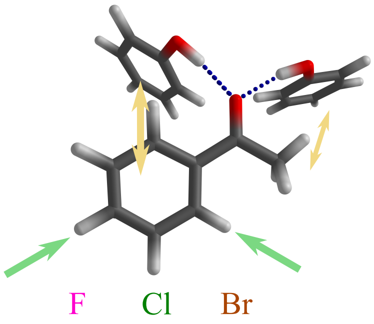
INVESTIGATING SUBSTITUENT EFFECTS IN DISPERSION-CONTROLLED ACETOPHENONE-PHENOL BALANCES

C. ZIMMERMANN, MARTIN A. SUHM, *Institute of Physical Chemistry, Georg-August-Universität Göttingen, Göttingen, Germany*.

The carbonyl oxygen of the asymmetrically substituted ketone acetophenone exhibits two hydrogen bond docking sites, where in combination with a phenol molecule two competing isomers can be formed. The two conformers can be probed experimentally by analyzing the differences in the OH-stretching frequency via FTIR spectroscopy in a supersonic jet and determining their abundance ratio at low temperatures. [a] This allows for the experimental benchmarking of theoretically predicted relative conformational energies on a kJ mol^{-1} or even finer scale. [bc] By halogenating the second or fourth position in the phenyl-ring of the acetophenone molecule with fluorine, chlorine or bromine, six closely related systems are formed, allowing to probe the influence of substituent effects on the favored docking site in addition to the London dispersion attraction and steric hindrances.



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[a] C. Zimmermann et al., *Phys. Chem. Chem. Phys.*, **2020**, *22*, 2870.

[b] H. C. Gottschalk et al., *J. Chem. Phys.*, **2018**, *148*, 014301.

[c] A. Poblotzki et al., *J. Phys. Chem. Lett.*, **2017**, *8*, 5656.