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:ภาษาอังกฤษ Crystal Structures of Supramolecular Metavanadate Compounds

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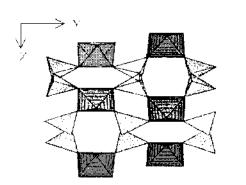
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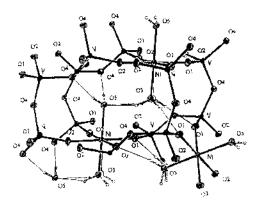
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The isomorphous  $MV_2O_6.2H_2O$  ( $M = Ni^{2-}$ ,  $Co^{2-}$ ) compounds crystallize in the orthorhombic space group Pnma and consist of  $VO_4$  tetrahedra linked through two of the oxygen atoms into chains propagating approximately along the (100) direction. Adjacent  $VO_4$  chains are interconnected by  $MO_6$  octahedra where each of the four equatorial oxygen atoms is shared with a  $VO_4$  oxygen atom of a different chain, and the axial oxygen atoms are waters of hydration. A polyhedral representation of the 011 plane is given below left.

The oxygen atom of one water molecule lies on the mirror plane with both H atoms forming mirror related strong hydrogen bonds with oxygen atoms linking adjacent VO<sub>4</sub> tetrahedra. The oxygen atom of the second water molecule is disordered with respect to the mirror plane. Both hydrogen atoms are again involved in O-H O hydrogen bonds, one strong hydrogen bond to the lone pair of the first water molecule in an adjacent unit and the second weak bond to one oxygen atom linking a VO<sub>4</sub> tetrahedra to a MO<sub>6</sub> octahedra. The lone pair of the second water does not participate in hydrogen bonding. The waters of hydration thus occur as hydrogen bonded pairs as illustrated below right, which if removed leave porous channels in the (010) direction.





 $CaV_2O_6$  is a modulated structure that can be described in term of a parent structure in space group C2/m. The parent structure consists of  $CaO_6$  octrahedra and  $VO_5$  trigonal bipyramids (Tb). The  $VO_5$  trigonal bipyramids are edge connected using one equatorial O atom and the two axial O atoms to form parallel zigzag chains propagating approximately along the (010) direction. Each of the chain oxygens thus connects to the three V atoms of three  $VO_5$  trigonal bipyramids, functioning as one of the equatorial O atoms in one Tb and the top apical O atom of the Tb below and the bottom apical O atom of the Tb above. Adjacent  $VO_5$  chains are interconnected by  $CaO_6$  octahedra sharing the remaining two equatorial O atoms of the  $VO_5$  Tb. The oxygen atoms have different environments, one being two coordinate linking one V atom to one Ca atom, while the other is three coordinate linking the V atom to two adjacent C-center related Ca atoms. The cross-channel O-O contact distances are 3.125 and 3.561 Å for the Oh-Tb-Oh-Tb-Tb and the Oh-Tb-Oh-Tb channels respectively.