

研究论文

4-(1,2,4-三唑-5-酮-4-基)-3-硫代脲酸乙酯的合成、晶体结构及理论计算

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摘要 4-氨基-1,2,4-三唑-5-酮(ATO)与硫氰酸钾、氯甲酸乙酯在乙酸乙酯中反应,合成了4-(1,2,4-三唑-5-酮-4-基)-3-硫代脲酸乙酯,在室温下采用缓慢蒸发溶剂二甲基甲酰胺得到合适的可用于X射线衍射的单晶.

晶体属六方系,空间群为 $R\bar{3}$,晶体结构参数为 $a=2.60524(7)$ nm, $b=2.60524(7)$ nm, $c=0.82579(6)$ nm, $\gamma=120^\circ$, $V=4.8540(4)$ nm³, $D_c=1.442$ g/cm³, $\mu=0.300$ mm⁻¹, $F(000)=2190$, $Z=18$, $R_1=0.0569$, $wR_2=0.1424$.

选取标题化合物的一个结构单元作为初始模型,运用Gaussian 03程序对化合物进行了HF/6-311G, MP2/6-311G和B3LYP/6-311G水平的几何全优化,并对其原子电荷及自然键轨道(NBO)进行了分析.

关键词 [4-氨基-1,2,4-三唑-5-酮](#) [乙氧酰基硫脲](#) [晶体结构](#) [理论计算](#) [自然键轨道](#)

分类号

Synthesis, Crystal Structure and Theoretical Calculation of 4-(1,2,4-Triazole-5-one-4-yl)-3-thiourea Carboxylic Acid Ethyl Ester

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Abstract 4-(1,2,4-Triazole-5-one-4-yl)-3-thiourea carboxylic acid ethyl ester was synthesized by mixing 4-amino-1,2,4-triazole-5-one (ATO), potassium thiocyanate and ethyl chloroformate in ethyl acetate. Single crystals suitable for X-ray measurement were obtained by slow evaporation of the solvent dimethylformamide at room temperature. The crystal belongs to rhombohedral symmetry with space group $R\bar{3}$ and crystal parameters of $a=2.60524(7)$ nm, $b=2.60524(7)$ nm, $c=0.82579(6)$ nm, $\gamma=120^\circ$, $V=4.8540(4)$ nm³, $D_c=1.442$ g/cm³, $\mu=0.300$ mm⁻¹, $F(000)=2190$, $Z=18$, $R_1=0.0569$, $wR_2=0.1424$. A crystal unit of the title compound was selected as the initial structure, and it was fully optimized by HF/6-311G, MP2/6-311G and B3LYP/6-311G methods in Gaussian 03 package, and the atomic charges and natural bond orbital (NBO) analysis were also discussed.

Key words [4-amino-1,2,4-triazole-5-one](#) [ethoxylacylthiourea](#) [crystal structure](#) [theoretical calculation](#) [natural bond orbital](#)

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