

Review Form 1.6

Journal Name:	Asian Journal of Research and Reviews in Physics
Manuscript Number:	Ms_AJR2P_77309
Title of the Manuscript:	THEORETICAL STUDY OF SOLVENT EFFECTS ON THE ELECTRONIC AND THERMODYNAMIC PROPERTIES OF TETRATHIAFULVELENE (TTF) MOLECULE BASED ON DFT
Type of the Article	Original Research Article

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This journal's peer review policy states that **NO** manuscript should be rejected only on the basis of '**lack of Novelty**', provided the manuscript is scientifically robust and technically sound. To know the complete guideline for Peer Review process, reviewers are requested to visit this link:

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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	<p>The sections 4.3 (GCRD), 4.4 (Thermodynamics properties) 4.5 (NLO) and 4.7 (IR intensities) should be explained in more depth. In these sections, the interpretation of the results should be more justified. Currently, the authors only show the orders of TTF reactivity based on the solvents studied. The authors have very attractive information that they could communicate to the scientific community.</p> <p>For example one should expect that the polarizability of TTF increases with decreasing polarity of the solvents, while the anisotropic polarizability behaves the opposite.</p> <p>Although the TTF molecule has been studied previously, the authors should include a figure showing the chemical structure and the enumeration used. In this way, the results of bond distances and angles can be better understood.</p> <p>Currently there are other previous works focused on the same molecule, however, these works could be used to revalue the results presented in this manuscript. In this sense, it could be confirmed if the statement " <i>Interestingly, the order of stability increases with an increase in polarity of the solvents</i> " is extensible for all the solvents studied, or only that order is for the solvents studied by these authors.</p>	
Minor REVISION comments	<p>There are several abbreviations that are not defined, such as OPDOS or IRPAL, please include the definition when the term is first introduced.</p> <p>Check the numbering of sections 4.x they are not well indicated.</p> <p>On page 7, authors should check the phrase: "The HOMO-LUMO gap of 3.6330 eV obtained in the gas phase is found to be very close to 3.6300 eV of an isolated TTF molecule reported by [18]" because it is not correct.</p>	
Optional/General comments	<p>In general, the manuscript is well structured, but a revision is required to extract valuable information contained in the results and should be reflected in the manuscript.</p>	

PART 2:

	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)
Are there ethical issues in this manuscript?	<i>(If yes, Kindly please write down the ethical issues here in details)</i>	

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