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Department of Chemistry

Moscowitz Memorial Lectureship

9:45 a.m. Tuesday, October 11 • 331 Smith Hall

Professor

Marsha Lester

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Dynamical Outcomes of Quenching: Reflections on a Conical Intersection

Website: http://www.chem.upenn.edu/chem/research/faculty.php?id=25

Abstract

Hydroxyl radicals are important in combustion and atmospheric environments, where they are often detected by laser-induced fluorescence (LIF) on the $A^2\Sigma^+ - X^2\Pi$ band system. However, collision partners known to quench electronically excited OH $A^2\Sigma^+$ radicals are ubiquitous in these environments. Thus, great effort has been made to quantify the rates and/or cross sections for collisional quenching, so that its effects on LIF signals may be taken into account to allow an accurate determination of OH concentrations. Despite extensive kinetic measurements, fundamental questions remain regarding the fate of the collisionally quenched molecules and the ***mechanism*** by which these nonadiabatic processes occur. This presentation will overview fundamental chemical dynamics studies aimed at understanding the quenching of OH $A^2\Sigma^+$ by molecular partners (M = H_2, N_2, O_2, CO, CO_2). Recent experimental and theoretical studies reveal efficient quenching of OH $A^2\Sigma^+$ arising from strong nonadiabatic coupling in the vicinity of a conical intersection, resulting in nonreactive quenching that returns OH to its ground $X^2\Pi$ electronic state and reactive quenching that yields new products. The branching between these outcomes and the quantum state distributions of the products reflect the unique properties of the conical intersection region. Finally, a new UV+VUV photoionization scheme for sensitive detection of OH radicals, using readily available wavelengths and a well-characterized resonant transition, will be introduced that is expected to be widely applicable for molecular reaction dynamics.

The Moscowitz Memorial Lectureship in Chemistry was established by friends and colleagues of Professor Albert Moscowitz (1929-1996) to honor his many contributions to molecular spectroscopy. He was known for his research on the interpretation of optical rotation and circular dichroism spectra in terms of the structures of chiral molecules. In collaboration with colleagues in the medical sciences, he developed important applications of his methods to biomedical systems. Throughout his career, Moscowitz held numerous visiting professorships at other universities, and served on the editorial boards of the leading journals in chemical physics. His work was honored by election as Foreign Member of the Danish Royal Academy of Sciences and Letters, and as a Fellow of the American Physical Society.

Marsha I. Lester received her doctorate from Columbia University in 1981. She has risen through the academic ranks at the University of Pennsylvania, where she is currently the Edmund J. Kahn Distinguished Professor in the Department of Chemistry of the School of Arts & Sciences. She recently completed a four-year term as chair of the Department of Chemistry. Lester has received many honors and awards, including her election to Fellowship in the American Academy of Arts & Sciences, the Bourke Lectureship of the Faraday Division of the Royal Society of Chemistry, a John Simon Guggenheim Memorial Foundation Fellowship, Fellow of the American Association for the Advancement of Science, the American Chemical Society, and the American Physical Society, an Alfred P. Sloan Research Fellowship, and the Camille and Henry Dreyfus Teacher-Scholar Award. She has recently been appointed editor-in-chief of *The Journal of Chemical Physics*.

Research

Lester's research group has developed innovative methods for generating open-shell complexes between a free radical and a reactive partner, such as OH-H_2 and OH-CO, now known as entrance channel complexes, and for stabilizing intermediates; e.g., HOONO and HOOO, of key chemical reactions. Her group has employed novel spectroscopic methods, including pump-probe and double resonance techniques, to rigorously characterize important, yet previously uncharted, regions of chemical reaction pathways. Her pioneering experimental studies and closely coupled theoretical computations focus on reactions of the hydroxyl radical, the key initiator of oxidation chemistry in atmospheric and combustion environments.

Host: Associate Professor David Blank
Refreshments will be served prior to the seminar.