

# $\text{Ca}_2(\text{Mn,Ti})\text{O}_4$ , a potentially new mineral with the Ruddlesden-Popper structure

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A potentially new mineral  $\text{Ca}_2(\text{Mn,Ti})\text{O}_4$ , was found within the xenolith sample from the Bellerberg volcano in Germany. It is an accessory phase in partially altered xenolith composed mainly of cuspidine, fluorapatite, and gehlenite. It forms flat plate dark-brown crystals up to 100  $\mu\text{m}$  in size. The empirical formula, established by electron microprobe analyses, is  $(\text{Ca}_{1.98}\text{Ce}_{0.06})_{\Sigma 2.04}(\text{Mn}^{4+}_{0.36}\text{Ti}_{0.35}\text{Fe}^{3+}_{0.19}\text{Al}_{0.09})_{\Sigma 0.99}\text{O}_4$ .

This mineral exhibits a Ruddlesden-Popper type structure characteristic for perovskite-like layered oxides of general formula  $A_{n+1}M_n\text{O}_{3n+1}$ , where  $A$  is typically an alkaline or rare earth ion, and  $M$  is a transition or post-transition metal ion (Ruddlesden and Popper, 1957). The diffraction pattern of the analysed crystal reveals a tetragonal lattice with unit cell parameters  $a = 3.7666(2)$  Å,  $c = 11.9861(8)$  Å, and volume  $V = 170.050(17)$  Å<sup>3</sup>. The  $A$  site was refined with  $\text{Ca}^{2+}$  and  $\text{Ce}^{3+}$  scattering factors, whereas for the  $M$  site, a mixed scattering curve was used (0.55 Mn/Fe + 0.36 Ti + 0.09 Al) according to the chemical analyses. The final structure refinement converged to  $R = 2.74\%$ . The crystal structure of  $\text{Ca}_2(\text{Mn,Ti})\text{O}_4$  exhibits a modular nature and consists of  $\text{Ca}(\text{Mn,Ti})\text{O}_3$  perovskite layers, which are packed between  $\text{CaO}$  rock-salt layers arranged along the  $c$ -axis (Fig. 1).

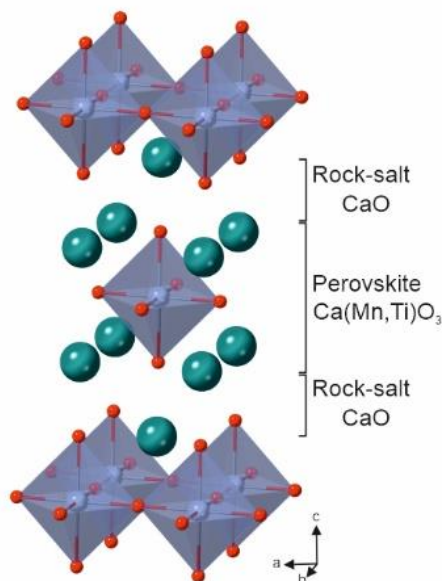


Figure 1. The  $\text{Ca}_2(\text{Mn,Ti})\text{O}_4$  phase with Ruddlesden-Popper structure, comprising rock-salt ( $\text{CaO}$ ) and perovskite layers  $\text{Ca}(\text{Mn,Ti})\text{O}_3$  build by Ca-green spheres and  $(\text{Mn,Ti})\text{O}_6$  octahedra.

Previous reports indicate that Ruddlesden-Popper calcium manganates exhibit functional electronic properties and are interesting for various electronic phenomena, such as insulator-to-metal transitions, charge-ordering, and colossal magnetoresistance effect (Fawcett et al. 1998; Autret et al. 2004).

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