

胍基硫代甲酸酯配合物的合成、晶体结构、光谱及三阶非线性光学性质研究

吴杰颖, 田玉鹏, 谢复新, 倪诗圣, 张银汉, 段春迎

安徽大学化学系, 合肥(230090); 中国科学技术大学应用化学系, 合肥(230026)

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摘要 报道三种有推拉电子基团的胍基硫代甲酸酯衍生物配体

(HL¹~³)。此类配体与二价过渡金属离子配位时脱去一质子, 形成D-M-D和A-M-A(D=给体, M=金属, A=受体)类型、含有共轭体系的中性配合物。本文集中研究了该类配体的镍、铜、钯、铂配合物的IR、磁化率、ESR谱, 电子光谱和三阶非线性光学性质, 通过光谱研究初步确定了它们均为平面正方形构型配合物, 文中还报道了CuL₂的晶体结构。晶体属P1空间群, a=0.7835(2), b=1.0530(2), c=1.1816(2)nm, α=100.61(3), β=92.38(3), γ=110.00(3)°, Z=1, 最终的R因子为0.063。通过晶体结构测试, 进一步确定铜配合物的结构为平面构型。

关键词 [硫代甲酸P](#) [胍基](#) [络合物晶体结构](#) [非线性光学晶体](#) [镍络合物](#) [铜络合物](#) [钯络合物](#) [铂络合物](#)

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Synthesis, crystal structure, spectroscopic and third-order nonlinear optical property studies on some dithiocarbazate complexes

Wu Jieying, Tian Yupeng, Xie Fuxin, Ni Shisheng, Zhang Yinhan, Duan Chunying

Anhui Univ, Dept Chem, Hefei(230090); Univ Sci & Technol China, Dept Appl Chem, Hefei(230026); Nanjing Univ, Coordinat Chem State Key Lab. Nanjing(210008)

Abstract Three SN Schiff base ligands derived from dithiocarbazate were prepared. Their neutral bisligand chelates, ML₂ [M=Ni(II), Cu(II), Pd(II) and Pt(II)], forming D-M-D and A-M-A type complexes were also prepared and characterized (D=donor, M=metal A=acceptor). Magnetic and spectroscopic data suggest a square-planar structure for the complexes. ESR spectra and variable-temperature magnetic susceptibility data supported a square-planar structure of Cu(II) chelate too. Single crystal X-ray diffraction analysis of the copper (II) chelate established that the Schiff base ligand lost a proton from its tautomeric thiol form and coordinated to metal via the mercapto sulfur and β-nitrogen. The geometry around Cu(II) is square-planar with two equivalent Cu-N and Cu-S bonds, forming an electronic delocalization system. The third-order NLO properties of them were also studied. The results show that the electro-donation group is quite helpful for the complexes exhibit higher third-order response.

Key words [METHANETHIOIC ACID P](#) [CRYSTAL STRUCTURE OF COMPLEX](#) [NON LINEAR OPTIC CRYSTAL](#) [NICKEL COMPLEX](#) [COPPER COMPLEX](#) [PALLADIUM COMPLEX](#) [PLATINUM COMPLEX](#)

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