RRKM/master equation calculations for some typical combustion reactions and the uncertainty analysis

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Rate constant parameters are important components of chemical kinetic mechanisms, which are required by numerical simulations of combustion. With the development of computational techniques including quantum chemistry methods and kinetic theories, rate constants from theoretical predictions, especially RRKM/master equation modeling, have been well accepted to build combustion kinetic models. Recently we have employed RRKM/master equation methods to compute the temperature and pressure-dependent rate coefficients with the high level potential energy surfaces for a series of C4 hydrocarbons including C_4H_7, C_4H_6 and C_4H_5, which will be reviewed here.

The uncertainties of rate constants are crucial to evaluate and minimize the uncertainty of modeling predictions. With the help of global uncertainty analysis, we are be able to explore the uncertainty of the rate constants predicted by RRKM/master equation calculations. Taking our computations on the C_4H_7 reaction system as a prototypical case, the uncertainty propagation behavior during the RRKM/master equation modeling will be discussed.