

4-(2-羟基苯基)-亚胺基-戊-2-酮的晶体结构和谱学性质研究

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摘要 通过邻氨基苯酚与乙酰丙酮反应,合成Schiff碱4-(2-羟基苯基)-亚胺基-戊-2-酮,获其单晶,测定晶体结构,用UV-Vis,IR,¹H NMR谱对其进行了表征。其晶体属正交晶系,空间群P2₁-12₁-1,晶胞参数:a=0.8840(10) nm,b=1.05250(10)nm,c=1.12260(10)nm。V=1.0450(2)nm³,Z=4,结构偏离因子R=0.0320,ωR=0.0669,吻合因子S=0.949存在较强的分子间氢键,O(1)与相邻分子的O(2)之间的平均距离为0.2640nm。晶体结构分析和谱学性质研究表明,化合物存在亚胺烯醇式和烯胺酮式两种异构平衡。

关键词 [晶体结构](#) [谱学性质](#) [表征](#) [氨基苯酚P](#) [乙酰丙酮](#) [席夫碱](#) [亚胺基](#)

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Studies on the crystal structure and spectroscopic properties of 4- [2-hydroxyphenyl]imino]-pentan-2-one

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Abstract By the reaction of o-Aminophend and Acetylacetone in absolute alcohol in the molar ratio of 1:1, 4-[(2-hydroxyphenyl)imino]-2- pentanone was synthesized and its single crystals were obtained. The crystal structure has been determined by X-ray diffraction method and its spectroscopic properties have been studied by UV-Vis, IR and ¹H NMR. The crystal is belong to orthorhombic system, space group P2₁-12₁-1 with unit cell parameters, a=0.8840(10) nm, b=1.05250(10)nm, c=1.12260(10)nm, V=1.0450(2)nm³, Z=4, final R=0.0320, ωR=0.0669, S=0.949. Rather strong hydrogen bond exists in the crystal, the average distance of O(1)...O(2) is 0.2640nm. The analytical results of crystal structure and spectroscopic properties of the title compound show that two kinds of isomerization equilibrium between imine-enol mode and enamine-ketone mode exist in the title compound.

Key words [CRYSTAL STRUCTURE](#) [CHARACTERIZATION](#) [ACETOPREPANONE](#) [SCHIFF BASE](#) [IMINO GROUP](#)

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