

Review Form 1.6

Journal Name:	International Research Journal of Pure and Applied Chemistry
Manuscript Number:	Ms_IRJPAC_83870
Title of the Manuscript:	Computational study of some heterocyclic compounds as corrosion inhibitors for aluminum using the DFT method
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.journalirpac.com/index.php/IRJPAC/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	<ul style="list-style-type: none"> -Generally, in all the text the sentences are either pasted or separated due to the change of word version or problem of typescript (the authors must check them). -In the part of computational studies, the authors must quote some references on this method used in the corrosion like: <ul style="list-style-type: none"> - Attar, T., Nouali, F., Kibou, Z. et al. Corrosion inhibition, adsorption and thermodynamic properties of 2-aminopyridine derivatives on the corrosion of carbon steel in sulfuric acid solution. J Chem Sci 133, 109 (2021). https://doi.org/10.1007/s12039-021-01971-w - Benchadli, A. Attar, T., Messaoudi, B., Choukchou-Braham, E. (2021). Polyvinylpyrrolidone as a Corrosion Inhibitor for Carbon Steel in a Perchloric Acid Solution: Effect of Structural Size. <i>Hungarian Journal of Industry and Chemistry</i>, 49(1), 59–69. https://doi.org/10.33927/hjic-2021-08 - Attar, T., Benchadli, A, Mellal T et al. Use of Experimental Designs to Evaluate the Influence of Methyl Green Dye as a Corrosion Inhibitor for Carbon Steel in Perchloric Acid. <i>Malaysian Journal of Chemistry</i>, 2021, Vol. 23(1), 60-69 - N. Benhadria, B. Messaoudi, T. Attar, The Study of the Correlation between the Detection Limit and the Energy Stability of Two Antimony Complexes by Means of Conceptual DFT. <i>Malaysian Journal of Chemistry</i>, 2020, 22(2), 111-120 In Results and Discussion: where the ionization potential (I) and the electron affinity (E) (Affinity is A instead of E) -The reference [18] is not necessary to show the Hartrees to ev conversion (it is known). -The references should be written following the instruction of the journal. -Authors should show agreement between inhibitory efficacy (IE%) and theoretical calculations in Table 3. -Figure 2 must move and interpret in the result and discussion part. We do not put a figure or table in the conclusion. -The conclusion should be reformulated for to show the importance of this work. 	
Minor REVISION comments		
Optional/General comments		

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>	

Reviewer Details:

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