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论文

稀土配合物{La［o-$C_6H_4(NO_2)(CO_2)$］$_3$·$(DMF)_2$}$_2$的晶体结构及其荧光性能

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摘要:

合成了一种新的双核倒反中心的稀土镧配合物{La［o-$C_6H_4(NO_2)(CO_2)$］$_3$·$(DMF)_2$}$_2$. 通过元素分析、 核磁共振谱和红外光谱对配合物的组成和结构进行了表征, 用热重分析研究了该配合物的热稳定性, 用X射线单晶衍射法测定了其晶体结构. 镧配合物{La［o-$C_6H_4(NO_2)(CO_2)$］$_3$·$(DMF)_2$}$_2$晶体属三斜晶系, 空间群P1, 晶胞参数 a=1.902(2) nm, b=1.245 0(2) nm, c=1.298 7(2) nm, α=64.555(2)°, β=66.348(2)°, γ=71.920(2)°, V=1.569 5(5) nm3, Dc=1.658 Mg/m^3, Z=2, μ=1.437 mm-1, F(000)=784. 配合物中有2个La(Ⅲ)被4个邻硝基苯甲酸的羧酸根的负氧离子桥联, 每个La(Ⅲ)的中心离子配位数为9, 配位原子分别来自于7个邻硝基苯甲酸的羧酸根的负氧离子和2个DMF的羰基氧原子. 化合物中的氢键和π…π堆积作用使其成为三维立体结构. 同时发现了标题化合物固体具有光致发光现象, 发光性能测试表明, 配合物具有很好的荧光性质.

关键词: 镧配合物; 合成; 晶体结构; 荧光

Crystal Structures and Fluorescence Property of Rare Earth Complexes {La［o-$C_6H_4(NO_2)(CO_2)$］$_3$·$(DMF)_2$}$_2$.

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Abstract:

The o-nitro-benzoic acid($C_7H_5O_4N$) and N,N-dimethylformamide(DMF) coordinate with La(Ⅲ) to form a dinuclear complex The o nitro benzoic acid($C_7H_5O_4N$) and N,N dimethylformamide(DMF) coordinate with La(Ⅲ) to form a dinuclear complex The o nitro benzoic acid(C7H5O4N) and N,N dimethylformamide(DMF) coordinate with La(Ⅲ) to form a dinuclear complex La［o C6H4(NO2)(CO2)］3·(DMF)2}2. The complex resides on an inversion center. The structure of the complex is characterized by IR, ^{1}H NMR, ^{13}C NMR, UV and fluorescent emission spectra. The results show that the complex crystallizes in a triclinic system, space group P1, cell parameter a=1.902(2) nm, b=1.245 0(2) nm, c=1.298 7(2) nm, α=64 555(2)°, β=66 348(2)°, γ=71.920(2)°, V=1.569 5(5) nm3, Dc=1.658 Mg/m^3, Z=2, μ=1.437 mm^{-1}, F(000)=784. In the complex, two La(Ⅲ) are bridged by four o nitro benzoic acids liganding with their carboxyl. The coordination number of La(Ⅲ) is nine and the coordinated atoms are all oxygen from the carboxyl and carbonyl. Nine oxygen atoms(seven from a carboxyl of o nitro benzoic acid and two from DMF molecule) occupy the nine coordination sites around La(Ⅲ), respectively. Hydrogen bonds and aromatic π…π stacking interactions assemble the title complex into a three dimensional network. Luminescence measurement shows that the complex emits fluorescence. . The complex resides on an inversion center. The structure of the complex is characterized by IR, ^{1}H NMR, ^{13}C NMR, UV and fluorescent emission spectra. The results show that the complex crystallizes in a triclinic system, space group P1, cell parameter a=1.902(2) nm, b=1.245 0(2) nm, c=1.298 7(2) nm, α=64.555(2)°, β=66.348(2)°, γ=71.920(2)°, V=1.569 5(5) nm^3, Dc=1.658 Mg/m^3, Z=2, μ=1.437 mm^{-1}, F(000)=784. In the complex, two La(Ⅲ) are bridged by four o-nitro-benzoic acids liganding with their carboxyl. The coordination number of La(Ⅲ) is nine and the coordinated atoms are all oxygen from the carboxyl and carbonyl. Nine oxygen atoms(seven from a carboxyl of o-nitro-benzoic acid and two from DMF molecule) occupy the nine coordination sites around La(Ⅲ), respectively. Hydrogen bonds and aromatic π…π stacking interactions assemble the title complex into a three dimensional network. Luminescence measurement shows that the complex emits fluorescence. The complex resides on an inversion center. The structure of the complex is characterized by IR, ^{1}H NMR, ^{13}C NMR, UV and fluorescent emission spectra. The results show that the complex crystallizes in a triclinic system, space group P1, cell parameter a=1.902(2) nm, b=1.245 0(2) nm, c=1.298 7(2) nm, α=64.555(2)°, β=66.348(2)°, γ=71.920(2)°, V=1.569 5(5) nm3, Dc=1.658 Mg/m3, Z=2, μ=1.437 mm-1, F(000)=784. In the complex, two La(Ⅲ) are bridged by four o-nitro-benzoic acids liganding with their carboxyl. The coordination number of La(Ⅲ) is nine and the coordinated atoms are

all oxygen from the carboxyl and carbonyl. Nine oxygen atoms(seven from a carboxyl of o-nitro-benzoic acid and two from DMF molecule) occupy the nine coordination sites around La(Ⅲ), respectively. Hydrogen bonds and aromatic π…π stacking interactions assemble the title complex into a three dimensional network. Luminescence measurement shows that the complex emits fluorescence.

Keywords: Lanthanide complex; Synthesis; Crystal structure; Fluorescence

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