

$\text{Ca}_{10}\text{V}_{5.2}\text{Fe}_{0.8}\text{O}_{24}$, a Novel Oxometalate with Discrete Complex Anions

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Lustrous needle shaped prismatic single crystals of the new compound $\text{Ca}_{10}\text{V}_{5.2}\text{Fe}_{0.8}\text{O}_{24}$ were obtained out of a sample with nominal composition $\text{Ca}_2\text{Fe}_{1.6}\text{V}_{0.4}\text{O}_5$ prepared at 1400 °C. The crystals are opaque and stable to humid air. $\text{Ca}_{10}\text{V}_{5.2}\text{Fe}_{0.8}\text{O}_{24}$ crystallizes with a new structure type, space group *Pnma* with $a = 6.803(3)$, $b = 16.015(8)$, $c = 10.418(7)$ Å, $Z = 2$, $R = 0.041$. The crystal structure is characterized by two mononuclear tetrahedral species, MO_4 , which differ significantly from each other with respect to their M–O bond lengths. One with an average bond distance of 1.709(8) Å represents an orthovanadate ion. The other with a significantly larger value $d(\text{M–O}) = 1.744(6)$ Å corresponds to a mixed occupation of its centre according to $[\text{V}_{0.8}\text{Fe}_{0.2}\text{O}_4]^{3.5-}$. In the crystal structure the complex anions are arranged in separate sheets parallel to the (010) plane. They are separated from each other by three crystallographically independent Ca^{2+} ions which are each coordinated by 7 oxygen atoms in distorted pentagonal bipyramidal and trigonal prismatic configurations, respectively.

Key words: Complex Oxides, Vanadium, Iron