Title: Theory and application of optical spectroscopic methods for structural molecular studies

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Abstract:
In the thesis, methods of the chiroptical spectroscopy (Raman optical activity, electronic and vibrational circular dichroism, circularly polarized luminescence) were utilized to obtain information on structure of chiral molecules. In four main projects, we focused on improving accuracy of quantum-chemical computations used for interpretation of experimental spectra by including anharmonic effects, solvent, molecular flexibility and dynamics. In the first project, the normal mode geometry optimization method was investigated and a suitable frequency limit providing realistic vibrational band broadening was found. Then the ability of harmonic and anharmonic computational approaches to describe the C-H stretching vibrations was explored for three terpene molecules and four spectroscopic methods. In the third project, we estimated the role of dispersion forces and different organic solvents for conformer equilibria and dynamics of cyclic dipeptides containing tryptophan. In the last project, circularly polarized luminiscence spectra, which were sensitive to the position of histidine in the peptide chain, could be rationalized by free energies obtained from molecular dynamics simulations.

Keywords: chiroptical spectroscopy, Raman optical activity, quantum-chemical calculations, conformational flexibility, anharmonic corrections