Molecular Modeling in Process Engineering

2023/2024

Project 5

Estimation of the equilibrium constant from the molecular partition function

The purpose is to learn how to compute partition functions and an equilibrium constant from the data determined using electronic structure calculations.
It is requested to determine for all species involved in the reaction, in the 300-2000K temperature regime the following quantities:

- translational partition function
- vibrational partition function
- rotational partition function
- electronic partition function

And calculate the equilibrium constant of the following reaction:

CH4 $\leftrightarrow$ CH3 + H
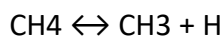
All the necessary data can be evaluated through optimization following by frequency calculation for each considered molecule. Useful equations, together with their derivation, are reported in chapter 4 of the ACK lecture notes, that you can find on BEEP. It is requested to perform all the calculations using an excel worksheet. (to validate the implemented equations through comparison with the data determined using quantum chemical calculations)