How accurately can we determine rate coefficients for elementary chemical steps?

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Typical reaction mechanisms for the combustion of organic fuels nowadays consist of several hundreds to several thousands of elementary chemical steps interconnecting a similar number of different species. Leaving aside the important question of sensitivity/uncertainty analysis of these complex mechanisms [1], we will review specific methods to obtain rate coefficients for elementary chemical steps in the gas phase for combustion-relevant conditions.

The accuracy of rate coefficients determined with different experimental setups like shock tubes and slow-flow reactors will be discussed in terms of examples from the literature and from our own work. Furthermore, we will examine the uncertainty of rate coefficients predicted from microscopic kinetic theories [2] on the basis of data from quantum chemical calculations [3]. Different types of reactions will be considered: unimolecular reactions, direct bimolecular reactions, and complex-forming bimolecular reactions. Finally, we will examine how the temperature and pressure ranges can be extended by extrapolations and how the quality of kinetic data can be improved from a combination of experiment and theory.

[1] A.S. Tomlin, T. Turányi, in: F. Battin-Leclerc, J.M. Simmie, E. Blurock (Eds.), *Cleaner Combustion: Developing Detailed Chemical Kinetic Models*, Springer, London, U.K., 2013, p. 411.
[2] M. Olzmann, in: F. Battin-Leclerc, J.M. Simmie, E. Blurock (Eds.), *Cleaner Combustion: Developing Detailed Chemical Kinetic Models*, Springer, London, U.K., 2013, p. 549.
[3] E. Goos, G. Lendvay, in: F. Battin-Leclerc, J.M. Simmie, E. Blurock (Eds.), *Cleaner Combustion: Developing Detailed Chemical Kinetic Models*, Springer, London, U.K., 2013, p. 515.