemical species, that species was nitrogen dioxide; it reached center stage in 1958 with his eleventh publication and featured also in one of his last, in 1985.

Throughout his career he puzzled over the strong fluorescence from the lowest group of electronically excited state of NO_2. First, he established the mechanism of combination of oxygen atoms and nitric oxide into these states, discovering the intricate competition between radiation by these states and their collisional deactivation to lower energy, non-emitting states. Beginning in 1966 his group populated the same states by exciting nitrogen dioxide with visible light, later using the temporal development of the fluorescence to gain analogous information but in more detail. These were among the first investigations of the mysterious communication between quantum states, later known as IVR (intramolecular vibrational relaxation), and thus Kaufman helped set the scene for one of the major research fields of the 1980s. Ironically, although (with sulfur dioxide) among the first molecules to be studied in this way and although the subject of a vast number of investigations, nitrogen dioxide still conceals many of the secrets of the dynamical properties of these excited states.

Another area that Kaufman entered relatively late but exploited to bequeath future generations a fascinating array of still poorly understood data was that of infrared chemiluminescence of the products of chemical reactions. Initially set up to study infrared emission from nitrogen dioxide from reactions of nitric oxide with oxygen atoms and with ozone, this system was used to measure rates of vibrational relaxation of many vibrational states of hydrogen chloride and hydrogen fluoride and deuterated analogues in collision with various molecular species. In agreement with well-established theoretical models the probability per collision of relaxing the first excited level was quite small for most collisional partners. However, the probability was observed to increase with vibrational quantum number to near unity for most polyatomic relaxers. This unexpected behavior remains a challenge to theorists; there is a strong implication that IVR is efficient in the collision complex.

It is perhaps surprising that Kaufman did not extend his research to include theoretical calculations beyond minor incursions into transition-state theory and the bond energy-bond order model. He doubtless felt that it was his role to obtain the relevant mechanistic information experimentally and he gained much insight into particular reactions through ingenious use of isotopic substitution or careful searches for key reaction products. Although he referred in print to his nontheorist mind, he was keenly aware of the status of theory regarding thermal reaction rates. His graduate course on chemical kinetics was dominated by description and critical discussion of theories of bimolecular and unimolecular reactions. The phrase “critical discussion” perhaps expresses well his approach: just as we have seen that he expected experimentalists to defend their experimental approach and critically to assess the reliability of their conclusions, so he wished to apply the same standards to the work of theorists, in particular regarding the validity of conclusions drawn from theoretical calculations. This constituted an almost impossible demand on theorists and led to a slight prickliness in his relations with some in that community. However, in the late 1970s when his concern led him to organize a symposium around this subject, the response was overwhelming and the three-day event attracted a brilliant group of experimentalists and theorists. The symposium was titled: "Current Status of Kinetics of Elementary Gas Reactions: Predictive Power of Theory and Accuracy of Measurement." It also paid special attention to the compilation and critical evaluation of rate data. This unusual occasion, with its sharp focus on the general subject of thermal rate data, was clearly a great success, as measured by developments in the 1980s. Thus, in this area as in so many others the colossal influence of Fred Kaufman is felt, and it is appropriate to end this account with his introductory remarks in the *Journal of Physical Chemistry*,[1] which reported on this meeting. They are as valid fifteen years on as they were at the time.

> My reason for calling this meeting was the need to take stock of the present state of the field of elementary gas reaction kinetics: to assess the accuracy of measurement techniques; to discuss the compilation and evaluation of rate data; and, most importantly, to examine the predictive power of theory. The stock-taking was stimulated by recent advances in the direct experimental measurement of elementary atom or radical reaction kinetics and by the preoccupation of theorists with problems of detailed state-to-state dynamics at a time when the demand for rate constants, measured, calculated or guessed, is growing rapidly in such diverse fields as atmospheric chemistry, combustion, and pollution. For these reasons, the subject matter of the symposium was sharply focused on thermal reaction rates of neutral (electronic) ground-state species, not because state-to-state dynamics or excited state reactions or ion reactions are any less interesting, but because thermal reactions have recently been treated with much benign neglect. They did, after all, form the foundation of reaction rate theory in the 1920s and 1930s, yet have only recently become open to direct experimental measurement of good accuracy.
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> A large number of key questions ought once again to be asked and

their answers examined in the light of laboratory results. They include the following: validity and the limitations of transition state theory; potential energy surfaces, how to calculate them (ab initio versus semiempirical) and what detail is required (in a cost-benefit analysis sense); classical trajectory calculations; quantum corrections based on one-, two-, and three-dimensional theory; nonequilibrium effects in two-body reactions; energy transfer in dissociation/recombination reactions and its dependence on excitation energy, molecular complexity, and temperature; prediction of rate parameters over large temperature ranges for widely different molecular complexity or for series of reactants differing only in substituent effects; implication of energy disposal information for thermal rate constants; critical test cases presently available or to be developed for theory-experiment comparison.

