

九配位K₃[Ho(NTA)₂(H₂O)]·5H₂O和八配位NH₄[Ho(cDTA)(H₂O)₂]·4.5H₂O配合物的合成及结构

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摘要 报道了稀土金属Ho(III)离子氨基多羧酸(NTA=氨基三乙酸, cDTA=反式-1, 2-环乙二氮四乙酸)配合物的合成及分子结构和晶体结构的测定。具体结果如下: (a)分子式K₃[Ho(NTA)₂(H₂O)]·5H₂O, 单斜晶系, C2/c空间群, a = 1.5364(8) nm, b = 1.2881(7) nm, c = 2.6163(13) nm, β = 96.140(9)°, V = 5.416(5) nm³, Z = 8, D_c = 1.932 g/cm³, μ = 3.635 mm⁻¹和F(000) = 2944。其R和R_w值分别为0.0310和0.0675(对4509个独立的衍射点), R和R_w值分别为0.0442和0.0707(对所有10336个衍射点)。K₃[Ho(NTA)₂(H₂O)]·5H₂O配合物中, Ho(III)N₂O₇部分是一个九配位单帽四方反棱柱体结构。(b)分子式NH₄[Ho(cDTA)(H₂O)₂]·4.5H₂O, 三斜晶系, P1, 空间群, a = 0.8636(3) nm, b = 1.0072(3) nm, c = 1.4457(5) nm, α = 88.382(5)°, β = 75.275(5)°, γ = 88.382(5)°, V = 1.2154(7) nm³, Z = 2, D_c = 1.657 g/cm³, μ = 3.315 mm⁻¹和F(000) = 606。其R和R_w值分别为0.0283和0.0708(对4203个独立的衍射点), R和R_w值分别为0.0325和0.0730(对所有4595个衍射点)。NH₄[Ho(cDTA)(H₂O)₂]·4.5H₂O配合物中Ho(III)N₂O₆部分是一个八配位四方反棱柱体结构。

关键词 钛络合物 氨基三乙酸 晶体结构

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Synthesis and Structures of Nine-Coordinated K₃[Ho(NTA)₂(H₂O)]·5H₂O and Eight-Coordinated NH₄[Ho(cDTA)(H₂O)₂]·4.5H₂O

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Abstract The crystal structures of two Ho(III) complexes with nta (nitrilotriacetic acid) and cDTA (trans-1,2-cyclohexanediaminetetraacetic acid) ligands have been reported, respectively. The crystal data are as follows: (a) K₃[Ho(NTA)₂(H₂O)]·5H₂O, monoclinic system, C2/c space group, a = 1.5364(8) nm, b = 1.2881(7) nm, c = 2.6163(13) nm, β = 96.140(9)°, V = 5.416(5) nm³, Z = 8, D_c = 1.932 g·cm⁻³, μ = 3.635 mm⁻¹, F(000) = 2944, R = 0.0310, R_w = 0.0675 for 4509 unique reflections and R = 0.0442, R_w = 0.0707 for all 10336 reflections. The Ho(III)N₂O₇ part in the complex anion [Ho(NTA)₂(H₂O)]³⁻ is a pseudo-monocapped square antiprismatic nine-coordinated structure. (b) NH₄[Ho(cDTA)(H₂O)₂]·4.5H₂O, triclinic system, P1 space group, a = 0.8636(3) nm, b = 1.0072(3) nm, c = 1.4457(5) nm, α = 88.382(5)°, β = 75.275(5)°, γ = 88.380(5)°, V = 1.2154(7) nm³, Z = 2, D_c = 1.657 g/cm³, μ = 3.315 mm⁻¹, F(000) = 606, R = 0.0283, R_w = 0.0708 for 4203 unique reflections and R = 0.0325, R_w = 0.0730 for all 4595 reflections. The Ho(III)N₂O₆ part in the complex anion [Ho(cDTA)(H₂O)₂]⁻ is a pseudo square antiprismatic eight-coordinated structure.

Key words [HOLMIUM COMPLEX](#) [nitrilotriacetic acid](#) [CRYSTAL STRUCTURE](#)

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