

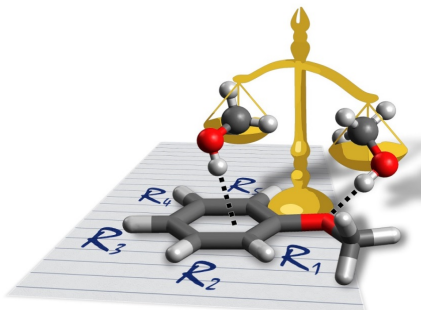
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 Building 99, Seminar Room I+II (EG)

Martin A. Suhm

Georg-August-Universität Göttingen

Low Temperature Molecular Docking Balances from an Infrared Spectroscopy Perspective

Extended molecules can be solvated at various inequivalent sites and it is useful to learn from experiment on a kJ/mol accuracy scale which solvent docking site is energetically more attractive. Theoretical relative energy predictions are rather easy to make and could thus be rigorously benchmarked by such experimental ratings of docking sites. However, experimental comparison of solvent-solute pair binding energies is not trivial, because it requires low temperature for complex stabilization but still sufficiently high mobility for equilibration. For the class of simple aromatic ethers solvated by methanol, the docking competition is very subtle [1] and we were able to tune it by chemical substitution, switching at will between classical OH-O and more diffuse OH- π docking preferences [2]. This new docking balance experiment profits from linear infrared absorption spectroscopy in supersonic jets [3] and allows for a fairly rigorous test of state-of-the-art quantum chemical predictions for relative hydrogen bond energies. The popular M06-2X density functional is shown to fail quite badly.



[1] M. Heger, J. Altnöder, A. Poblitzki, and M. A. Suhm, To π or not to π – how does methanol dock onto anisole? *Phys. Chem. Chem. Phys.* 17 (2015) 13045-13052

[2] H. C. Gottschalk, J. Altnöder, M. Heger, M. A. Suhm, Control over the hydrogen bond docking site in anisole by ring methylation, *Angew. Chem. Int. Ed.* 55 (2016) 1921-1924

[3] M. A. Suhm, F. Kollipost, Femtosecond single-mole infrared spectroscopy of molecular clusters, *Phys. Chem. Chem. Phys.* 15 (2013) 10702-10721