The reader of this journal issue must decide which of these and other issues have been brought closer to successful resolution. My own brief appraisal would begin with the statement that the meeting seemed a useful and successful exercise, that it should probably be repeated in a few years, and possibly become a regularly scheduled event, albeit an infrequent one.

In assessing the present state of affairs in the three topical areas, it is probably fair to say that the greatest progress has been achieved in the first area under discussion, that of experimental measurements. Here the wide use of highly sensitive detection techniques (resonance fluorescence, laser induced fluorescence, laser magnetic resonance, molecular beam sampling mass spectrometry, etc.) and the wide range of atom or radical generation techniques (photolytic, discharge, thermal, chemical, etc.) has made it possible to make measurements on vastly more reaction systems than ever before, and to do so in a direct manner (i.e., without recourse to classical methods of fitting analytical data to proposed mechanisms). The major experimental methods, flash photolysis and discharge-flow for the low temperature range and shock tube for high temperatures, continue to dominate the scene. Other methods (e.g., very low pressure pyrolysis [VLPP]) are making major contributions, especially for bond fission reactions of large molecules. Hybrid techniques (e.g., discharge flow shock tube and extensions to high temperatures [high temperature fast flow reactor]) are successfully bridging the gap between the widely separated temperature regimes of earlier studies. The realistic appraisal of experimental error still leaves much to be desired and we are fortunate in having the fine review paper by Cvetanovic, Singleton, and Paraskevopoulos to help us put our house in order. Experimental rate measurements of elementary reactions have certainly “arrived” and their future looks very bright indeed, both in regard to improved accuracy and to wide applicability to reaction systems.

The second topical area, compilation and critical evaluation of rate data, suffers greatly from being underfunded. The papers devoted to this field and the ensuing discussion show the urgent need for increased support. This is due both to the proliferation of experimental studies and to increased “user” pressure, mainly for modeling calculations in atmospheric chemistry, combustion, or pollution studies. Rate data evaluation is a relatively small, inexpensive activity, but it is in great demand by many groups: by experimentalists to keep abreast with the field; by theorists to have reliable results to guide and check their calculations; and by modelers to provide them with input parameters for computer codes. It is clear, of course, that compilation and evaluation spans a wide spectrum and that different “customers” may have very different requirements. Yet the overall need for faster progress on all fronts (i.e., for greater funding support) seems well substantiated.

The third area, predictive power of theory, makes up almost two-thirds of the symposium and of the published papers. It is also the most difficult to assess in a broad, overall sense. There has been clear progress on all fronts. Ab initio, three-dimensional, fully quantum calculations of the dynamics of some simple systems ($H + H_2$), routine three-dimensional classical trajectory calculations on many systems, ab initio and semiempirical potential energy surfaces, testing of various approximate theories against exact calculations in the easily accessible one-dimensional format (mainly for A + BC reactions), development of improved statistical theories of dissociation-recombination reactions, and continued application of transition state theory, particularly in its thermochemical variant (Benson, Golden), with excellent success to a host of complicated systems. To my nontheorist mind, many major questions remain unsettled: How extrapolatable are one-dimensional concepts and findings to the real world? What is the present and near-future accuracy of ab initio potential energy surface calculations and what impact can they be expected to have on elementary reaction rate calculations? How many and what kind of scaling parameters are needed in the characterization of semiempirical surfaces for thermal rate constant calculations? How are quantum (tunneling) effects best approximated in complex reaction systems? How serious are the necessary overestimates of equilibrium (transition state) theory rate constants due to “recrossing” effects, due to non-uniqueness of the transition state, due to specificity of energy disposal? What is a conservative estimate of the predictive power of thermochemical kinetics? As good as a factor of 2 or 3 in the Arrhenius A factor? The list of questions could be lengthened almost indefinitely, but enough. There is clearly much more work to be done. What impresses me, however, is the general usefulness and resilience of simple transition state theory which, after early triumphs went into a lengthy eclipse only to re-emerge as a surprisingly accurate (and sometimes as the only) tool of the gas phase kineticist.

Lastly, the symposium did achieve its major goal: to bring experimentalists and theorists together and to show that the field of thermal elementary reaction kinetics is alive and well.

NOTE

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