

Trirutiles as potential multiferroics: the case of Mn₂TeO₆

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The trirutile structure (A₂BO₆) is a superstructure of the standard rutile unit cell, involving a (2:1) ordering of A³⁺ and B⁶⁺, with *P4₂/mnm*. Compounds with A magnetic ions, such as Fe, Cr, V, and B non-magnetic ions, such as Te or W, were reported as potential multiferroics candidates [1]. Within this inverse trirutile system, Mn₂TeO₆ was first reported by Hund [2] and Fruchart et al. [3]. The fact that the structure of Mn₂TeO₆ was not determined precisely in these earlier works motivated us to revisit its crystal and magnetic structures, along with its physical properties. To this end, synchrotron powder X-ray (MSPD@ALBA, Spain), neutron powder (WISH@ISIS, UK and G4.1@LLB, France), TEM studied were performed.

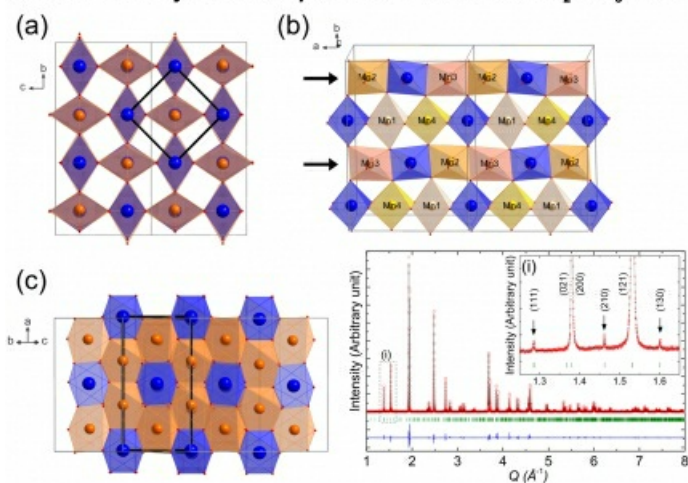
Like other inverse trirutile compounds, the high-temperature (from 700 to 420°C) crystal structure of Mn₂TeO₆ is tetragonal. Below 420°C, however, the phase transforms to a monoclinic phase (*P12₁/c1*) is with a doubling along *b*-axis (*a* = 9.103 Å, *b* = 13.05 Å, *c* = 6.466 Å, β = 90.03°.). It is evidenced by the superlattice reflections on the electron diffraction and synchrotron powder diffraction at room temperature. The refinement of the room temperature structure from synchrotron powder diffraction was carried out with an approach based on symmetry-adapted modes: the structural distortion is seen as a superposition onto the parent structure of symmetry breaking atomic displacements modes. Amongst the 7 basis modes that could be taken into account to describe the transition from tetragonal to monoclinic supercell, a single one, the Σ₃ representation, is found to be of predominant amplitude and is also sufficient to get a satisfactory refinement. The structure of Mn₂TeO₆ can be understood therefore as a distorted inverse trirutile structure: with respect to the parent tetragonal one, the Mn/Te (2:1) lines of edge-sharing octahedra running along *a* are now slightly puckered (Figure 1 (b), the lines indicate by black arrows.). This distortion is attributed to cooperative Jahn-Teller effects of Mn³⁺, which lead to both elongated (Mn(1) and Mn(3)) and compressed (Mn(2) and Mn(4)) octahedra.

[1] Horneich, R. M. (1969). *Solid State Commun*, **7**, 1081–1085.

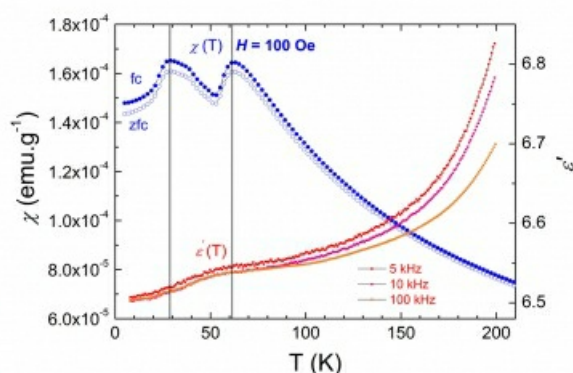
[2] Hund, F. (1971). *Naturwissenschaften*, **58**, 323.

[3] Fruchart, D. et al., (1980). *J. Phys. Fr*, **41**, 141–147.

Structure and synchrotron powder diffraction of Mn₂TeO₆ at RT



Magnetic susceptibility & dielectric constant



Keywords: [inverse trirutile](#), [symmetry-adapted structure refinement](#), [magneto-electric coupling](#)