



SDI Review Form 1.6

Journal Name:	Asian Journal of Chemical Sciences
Manuscript Number:	Ms_AJOCS_43438
Title of the Manuscript:	Theoretical Investigation of Spectroscopic, Electronic and Thermodynamic Properties of [2-Methoxy-4-(3-methyl-4,5-dihydro-1H-1,2,4-triazol-5-one-4-yl)-azomethinphenyl acetate molecule
Type of the Article	Original Research Article

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PART 1: 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)
Compulsory REVISION comments	The article is about theoreti,cal ctudy for [2-Methoxy-4-(3-methyl-4,5-dihydro-1H-1,2,4-triazol-5-one-4-yl)-azomethinphenyl acetate molecule with (DFT/B3LYP) and Hatree Fock (HF/B3LYP) methods. There were grammatical mistakes such as "Experimental data obtained from the literature", In the last year, thereotical properties of Schiff bases were investigated on a computer", These values for compound were given in the table 2, "IR spectrums were drawn with obtained values according to HF and DFT method. Theoretically IR values were compare with experimentally IR values.The result of this compare were found corresponding with each other of values. "Theoretically IR values were compare with experimentally IR values. And etc. There were some typo errors such as "atalysts" "exzamed" 1H-NMR and 13C-NMR should be written as otherwise it was used incorrectly. What means below sentence "There is such a relation ship between R2-values of the compound" Experimental C=O peak assigned at 1770, 1700 were calculated at 1740. Why is the reason? It is said according to the calculation the longest bond length is between C11-C12 atoms that this value is 1.50 Å. Why? The molecule is not big. Why is 6-31G(d,p) basis set used. It should use more accuracy basis set. In Figure 4. HOMO-LUMO energy of the molecule calculated with DFT were given twice. There is no explanation for Table 8, Table 9 and Figure 5	1. Grammatical mistakes corrected. 2. Some word errors such as "atalysts" "exzamed" corrected. 3. 1H-NMR and 13C-NMR corrected. 4. Experimental C=O peak assigned at 1770, 1700 but, vibration frequency of theoretical C=O peak calculated at 1740. This values are compatible with each other. 5. The highest bond length is between C11-C12 atoms that this value is 1.50 Å. Because this value is obtained with the theoretical calculation and is the highest value among all theoretic bond angles given in table 4. 6. I worked with the 6-311G(d,p) basis set but I could not finish it due to the problems that occurred in my computer. For this reason I did work again with 6-31G (d) basis set. This basic set gives results in less time and the results obtained by this set are supporting experimental values. 7. In Figure 4. corrected. 8. Explanation for Table 8, Table 9 and Figure 5 added. Necessary corrections were made and sent back to manuscript. Thank you...
Minor REVISION comments		
Optional/General comments		