

研究论文

## 新颖的咪唑官能化夹心型钨铋酸盐超分子化合物的合成与晶体结构

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**摘要** 在常规条件下合成了一个新颖的超分子化合物 $\text{Na}_8\text{H}[\{\text{Na}(\text{H}_2\text{O})\}_3\{\text{Mn}(\text{C}_3\text{H}_4\text{N}_2)\}_3(\text{BiW}_9\text{O}_{33})_2] \cdot 3\text{H}_2\text{O}$ , 通过X射线单晶结构分析、红外光谱及元素分析对该化合物进行了表征. 结果表明, 该化合物属六方晶系,  $P6(3)/m$ 空间群. 晶胞参数 $a=1.394\ 8(4)\ \text{nm}$ ,  $b=1.394\ 8(4)\ \text{nm}$ ,  $c=3.348\ 6(19)\ \text{nm}$ ,  $\gamma=120^\circ$ ,  $V=5.641(4)\ \text{nm}^3$ ,  $Z=12$ . 该化合物是以 $\alpha$ -B-BiW9钨铋酸盐为基本构筑单元的夹心结构化合物. 夹层中心3个 $\text{Mn}^{2+}$ 分别与3个咪唑分子配位形成无机-有机杂化材料. 3个 $[\{\text{Na}(\text{H}_2\text{O})\}_3\{\text{Mn}(\text{C}_3\text{H}_4\text{N}_2)\}_3(\text{BiW}_9\text{O}_{33})_2]^{9-}$ 多阴离子结构基元利用氢键(非典型氢键)沿 $ab$ 面构筑成具有三角形空穴的二维层状骨架结构. 这种二维层状结构利用氢键作用沿 $c$ 轴方向交错排列, 形成了含有一维六边形孔道的三维超分子结构.

**关键词** [多金属氧酸盐](#); [咪唑](#) [孔道](#) [超分子化合物](#)

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## Synthesis and Crystal Structure of a Novel Supermolecular Compound Based on Imidazole Functionalized Sandwich Type of Tungstobismutate

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**Abstract** A novel supermolecular compound,  $\text{Na}_8\text{H}[\{\text{Na}(\text{H}_2\text{O})\}_3\{\text{Mn}(\text{C}_3\text{H}_4\text{N}_2)\}_3(\text{BiW}_9\text{O}_{33})_2] \cdot 3\text{H}_2\text{O}$ , was synthesized under the open-air conditions, and characterized by X-ray single-crystal diffraction, IR spectra and elemental analysis. The crystal belongs to hexagonal system, space group  $P6(3)/m$  with  $a=1.394\ 8(4)\ \text{nm}$ ,  $b=1.394\ 8(4)\ \text{nm}$ ,  $c=3.348\ 6(19)\ \text{nm}$ ,  $\gamma=120^\circ$ ,  $V=5.641(4)\ \text{nm}^3$ ,  $Z=12$ . The crystal structure consists of two  $\alpha$ -B-BiW9 subunits and displays a sandwich type polyanion linked by three  $\text{Mn}^{2+}$  ions between the two  $\alpha$ -B-BiW9 units and the  $\text{Mn}^{2+}$  ions coordinate an imidazole molecule, respectively. Thus, this compound can be considered as a new kind of inorganic-organic hybrid materials. Moreover, three neighboring  $[\{\text{Na}(\text{H}_2\text{O})\}_3\{\text{Mn}(\text{C}_3\text{H}_4\text{N}_2)\}_3(\text{BiW}_9\text{O}_{33})_2]^{9-}$  polyanions form a triangle cavity through the nonclassical hydrogen bonds and such units extend further along  $ab$  plane to construct two-dimensional layered framework. Such two-dimensional layered structure further pack each other interlacedly along  $c$  axis to construct an interesting three-dimensional supermolecular framework containing a one-dimensional hexagonal channels.

**Key words** [Polyoxometalate](#) [Imidazole](#) [Channel](#) [Supermolecular compound](#)

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