



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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PART 2: Review Comments

	Reviewer's comment	Author's comment <i>(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)</i>
<u>Compulsory</u> REVISION comments	1. While the author studies the relative stability of different tautomers of 2-thiouracil, the determination of zero point vibrational energy as well as heat capacities in Table 2 makes very little sense. Even the author does not provide any discussion about these parameters in the results and discussion part and in conclusion. While the dipole moment is important for their polarisations in solvents, the other two parameters do not contribute to the overall conclusion. 2. The author determines the thermodynamic properties of tautomers such as Gibbs free energy, enthalpy and entropy. A better discussion on those parameters for the inter-conversion and the stability of some tautomers could be provided. Overall a proper analysis of the obtained data is missing in the whole manuscript. 3. Similarly, some trends on the equilibrium of different tautomers could be described in the last section of the manuscript, based the positive and negative values of equilibrium constants as obtained from the calculations shown in Tables 5 and 6. 4. Two important references on this topic are missing. (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'. The author can better use the same	1. As the reviewer comment the zero point vibrational energy as well as heat capacities in Table 2 are removed and in the text also. 2 and 3, the author, revised and give the detail discussion. 4. 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 accessible 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.



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	convention throughout the manuscript. 6. Lines 94-99: The sentence is too big and is not correct grammatically. The author should revise it by making it a meaningful discussion. 7. Line 102: The order of relative 'energies' should be replaced with 'stabilities'. 8. Line 116: 'movement' should be replaced with 'moment'. Please correct this in some other places as well. 9. Line 125: 'expect' to be corrected with 'except' 10. Line 139: 'Eq.5' should be 'Eq.6'. 11. Line 169-170: 'Table 4' must be corrected with 'Table 5'. 12. All the Tables 1-6 should be revised carefully. The order of parameters should be followed uniformly starting from....gas phase.....water....acetonitrile. This is different in Table 1. In all the Tables, the columns are not aligned properly, making the data sets very difficult to understand. The author should make proper columns with appropriate column headings for the data.	(b) Andrzej Leit and Ludwik Adamowicz, 'Tautomerism of 2- and 4-Thiouracil. Ab Initio Theoretical Study' J. Am. Chem. Soc., 1990, 112, 1504. Justification: The author mainly concentrates on the molar gibbs free energy of salvation and interconversion of tautomers. So there are no literature values of above calculations. 6. Lines 94-96: corrected as From the table 1 shows that the mono-enol tautomers of thio-enol (2TU11&2TU12) and keto-enol (2TU9&2TU10) tautomers have highest energy, with relative energy about 20-25 kcal mol⁻¹. Because of the possibility of migration of hydrogen atoms, and eliminating the simultaneous transfers little likely of more than atom, only the exchange of hydrogen atom between heteroatom spatially close and separate by more than two atoms can be carried out. 7. Line 102: corrected , 8. line 116: corrected, 9. Line 125: corrected, 10. Line 139 corrected, 11. line: 169-170: corrected, 12. All the tables sre revised.
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Minor REVISION comments	1. There are many spelling mistakes and problems with the proper construction of sentences throughout the manuscript. Author should revise the manuscript carefully making the sentences shorter in some cases, with scientific language and clearer to the readers.	All spelling mistakes and grammatical mistakes are corrected.
Optional/General comments	The theoretical study by N. S. Babu describes the tautomerism and the relative stability of different conformers of 2-thiouracil. Similar study has been reported earlier by different authors starting back 1990s. As the present study considers more number of tautomers for comparison with determination of different thermodynamic parameters, the manuscript can be published in ACSJ but only after a major revision.	