

Abstract

The main target of this bachelor's thesis is the preparation and characterization of novel compounds with expected non-linear optical properties. Starting material for the preparation of new salts was 2,4-diamino-1,3,5-triazine. These salts or co-crystals were prepared by the crystallization with selected inorganic and organic acids. The methods of infrared and Raman spectroscopy along with X-ray diffraction methods were used to characterize the prepared materials. Moreover, the NLO potential of selected molecules was proven by quantum – chemical calculations. These calculations were also used for the interpretation of the vibrational spectra. Finally, the structures with non-centrosymmetric assembly were examined for the second harmonic generation efficiency in powdered samples.

Keywords: non-linear optics, 2,4-diamino-1,3,5-triazine, vibrational spectroscopy, structural analysis