Quantification of dispersion interactions with the help of thermochemistry: substituted benzophenones

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Dispersion is the superordinate concept for attractive forces which act between separated molecules or molecular fragments even in the absence of charges or permanent electric moments. These interactions are generally responsible for the thermodynamic stability and the structuring of the solid and the liquid state. Dispersion forces between molecules are much weaker than the covalent bonds within molecules. Due to this reason, it is not easy to give a quantitative interpretation of dispersion, because the size of the attraction varies considerably with the size of interacting molecules and their shape.

In this project we want to increase the understanding and to quantify the dispersion forces in large molecular systems by means of experimental thermodynamic methods (calorimetry: DSC, combustion, solution, as well as with thermogravimetry, vapour pressure determination with combined Quartz Crystal Microbalance Langmuir method, Knudsen method, transpiration technique, static method); high level *ab initio* methods as well as correlation approaches between energetic properties and the structure of the molecules.

In the focus of this study are substituted benzophenones, where attractive forces between π–π orbitals of benzene rings could stabilize energetics of the molecule. The combination of experimental methods for determination of the interaction in the condensed phase with theoretical methods allows quantifying dispersion interactions in the condensed phase and, this way, to start building the bridge between gaseous and condensed phase for better quantitative description of them. That is extremely important due to the fact that the vast majority of chemical and biological processes take place in the liquid phase or in solution.

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