

Ni[H₂NC(CH₂OH)₃]₂·(H₂O)₂·(Pic)₂的合成、晶体结构与量子化学研究

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摘要 三羟甲基氨基甲烷与苦味酸(Pic)镍在乙醇水混合液中反应,制得少见的半对称分叉氢键连接的超分子化合物Ni[H₂NC(CH₂OH)₃]₂·(H₂O)₂·(Pic)₂,晶体属三斜晶系,空间群为P(1-bar),晶胞参数为a=0.6912(1) nm, b=0.8190(1) nm, c=1.3595(2) nm, α=79.59(1)°, β=83.69(1)°, γ=83.77°, V=0.74925(18) nm³, Z=2, F(000)=410。在配合物的结构单元中, Ni⁽²⁺⁾位于对称中心,分别与两个四齿配体(三羟甲基氨基甲烷)中的两个-OH,一个-NH₂,三齿配位,呈笼状螯合。而另一个-OH,因配体和中心离子构型的限制,不参与配位。运用Gaussian 98量子化学程序包,对该配合物进行从头算研究,探讨了此配合物的稳定性、原子净电荷分布,并对分子识别、分子间与分子内交互作用进行了讨论,为该类配合物的合成、分子组装研究提供理论参考。

关键词 [镍络合物](#) [晶体结构](#) [氢键](#) [从头算法](#) [甲烷 P](#) [苦味酸](#)

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Preparation, Crystal Structure and Quantum Chemical Investigation of Ni[H₂NC(CH₂OH)₃]₂·(H₂O)₂·(Pic)₂

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Abstract Supramolecular complex Ni[H₂NC(CH₂OH)₃]₂·(H₂O)₂·(Pic)₂ was prepared by reaction of niacinamide and nickel picrate in aqueous ethanol solution and characterized by elemental analysis as well as IR spectroscopy. The crystal structure was determined by single crystal diffraction analysis: triclinic, space group P1-bar, a = 0.6912(1) nm, b = 0.8190(1) nm, c = 1.3595(2) nm, α = 79.59(1)°, β = 83.69(1)°, γ = 83.77°, V = 0.74925(18) nm³, Z = 2, F(000) = 410. Every [Ni(C₆H₆N₂O)₂(H₂O)₄](Pic)₂ unit forms nine hydrogen bonds (of two types: O-H...O and N-h...O) leading to a three-dimensional network. Applying Gaussian 98 software package, using STO-3G basis set, the population regularities of the atomic net charges have been discussed. Some results obtained may be useful as theoretical reference for synthesis of the transition metal complexes, molecular assembly analysis and study of the active site in enzymes and proteins, etc.

Key words [NICKEL COMPLEX](#) [CRYSTAL STRUCTURE](#) [HYDROGEN BONDS](#) [AB INITIO CALCULATION](#) [METHANE P](#) [TRINITROPHENOL P](#)

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