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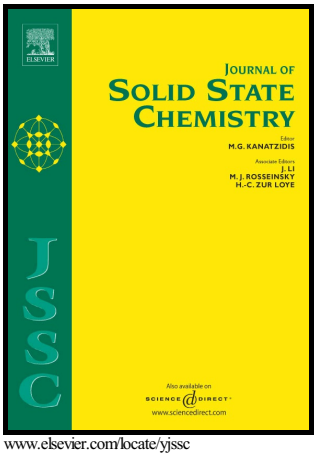

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$NaCa_4V_5O_{17}$ with Isolated V_2O_7 Dimer and V_3O_{10} Trimer Exhibiting a Large Birefringence

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Abstract

A new $NaCa_4V_5O_{17}$ 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, α = 84.597(3)°, β = 87.276(3)°, γ = 86.860(3)°, and Z = 2. $NaCa_4V_5O_{17}$ is the first compound in alkali and alkaline earth metal vanadate system with isolated V_2O_7 dimers and V_3O_{10} trimers. The UV–Vis–NIR diffuse reflectance spectrum shows that $NaCa_4V_5O_{17}$ 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 $NaCa_4V_5O_{17}$.

Graphical abstract: