Measuring reactions of key intermediates in hydrocarbon oxidation

Craig A. Taatjes

Combustion Research Facility, Sandia National Laboratories, MS 9055, Livermore, CA 94551-0969, USA

The oxidation of hydrocarbons in combustion or other systems involves a complicated web of chemical transformations, passing through multiple unstable intermediates. Modeling the oxidation process requires understanding how these intermediates react. However it is unsettlingly common that critical intermediate species cannot be readily interrogated, and that the kinetics of key reactions must be inferred from indirect measurements. I will discuss recent combinations of experiment and theory that indirectly reach inside the "black box" of oxidation processes to probe the underlying mechanisms of important reactions, with particular emphasis on understanding the fundamental chemistry relevant to autoignition of traditional, non-traditional, and alternative fuels. Moreover I will highlight recent progress towards *direct* measurement of the kinetics of some elusive intermediates in combustion and tropospheric chemistry.

This work is supported by the Division of Chemical Sciences, Geosciences, and Biosciences, the Office of Basic Energy Sciences, and the U.S. Department of Energy, and by the Laboratory Directed Research and Development (LDRD) program at Sandia National Laboratories. Sandia is a multi-program laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the National Nuclear Security Administration under contract DE-AC04-94-AL85000.