

# Poster Presentations

## [MS19-P07] Synthesis and Crystal Structure of $\text{Pb}_4(\text{V}_3\text{O}_8)_2(\text{SeO}_3)_3$

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Crystals of  $\text{Pb}_4(\text{V}_3\text{O}_8)_2(\text{SeO}_3)_3$  (**I**) were obtained by hydrothermal method from aqueous solution and  $\text{PbO}$ ,  $\text{V}_2\text{O}_5$ ,  $\text{SeO}_2$  in ratio 1:2:10. The reaction was performed in 23 mL Teflon-lined Parr reaction vessel heated in Thermo Scientific mechanical convection oven up to 210°C and hold over 96 hours. Afterward the vessel was cooled to room temperature at a rate of 5°C/h. Products consisted of orange platy crystals of **I** up to 300  $\mu\text{m}$  in maximal dimension.

Crystals selected for data collection were mounted on a Bruker DUO four-circle diffractometer equipped with an APEX II CCD detector and monochromated  $\text{MoK}\alpha$  radiation. The structure of **I** was solved by direct methods. The following twinning matrix was applied during the refinement [-100 0-10 -0.80-1]. **I** is triclinic,  $P-1$ ,  $a=7.1337(3)\text{Å}$ ,  $b=7.1869(3)\text{Å}$ ,  $c=21.5324(10)\text{Å}$ ,  $\alpha=90.138(2)^\circ$ ,  $\beta=98.139(2)^\circ$ ,  $\gamma=94.775(2)^\circ$ ,  $V=1088.92(8)\text{Å}^3$ ,  $R_1=0.0640$  for 4721 unique reflections with  $|F_o| \geq 4\sigma_F$ .

There are six symmetrically inequivalent V sites in the structure of **I**. V–O distances vary in the range of 1.604–2.634 Å and 1.606–2.080 Å in  $\text{VO}_6$  octahedra and  $\text{VO}_5$  square pyramids, respectively. Se–O bonds are in the range of 1.676–1.739 Å. The structure of **I** contains four symmetrically distinct  $\text{Pb}^{2+}$  cations. All Pb–O bonds  $\leq 3.5\text{Å}$  were taken into consideration. Coordination of Pb atoms is distorted and variable due to the

stereochemical activity of lone electron pair.

The structure of **I** is based on ‘vanadium bronzes’ derivative chains formed by edge- and corner-sharing  $\text{VO}_6$  octahedra,  $\text{VO}_5$  square pyramids and  $\text{SeO}_3$  trigonal pyramids.  $[(\text{V}_3\text{O}_8)_2(\text{SeO}_3)_3]^{8-}$  chains are oriented along [100] and interconnected by  $\text{Pb}^{2+}$  cations into 3D framework. Comparison with the other similar compounds is given.

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