MS14-P2 The crystal structure of a davidite related ternary oxide $La_{1.78}Mn_{6.6}Ti_{13.62}O_{38}$

Amalija Golobič[1], Maja Vidmar[1], Srečo D. Škapin[2], Danilo Suvorov[2], Anton Meden[1]

1. University of Ljubljana, Faculty of Chemistry and Chemical Technology, Večna pot 113, 1000 Ljubljana, Slovenia
2. Jožef Stefan Institute, Jamova 39, 1000 Ljubljana, Slovenia

email: amalija.golobic@fkkt.uni-lj.si

The title compound is a new ternary oxide in the La_2O_3–Mn_2O_3–TiO_2 pseudo-ternary system. It was synthesized by wet precipitation technique using manganese (III) oxide and lanthanum nitrate diluted in citric acid and the water solution of titanium (IV) isopropoxide. The product was calcined at 750°C in air and sintered at 1100°C for 20 h. After the heat treatment, the sample was cooled by quenching to room temperature. The formula of the obtained single phase product is $La_{1.78}Mn_{6.6}Ti_{13.62}O_{38}$ which is in accordance to the synthetic ratio of metals and supported by scanning electron microscopy (SEM) using wavelength-dispersive (WDS) and energy-dispersive spectroscopy (EDS). The compound is isostructural with naturally occurring crichtonite group minerals, which crystallize in trigonal system in *R*–3 space group. It conforms to the general formulae $AM_{21}O_{38}$, where *A* is occupied by a large cation: Ca, Sr, xRb, K, Na and rare-earth elements – RE. The minerals with RE on A site are called davidites.

The X-ray powder diffraction pattern was collected on a PANalytical X'Pert PRO MPD diffractometer in reflection geometry using $CuK_{\alpha 1}$ in range from 10° to 120° 2θ. Crystal structure was determined using Rietveld method incorporated in TOPAS-Academic program taking a structure of $Ca_2Zn_4Ti_{16}O_{38}$ [1] as a starting model. The Ca^{2+} on cuboctahedral site *A*, surrounded by 12 O^{2-} anions, is replaced by La^{3+}. The Ca^{2+} on octahedral *M*(1) site is replaced by La^{3+} and Mn^{2+} (La/Mn)2. Mn^{2+} is additionally disposed over tetrahedral site *M*(2) (instead of Zn^{2+}, Mn3), while the rest of Mn^{2+} is sharing the octahedral *M*(3) site with Mn^{3+} and Ti^{4+} (Ti/Mn)1. Sites M(4) and M(5) are fully occupied by Ti^{4+} (Ti2, Ti3). Sites A and M(1) lie on 3-fold rotoinversion axis, M(2) lies on 3-fold axis, M(3), M(4) and M(5) lie on general positions. a=9.28107(7) Å, α=68.4560(5)°, V=666.237(15) Å^3, 34 structural and 9 profile parameters, R_p = 2.82, R_{wp}=3.56, R_p = 16.80, R_{wp}=12.75.

[1] Gatehouse, B. & Grey, I.. *J. Solid State Chem.* **46,** 151–155 (1983).

Financial support of the Ministry of Education, Science and Sport of the Republic of Slovenia is gratefully acknowledged (grants P1-0175, P2-0091, MR-33158).

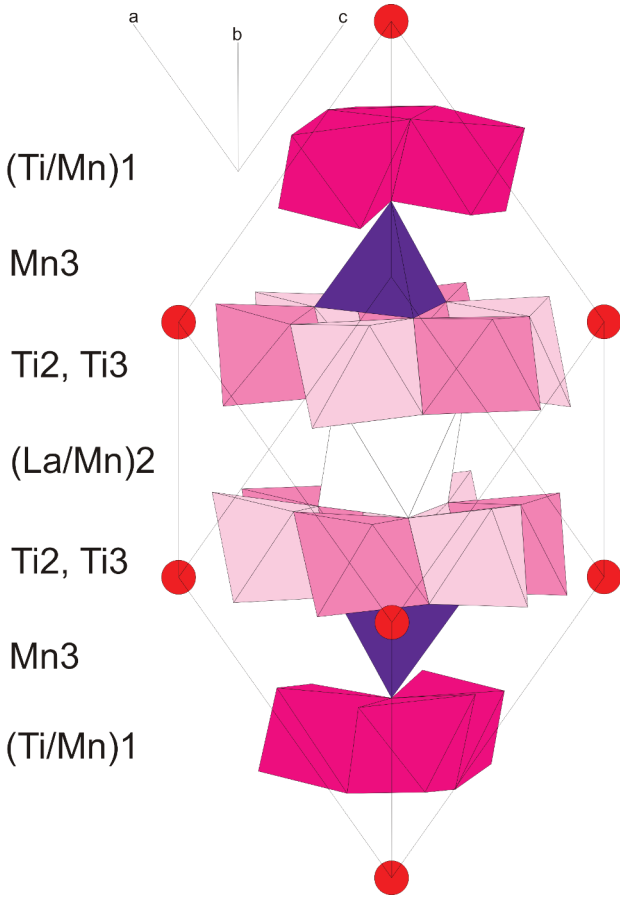

Figure 1. Unit cell of title compound extended to complete polyhedra.

Keywords: powder diffraction, ternary oxide, ceramics, davidite, Rietveld refinement,