Hydrothermal Synthesis and Characterization of Sodium Manganese Oxo-Phosphate $Na_2Mn_2O(PO_4)_2{\cdot}H_2O$, a Novel Octahedral-Tetrahedral Open Structure Network

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Beamline(s): **X7B**

Introduction: Transition-metal-containing zeolite-like materials are of academic and practical interests because of the integration of molecular sieving characteristics of zeolites and redox chemistry of transition metals.

Methods and Materials: Sodium manganese oxo-phosphate, $Na_2Mn_2O(PO_4)_2{\cdot}H_2O$ (OTMS-1) is obtained from a mixed solution of Mn^{2+}, MnO_4^- and PO_4^{3-} by hydrothermal methods. The structure of OTMS-1 is resolved from single crystal diffraction data collected at NSLS beam line X7B with an 80 X 15 X 15 μm crystal.

Results: The OTMS-1 space group was determined to be P2(1)/m. All manganese ions have an elongated octahedral environment. As shown in **Figure 1**, each MnO_6 octahedron shares two edges with two other MnO_6 octahedra to form a zigzag chain. The zigzag chains are connected by PO_4 tetrahedra to form 2-dimensional planes, between which sodium ions are located. Water molecules reside in the one-dimensional microporous voids surrounded by the 2-dimensional planes and sodium ions (**Figure 2**).

Conclusions: Novel synthetic approaches have been developed to prepare OTMS-1, a new Octahedral-Tetrahedral Molecular Sieve. There exists a unique feature of zigzag edge-sharing MnO_6 chains in the OTMS-1 structure. There are also microporous one-dimensional voids in the framework. OTMS-1 and its derivatives may find catalytic applications in partial oxidation reactions.

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References: R.C. Haushalter *et al*, J. Solid State Chem. **108**, 128 (1994), J Escobal *et al*, J. Mater. Chem. **9**, 2691 (1999), M.A.G. Aranda *et al*, Angew. Chem. Int. Ed. Engl. **31**, 1090 (1992),

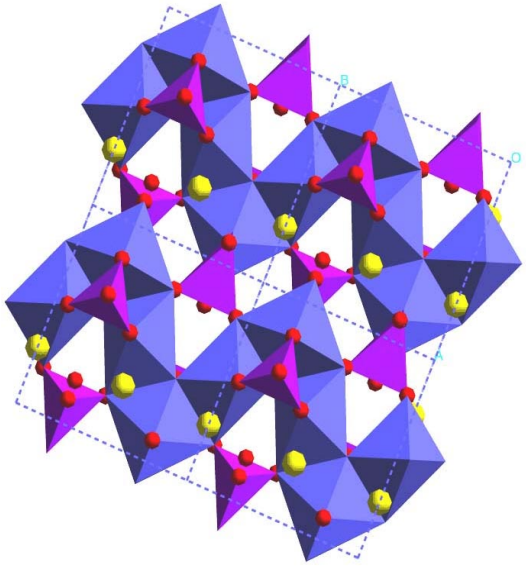

Figure 1. MnO_6 octahedra (blue) form zigzag chain bridged by PO_4 polyhedra(purple)

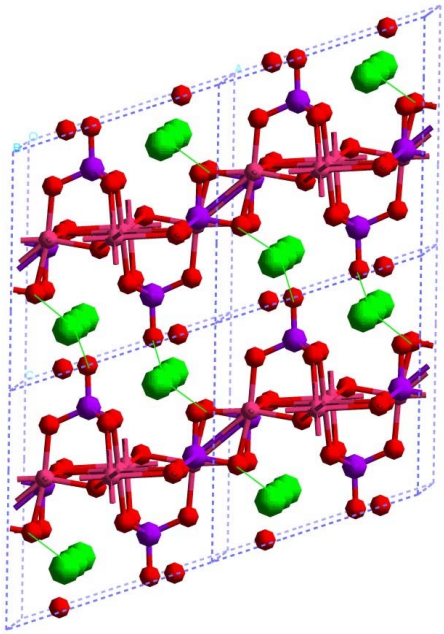

Figure 2. Channels formed from MnO_6 sheets and Na cation bridges contain water molecules. figure, delete this box