

研究论文

## 5-氟胞嘧啶互变异构的密度泛函理论计算

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**摘要** 采用BH-HLYP/6-311+G\*\*方法对10种气相和水相中可能存在的5-氟胞嘧啶互变异构体进行了几何全优化,并计算出它们的总能量和吉布斯自由能. Onsager反应场溶剂模型用于水相的计算. 计算结果表明, 5-氟胞嘧啶在气相中主要以烯醇式-氨基式形式存在, 在水相中主要以酮式-氨基式形式存在.

溶剂化自由能与异构体的气相偶极矩存在相关性. 进一步求得互变异构化以及构象异构化和顺反异构化的过渡态, 探讨异构化过程中的几何结构和能量的变化.

**关键词** [5-氟胞嘧啶](#) [互变异构](#) [密度泛函理论方法](#) [自洽反应场方法](#) [过渡态](#)

分类号

## Density Functional Theory Calculations on Tautomerism of 5-Fluorocytosine

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**Abstract** The preference conformations of 10 possible tautomers of 5-fluorocytosine were calculated by the BH-HLYP/6-311+G\*\* method, in both the gas and aqueous phases, with full geometry optimization. The Onsager solvation model was employed for aqueous solution calculations. The total energy, standard enthalpy, standard entropy and standard free energy were obtained. The calculations show that 5-fluorocytosine to exist as the enol-amino form is the predominant isomer in the gas phase, while the keto-amino form is the predominant isomer in the aqueous phase. The entropy effect on the Gibbs free energy of 5-fluorocytosine is very small and there is little significance for the tautomeric equilibria. The enthalpic term is dominant in the determination of tautomeric equilibria. The free energy of solvation was well correlated with the dipole moments of 5-fluorocytosine tautomers. In addition, the structure and mechanism of isomerization of 5-fluorocytosine were also studied by DFT method at BH-HLYP/6-311+G\*\* level.

**Key words** [5-fluorocytosine](#) [tautomerism](#) [density functional theory method](#) [self-consistent reaction field method](#) [transition state](#)

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