Abstract
The thesis is focused on quantum-chemistry investigation of non-covalent: hydrogen bonded complexes of phenylacetylene with various molecules: water, ammonia, methanol, methylamine, borane trimethylamine. Mainly explain methyl induced switching of the binding motif. First chapter describes properties of the phenylacetylene molecule, mainly its multifunctionality according to present binding motifs in different complexes. Chapter number two treats the experimental background of the thesis, cite used spectroscopic methods. Interpretation of experimentaly observed spectra is also presented. Third chapter shows metodology used to find local minimas at potential energy surface. Transition from interaction energy to Gibbs free energy is also presented. Chapter also include proper describtion of some of the computational methods for example: DFT-SAPT. Last chapter presents results and interprets connection between theory and experiment, which leads to better understanding of observed phenomena.