

The main issue of this bachelor thesis is investigation of new compounds of 2-aminopyrimidine and aminopyrazine in consideration of their potential usage in the field of nonlinear optics. The focus of this thesis was preparation of salts and cocrystals combining 2-aminopyrimidine or aminopyrazine with boric acid and other 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.