World Academy of Science, Engineering and Technology
International Journal of Chemical and Molecular Engineering
Vol:18, No:04, 2024

Fuel Oxidation Reactions: Pathways and Reactive Intermediates Characterization via Synchrotron Photoionization Mass Spectrometry

Authors : Giovanni Meloni

Abstract : Recent results are presented from experiments carried out at the Advanced Light Source (ALS) at the Chemical Dynamics Beamline of Lawrence Berkeley National Laboratory using multiplexed synchrotron photoionization mass spectrometry. The reaction mixture and a buffer gas (He) are introduced through individually calibrated mass flow controllers into a quartz slow flow reactor held at constant pressure and temperature. The gaseous mixture effuses through a 650 µm pinhole into a 1.5 mm skimmer, forming a molecular beam that enters a differentially pumped ionizing chamber. The molecular beam is orthogonally intersected by a tunable synchrotron radiation produced by the ALS in the 8-11 eV energy range. Resultant ions are accelerated, collimated, and focused into an orthogonal time-of-flight mass spectrometer. Reaction species are identified by their mass-to-charge ratios and photoionization (PI) spectra. Comparison of experimental PI spectra with literature and/or simulated curves is routinely done to assure the identity of a given species. With the aid of electronic structure calculations, potential energy surface scans are performed, and Franck-Condon spectral simulations are obtained. Examples of these experiments are discussed, ranging from new intermediates characterization to reaction mechanisms elucidation and biofuels oxidation pathways identification.

Keywords : mass spectrometry, reaction intermediates, synchrotron photoionization, oxidation reactions
Conference Title : ICFRC 2024 : International Conference on Free Radical Chemistry
Conference Location : Boston, United States
Conference Dates : April 22-23, 2024