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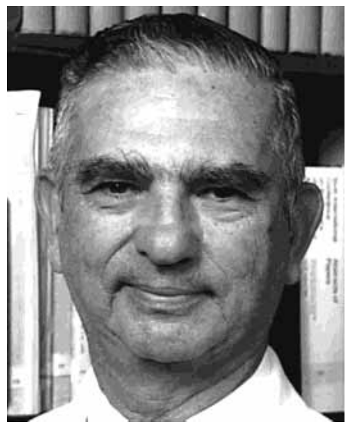

Tribute to Aron Kuppermann†

We and all of his colleagues who contributed to this special issue of *The Journal of Physical Chemistry A* are pleased to dedicate it to Aron Kuppermann on the occasion of his 75th birthday. Few scientists have had as significant an impact on both theoretical and experimental advances in a scientific discipline as Aron Kuppermann has had on the study of chemical dynamics. Over his career, Aron was first one of the leaders in bringing modern chemical physics to bear on the field of radiation chemistry, then he was an influential pioneer in the development and application of experimental electron impact spectroscopy; he has also has been one of the leaders in the development of theoretical approaches to the study of chemical reactions using accurate quantum mechanical techniques, and he was a major contributor to the application of variable angle photoelectron spectroscopy to a broad range of molecules. He has also contributed extensively to the study of intermolecular properties using crossed molecular beams. Aron has been at the forefront of the integration of high end computers into chemical research, and has been able to combine his interests in computation and chemistry to facilitate the completion of new science that would not have been possible with traditional computers and computing arrangements. Working at both the University of Illinois and the California Institute of Technology, Aron has contributed to the education of a whole generation of chemical physicists and he has worked to improve conditions for scientific research around the world, most notably in his native Brazil, and also in developing countries.

Briefly summarizing his many accomplishments is a challenging task. He helped develop some of the first exact methods for collinear atom−diatom reactions and helped to characterize the existence and properties of dynamical resonances in these systems. While applying the techniques he developed to an ever increasing family of triatomic chemical reactions, he led the development of techniques that extended the quantum mechanical treatment of reactions through coplanar and, finally, fully three-dimensional reactions. He helped develop and apply new methods, such as the quantum mechanical streamlines and collision-lifetime matrix analysis, that led to improved understanding and development for conceptual intuition about the details of the dynamics of the reactions. He also perceptively recognized the limitations of methods he helped develop, and worked to implement alternate approaches, such as the hyperspherical coordinate approach that facilitated the study of three-body dissociative reactions and the transfer of light atoms between heavier atoms. More recently, he pioneered more detailed studies of geometric phase effects in chemical reactions. Through all these efforts, he maintained a clear emphasis on exact treatments that have been used for many years as a benchmark for approximate studies carried out by other computational scientists as well as for experimental studies carried out in the laboratory.

His experimental studies reflect a strong emphasis on understanding the details of the dynamical processes involving molecular collisions with electrons, photons, and other molecules. The angular dependence of the products in these collisions became a focus of his studies, and this information

† Part of the special issue "Aron Kuppermann Festschrift".

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was used to provide insight into the nature of the interactions involved in these collisions. In particular, his group characterized the existence of excited triplet states for a large number of molecules using the angular dependence of the electronic products in electron impact spectroscopy before this information became available from laser techniques. Excited quartet states have also been examined. New instrumentation has further allowed the characterization of excited states in transient species in addition to the stable molecules that had been studied in the past.

In doing his work, Aron combined a chemist's intuition for the way that reactions take place, with a physicist's knowledge of quantum mechanics, an engineer's insight into how to construct and maintain complex instrumentation, and an applied mathematician's interest in efficient and accurate numerical approaches for computational work—both for the theoretical work and the analysis needed to interpret experimental observations. He has approached all his work with a high degree of intellectual rigor, and has taken great care to ensure that all the complexities and subtleties that nature provides in the form of quantum mechanics are carefully represented in his efforts. Aron is a tireless worker; members of his group can all recall his providing very detailed notes that he would write up for attacking problems of current interest, usually with the times he did that noted on them (frequently well into the middle of the night).

The recognition that the ability of chemical physicists to study reaction dynamics from first principles hinged on both the availability of computing and the development of appropriate numerical methods is something that came early to Aron (while at the University of Illinois), and he was always innovative in finding and using the needed computational resources. His arrangement to use the then-state-of-the-art IBM 360 computer at Ambassador College was a particular boon to the early three-dimensional reactive scattering studies. Indeed, it is not clear how the full range of "production runs" for the first 3-D H + H_2 studies could have been done affordably without this arrangement. Later on, Aron worked with his colleagues at Caltech to bring one of the first "superminicomputers" to campus (a VAX 11/780) as part of the Dreyfus-NSF Theoretical Chemistry Computing Center. More recently, he and members of his group have been among the most aggressive users of massively parallel machines at Caltech and elsewhere, and Aron has taken on leadership roles in the management of these systems.

It does a disservice to Aron to focus solely on his scientific contributions, numerous though they have been. Aron had the opportunity to mentor a large number of students, postdoctoral fellows, and undergraduate students over the years, and many of them have gone onto great success, not only in the field of chemical physics, but also in related areas ranging from law to medicine to business. The focus on intellectual rigor and attention to the basic principles involved in one's work became guiding principles for his many students, and they have brought that to their various chosen fields.

Aron also took great pains in the classes that he taught. His lectures were models of careful presentation; for example, students taking his scattering theory course could not only be sure that the complex algebraic manipulations were always accurately described as he wrote them on the blackboard, but that they would be accompanied by insightful explanations of the physics and chemistry behind them.

Aron provided his students with a high degree of autonomy in how they went about their work, and he also showed great trust in both their competence and their work ethic. This led not only to a high degree of enthusiasm among his students, but also to a strong sense of community among the members of his group. He respected the outside interests and family commitments of the members of his group. Aron's involvement in his own family (wife – Roza, and 4 children – Baruch, Nathan, Miriam, and Sharon), as well as in religious and community activities, sent a clear message to the members of his group about the importance of leading a balanced life. He helped bridge these very important aspects of his life in several ways, most notably through hosting group meetings at his house. Countless Kuppermann-group members recall with great fondness the warmth that he and Roza extended to them over the years—not just while working with Aron, but afterward as well. The pride that Aron took in both the personal and professional growth of his students is clearly evident.

Aron displays a sense of humor that may surprise people who see him only in a "scientific" way, but his close collaborators have all seen it. Although he takes his science very seriously, he does not take himself seriously. He has maintained an uncanny ability to laugh at himself over the years, even in the face of occasional pranks carried out by his students.

It is with great pleasure and with a sense of privilege for having been able to work with and learn from Aron as part of our own education that we dedicate this edition of *The Journal of Physical Chemistry A* to Prof. Aron Kuppermann.

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