

Sharon G. Lias: 1935–2004



Sharon Garrison Lias (January 16, 1935–November 30, 2004) made pioneering research contributions to ion chemistry, and also authored definitive evaluations of the thermochemistry of ions and of mass spectra. Her work led to the NIST Ion Energetics and NIST Mass Spectrometry Databases that are vital resources for researchers and for chemical analysis.

Sharon Lias obtained a B.S. in Chemistry from the College of William and Mary, Virginia, (1957), M.S. (1965), and Ph. D. (1972) in Physical Chemistry from the American University in Washington.

The scientific career of Dr. Lias was centered at the National Institute of Standards and Technology (previously National Bureau of Standards) in Gaithersburg, Maryland. She first joined NBS in 1954 as a summer student, was a member of the scientific staff from 1956 to 1995, and continued as Scientist Emeritus through 2001. Much of her 47-year career at NBS/NIST was shared with Dr. Pierre Ausloos, a collaboration that lasted through both of their careers. Her contributions were recognized by the U.S. Department of Commerce Silver Medal in 1978 and Gold Medal 1985. The work of Dr. Lias resulted in 116 articles, book chapters, edited books, and databases.

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Dr. Lias was a member of the American Society of Mass Spectrometry (ASMS) Board of Directors, 1995–1997; chair of the ASMS Committee on Standards and Measurements, 1995–1996; member of the Editorial Board of the series, “Molecular Structure and Energetics”, VCH Publishers, Inc.; member of the Executive Council of the Joint Committee on Atomic and Molecular Physical Data, and of the American Institute of Physics Subcommittee on Numerical Data Bases; member of the Advisory Committee for the Clearinghouse for Digital Infrared Spectra; and coeditor of “Structure/Reactivity and Thermochemistry of Ions”, D. Reidel Publishing Co.

Most of Sharon’s ion chemistry work used the low-pressure ion cyclotron resonance method. She also collaborated with Professor Frank H. Field, 1971–1973, at Rockefeller University in New York, using high-pressure mass spectrometry.

An early focus of Dr. Lias concerned the radiolysis of hydrocarbons. This interest led to studies of ion-molecule reactions, both in the condensed phase and gas phase, resulting in pioneering contributions to this field. The studies on hydrocarbon ions continued throughout Dr. Lias’ work and were also extended to halogenated hydrocarbons and other functionalized species.

These studies lead to results that are fundamental to ion chemistry in general. Her research concerned the

reaction rates and the attainment of equilibrium for a large variety of ion-molecule reactions. She greatly enhanced the versatility of the ion cyclotron resonance mass spectrometer by providing a capability for studying the temperature dependence of ion-molecule reaction rates and equilibria. She made the first systematic determinations of the entropy changes associated with ionic equilibria, and by a detailed accounting for the entropy factor, she verified her proposal that the intermolecular potentials contribute to charge transfer equilibria.

An early contribution to ion thermochemistry through equilibrium measurements was the determination of ionization potentials for some 40 organic compounds through charge transfer equilibrium constants, and an analysis of the relationship of these results to adiabatic ionization potentials. Because those were the first studies of the temperature dependence of ion-molecule equilibria carried out in a low-pressure mass spectrometer, Dr. Lias' results generated an unusual amount of interest among mass spectrometrists. Dr. Lias also worked on the determination and evaluation of proton affinities.

In kinetics, she contributed some of the first observations of slow ion-molecule reactions that are exothermic but nevertheless proceed orders of magnitude slower than the collision rate. This was an essential step toward the development of the now well established Brauman double-well model of ion-molecule kinetics. Another original contribution concerned the use of ion-molecule reactivities to differentiate between isomeric ions.

Other basic contributions related to the nature of reaction complexes, for example, the relations between binding energies and intracomplex reactions as reflected in isotope exchange, and the relations between structures of complexes and reactions into competing channels.

While Dr. Lias made basic research contributions, of equal significance was her dedication to ion energetics databases and other activities of general benefit to the field, including the organizing of conferences and editing books.

The database work of Dr. Lias included an early compilation of rate coefficients of hydrocarbon ion reactions (together with Dr. L. W. Sieck, 1976); the earliest compilation of proton affinity literature (with K. Hartman, P. Ausloos, H. M. Rosenstock, and S. S. Schroyer, 1976 and 1979); of ionization potential and appearance potentials (with R. D. Levin, 1982); gas-phase basicities and proton affinities (with J. F. Liebman and R. D. Levin, 1984, and with E. P. Hunter, 1998); positive and negative ion energetics (with S. E. Stein and J. E. Bartmess, 1993).

A major compilation is "Gas-Phase Ion and Neutral Thermochemistry" ("Giant Tables") (with J. E. Bartmess, J. F. Liebman, J. L. Holmes, R. D. Levin, W. G. Mallard. *J. Phys. Chem. Ref. Data* **1988**, *17*, 1–861) that received over 4000 citations. This further led to major

portions of the NIST Chemistry WebBook, (P. J. Linstrom and W. G. Mallard, Editors). Dr. Lias was a major originator of this database and contributed to it substantial compilations of ionization energies, ion energetics, proton affinities, and cluster ion binding energies. This compilation contains the gas phase ion energetics of 15,600 species, and is considered to be the authoritative source of ion thermochemistry data. These data are essential to the synthesis and characterization of chemicals, the modeling of flames, plasmas, and planetary atmospheres, as well as in laser design and pollutant identification.

Dr. Lias also made important contributions to the NIST Mass Spectrometry Database (with S. E. Stein and P. Ausloos), which is a major resource in analytical mass spectrometry.

In addition to her research and database activities, Dr. Lias had management positions at NIST that included: Director of the Ion Energetics Data Center, 1979; Ionizing Radiation and Aqueous Kinetics group leader, 1983; program manager for Physical Data, Standard Reference Data Program, 1986–1987; chief, Chemical Kinetics and Thermodynamics Division, 1988–1991. In these positions, Sharon is remembered for her competence as a manager and for her compassion for employees who needed help. Amongst these actions was her care for Dr. Henry Rosenstock, another NBS pioneer of ion chemistry.

Together with Dr. Pierre Ausloos, Sharon Lias was one of the pioneers of ion chemistry from its earliest years. Her selfless dedication to databases gave researchers in ion chemistry an invaluable resource. Her research results, and the repository of knowledge in the ion chemistry databases that Sharon Lias contributed to the ion chemistry community, will remain a lasting legacy of this valuable scientist and outstanding human being.

Selections from Dr. Lias' 116 publications:

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