

新型磷酸钒孔道结构化合物(H₃NCH₂CH₂NH₃)₃·[(VO)₄(PO₄)₂(HPO₄)₄]的水热合成及结构表征

杜洪兵,廖立兵,杨赞中,马哲生,熊明

中国地质大学材料科学与工程学院

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摘要 以有机分子乙二胺作为模板剂合成了新型磷酸钒孔道化合物(H₃NCH₂CH₂NH₃)₃·[(VO)₄(PO₄)₂(HPO₄)₄], 并通过X射线单晶衍射实验进行了结构表征, 晶体学数据为: C₂/c,a=1.8505(9)nm,b=0.7089(4)nm,c=2.3304(10)nm,β=96.43(3)°, V=3.038(3)nm³,Z=8,R=0.067,Rw^b=0.1635,

该化合物具有非常独特和规整的二维孔道骨架结构, 进一步的晶体化学研究表明该化合物为一新的VPO物相。

关键词 [磷酸盐](#) [钒化合物](#) [钒酰络合物](#) [孔道](#) [晶体结构](#) [水热法](#) [模板](#) [结构表征](#)

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Hydrothermal synthesis and structure characterization of a novel open-framework vanadium phosphate (H₃NCH₂CH₂NH₃)₃ [(VO)₄(PO₄)₂(HPO₄)₄]

Du Hongbing,Liao Libing,Yang Zanzhong,Ma Zhesheng,Xiong Ming

Abstract A novel ethylenediamine templated open-framework vanadium phosphate (H₃NCH₂CH₂NH₃)₃·[(VO)₄(PO₄)₂(HPO₄)₄] has been hydrothermally synthesized and characterized by single-crystal X-ray diffraction. Green needle-like compound crystallized in monoclinic space group C₂/c with a=1.8505(9) nm,b=0.7089(4) nm, c=2.3304(10) nm, β=96.43(3)°, V=3.038(3) nm³,Z=8, R=0.067 for 1912 unique reflections. The structure consists of layers constructed of corner-sharing V(IV) octahedra, V(IV) trigonal bipyramids, (PO₄)³⁻ and (HPO₄)²⁻ tetrahedra, which are held together by hydrogen bonding interaction to form the tunnels paralleled to the c axis and the (110) direction. Studies of crystal structure and crystal chemistry shows that this compound is a new VPO phase with a unique and topotactic two dimensional open framework structure.

Key words [PHOSPHATE](#) [VANADIUM COMPOUNDS](#) [VANADYL COMPLEX](#) [HOLE CHANNELS](#) [CRYSTAL STRUCTURE](#) [HYDRO-THERMAL METHOD](#) [FORMWORK](#) [STRUCTURE CHARACTERISTICS](#)

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