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**

General guideline for Peer Review process:

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	**Author(s) should eenly address issues : 1-9 in the reviewer's comments, in addition to the highlighted issues with suggestions in the Ms word manuscript review format(see attachment)**	
Minor REVISION comments	The suggested modifications and editing owing to typo errors, equations, slight grammatical errors and omission should be addressed.	
Optional/General comments	- Author(s) present(s) an extended study on the properties of the Tetrathiafulvelene (TTF) compound. This compound has been extensively studied in the past theoretically, but almost all studies concern on the structural, effect of solvents (water, acetone, Tetrahydrofuran (THF), Carbon tetrachloride (CCl4), and benzene) polarity on the frontier molecular orbitals energy gap and global chemical reactivity of TTF in order to understand its stability and reactivity in a different solvents. Authors in the present study first reproduce some of these results and then use them to extract some other useful information like bond lengths and bond angles, optoelectronic properties, density of states (DOS), nonlinear optical (NLO) properties, IR spectra analysis and thermodynamic responses in gas phase and in toluene, dichloromethane ,acetone and acetonitrile solvents using Gaussian 03 simulation package . **Thus, the manuscript contains novel results and deserves publication.** **But prior to acceptance several issues should be resolved**. The author(s) can consider the following points **in addition to the overall modifications and editing raised in the attachment manuscript in reviewed format:** 1- TITLE: The title reflects exactly the content of submission, but needs some modifications as indicated in the reviewed format of the manuscript (see attachment) 2- KEY WORDS: OK 3- SUITABILITY OF PUBLICATION IN THE JOURNAL: The submission is relevant. 4- ABSTRACT: Well written, but needs some editing as indicated in the reviewed format(see attachment) and in the line 3 of the abstract, the compound word should be- 'density functional theory' not density functional study. 5-' Titled compound' appeared severally in the report, change to TTF compound / TTF molecule 6- Several modifications and editing owing to typo errors, technical issues, etc have been suggested(see as attachment, the reviewed format of the manuscript. 7- The optimization parameters used for the relaxation of the structure are not stated in the report. 8- Pls, show relaxed crystallographic structures of the TTF need, if possible in	

	configurations of the considered solvents.(the materials studio or Xcrysden would help). 9- Pls, discuss the correlation between stability and reactivity.	

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?	*(If yes, Kindly please write down the ethical issues here in details)*	

Reviewer Details:

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