

Pyrolysis of Diethyl Ether: A Shock-Tube H-ARAS/TOF-MS and Modeling Study

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Diethyl ether can serve as a model compound to investigate safety-relevant issues of ignition processes e.g., at hot surfaces.¹ For an adequate modeling, the chemical mechanism and the corresponding kinetic data have to be known. A detailed pyrolysis and oxidation mechanism for diethyl ether was recently published by Yasunaga et al.²

In our poster contribution, we will report on shock-tube studies of the pyrolysis of diethyl ether in the temperature range 1200-1500 K at pressures of around 1 and 5 bar. We used hydrogen atom resonance absorption spectroscopy and time-of-flight mass spectrometry for species detection. Concentration-time profiles of H atoms, diethyl ether, acetaldehyde, formaldehyde, C₂H_n (*n* = 2, 4, 6), carbon monoxide, and methane were obtained and compared with simulation results from the pyrolysis/oxidation mechanism of ref. 2. A good agreement was found.

From the initial slopes of the measured H-atom concentration-time profiles, we were able to determine the overall rate coefficients of the two simple bond-fission reactions C₂H₅OC₂H₅ + M → C₂H₅O + C₂H₅ + M and C₂H₅OC₂H₅ + M → C₂H₅OCH₂ + CH₃ + M. To verify these data and to also account for the molecular elimination channel C₂H₅OC₂H₅ + M → C₂H₅OH + C₂H₄ + M, we also calculated temperature- and pressure-dependent rate coefficients by solving a thermal multichannel master equation on the basis of molecular data from high-level quantum chemical methods. The experimental and theoretical results of this work are in good agreement with the data used in ref. 2, which were estimated from the rate coefficients of the reverse reactions via detailed balancing or consideration of analogous reactions.

References

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- (2) Yasunaga, K.; Gillespie, F.; Simmie, J.M.; Curran, H.J.; Kuraguchi, J.; Hoshikawa, H.; Yamane, M.; Hidaka, Y. *J. Phys. Chem. A* **2010**, 114, 9098-9109.