Molecular Modeling in Process Engineering

2023/2024

Project 4

Quantum Chemical based Calculation of partition functions and related quantities

The purpose is to learn how to compute partition functions and related properties from the data determined using electronic structure calculations.
It is requested to determine, in the 300-2000K temperature regime the following quantities:

- translational partition function
- vibrational partition function
- rotational partition function
- electronic partition function
- heat capacity
- entropy

for the following molecules:

CH4, C2H6, H2O, CO, NO2

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)