Structure and Phase Transition of $[(CH_2OH)_3CNH_3]_2SiF_6$

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Single crystals of $(TRIS)_2SiF_6$ were grown and characterised by X-ray analysis, differential scanning calorimetry (DSC) and optical investigations. They were bond to be trigonal, space group $P\bar{3}$, with the unit cell dimensions $a = 7.699(1)$, $c = 7.818(2)$ Å. The SiF_6^{2-} anions, located in large cavities formed by hydrogen bonded cations, are strongly disordered at room temperature. The DSC measurements revealed a first-order phase transition at $T_C \approx 177$ K with a hysteresis of 4 K. The nature of the transition was confirmed by a sharp increase of the linear birefringence below T_C. Optical observations under a polarizing microscope showed a domain structure of the low temperature phase, characteristic of ferroelastic materials.

Key words: Phase Transition; X-ray Crystal Structure; Birefringence Domain Structure.