International Conference on Numerical Combustion
Rome, Italy, October 14-17, 2025
www.icnc2025.com

Accurate Rate Coefficients for $\dot{N}H_2$ + n-Butanol Reactions: A Theoretical Basis for Ammonia–Alcohol Combustion Mechanisms

Zimu Wang[1]*, Yueying Liang[1], Liang Yu[1], Xingcai Lu[1]
*lead presenter: wangzimu@sjtu.edu.cn
1 Key Laboratory for Power Machinery and Engineering of M. O. E., Shanghai Jiao Tong University, Shanghai 200240, P.R. China

n-Butanol, a second-generation biofuel, is a promising reactive green additive for blending with ammonia in advanced combustion engines, with potential to mitigate greenhouse gas emissions. In ammonia-based fuel blends, H-atom abstraction reactions by $\dot{N}H_2$ radicals play a key role in the overall combustion kinetics. However, due to the lack of direct experimental and theoretical investigations, the rate constants for these reactions involving n-butanol have typically been estimated by analogy with lower chain alcohols or alkanes. In this study, the kinetics of H-atom abstraction reaction from n-butanol by $\dot{N}H_2$ radicals are systematically studied using high-level quantum chemical methods. Geometries and vibrational frequencies of all relevant species were obtained at the QCISD(T)/CBS//M06-2X/6-311++G(d,p) level, while single-point energies were computed using QCISD(T)/cc-pVDZ and QCISD(T)/cc-pVTZ levels with basis set extrapolation corrections via MP2/cc-pVDZ, MP2/cc-pVTZ, and MP2/cc-pVQZ methods. One-dimensional hindered rotor potentials were obtained with 10° increment at the M06-2X/cc-pVTZ level. High-pressure limit rate constants for all reaction channels were calculated using conventional transition state theory coupled with Master Equation System Solver (MESS) over the temperature range of 300-2000 K. The results provide reliable theoretical data for constructing detailed kinetic mechanism of the ammonia/n-butanol fuel system, supporting their application in engine simulations, emission reduction strategies, and sustainable fuel development.