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Structural Evolution of Na6Mn(SO4)4 from High-Pressure Synchrotron Powder X-ray Diffraction

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Abstract : Compounds with the Vanthoffite crystal structure having general formula $Na6M(SO_4)_4$ (M= Mg, Mn, Ni , Co, Fe, Cu and Zn) display a variety of intriguing physical properties intimately related to their structural arrangements. The compound Na6Mn(SO4)4 shows antiferromagnetic ordering at low temperature where the in-plane Mn-O•••O-Mn interactions facilitates antiferromagnetic ordering via a super-exchange interaction between the Mn atoms through the oxygen atoms . The inter-atomic bond distances and angles can easily be tuned by applying external pressure and can be probed using high resolution X-ray diffraction. Moreover, because the magnetic interaction among the Mn atoms are super-exchange type via Mn-O•••O-Mn path, the variation of the Mn-O•••O-Mn dihedral angle and Mn-O bond distances under high pressure inevitably affects the magnetic properties. Therefore, it is evident that high pressure studies on the magnetically ordered materials would shed light on the interplay between their structural properties and magnetic ordering. This will indeed confirm the role of buckling of the Mn-O polyhedral in understanding the origin of anti-ferromagnetism. In this context, we carried out the pressure dependent X-ray diffraction measurement in a diamond anvil cell (DAC) up to a maximum pressure of 17 GPa to study the phase transition and determine equation of state from the volume compression data. Upon increasing the pressure, we didn't observe any new diffraction peaks or sudden discontinuity in the pressure dependences of the d values up to the maximum achieved pressure of ~17 GPa. However, it is noticed that beyond 12 GPa the a and b lattice parameters become identical while there is a discontinuity in the β value around the same pressure. This indicates a subtle transition to a pseudo-monoclinic phase. Using the third order Birch-Murnaghan equation of state (EOS) to fit the volume compression data for the entire range, we found the bulk modulus (B0) to be 44 GPa. If we consider the subtle transition at 12 GPa, we tried to fit another equation state for the volume beyond 12 GPa using the second order Birch-Murnaghan EOS. This gives a bulk modulus of ~ 34 GPa for this phase.

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