

Title: Molecular crystals for NLO applications – compounds of 1*H*-pyrazole-carboxamide

Author: Bc. Soňa Kohúteková

Department: Department of Inorganic Chemistry

Supervisor: prof. RNDr. Ivan Němec, Ph.D.

Abstract: The aim of this diploma thesis is preparation and characterisation of novel compounds of 1*H*-pyrazole-carboxamide in consideration of their potential application in the field of nonlinear optics. This thesis is focused on preparation of crystalline salts or adducts combining 1*H*-pyrazole-carboxamide with selected inorganic and organic acids. Prepared materials were characterised mainly by the means of vibrational spectroscopy and X-ray diffraction analysis. Quantum-chemical calculations were used for a prediction of nonlinear optical properties as well as for interpretation of measured vibrational spectra. Four different approaches of calculations were used for an optimisation of computing time together with accuracy of the fit of calculated and measured spectra. Finally, measurements of second harmonic generation efficiency of two powder samples with non-centrosymmetric crystal structures were performed.

Key words: NLO, vibrational spectroscopy, crystal structure, quantum-chemical calculations