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Full Papers

新颖有机/无机杂化配位聚合物$[(DBU-H)(PbI_3)]_n$的合成、晶体结构和量子化学研究

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摘要 在室温，pH 值6.0条件下由DBU与PbI_2自组装反应合成得到一种新颖有机/无机杂化配位聚合物$[(DBU-H)(PbI_3)]_n$

(DBU=1,8-二氮杂双环[5,4,0] -7-十一烯)，并用单晶X射线衍射方法确定其结构。该化合物属于单斜晶系，空间群$P2_1/c$，晶体学参数：a = 1.1940(2)，b = 1.7409(4)，c = 0.81347(16)

nm， β = 100.32(3)°，$C_9H_{17}N_2I_3Pb$，M_r = 741.15, V = 1.6635(6)

nm^3， Z = 4，D_c = 2.959 g/cm^3，$F(000)$ = 1304， μ(Mo Kα) = 15.687 mm^{-1}， R_1=0.0389，wR_2=0.0635。结构解析表明，单胞中包含由扭曲PbI_6八面体共面形成的$(PbI_3)_n^{n-}$无限链及质子化的$(DBU-H)^+$阳离子。无机链和$(DBU-H)^+$阳离子通过静电作用结合在一起形成有机/无机杂化结构。依据晶体结构数据，采用G03程序在DFT/B3LYP水平上计算了标题化合物的电子结构。

关键词 有机/无机杂化, 模板合成, 铅(Ⅱ)聚合物, 量子化学计算

分类号

Novel Organic-inorganic Hybrid Coordination Polymer $[(DBU-H)(PbI_3)]_n$: Synthesis, Crystallographic Structure and Quantum Chemical Investigation

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Abstract The coordination polymer $[(DBU-H)(PbI_3)]_n$ (DBU＝catena-(1,8-diazabicyclo[5,4,0]-undec-7-ene) was synthesized by self-assembly reaction of DBU and PbI_2 at room temperature with pH＝6.0 and structurally characterized by means of X-ray single crystal diffraction. It crystallizes in monoclinic system with space group$P2_1/c$and crystal parameters a＝1.1940(2) nm, b＝1.7409(4) nm, c＝0.81347(16) nm, β＝100.32(3)°, chemical formula $C_9H_{17}N_2I_3Pb$and M_r＝741.15, V＝1.6635(6) nm^3, Z＝4, D_c＝2.959 g/cm^3, $F(000)$＝1304, μ(Mo Kα)＝15.687 mm^{-1}, the final R＝0.0389 and wR＝0.0635 for 2279 observed reflections with $I>2\sigma(I)$. Structure analysis shows that the inorganic anion chain consists of distorted PbI_6 octahedra, which shares the same faces with adjacent PbI_6 units to form one-dimensional infinite chains along the c-axis. Anion chains are surrounded by protonated $(DBU-H)^+$ cations. Anion chains and cations are in combination with each other by static attracting forces in the crystal to form so-called organic-inorganic hybrid structure. According to the crystal structure data, quantum chemical calculation with DFT at B3LYP level was used to reveal the electronic structure of title compound.

Key words organic-inorganic hybrid template synthesis lead(Ⅱ) iodide quantum chemical calculation

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