

**Abstract**

The main issue of this master thesis is investigation of new compounds of aminopyrazine and 3-amino-1,2,4-triazine in consideration of their potential usage in the field of nonlinear optics. The focus of this thesis was finishing of characterisation of an adduct of aminopyrazine and boric acid prepared as a part of previous bachelor thesis, as well as preparation of salts and cocrystals combining 3-amino-1,2,4-triazine with selected acids.

Prepared materials were characterised mainly by the means of vibrational spectroscopy and x-ray diffraction analysis. Prediction of nonlinear optical properties of selected molecules and interpretation of recorded vibrational spectra was based on quantum chemical calculations. Finally, measurements of second harmonic generation efficiency of selected powder samples were performed.