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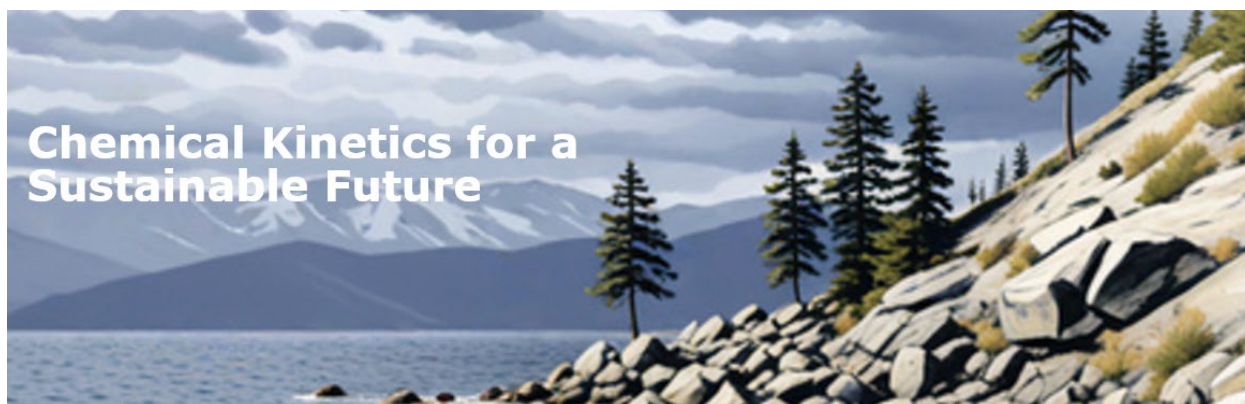
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Book of Abstracts

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Constraining the low-temperature oxidation mechanism of *n*-hexanol through the detection and identification of C₆ elusive intermediates

Y. Zhai^a, A. C. DeCecco^a, A. W. Jasper^b, N. Hansen^c, P. Dagaut^d, G. Villalobos^a, and D. M. Popolan-Vaida^a

^a Department of Chemistry, University of Central Florida, Orlando, FL 32816, USA
(Yitong.zhai@ucf.edu)

^b Chemical Sciences and Engineering Division, Argonne National Laboratory, Lemont, IL 60439, USA

^c Combustion Research Facility, Sandia National Laboratories, Livermore, CA 94551, USA

^d Centre National de la Recherche Scientifique (CNRS), ICARE, 1C Avenue de la Recherche Scientifique, 45071 Orléans Cedex 2, France

Alcohol-based fuels are currently considered viable energy carriers for the transportation sector. Consequently, a comprehensive mechanistic understanding of the low-temperature oxidation of alcohols is essential for application in advanced low-temperature compression engines. A multidimensional approach involving experimental investigations, kinetic modeling, and theoretical calculations was used to provide new insights into the low-temperature oxidation mechanism of a C₆ alcohol, *n*-hexanol (CH₃(CH₂)₅OH), through the detection and identification of elusive C₆ intermediates. The oxidation of *n*-hexanol was investigated in a jet-stirred reactor (JSR) under stoichiometric conditions ($\phi = 1.0$), an initial fuel concentration of 2%, a residence time of 2 s, a temperature range between 500 K - 660 K, and a pressure of 700 Torr. The reactants, intermediates, and final products were detected and identified by means of molecular-beam mass spectrometry coupled with single-photon ionization employing tunable synchrotron-generated vacuum ultraviolet radiation. Chemical kinetic simulations were performed using a previously published kinetic model (Togbé et al., *Energy Fuels* 11, 5859–5875, (2010)) to predict the reactivity of *n*-hexanol and elucidate the predominant formation pathways of the observed low-temperature species. Experimental photoionization efficiency curves in conjunction with *ab initio* calculations, enabled the identification of important low-temperature species, such as C₆ unsaturated alcohols, C₆ olefinic hydroperoxides, C₆ cyclic ethers, C₆ diones, and C₆ ketohydroperoxides. The results of this study provide valuable insight into the mechanism of low-temperature oxidation chemistry of *n*-hexanol, contributing to the development of kinetic models for the low-temperature oxidation of *n*-hexanol and other long-chain linear alcohols.