MAR09-2008-002289

Abstract for an Invited Paper
for the MAR09 Meeting of
the American Physical Society

Earle K. Plyler Prize Talk: Using High Resolution Electronic Spectroscopy to Probe Reactive Chemical Intermediates

TERRY MILLER, Ohio State University

Gas phase chemical reactions, such as occur in atmospheric chemistry, combustion, plasma processing, etc. are of great importance to our economy and society. These reactions are typically very complex involving up to 1000's of elementary steps with a corresponding number of reactive chemical intermediates. Spectrospic diagnostics, based upon well analyzed and well understood spectra of the intermediates, are crucial for monitoring such reactions and unraveling their mechanisms. These spectral analyses often benefit from the guidance provided by quantum chemical calculations and conversely the molecular parameters, experimentally determined from the spectra, serve as "gold standards" for benchmarking such calculations. Such standards are especially valuable for reactive intermediates whose electronic or geometric structure is particularly complex because of electron-spin interactions, Jahn-Teller effects or other vibronic interactions, hindered internal motions, large molecular size and weight, etc. The organic alkoxy, RO$\cdot$, and peroxy, $RO_2\cdot$, (R=alkyl group) free radicals are excellent examples of such species. The talk will focus on our recent characterization of these radicals via their "high-resolution," mostly rotationally resolved, electronic spectra utilizing the techniques of laser induced fluorescence, stimulated emission pumping, and cavity ringdown spectroscopy. Selected spectra, their analysis, and the molecular information resulting therefrom will be discussed.