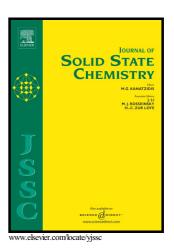
### Author's Accepted Manuscript

 $NaCa_4V_5O_{17}$  with Isolated  $V_2O_7$  Dimer and  $V_3O_{10}$  Trimer Exhibiting a Large Birefringence

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#### **ACCEPTED MANUSCRIPT**

# $NaCa_4V_5O_{17}$ with Isolated $V_2O_7$ Dimer and $V_3O_{10}$ Trimer Exhibiting a Large Birefringence

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#### **Abstract**

A new NaCa<sub>4</sub>V<sub>5</sub>O<sub>17</sub> compound has been synthesized by the solid-state method. It crystallizes in the triclinic space group  $P\overline{1}$  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. NaCa<sub>4</sub>V<sub>5</sub>O<sub>17</sub> is the first compound in alkali and alkaline earth metal vanadate system with isolated V<sub>2</sub>O<sub>7</sub> dimers and V<sub>3</sub>O<sub>10</sub> trimers. The UV–Vis–NIR diffuse reflectance spectrum shows that NaCa<sub>4</sub>V<sub>5</sub>O<sub>17</sub> 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 NaCa<sub>4</sub>V<sub>5</sub>O<sub>17</sub>.

Graphical abstract:

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