



SDI Review Form 1.6

PART 1:

Journal Name:	American Chemical Science Journal
Manuscript Number:	2012_ACSJ_2905
Title of the Manuscript:	Theoretical Study of Stability, Tautomerism, Equilibrium Constants (pK_T) of 2-Thiouracil in Gas phase and Different solvents (water and Acetonitrile) by the Density Functional Theory Method

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- This form has total 9 parts. Kindly note that you should use all the parts of this review form.



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PART 2: Review Comments

	Reviewer's comment	Author's comment (if agreed with reviewer, correct the manuscript and highlight that part in the manuscript. It is mandatory that authors should write his/her feedback here)
<u>Compulsory</u> REVISION comments	This paper deals essentially only with quantum calculations. There is no comparison with experiment, and therefore there is no information whether the calculated data make any sense. I expect there will be experimental information available in literature. This should be incorporated. Purely theoretical work of this kind seems to make little sense, in my view.	The number papers in literature deals only with quantum calculations. In this paper we determine the molar transfer Gibbs energies and inter conversion of tautomers of 2-thiouracil are Presented in first time. So no literature values are available. Two important references on this topic are available but we are not accible this references because of this articles are paid articles. (a) Yekeler H. 'Ab initio study on tautomerism of 2-thiouracil in the gas phase and in solution' J Comput Aided Mol Des. 2000 Mar;14(3):243-50. (b) Andrzej Leit and Ludwik Adamowicz, 'Tautomerism of 2- and 4-Thiouracil. Ab Initio Theoretical Study' J. Am. Chem. Soc., 1990, 112, 1504. 5. Line 25: 'Tautomerisation' should be replaced with 'Tautomerism'.
<u>Minor</u> REVISION comments		



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<u>Optional/General</u> comments	Please note spelling errors, e.g. Line 8 dipole moments Line 14: solvnet -> solvent (see also, e.g, Table 4 same spelling issues) Two sentences in abstract do not run smoothly, I mean connection between first and second part of the sentences: The relative energy value indicates that tautomer 2TU1 is the most stable tautomer in both gas and solution phase and to calculate the inter conversion of equilibrium constants for all tautomers. In addition to calculate the thermodynamic properties and the values of $\Delta \Delta G^0(\text{solvnet1-solvent2})$, determines the solvent effect on the position of the equilibrium.	Line 8: corrected Line 14: corrected Table 4: corrected The two sentences in abstract are corrected, as All calculations indicate that the most stable tautomer for both species, in the gas phase as well as in solution, has the 2TU1 form. In addition to calculate the thermodynamic properties and the inter conversion equilibrium constants for all tautomers. The molar transfer Gibbs energies of $\Delta \Delta G_t^0(\text{solvent1- solvent2})$, determines the solvent effect on the position of the equilibrium.
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