

综述与进展

芳醛-*N*-(1-苯基-1*H*-四唑-5-巯基)乙酰肼的微波合成及其晶体结构

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收稿日期 2005-6-8 修回日期 2005-10-25 网络版发布日期 接受日期

摘要 在微波辐射下快速、高产率地合成了一系列含有四唑环的酰肼类化合物, 并对其进行了元素分析、红外以及核磁共振氢谱和碳谱表征. 对化合物**4a**的无色晶体进行了X射线晶体衍射. 结果表明, 该晶体属三斜晶系, 空间群 $P-1$, $V=0.80070(38) \text{ nm}^3$, $Z=2$, $D_c=1.404 \text{ g}\cdot\text{cm}^{-3}$, $a=0.7382(1) \text{ nm}$, $b=0.9992(2) \text{ nm}$, $c=1.1535(2) \text{ nm}$, $\alpha=81.41(2)^\circ$, $\beta=85.72(2)^\circ$, $\gamma=72.21(2)^\circ$, 分子结构呈反式构型, 通过分子间氢键组装成二聚体.

生物活性测试发现部分化合物具有抗菌活性.

关键词 [四唑](#) [酰肼](#) [微波辐射](#) [生物活性](#)

分类号

Microwave Assisted Synthesis and Crystal Structure of Arylal-dehyde- *N*-(1-phenyl-1*H*-tetrazole-5-yl)thiol Acetyl Hy-drazones

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Abstract A series of hydrazone compounds containing tetrazole ring were synthesized rapidly in high yields under the condition of microwave irradiation and confirmed by elemental analysis, IR, ^1H NMR and ^{13}C NMR spectra. The crystal structure of compound **4a** was determined by X-ray diffraction method. It belongs to triclinic system with space group $P-1$, $a=0.7382(1) \text{ nm}$, $b=0.9992(2) \text{ nm}$, $c=1.1535(2) \text{ nm}$, $\alpha=81.41(2)^\circ$, $\beta=85.72(2)^\circ$, $\gamma=72.21(2)^\circ$, $D_c=1.404 \text{ g}\cdot\text{cm}^{-3}$, $V=0.8007(38) \text{ nm}^3$, $Z=2$. The crystal structure shows that the compound has *trans* configuration and characteristic dimers connected by intermolecular hydrogen bond. The bioassay result indicates that some of the compounds have relatively low antibacterial activity.

Key words [tetrazole](#) [acylhydrazone](#) [microwave irradiation](#) [bioactivity](#)

DOI:

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