

# Crystal Structures of New Pyrovanadates $A_2\text{MnV}_2\text{O}_7$ ( $A = \text{Rb}, \text{K}$ )

Hamdi Ben Yahia, Etienne Gaudin, and Jacques Darriet

Institut de Chimie de la Matière Condensée de Bordeaux-CNRS, Université Bordeaux 1,  
87 avenue du docteur A. Schweitzer, 33608 Pessac Cedex, France

Reprint requests to Dr. E. Gaudin. Fax: (+33)540002761. E-mail: gaudin@icmcb-bordeaux.cnrs.fr

*Z. Naturforsch.* **2007**, 62b, 873 – 880; received March 3, 2007

*Dedicated to Dr. Bernard Chevalier on the occasion of his 60<sup>th</sup> birthday*

The new compounds  $A_2\text{MnV}_2\text{O}_7$  ( $A = \text{K}, \text{Rb}$ ) with structures related to the melilite-type have been synthesized by a solid state reaction route. The crystal structures of  $\text{K}_2\text{MnV}_2\text{O}_7$ ,  $\text{Rb}_2\text{MnV}_2\text{O}_7$  and  $\text{KRbMnV}_2\text{O}_7$  have been determined using X-ray single crystal diffraction data. The compound  $\text{K}_2\text{MnV}_2\text{O}_7$  crystallizes with a melilite-type structure with tetragonal unit cell parameters  $a = 8.609(3)$ ,  $c = 5.538(4)$  Å and space group  $P4_21m$ . The structures of  $\text{Rb}_2\text{MnV}_2\text{O}_7$  and  $\text{KRbMnV}_2\text{O}_7$  are derived from the melilite-type structure with space group  $P4_2/mnm$  and unit cell parameters  $a = 8.577(6)$ ,  $c = 11.809(6)$  Å, and  $a = 8.530(6)$ ,  $c = 11.466(5)$  Å, respectively. The three structures consist of  $[\text{MnV}_2\text{O}_7]^{2-}$  layers perpendicular to the  $c$  axis separated by  $A^+$  layers. The  $[\text{MnV}_2\text{O}_7]^{2-}$  layers feature corner-sharing  $\text{MnO}_4$  tetrahedra and  $\text{V}_2\text{O}_7$  pyrovanadate units, the linkage leading to rings of five tetrahedra. The doubling of the  $c$  parameter for  $\text{Rb}_2\text{MnV}_2\text{O}_7$  or  $\text{RbKMnV}_2\text{O}_7$  is explained by the existence of a mirror plane perpendicular to the  $[001]$  direction between two  $[\text{MnV}_2\text{O}_7]^{2-}$  layers. The  $A^+$  alkali cations occupy distorted square antiprisms of oxygen atoms in  $\text{K}_2\text{MnV}_2\text{O}_7$  and distorted square prisms of oxygen atoms in  $\text{Rb}_2\text{MnV}_2\text{O}_7$  and  $\text{RbKMnV}_2\text{O}_7$ .

*Key words:* Vanadate, Melilite, Crystal Chemistry, Single Crystal X-Ray Diffraction, Oxides