

Structure and Bonding in Thiooxovanadates $A_3VS_xO_{4-x}$ ($A = Na, K$; $x = 1 - 4$)

Simone Schnabel, Caroline Röhr, *Inst. f. Anorganische und Analytische Chemie, Universität Freiburg, Germany*. E-mail: simone@pyrite.chemie.uni-freiburg.de

Alkalithiooxovanadates(V) $A_3VS_xO_{4-x}$ ($A=Na,K$; $x=1-4$) [1-3], amongst them the new compounds K_3VS_3O (SG $P2_1/c$, $a = 1014$, $b = 685$, $c = 1195$ pm, $\beta = 93.2^\circ$, $R1=0.09$) and Na_3VSO_3 (SG $R3c$, $a = 863$, $c = 1235$ pm, $R1 = 0.02$) were synthesized via reactions in the melt starting from V, the alkaline metal (A), A_2S , A_2O and sulfur. The structures of all compounds contain similar ortho anions $[VS_xO_{4-x}]^{3-}$, each with a different ion packing. The bonding situation for all sodium compounds $Na_3VS_xO_{4-x}$ with $x=1-4$ was investigated by raman spectroscopy and DFT bandstructure calculations. In order to study the influence of cations, measurements and calculations of sodium vanadates are compared to corresponding potassium compounds.

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