MS21-2-1 Incommensurately modulated Rb_2ZnCl_4
#MS21-2-1

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Abstract
Rubidium zinc chloride (Rb_2ZnCl_4) is isostructural to β-K_2SO_4 and shows ferroelectric behaviour below 192K [1]. It belongs to A_2BX_4 crystal family and exhibits successive phase transitions which are characteristic of this family. At high temperature it has an orthorhombic structure with Pmcn as its space group with some disorder associated with $ZnCl_4$ tetrahedra, then an incommensurate modulation develops along c-axis at 303K with the wavevector q = (1/3 – δ) c*, where 'δ' is the parameter which shows the incommensurability and it decreases with decreasing temperature. At around Tc = 192K, 'δ' becomes zero and thus Rb_2ZnCl_4 goes from an incommensurately modulated structure to a commensurately modulated structure [2]. Finally, Rb_2ZnCl_4 undergoes an additional phase transition around 75K [3] with a probable monoclinic distortion and additional satellites in a*b* plane. In the incommensurate phase the modulation wave function goes from a harmonic sinusoidal function to a highly anharmonic function as it approaches lock-in phase transition at Tc. The modulation function in the incommensurate phase of Rb_2ZnCl_4 is not only given by displacive modulation but also by the modulations of atomic displacement parameters (ADPs) and anharmonic ADPs [4-5]. In the low temperature phase (T<75K), the additional modulation arises in the ab plane with the wavevector q = 0.5a*+0.5b*. The detailed structural analysis in each phase, especially near the lock-in transition along with the lattice dynamics studies help us to understand the relation between aperiodic order and physical properties.

References
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