Title: Theory and Applications of Optical Activity of Biomolecules

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Abstract:

This thesis describes how we used several chiroptical spectroscopic methods to study chiral molecules: vibrational circular dichroism (VCD), circularly polarized luminescence (CPL) and magnetic circular dichroism (MCD). VCD and induced lanthanide CPL were used to study the structure of amyloid protein fibrils. We found out that VCD is very sensitive to their structure and supramolecular chirality. It could be used to distinguish between various polymorphic fibrils. On the other hand, induced lanthanide CPL provided information on the local structure. VCD was also used to study the hydration polymorphism of nucleoside crystals. Due to the crystal packing, the VCD signal was strong and specific for different types of crystals. Finally, electronic structure of hydrated Ln^{3+} ions was studied by MCD. Molecular dynamics simulations together with crystal field theory (CFT) and multistate complete active space calculations with second order perturbation correction (MS-CASPT2) were used to interpret the spectra. CFT provided better electronic transition energies, while MS-CASPT2 method gave better spectral shapes.

Keywords: optical activity, chiroptical spectroscopy, vibrational circular dichroism, circularly polarized luminescence, lanthanides, amyloid fibrils, proteins, magnetic circular dichroism, quantum-chemical calculations