

Full Paper

N-(嘧啶-2-基)-*N'*-甲氧酰基硫脲的合成、晶体结构及量子化学研究

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摘要 用2-氨基嘧啶与硫氰酸钾、氯甲酸甲酯在乙酸乙酯中反应; 合成了*N*-(嘧啶-2-基)-*N'*-甲氧酰基硫脲; 在二甲基甲酰胺中培养出单晶。

通过X射线单晶结构分析法测定了分子结构和晶体结构; 晶体属三斜系; 空间群为*P*-1; 晶体结构参数为*a*=0.72152(4); *b* = 0.82056(4); *c* =0.90772(5); α =105.141(4)°; β =94.588(4)° γ =115.415(4)°; *V*=0.45704(4) nm³; *D*_c=1.542g/cm³; μ =0.333 mm⁻¹; *F*(000)=220; *Z*=2. 采用DFT-B3LYP/6-311G、HF/6-311G和MP2/6-311G方法对标题化合物进行几何全优化; 并对其成键情况、原子电荷分布、分子轨道能量进行了分析。

关键词 [2-氨基嘧啶](#); [硫脲](#); [合成](#); [晶体结构](#); [量子化学研究](#)

分类号

Preparation, Crystal Structure and Theoretical Calculation of *N*-(Pyrimidin-2-yl)-*N'*-methoxycarbonyl-thiourea

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Abstract The compound, *N*-(pyrimidin-2-yl)-*N'*-methoxycarbonyl-thiourea, has been synthesized. The single crystal structure has been determined by an X-ray diffractometer. The crystal belongs to triclinic with space group *P*-1 and *a*=0.72152(4) nm, *b*=0.8056(4) nm, *c*=0.90772(5) nm, α =105.141(4)°, β =94.588(4)°, γ =115.415(4)°, *F*(000)=220, the unit cell volume *V*=0.45704(4) nm³, the molecule number in one unit cell *Z*=2, the absorption coefficient μ =0.333 mm⁻¹, the calculated density *D*_c=1.542 g/cm³. The theoretical investigation of the title compound was carried out with B3LYP/6-311G, HF/6-311G and MP2/6-311G methods, and the atomic charges and natural bond orbital analysis were also discussed.

Key words [2-aminopyrimidine](#) [thiourea](#) [synthesis](#) [crystal structure](#) [quantum chemical investigation](#)

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