TKJ4205/KJ8902 Molecular Modelling
Exam 15.12.2011, 09.00-13.00

Norges Teknisk-Naturvitenskapelige Universitet (NTNU)
Code A: All printed and hand-written texts are allowed. All calculators are allowed.
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NB: The tasks are not weighted equally. The weight for each task is given in parenthesis after the task number. The weights sum up to 100. The expected length of the answer on each subtask is around 1/2 page with a normal style of hand-writing, which indicates the expected level of detailness of each answer.

Exercise 1 (15,15)

a) Describe the general features of the Hartree-Fock model in quantum chemistry (without mathematical derivations). How is it built up and what are the approximations?

b) How is electron correlation defined, and what is our physical interpretation of electron correlation? How is electron correlation included in molecular orbital and density-functional theory calculations, respectively?

Exercise 2 (15)

The solvation effect on a molecule can be calculated by a "full quantum chemical calculation" by including the solute and all the solvent molecules on the same level of theory. Discuss three solvation models where the solvent is treated with a more simple model. What are the main features of each model, their respective advantages and disadvantages as compared to a "full quantum chemical model"?

Exercise 3 (15)

What do we mean by liquid structure (e.g. compared to gases and solids)? How is it calculated in molecular simulations?

Exercise 4 (10,10,10,10)

Your fellow student comes around and asks you about some problems he/she has. You realize that molecular modelling would be useful and you vigorously offer to do some calculations. Which strategy would you suggest in the following cases:

a) To predict the positions of the peaks in a UV/VIS spectrum of a coloured liquid.

b) To calculate the diffusion constant of small molecules (e.g. CO_2) in a porous medium (e.g. a zeolite).

c) To calculate which is the most stable conformation in a small organic molecule (10-20 atoms) and in a macromolecule (e.g. a biopolymer with thousands of atoms), respectively.

d) To suggest which molecule in a series of ligands ($L_1, \ldots, L_{30}$) that is most efficient in inhibiting an enzyme.