Temperature dependent structural studies of incommensurately modulated Rb$_2$ZnCl$_4$

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Rubidium tetrachloro zinicate (Rb$_2$ZnCl$_4$) belongs to A$_2$BX$_4$ crystal family with the β-K$_2$SO$_4$ structure type [1], which are known for their ferroelectric properties and successive phase transitions. Rb$_2$ZnCl$_4$ 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$_2$ZnCl$_4$ 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 $\delta$ 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$_2$ZnCl$_4$ 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$_2$ZnCl$_4$ 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.


**Keywords:** Aperiodic crystals; Incommensurate structures; modulation wavefunction; lock-in transition; single crystal XRD

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