Molecular Modeling in Process Engineering

2023/2024

Project 10

1) Estimation of quantum tunneling partition function

The purpose is to compute the quantum tunneling for the reactions investigated in project 9.

- Download the folder "Eckart_cc_1.1.tar" from Webeep
- Upload the folder in your work directory and extract the content with the command untar -xvf name_archive.tar
- Follow the instructions in readme file
- Insert correct forward/backward energy barriers and imaginary frequency in input data
- Calculate quantum tunneling partition function

2) Calculation of ΔG solvation

It is required to estimate the ΔG solvation of the following ions:

HO_2^-, NH_2^-, CH_3O^-

Calculate the energy of different molecules in the solution and the gas phase using an appropriate level of theory and basis sets.
Determine the ΔG solvation and compare it with data reported in the literature.

3) Determination of pKa in aqueous solutions

Now that you are a master at calculating the ΔG solvation of small ions, try determining the pKa of the following acids:

formic acid, acetic acid and sulphuric acid

Each student must perform calculations for a single molecule. Don't all make the same molecule.
The definition and steps required to calculate pKa are in the literature article uploaded on webeep.
As usual, compare the value obtained with the available experimental data.