Phase Transition and Charge Density Study of the m-carboxy-phenyl ammonium phosphite

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Hybrid materials resulting from the association of amino acids with phosphorous acid have a great importance in industry (frequency doubling; can be used as infrared detector and pyroelectric devices). The structure determination, thermal behaviour and the charge density of a new hybrid material of this family (m-carboxy phenyl ammonium monohydrogenphosphite $C_7H_8NO_2^+$, $H_2PO_3^-$ (m-CPAMP) at low and high temperature phases (LTP) and (HTP) respectively will be presented and discussed**.** this study will improve the understanding of the phase transition mechanism

Crystals of m-CPAMP, space group $P2_1/c$, grown from aqueous solution undergo a reversible phase transition as evidenced by the behaviour of the unit-cell parameters versus temperature and by DSC measurements at about T_c = 246 ±2 K. The reported phase transition appears to be first order type according to the thermal hysteresis, 3.6 K, and the observed abrupt jumps of the unit-cell parameters.

Using accurate X-ray single crystal investigations between 100 and 320 K**,** we were able to describe the transition by the rotation of both cations and anions by *ca* 4.6° around the crystallographic b axis induced by their translation along the b direction**.** We also will show how the precise description of the electron charge density and its topology modelled from high resolution X-ray diffraction helps in the description of the phase transition.

Keywords: hybrid materials, phase transitions, charge density