The effect of the alicyclic amine dynamics on physicochemical properties of their organic-inorganic hybrids

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The aim of the presented dissertation was the synthesis, single crystal growth and physicochemical characterization of the crystals from the group of the organic-inorganic hybrids containing organic cations in their crystal structure. The cations exhibit the conformational equilibria in the solid state. In the realization of the work the cations of organic alicyclic amines with a seven-, six- and five-membered ring were used. These organic cations reveal a dynamic equilibrium between two or more conformations. Such a dynamical conformation equilibrium can be an origin of the interesting electrical and optical properties.

Achieving these objectives require the elaboration of the synthesis and single crystal growth. Subsequently, the organic-inorganic hybrid crystals obtained have been characterized by the X-ray methods to determine their crystal structures. Moreover, the application of complementary methods, sensitive to the dynamics of molecules or fragments of these molecules, allowed us to observe the macroscopic effects associated with the change of the cationic conformation, on cooling/heating the samples (dielectric spectroscopy, ^{1}H NMR in solid state, infrared (IR) and Raman spectroscopies and measurements of the alternating (*ac*) and direct current (*dc*) conductivity. The methods applied to detect phase transformations in the solid state (TGA/DTA and DSC) as well as optical methods, like UV-Vis spectroscopy and Second Harmonics Generation (SHG) have been also used.

In this work 16 organic-inorganic hybrids were synthesized, of which 11 were obtained and characterized for the first time in the literature. In the group of the hybrids obtained, the five compounds exhibit structural instability. Based on the research results, the molecular and structural mechanisms of the phase transitions of these hybrids were proposed. Some of the crystals characterized exhibit the semiconductor properties. Moreover, seven (7) compounds have optically non-linear properties, which have been confirmed by the second harmonic generation (SHG) experiments. The combination of such semiconductor and optical properties creates an opportunity to apply the described hybrids for example in photovoltaics or optoelectronics.