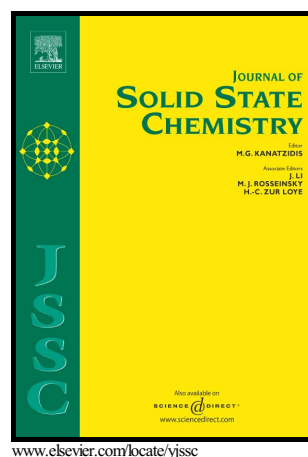


Three New d^{10} Transition Metal Selenites
Containing PO_4 Tetrahedron:
 $\text{Cd}_7(\text{HPO}_4)_2(\text{PO}_4)_2(\text{SeO}_3)_2$,
 $\text{Cd}_6(\text{PO}_4)_{1.34}(\text{SeO}_3)_{4.66}$ and $\text{Zn}_3(\text{HPO}_4)$
 $(\text{SeO}_3)_2(\text{H}_2\text{O})$

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Three New d^{10} Transition Metal Selenites Containing PO_4 Tetrahedron: $\text{Cd}_7(\text{HPO}_4)_2(\text{PO}_4)_2(\text{SeO}_3)_2$, $\text{Cd}_6(\text{PO}_4)_{1.34}(\text{SeO}_3)_{4.66}$ and $\text{Zn}_3(\text{HPO}_4)(\text{SeO}_3)_2(\text{H}_2\text{O})$

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Abstract

Three new d^{10} transition metal selenites containing PO_4 tetrahedron, namely, $\text{Cd}_7(\text{HPO}_4)_2(\text{PO}_4)_2(\text{SeO}_3)_2$ (**1**), $\text{Cd}_6(\text{PO}_4)_{1.34}(\text{SeO}_3)_{4.66}$ (**2**) and $\text{Zn}_3(\text{HPO}_4)(\text{SeO}_3)_2(\text{H}_2\text{O})$ (**3**), have been synthesized by hydrothermal reaction. They feature three different structural types. Compound **1** exhibits a novel 3D network composed of 3D cadmium selenite open framework with phosphate groups filled in the 1D helical tunnels. The structure of compound **2** displays a new 3D framework consisted of 2D cadmium oxide layers bridged by SeO_3 and PO_4 groups. Compound **3** is isostructural with the reported solids of $\text{Co}_3(\text{SeO}_3)_{3-x}(\text{PO}_3\text{OH})_x(\text{H}_2\text{O})$ when x is equal to 1.0. Its structure could be viewed as a 3D zinc oxide open skeleton with SeO_3 and HPO_4 polyhedra attached on the wall of the tunnels. They represent the only examples in metal selenite phosphates in addition to the above cobalt compounds. Optical diffuse reflectance spectra revealed that these solids are insulators, which are consistent with the results of band structure computations based on DFT algorithm.

Graphical Abstract

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