Temperature dependent structural studies of incommensurately modulated Rb_2ZnCl_4

S. R. Kotla[1], A. M. Schaller[1], T. Rekis[1], S. Ramakrishnan[1], J. Bao[1], L. Noohinejad[2], S. van Smaalen[1], G. de Laitre[3], M. de Boissieu[3]

[1]Laboratory of Crystallography, University of Bayreuth, 95447 Bayreuth, Germany,
[2]DESY, Notkestrasse 85, 22607 Hamburg, Germany,
[3]Univ. Grenoble Alpes, CNRS, Grenoble INP, BP 75, 38402 Saint Martin d'Hères Cedex, France.

smash@uni-bayreuth.de

Rubidium tetrachloro zincate (Rb_2ZnCl_4) belongs to A_2BX_4 crystal family with the β-K_2SO_4 structure type [1], which are known for their ferroelectric properties and successive phase transitions. Rb_2ZnCl_4 has an orthorhombic crystal structure with *Pmcn* as its space group in its normal phase and goes from a normal disordered structure to incommensurately modulated structure along its *c*-axis at 303 K, then goes to a commensurately modulated structure around 192 K (T_c) [2]. Here we report the temperature dependent crystal structure of Rb_2ZnCl_4 in an attempt to elucidate the relation between structure and physical properties of this compound.

In the incommensurate phase the modulation wave vector is given by $q = (1/3 - \delta)\ c^*$, where δ is the parameter which changes with temperature, it decreases with decrease in temperature and finally becomes zero at the lock-in phase transition temperature T_c [3]. In Rb_2ZnCl_4 the modulation wave function changes from a sinusoidal harmonic function just below the incommensurate phase transition (303K) to a strongly anharmonic function near the lock-in phase transition at T_c. The modulation function in the incommensurate phase of Rb_2ZnCl_4 is not only given by displacive modulation but also modulations of atomic displacement parameters (ADPs) and anharmonic ADPs [4-5]. The structural analysis together with the lattice dynamics studies help us to understand the relation between aperiodic order and physical properties.

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