

Graduate School IUAP V-03

FUNDP
June 12 2006

S KENMERK
UW KENMERK
LEUVEN

Lecture

Dr. NADEZHDA MARKOVA

Bulgarian Academy of Sciences, Sofia

**Theoretical investigations on tautomeric equilibria
in organic molecules taking into account the
specific solvent effects**

The tautomeric equilibria of formamide, its chalcogen analogues (thioformamide and selenoformamide), 2-aminothiazolidine-4-on, 4-aminothiazolidine-2-on and 5-fluorouracil were studied in the gas phase and in water solution using post-Hartree-Fock ab initio quantum chemical calculations. The values of proton transfer barriers in the isolated, mono- and polyhydrated tautomers of studied compounds were calculated for two different mechanisms of tautomerisation. In the absence of water, the process of proton transfer should not occur. Addition of water molecules decreases the barrier making the process faster, as the participation of two water molecules in a proton transfer reaction is more favourable than the participation of only one water molecule. The solvent effects were considered by explicit inclusion of three (four) water molecules, which model a first hydration shell around the solute. To estimate the effect of the medium (water) on the relative stabilities of the tautomers of the studied compounds we applied the polarizable continuum model. The basis set and electron correlation effects on the energy barriers of tautomerization and the energy differences between tautomers were analyzed.

When and where:

Monday June 12 2006 at 11:00
FUNDP, Rue Grafé 2, B-5000 Namur
Faculty of Sciences,
Chemistry & Physics buildings
3rd floor, room 313