CFEL SCIENCE

SEMINAR

16h May 2024 - 10:00 h

CFEL – Building 99, seminar room IV (first floor)

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Roskilde University

Hydrogen Bonding. An important physico-chemical parameter

The talk will concentrate on intramolecular hydrogen bonding and primarily on liquid state phenomena but a comparison is made to solid state phenomena. The primary experimental technique will be NMR and in this context deuterium isotope effects on chemical shifts. This will be complemented by DFT calculations. Resonance assisted hydrogen bonding is discussed in terms of bond lengths and deuterium isotope effects on ^{13}C chemical shifts and use of nuclear quadrupolar coupling constants wil be mentioned.

Tautomeric equilibria of intramolecular hydrogen bonded sysstems are investigated using low temperature NMR to obtain thremodynamic parameters. Liquid and solid state data are compared.

The talk will briefly touch upon calculationns of Infra Red NH sretching frequencies.

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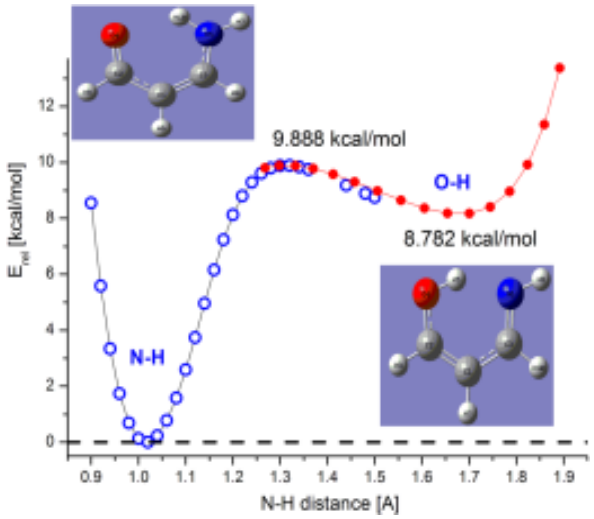

Host: Melanie Schnell / CFEL Molecular and Ultrafast Science Seminar