Review Form 1.6

Journal Name:	**Journal of Energy Research and Reviews**
Manuscript Number:	**Ms_JENRR_84391**
Title of the Manuscript:	**ELECTRONIC STRUCTURE AND IR SPECTRA ANALYSIS OF TETRATHIAFULVELENE (TTF) USING RHF AND DFT QUANTUM MECHANICAL METHODS**
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:

(https://www.journaljenrr.com/index.php/JENRR/editorial-policy)

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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 manuscript describes a set of calculations on the pure molecule of TETRATHIAFULVELENE (TTF), with the RHF and DFT methods. Strictly speaking, there is nothing new in the results presented, since the first generation of this molecule was discovered 50 years ago and, in the meantime, more than 10,000 articles have been published on the most varied aspects of its structure. At present, the main research focus has been on chemical variations of TTF including doping by other atoms, for the production of semiconductor materials for application in micro-electronics.** **The authors claim that their calculations with RHF are pioneering as far as they know, but there are many calculations available in the literature with this method in derivatives of the TTF, see for example Ref.[1]; so it would be interesting for the authors to comment on this reference and if they plan to address doped molecules in the future.** **The major current trend in the use of the DFT method is due to its faster convergence, which is due to the disadvantage of the RHF method, which depends on a more precise prior knowledge of the shapes of the wave functions integrating the orbitals that form the bases for implementing the computation of the parameters of the molecule. However, the material may be published, provided that a number of glaring deficiencies in the manuscript are corrected, namely:** **1. There are several mistakes in the writing of the formulas, which is a very serious issue in an article in a high-precision field (highlighted with a yellow marker in the revised manuscript). In the introduction itself, the chemical formula of TTF is wrongly written as C6H4C2, which should be corrected to C6H4S4. Further down are several sign errors in the definitions of electronegativity and chemical potential. The correct definitions can be obtained from Ref.[1], formulas 7 to 12.** **2. There are a huge amount of grammatical mistakes in the text (highlighted with a yellow marker and corrected in red ink in the revised manuscript), mainly a lack of definite or indefinite articles, verbs with wrong tenses, wrong commas, and missing adverbs (aside from some old-fashionable English, though there be a matter of style). This type of mistake requires the authors to submit the manuscript for review by a native English speaker so that it conforms to the grammatical norms of standard English.** **Other than that and the lack of novelty aside, the rest of the material is in the correct format, so as long as the aforementioned corrections are made, I recommend it for publication.** **Reference.** **[1] G.F. Olinga Mbala, M.T. Ottou Abe, Z. Ntieche, G.W. Ejuh, J.M.B. Ndjaka, Heliyon 7 (2021) e07461, 1-30.**	
Minor REVISION comments		
Optional/General comments		

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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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