

# Molecular Modeling in Process Engineering

2023/2024

## Project 9

Determination of rate constants of abstraction reactions using transition state theory

Determine the rate constant for the following reactions in the forward and the backward direction using transition state theory in the temperature interval 300-2000 K. Report in an excel file the values of the partition functions, the energy barrier, and the parameters used to compute the partition functions (electronic degeneracy, symmetry numbers, inertia moments, masses, ...). Compare the calculated rate constants with literature values (see <https://kinetics.nist.gov>). Perform calculations using a 'reasonable' choice of density functional. Consider about using both gaussian and molpro.

Reaction 1:  $\text{CH}_4 + \text{H} \leftrightarrow \text{CH}_3 + \text{H}_2$

Reaction 2:  $\text{NH}_3 + \text{H} \leftrightarrow \text{NH}_2 + \text{H}_2$

Answer the following question:

How can quantum tunnelling contributions be accounted for?