Structural Phase Transitions and Hydrogen bonding in $Rb_3H(SO_4)_2$

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Compounds of the type $A_3H(XO_4)_2$, where A = Li^+, Na^+, K^+, Rb^+, Cs^+, $(NH_4)^+$ and X = S, Se are known ferroelectric and paraelectric materials. Recently, structural phase transition in $(NH_4)_3H(SO_4)_2$ have been studied in detail [1]. We have investigated the phase transition in the analogous $Rb_3H(SO_4)_2$, the structure of which at room temperature was determined by Fortier *et al.*[2]. in 1985, at four different temperatures to follow the phase transition behavior. The data were collected on a Bruker Smart Apex CCD system equipped with an Oxford cryostat at 293K, 100K, 393K and 425K respectively. The hydrogen atom is localized at the midpoint at 100K with respect to the sulfate tetrahedra while at room temperature it is connected with one of the oxygen atoms. DSC studies on a single crystal of the compound indicate phase transitions around 399K and 425K. The crystal structures of $Rb_3H(SO_4)_2$ at four different temperatures show subtle conformational and packing changes and the geometry around the Rb atoms shows different coordination with respect to temperature.

[1] Dominiak P. M., Herold J., Kolodziejski W., Woz´niak K.,I*norganic Chemistry*, 2003, **42**, 1590. [2] Fortier S., Fraser M.E., Heyding R.D., *Acta Cryst*., 1985, **C41,** 1139.

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