Abstract
The topic of the diploma thesis is calculations with single-reference and Brillouin-Wigner multireference coupled clusters methods. In the beginning, the brief overview of the theory of selected quantum chemical methods with emphasis on the theory of coupled clusters (single reference as well as multireference) is presented.

Third chapter deals with calculations of the lowest lying singlet and triplet states of boron nitride molecule (BN). The lowest singlet state ($^1\Sigma^+$) exhibits multireference character and this molecule is thus a suitable candidate for testing of newly developed computational methods. Vibrational frequencies, anharmonicities and singlet-triplet energy splitting were calculated with different variants of multireference Brillouin-Wigner coupled clusters method (MR BWCC). The results were compared with experimental values and the results of single-reference and reduced multireference coupled clusters.

The fourth and fifth chapters present the study of a series of seven small fused cyclopentanes of the formula C_5H_{2n} (n = 0 - 4) [1]. The existence of local minima of all seven structures was verified at the CCSD(T)/cc-pVTZ level. Their stability was predicted according to enthalpies of formation and strain energies. ^{1}H and ^{13}C NMR spectra (chemical shifts), IR and Raman spectra were calculated at the CCSD(T)/cc-pVTZ level. Also the isomerization of one of them – tricyclopentane to 1,3-diene, which goes through biradical transition state, was studied. The results of reaction and activation enthalpies and vertical singlet-triplet splitting of the transition state were compared with the results of previous theoretical studies.

Keywords: *Ab initio* calculations, single-reference and multireference coupled clusters, boron nitride, polycyclopentanes

References
[1] Veis L.; Čársky P.; Pittner J.; Michl J. *Collect. Czech. Chem. Commun.* **2008**, 73, 1525-1551