# Abstract

The aim of this thesis is to investigate strength and origin of the stabilization for various types of noncovalent interactions. As this knowledge could lead to a deeper understanding and rationalization of the binding phenomena. Further, to participate on the development of new noncovalent data sets, which are nowadays inevitable in the process of parametrization and validation of new computational methods.

In all the studies, different binding motifs of model complexes, which represent usually crystal structures, structures from unrelaxed scans or the local minima, were investigated. The calculations of the reference stabilization energies were carried out at *ab initio* level (e.g. CCSD(T)/CBS, QCISD(T)/CBS). Further, the accuracy of more approximate methods (e.g. MP2.5, DFT-D or SQM methods) toward reference method, was tested. In order to obtain the nature of the stabilization the DFT-SAPT decomposition was frequently utilized.

In the first part of the thesis, the importance and basic characteristics of different types of noncovalent interactions (e.g. halogen bond, hydrogen bond, $\pi\cdots\pi$ interaction *etc.*), are discussed. The second part provides the description of computational methods which were essential for our investigation. The third part of the thesis provides an overview for part of our research during my PhD studies, relevant to the topic of the thesis.