QUANTIFICATION OF DISPERSION INTERACTIONS BY USING THERMOCHEMICAL METHODS

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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 lecture we show our understanding of dispersion forces in large molecular systems and quantify them using experimental thermodynamic methods. Experimental methods: combustion calorimetry, differential scanning calorimetry, solution calorimetry, as well as with thermogravimetry and vapour pressure determination using Quartz Crystal Microbalance method, Knudsen method, transpiration technique, and static method). Theoretical methods: 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 aromatic hydrocarbons, where attractive forces between $\pi-\pi$ orbitals of benzene rings could stabilize energetics of the molecule. Moreover, dispersion forces are analyzed in homologous series of the molecular and ionic compounds. The combination of experimental methods for determination of the interaction in the condensed phase with theoretical methods allows for quantification of dispersion interactions in the condensed phase and in gas-phase.

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