

Abstract Submitted  
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**Two-State Reactivity in Hydrocarbon Oxidation by FeO<sup>+</sup>: New Insight through Temperature Dependent Kinetics** SHAUN ARD, JOSH MELKO, NICK SHUMAN, ALBERT VIGGIANO, AFRL — Oxidative activation of C-H and C-C bonds is the rate limiting step in many catalytic applications. Transition metals and their oxides are the active component in numerous catalysts as they have proven to be efficient in the activation of these bonds. We report the temperature dependence of reaction kinetics from 120-700K for reactions of FeO<sup>+</sup> with CH<sub>4</sub>, C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>4</sub>, and C<sub>2</sub>H<sub>6</sub> for the first time, in an effort to improve the mechanistic understanding, and from that the efficiency of these important reactions. The rate constants were found to decrease smoothly with temperature for each hydrocarbon, except for that with methane which displayed an abrupt change in temperature dependence. The branching fractions for the alcohol producing channels were also found to decrease with temperature for each hydrocarbon, with the exception of ethane where it remained constant. Implications of these results towards catalytic applications and theoretical modeling of these systems will be discussed. Specifically, the role of spin orbit coupling in determining the probability of spin inversion, and thus the importance of the “two-state reactivity” model applied to many transition metal oxide and hydrocarbon reactions will be addressed.

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