一种新型磷酸铍微孔晶体的合成与表征

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摘要 水热晶化法合成并培养一种新型磷酸铍微孔晶体。经多晶X射线衍射,四圆X射线单晶结构分析,红外光谱等测定,其骨架结构是由磷氧四面体和铍氧四面体交替的,通过共用顶点氧原子(氧桥形式)构成的阴离子骨架。晶体属正交晶系,空间群为Pna21, 晶胞参数a=0.8699(1)nm, b=0.856(1)nm, c=0.4953(2)nm,晶胞体积V=0.3691(7)nm^3。Z=4,求解结构中最后R=0.054, Rw=0.048。微孔体系由4,6和8元环组成。水分子和平衡阴离子骨架电荷的质子位于平行(100)方向的六元环通道中,研究其热稳定性能。关键词 红外分光光度法 晶体结构 X射线衍射分析 热稳定性 磷酸铍 分类号 0612

The synthesis and characterization of a novel beryllophosphate microporous crystal

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Abstract A novel beryllophosphate microporous crystal was synthesized hydrothermally, and the bigger singlg crystal was also obtained. The framework structure was found consisting of alternating PO4 tetrahedral and BeO4 tetrahedral by means of X-ray powder diffraction, four circle X-ray structural analysis, IR spectroscopy and etc. The crystal was crystallized in orthorhombic, space group Pna21. The unit cell parameter a=0.8699(1)nm, b=0.8567(1)nm, c=0.4953(2) nm, Z=4, the unit cell volume is 0.3691(7)nm^3. The final discrepany factor is R=0.054, and Rw=0.048. The microporous system is composed of four-, six- and eight-membered rings. The water molecules and the protons which balance the negative charges of anionic framework are located in the six-membered ring channel parallel to (100) direction. The thermal stability of the product was also studied.

 Key words
 INFRARED SPECTROPHOTOMETRY
 CRYSTAL STRUCTURE
 X-RAY DIFFRACTION

 ANALYSIS
 THERMAL STABILITY

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