

Review Form 1.6

Journal Name:	Journal of Energy Research and Reviews
Manuscript Number:	Ms_JENRR_92704
Title of the Manuscript:	Effects of mono-halogen-substitution on the Electronic and Non-Linear Optical Properties of Poly(3-hexylthiophene-2,5-diyl) for Solar Cells Applications: A DFT Approach
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>)

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	Thermodynamic Properties The thermodynamic parameters presented in Table 5 are zero-point vibrational energy (ZPVE), total entropy (S) and molar heat capacity (Cv), which arise from contributions of electronic, translational, rotational constants and vibrations. They were calculated at constant temperature and pressure of about and respectively. The analysis of thermodynamic parameters is important in the estimation of the outcome of a chemical reaction [40] How calculate these parameters and calculate the activation energy.	
Minor REVISION comments	Give detail discussions about thermodynamic properties and the role of activation energy and entropy	
Optional/General comments	I strongly accept this paper to publish in this journal minor revision after give detail discussion of thermodynamic properties and degree of purity Poly(3-hexylthiophene-2,5-diyl) with the acronym P3HT and its derivatives	

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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