Temperature induced structural phase transition in hydrated minerals $\text{Na}_6\text{M}({\text{SO}_4})_4(M=\text{Co, Ni})$

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Minerals, in particular bimetallic sulfates, are important multifunctional materials which show properties like fast-ion conductor, ferroelectric and magnetism with variation in temperature.$^1$ $^2$ $^3$ These properties are generally associated with structural phase transition and hence provide a pathway for the design of futuristic materials from easily available rich mineral sources. Several new futuristic materials have been synthesized based on mineral structures. In this context, hydrated vanthoffite mineral, $\text{Na}_6\text{Ni}({\text{SO}_4})_4.2\text{H}_2\text{O}$ (DHNANI) and $\text{Na}_6\text{Ni}({\text{SO}_4})_4.4\text{H}_2\text{O}$ (THNANI), $\text{Na}_6\text{Co}({\text{SO}_4})_4.2\text{H}_2\text{O}$ (DHNACO) and $\text{Na}_6\text{Co}({\text{SO}_4})_4.4\text{H}_2\text{O}$ (THNACO) are targeted in the present work. Their thermal property followed by phase transition have been investigated. DHNANI and THNANI crystallize concomitantly having space group $\text{P-1}$ ($Z=1$) with different cell parameter so as DHNACO and THNACO and are isostructural to DHNANI and THNANI respectively. These crystals on heating above $200^\circ\text{C}$ loose the water molecule and the anhydrous phase has a space group $\text{P2}_1/\text{c}$ ($Z=2$). The structure analyses indicate the presence of channels for $\text{Na}^+$ ions to migrate leading to the generation of solid electrolyte.


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