

研究论文

5-氟尿嘧啶和5-氯尿嘧啶及其互变异构体的理论计算研究

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摘要 采用HF/3-21G方法,对6种气相和水相中可能存在的5-氟尿嘧啶(和5-氯尿嘧啶)互变异构体进行了构象分析.采用B3LYP/6-311+G**方法对处于优势构象时的各互变异构体进行了几何全优化,并计算出它们的总能量、焓、熵、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-氟尿嘧啶和5-氯尿嘧啶在气相中和水相中主要以双酮形式存在. 5-氟尿嘧啶和5-氯尿嘧啶的熵效应小,对互变异构平衡没有显著的影响,而焓变对互变异构产生了主要的影响. 讨论了水溶剂化作用对异构体的能量、电荷分布和偶极矩的影响. 溶剂化自由能与异构体的气相偶极矩存在相关性. 另外,详细地将5-氟尿嘧啶和5-氯尿嘧啶与尿嘧啶进行了对比,获得三者最稳定异构体间电子结构异同的有用信息.

关键词 [5-氟尿嘧啶](#) [5-氯尿嘧啶](#) [互变异构体](#) [密度泛函理论方法](#) [自洽反应场方法](#) [偶极矩](#)

分类号

Theoretical Studies on Tautomers of 5-Fluorouracil and 5-Chlorouracil

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Abstract The conformational properties of 6 possible tautomers of 5-fluorouracil or 5-chlorouracil were studied by using HF/3-21G method. On this basis, preference conformations of tautomers were calculated by the B3LYP/6-311+G** method, both in the gas and aqueous phases, with full geometry optimization. The Onsager solution theory 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-fluorouracil and 5-chlorouracil existing as the dione forms are the predominant isomers in the gas and aqueous phases. The entropy effect on the Gibbs free energy of 5-fluorouracil and 5-chlorouracil 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 is well correlated with the dipole moments of 5-fluorouracil and 5-chlorouracil tautomers. In addition, the electronic structural parameters of 5-fluorouracil and 5-chlorouracil were compared with those of their parent uracil to obtain some valuable information.

Key words [5-fluorouracil](#) [5-chlorouracil](#) [tautomer](#) [density functional theory method](#) [self-consistent reaction field method](#) [dipole moment](#)

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