

REVIEWER'S REPORT

Manuscript No.: IJAR-54149

Date: 03/09/2025

Title: Corrosion inhibition properties of 2-methylchromeno[2,3-c]pyrazol-3(2H)-one for Aluminum in sulfuric acid medium: Gravimetric and Quantum Chemical Studies

Recommendation:

Accept as it is

Accept after minor revision.....

Accept after major revision

Do not accept (*Reasons below*)

Reviewer Name: Dr Gulnawaz

Detailed Review Report

The manuscript investigates the inhibition efficiency of 2-methylchromeno[2,3-c]pyrazol-3(2H)-one (MCP) for aluminum corrosion in sulfuric acid medium through gravimetric methods supported by density functional theory (DFT) calculations. The study is relevant for corrosion science and materials chemistry, with strong emphasis on both experimental and theoretical insights. The results demonstrate that MCP is an effective green inhibitor, and the adsorption follows Langmuir isotherm with mixed physical–chemical character.

The work is original, methodologically sound, and provides comprehensive data. However, the manuscript would benefit from **structural refinement, language polishing, and improved figure/table referencing** before publication.

Major Comments

1. Abstract

- The abstract is lengthy and contains too many details (e.g., exact IE% values at different temperatures). It should be shortened to highlight **background, methods, main findings, and novelty**.

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2. Introduction

- Well written but repetitive in some parts (e.g., inhibitor types and adsorption mechanisms). This could be streamlined for better clarity.
- Please cite more recent studies (2021–2024) on aluminum corrosion inhibitors, especially heterocyclic compounds, to strengthen the literature context.

3. Materials and Methods

- The synthesis description is clear but lacks a reaction scheme. A **figure showing the structure of MCP** should be included early in this section.
- Details on **replicates and statistical treatment of gravimetric data** should be explicitly stated (e.g., average of three measurements with \pm SD).
- DFT section: specify the **basis set and functional** clearly in one sentence without repetition.

4. Results and Discussion

- Figures (mass loss vs. time, IE% vs. concentration, adsorption isotherms, etc.) must be **clearly referenced and numbered sequentially**.
- Activation parameters: clarify the role of enthalpy/entropy in terms of adsorption nature.
- Some results are repeated (e.g., Langmuir fitting and mixed adsorption mechanism appear multiple times). Please condense.

5. Computational Studies

- The discussion of frontier orbital energies and global reactivity descriptors is comprehensive, but could be **shortened** and more directly linked to experimental inhibition efficiency.
- Provide a **figure of HOMO and LUMO plots** for MCP (if available).

6. Conclusion

- The conclusion is informative but verbose. It should be reduced to **3–4 strong take-home points**.

Minor Comments

- Correct typographical errors:
 - "inhiibitor" → "inhibitor"
 - "Sufuric" → "Sulfuric"

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- "efficiency of corrosion inhibition **can increase** as a result of adsorption" (grammar correction).
- References need uniform formatting (journal abbreviations, volume/issue, page numbers).
- Units: Write consistently as °C, g/L, cm², etc.
- Ensure all acronyms (e.g., IE%, DFT, HOMO, LUMO) are defined at first use.