

## Exercise 7

In this exercise you are to study the interactions of acetic acid molecules in different environments. For this purpose you will need to run MD simulations of acetic acid in vacuum, aqueous solution and butanol solution. The files required for this exercise are to be found on the course homepage under the name Ex7.tar.gz.

In the file „AcOH.gro” the coordinates of a single acetic acid molecule are found. Using the `genbox` command (see below for details) you can generate a box with a given number of randomly placed acid molecules from this file (around 40 molecules for a 4x4x4 nm<sup>3</sup> box works well). From the such generated coordinates, you can also generate the coordinates of the solutions in a second step using the `genbox` command. You might need to perform an energy minimisation on the generated coordinates in order to remove bad contacts – this can be done with the file „em.mdp”.

In order to run the simulation you need to adapt the file „acidbox.top” by adding the number of acetic acid and butanol molecules contained in the system to be simulated at the end of the file (in case of water this should be added automatically by `genbox` if the topology file is given in the input). The „run0.mdp” file needs to be completed with information about temperature and pressure control. Choose whether and which you want to use and add the corresponding information at the end of the file (see Exercise 5; using a barostat for the solvent-free simulation is, however, not recommendable)! Remember to document all choices you make for the assistant!

## Questions

1. Inspect the obtained trajectories. What kind of complexes are formed between molecules of acetic acid?
2. Calculate the equilibrium constant for the hydrogen bond formation between two molecules of acetic acid in the three different environments!
3. How is the equilibrium constant related to the free energy (which free energy function is the appropriate one to use for your modelled systems)? What values for the change in free energy do you obtain from your equilibrium constants? Do these values seem reasonable?

4. Simple force fields as the one used in this exercise do not cover chemical reactions. Which reaction would be relevant in the systems modelled in this exercise? Give an estimate as to how much this may affect the results.

## Code details

For production of a box containing 40 acetic acid molecules:

```
genbox -nmol 40 -ci AcOH.gro -o acidbox.gro -p acidbox.top -box 4  
4 4
```

For solvation of the box containing acetic acid (this should work as it is for water; for butanol add „butbox\_288.gro” after the -cs option):

```
genbox -cp acidbox.gro -cs -p acidbox.top -o solvatedbox.gro
```