

## 双缩二氨基硫脲类化合物的合成与结构

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**摘要** 合成了1, 5-二(4-甲氧基苯甲醛)双缩二氨基硫脲(1), 1, 5-二(对二甲氨基苯甲醛)双缩二氨基硫脲(2), 1, 5-二(2-呋喃甲醛)双缩二氨基硫脲(3)三个化合物, 并通过元素分析、红外光谱、核磁共振、质谱进行了结构表征。首次报道了双缩二氨基硫脲类化合物的<sup>13</sup>C NMR数据, 并发现在溶液中由于构象异构体或二聚体的存在, 该类化合物的部分<sup>13</sup>C NMR谱峰出现矮而宽、不易检测的特征。配体1形成的晶体为单斜晶系, 具有P2<sub>1</sub>/c空间群, a=1.4363(3)nm, b=1.2622(2)nm, c=1.0970(2)nm, β=101.730(10)°, V=1.9472(6) nm<sup>3</sup>, Z=4, D<sub>c</sub>=1.318g/cm<sup>3</sup>, μ=0.193mm<sup>-1</sup>, F(000)=816, R<sub>1</sub>=0.0560, ωR<sub>2</sub>=0.1496。由于分子间弱氢键力的作用, 在晶体中以二聚体的形式存在。

**关键词** [缩氨基硫脲 P](#) [晶体结构](#) [二聚体](#) [苯甲醛 P](#) [甲氧基](#) [元素分析](#) [红外分光光度法](#) [核磁共振谱法](#) [质谱法](#)

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## Synthesis and Crystal Structure of Some Dithiocarbohydrazones

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**Abstract** Novel 1,5-bis(4-methoxybenzaldehyde)-dithiocarbohydrazone (1), 1,5-bis(p-dimethylaminobenzaldehyde)-dithiocarbohydrazone (2) and 1,5-bis(2-furaldehyde)-dithiocarbohydrazone (3) have been synthesized and characterized by elemental analysis, IR, NMR and MS spectra. The <sup>13</sup>C NMR data of the dithiocarbohydrazones was initially reported. It was found that the partial <sup>13</sup>C NMR signals of the title compounds presented small and broad, and were difficult to be detected as the result of different conformers or dimers formed in solution. The crystal structure of compound 1 was determined by X-ray single crystal diffraction analysis. Crystal structure of compound 1 belongs to monoclinic system with space P2<sub>1</sub>/c. The unit cell parameters are a = 1.4363(3) nm, b = 1.2622(2) nm, c = 1.0970(2) nm, β = 101.730(10)°, V = 1.9472(6) nm<sup>3</sup>, Z = 4, D<sub>c</sub> = 1.318 g/cm<sup>3</sup>, μ = 0.193 mm<sup>-1</sup>, F(000) = 816, R<sub>1</sub> = 0.0560, ωR<sub>2</sub> = 0.1496.

**Key words** [THIOSEMICARBAZONE P](#) [CRYSTAL STRUCTURE](#) [DIMER](#) [BENZALDEHYDE P](#) [METHOXY GROUP](#) [ELEMENTAL ANALYSIS](#) [IR](#) [<sup>13</sup>C NMR](#) [MS](#)

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