

研究论文

2,6-二(2-苯并咪唑基)吡啶与稀土苦味酸盐配合物的合成、晶体结构及荧光性质研究

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摘要 合成了稀土苦味酸盐(pic)与配体2,6-二(2-苯并咪唑基)吡啶(L)的配合物,通过元素分析、红外光谱及电子光谱对配体及配合物进行了表征,并用X射线单晶衍射测定了配合物[CeL₂(pic)₂](pic)•(CH₃OH)₃的晶体结构.配合物属于三斜晶系,空间群为P $\bar{1}$,晶胞参数 $a=1.3795(3)$ nm, $b=2.1292(5)$ nm, $c=2.5651(6)$ nm, $\alpha=105.847(3)^\circ$, $\beta=100.150(3)^\circ$, $\gamma=107.893(3)^\circ$, $Z=2$, $R=0.0519$, $wR=0.1255$.

晶体中一个不对称单元内有两个结晶学上独立的分子,这两个分子的构型基本相同,中心Ce³⁺

⁺均与两个三齿配位的配体及两个双齿配位的苦味酸根配位,配位数为10.中心Ce³⁺

⁺的配位多面体为变形双帽四方反棱柱,两个分子之间以 π - π 堆积连接,生成一个非中心对称的二聚体.

整个晶体则是由这些二聚体以分子间氢键作用连接成三维网状超分子结构.室温下,在紫外光激发下Eu(III)

配合物固体和溶液均表现出中心离子的特征荧光发射.

关键词 [2,6-二\(2-苯并咪唑基\)吡啶](#) [稀土苦味酸盐配合物](#) [合成](#) [晶体结构](#) [荧光性质](#)

分类号

Synthesis, Crystal Structure and Luminescent Properties of Rare Earth Picrates Complexes with 2,6-Bis(benzimidazol-2-yl)pyridine

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Abstract Solid complexes of rare earth picrates (pic) with the ligand 2,6-bis(benzimidazol-2-yl)pyridine (L) have been synthesized and characterized by elemental analysis, IR and electronic spectra. The crystal and molecular structures of the complex [CeL₂(pic)₂](pic)•(CH₃OH)₃ have been determined by single crystal X-ray diffraction. The crystal structure indicates that the complex crystallizes in the triclinic space group P $\bar{1}$ with parameters: $a=1.3795(3)$ nm, $b=2.1292(5)$ nm, $c=2.5651(6)$ nm, $\alpha=105.847(3)^\circ$, $\beta=100.150(3)^\circ$, $\gamma=107.893(3)^\circ$, $Z=2$, $R=0.0519$, $wR=0.1255$. The crystal consists of two similar but independent molecules in the asymmetric unit and the Ce(III) ion coordinated toward ten donor atoms, six of which belong to the nitrogen atoms of two tridentate ligands and four oxygen atoms from two bidentate picrates. The coordination polyhedron around Ce³⁺ is a distorted square antiprism, and the two independent molecules are connected by π - π stacking interactions to form a noncentrosymmetric dimer. The crystal structure is built of a packing of these dimers via intermolecular hydrogen bonding to yield an infinite three-dimensional supramolecular network. At room temperature, under UV light excitation the Eu(III) complex exhibited characteristic emission of the central metal ions both in solid state and in solutions.

Key words [2,6-bis\(benzimidazol-2-yl\)pyridine](#) [rare earth picrates complex](#) [synthesis](#) [crystal structure](#) [luminescent property](#)

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