Theoretical Investigation of the Hydrogen Abstractions from Furan and its Derivatives by HO_2 and OH Radicals

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The scarcity of fossil fuels in the transportation sector has motivated the interest in search of alternative energy resources. An important alternative is to use biomass derived fuels such as 2-methyltetrahydrofuran as they have a potential to significantly reduce pollutant emissions (1).

Our main objective is to develop detailed chemical kinetic models to predict the combustion behavior of Furan based biofuels in advanced engine such as HCCI. Presently in our group experiments have been performed to measure auto-ignition delay time over wide temperature and pressure range for Furans using shock tube and rapid compression machine. Predictive chemical kinetic models for auto-ignition are developed which demand high accuracy in rate parameters for H-abstraction reactions by OH and HO_2 radicals. The present work focuses on the computational investigation of H abstraction reactions from furans at MP2, G3MP2 and G3B3 level of theories for temperatures between 600-1500 K. Canonical variational transition state theory incorporating Wigner's, Eckart's symmetrical, Eckart's unsymmetrical and small-curvature tunneling corrections has been used in order to estimate accurate Arrhenius parameters for these abstraction reactions. Finally a detailed kinetic model is optimized considering these reactions and validated against experimental results.

References

(1) Andreas, J. J.; Florian, W. K.; Jan, H. B.; Martin, M.; Stefan, P.; Juergen K. *Energy Fuels* **2011**, 25, 4734–4744.