Vibrational spectroscopic aspects of thermal effects observed in the family of aminopyrimidium salts

Irena Matulková¹, Ivan Němec¹, Ivana Císařová¹, and Přemysl Vaněk²

¹ Department of Inorganic Chemistry, Faculty of Science, Charles University, Hlavova 2030/8, 128 40 Prague 2, Czech Republic, e-mail: ivan.nemec@natur.cuni.cz
² Department of Dielectric, Institute of Physics ASCR, v.v.i., Na Slovance 2, 182 21 Prague 8, Czech Republic

The most of physical properties (including the optical properties) of crystalline materials are intimately related to the symmetry of their crystal structures, and the eventual phase transitions are frequently accompanied by the changes of their physical properties. In addition to the “classical” phase transitions (i.e., first order transitions, second order and/or lambda transitions), other rarely observed effects, such as glass transitions and isostructural phase transitions [1], can occur in the family of molecular crystals based on aminopyrimidinium salts. Very interesting phenomenon of isostructural phase transitions is generally characterized by the discontinuity of the changes of the unit cell parameters and atomic coordinates connected with a temperature decrease or increase [2, 3].

This contribution deals with the detailed explanation of the thermal effects observed for several compounds belonging to the family of aminopyrimidinium salts (studied as a prospective molecular materials for nonlinear optics) by the combination of the vibrational spectroscopic (IR and Raman – see Fig. 1.), X-ray diffraction and calorimetric methods. Particular attention will be focused on the explanation of the temperature behaviour of diamino- and triaminopyrimidinium phosphates and dicarboxylates.

Fig. 1. Temperature dependent Raman spectra of triaminopyrimidinium hydrogen malonate.

Keywords: Vibrational Spectroscopy; Crystal Structure; Phase Transition

Acknowledgment

Financial support from the CUCAM project (project No. CZ.02.1.01/0.0/0.0/15_003/0000417) is gratefully acknowledged.

References