

Title: Novel Molecular Materials for Optics - Synthesis and Characterization of 5-aminotetrazole Salts

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Abstract: Nonlinear optics is currently an important field for the development of areas such as laser physics or telecommunications, and its understanding is essential for development of new technologies. Its development can also be aided by the investigation of various crystalline materials, such as salts containing cations and anions derived from polarizable organic molecules, exhibiting essential properties for nonlinear optics. This bachelor thesis is focused on preparation of crystalline forms of these compounds. These are salts of simple, nitrogen-rich bases with 5-aminotetrazole. Bigunidium 5-aminotetrazolate, guanidinium 5-aminotetrazolate and aminoguanidium 5-aminotetrazolate were prepared and further characterized. The structures of the latter salts were solved from X-ray diffraction data. The methods of spectral vibrational analysis supplemented with nuclear magnetic resonance and powder diffraction were applied to these prepared compounds. This thesis presents further findings for the continued research of aminotetrazole salts and for variants with other cations, which have similar properties.

Keywords: nonlinear optics; crystal structure; vibrational spectroscopy