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研究论文

$Eu(C_{10}H_9N_2O_4)(C_{10}H_8N_2O_4)(H_2O)_3]\cdot 0.5bipy\cdot 3H_2O$ 配合物的合成、晶体结构及荧光性质

武望婷，*，胡怀明，王尧宇，史启祯

(西北大学化学系 陕西省物理无机化学重点实验室 西安 710069)

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摘要 在水-乙醇混合体系中, 以2-羰基丙酸水杨酰腙($C_{10}H_{10}N_2O_4$)、2,2-联吡啶($C_{10}H_8N_2$, 简写bipy)与$Eu(NO_3)_3\cdot 4H_2O$反应, 首次培养出黄色单晶$[Eu(C_{10}H_9N_2O_4)(C_{10}H_8N_2O_4)(H_2O)_3]\cdot 0.5bipy\cdot 3H_2O$. 该晶体属三斜晶系, 空间群为*P*-1, 晶胞参数$a=0.93392(16)$ nm, $b=1.3100(2)$ nm, $c=1.3895(2)$ nm, $\alpha=97.205(3)°$, $\beta=105.411(2)°$, $\gamma=106.364(2)°$, $V=15.35(2)$ nm^3, $Z=2$, $\mu=2.118$ mm^{-1}, $D_c=1.686$ Mg/m^3, $F(000)=786$, $R=0.0116$, $wR=0.0507$, GOF=0.995. 晶体测试结果表明, 该单晶结构为铕的9配位配合物, 两个2-羰基丙酸水杨酰腙分别以负一价和负二价酮式和三个水分子同时参与配位; 每个2-羰基丙酸水杨酰腙中的羧基氧、酰胺基中的羰基氧和C=N中的氮与Eu^{3+}配位, 形成两个共边的稳定五元环, 另三个配位原子则分别来自三个水分子中的氧原子, 该配合物在空间呈扭曲的单帽四方反棱柱, 而在不对称单位中还有游离的一个2,2-联吡啶分子和三个水分子, 这些游离分子与配位分子之间存在大量分子内和分子间氢键, 整个分子在空间呈三维网状结构. 发光性能测试表明该配合物具有很好的荧光性质.

关键词 铕配合物 2-羰基丙酸水杨酰腙 2,2-联吡啶 晶体结构 荧光性

分类号

Synthesis, Crystal Structure and Fluorescence Property of $[Eu(C_{10}H_9N_2O_4)(C_{10}H_8N_2O_4)(H_2O)_3]\cdot 0.5bipy\cdot 3H_2O$

WU Wang-Ting, HE Shui-Yang*, HU Huai-Ming, WANG Yao-Yu, SHI Qi-Zhen

(*Shaanxi Key Laboratory of Physico-inorganic Chemistry, Department of Chemistry, Northwest University, Xi'an 710069*)

Abstract $Eu(NO_3)_3\cdot 4H_2O$ has reacted with 2-oxopropionic acid salicyloyl hydrazone ($C_{10}H_{10}N_2O_4$) and 2,2'-bipyridyl ($C_{10}H_8N_2$, bipy) to obtain a yellow prismatic crystal of the complex $[Eu(C_{10}H_9N_2O_4)$- $(C_{10}H_8N_2O_4)(H_2O)_3]\cdot 0.5bipy\cdot 3H_2O$ for the first time in H_2O-C_2H_5OH mixed solvent. The compound crystallized in the triclinic system with space group *P*-1 and parameters $a=0.93392(16)$ nm, $b=1.3100(2)$ nm, $c=1.3895(2)$ nm, $\alpha=97.205(3)°$, $\beta=105.411(2)°$, $\gamma=106.364(2)°$, $V=15.35(2)$ nm^3, $Z=2$, $\mu=2.118$ mm^{-1}, $D_c=1.686$ Mg/m^3, $F(000)=786$, $R=0.0116$, $wR=0.0507$ and GOF=0.995. In the structure, europium atom is 9-coordinated by carboxyl O and acyl O atoms and azomethine N atom of two tridentate $C_{10}H_{10}N_2O_4$ ligands negative univalent and bivalent and three water molecules to form two stable five-membered rings sharing one side in ketone form. The coordination polyhedron around Eu^{3+} was described as a single cap square antiprism. In the crystal cell, there are one free bipy and three water molecules connected with 2-oxopropionic acid salicyloyl hydrazone and coordinated water molecule by hydrogen bonds. The complex formed a three-dimensional super molecule in space through hydrogen bonds. The test of luminescence performance of the complex has shown it has good fluorescence property.

Key words europium(III) complex 2-oxopropionic acid salicyloyl hydrazone 2 2-bipyridyl crystal structure fluorescence

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通讯作者 何水样 xdchemistry411@126.com