The bachelor thesis deals with the study of the chiral molecule 3-aminoquinuclidine (AQN), which is an important pharmacophore. The derivates of this molecule form a basis for several biologically important molecules and drugs: serotonin receptors activity modulators, agents displaying neuronal activity and medicaments supressing side effects of chemotherapy administration (antiemetics). AQN is a chiral molecule and information on its absolute configuration and enantiomeric purity is crucial to the use of AQN in drug synthesis. AQN contains both primary and tertiary amine group and depending on pH value it can be found in three differently charged forms. This thesis presents characterization of AQN utilizing methods of vibrational spectroscopy – infrared absorption and Raman scattering, together with their variants – vibrational circular dichroism (VCD) and Raman optical activity (ROA), all these in combination with quantum chemical simulations. The attention was paid to a choice of the suitable solvents and settings of experimental conditions. Based on pH dependent Raman spectral series we determined pK_A dissociation constants associated with transitions between AQN´s protonated states, which were further characterized by ROA and VCD. The properties of AQN in various phases (aqueous solution, crystalline and glass phase) were also investigated. The quantum chemical simulations were focused on interpretation of experimental data, i.e. vibrational analysis of AQN spectra in aqueous solution, and study of effects of molecular flexibility and solvent model on the quality of the simulated spectra profiles.