

## عنوان مقاله:

DFT Investigation of transition state of tautomerism in 6-flourothymine in Cyclohexane

## محل انتشار:

ششمین کنگره ملی تحقیقات راهبردی در شیمی و مهندسی شیمی با تاکید بر فناوری های بومی ایران (سال: 1398)

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## خلاصه مقاله:

Studies of tautomerism phenomena have been valuable in many areas of chemistry a demonstrated by several reviews. [1,2,3,4. ] points of view, partly due tosuggestions that the presence of unusual tautomers may have important biological properties,such as mutagenesis.One hypothesis suggests that the frequency of mispairing in DNA andthus, mutagenesis is correlated with equilibrium constants for the keto-enol or amino±imino tautomerisation [5]. In the present work, a complete TS scheme for tautomers for FT (Fig. 1) were studied using B3LYP/6- 311++G(d,p) level of theory. In addition, From the calculations, thermodynamic properties of TS of tautomerism equilibrium in FT were obtained. Thence, the effects of solvent on the TS of equilibrium have been investigated using Cyclohexane as . solvent

## کلمات کلیدی:

Tautomerism, 6-flourothymine, SCRF, Cyclohexane, B3LYP, TS

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