

NaCa₄V₅O₁₇ with Isolated V₂O₇ Dimer and V₃O₁₀ Trimer Exhibiting a Large Birefringence

Zhiqing Xie, Shichao Cheng, Shuwei Li, Hanqin Ding



PII: S0022-4596(18)30400-6
DOI: <https://doi.org/10.1016/j.jssc.2018.09.016>
Reference: YJSSC20377

To appear in: *Journal of Solid State Chemistry*

Received date: 3 August 2018
Revised date: 7 September 2018
Accepted date: 11 September 2018

Cite this article as: Zhiqing Xie, Shichao Cheng, Shuwei Li and Hanqin Ding, NaCa₄V₅O₁₇ with Isolated V₂O₇ Dimer and V₃O₁₀ Trimer Exhibiting a Large Birefringence, *Journal of Solid State Chemistry*, <https://doi.org/10.1016/j.jssc.2018.09.016>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting galley proof before it is published in its final citable form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

NaCa₄V₅O₁₇ with Isolated V₂O₇ Dimer and V₃O₁₀ Trimer Exhibiting a Large Birefringence

Zhiqing Xie^a, Shichao Cheng^a, Shuwei Li^b, Hanqin Ding^{a*}

^a*School of Physics Science and Technology, Xinjiang University, Urumqi 830046, China*

^b*Xinjiang Oil Field Development Company of Chinese Petrol, Kelamayi 834000, China*

*E-mail: dinghq@xju.edu.cn.

Abstract

A new NaCa₄V₅O₁₇ compound has been synthesized by the solid-state method. It crystallizes in the triclinic space group $P\bar{1}$ with unit cell parameters $a = 6.9379(6)$ Å, $b = 6.9523(6)$ Å, $c = 15.5017(13)$ Å, $\alpha = 84.597(3)^\circ$, $\beta = 87.276(3)^\circ$, $\gamma = 86.860(3)^\circ$, and $Z = 2$. NaCa₄V₅O₁₇ is the first compound in alkali and alkaline earth metal vanadate system with isolated V₂O₇ dimers and V₃O₁₀ trimers. The UV–Vis–NIR diffuse reflectance spectrum shows that NaCa₄V₅O₁₇ exhibits wide transparent regions ranging from 345 nm to NIR. Thermal analysis and IR spectrum were also performed. In addition, band structure, density of states and birefringence of the title compound were calculated by the first-principles calculation for better understanding the structure-property relationships of NaCa₄V₅O₁₇.

Graphical abstract:

Download English Version:

<https://daneshyari.com/en/article/10154819>

Download Persian Version:

<https://daneshyari.com/article/10154819>

[Daneshyari.com](https://daneshyari.com)