Reviewer's Comment:

1. As the authors have not isolated the species from the mixture it is likely that each and every functional group present in the molecule under consideration would likely to accelerate or inhibit the corrosion of Aluminum. In so what will be net effect and the interpretation of the theoretical calculation made?	It is impossible to study the net effect theoretically. We deal with single molecule and not the bulk.	It is the hetero atoms/lone pairs/pai bonds mainly involved in the process of adsorption leading to the prevention of corrosion of a material. Whole molecule is rarely involved. How could they obtain/isolated single molecule to deal with? If it is not done so what is the sanctity of the work/data?
2.HOMO and LUMO values are with the negative sign (Table 1). How the authors could state HOMO is of higher value than LUMO and also how to expect the transfer of electron from HOMO to LUMO?	LUMO is higher value than HOMO and we substrate LUMO from HOMO to obtain the energy gap: LUMO-HOMO	OK
3.Explanation/reason provided for the Data of Table 2 is not sufficient. It is difficult to understand why the calculations (LUMO inh – HOMO Al (eV) LUMO Al – HOMO inh (eV)) are made and in what way it helps in stating that inhibitor is of anodic or cathodic type. What sort of inference can be drawn from LUMO inh – HOMO Al calculation? Method of evaluation of HOMO or LUMO is not available. Basis for the separation of different inhibitors into cathodic and anodic inhibitor is not available in the text. Can it be decided just by free energy value?	The explanation is giving at the beginning of page 4 "The chemical reactivity is a function ……" line 87. Also, the explanation for interaction is given in lines before table 2. Mesembrenone shows strong interactions in the case of anodic and cathodic type. HOMO and LUMO for Al are obtained from Ref. 25.	It was asked to give relation/correlation between energy and cathodic/anodic corrosion prevention. What is the energy needed for the corrosion process? Is there any activation energy involved for the process?. If involved how do you call it as a spontaneous process? Without it the paper may not be of any interesting to the reader.
4. Method of evaluation of all the parameters of Table 3 is not known and moreover they have not been defined. Value of ΔN is too small and are almost equal (within the exptl.error?) to take any decision on the nature of bond present in the system (electrovalent or covalent), Electrophilicity value (ω) is the highest in case of Mesembren. It means it is a good acceptor of electron. Then how does the conclusion - Mesembren is a good inhibitor -arises?	Mesembrenone shows strong interaction in the case of cathodic 4.38 eV and anodic 4.98 eV (Table2) as compared to other three compounds. Thus Mesembrenone is considered to be a good inhibitor.	Method of evaluation of all the parameters of Table 3 is not known and moreover they have not been defined. So it is difficult for a reader to understand it.
5. Mesembrenone which has the lowest energy gap - Electron transfer is expected from HOMO of the species to LUMO of the metal. It is difficult to understand the authors decision that the largest inhibition efficiency is for the species Mesembrenone species?	Electron transfer from HOMO of the metal to LUMO of Mesembrenone to give strong interaction 4.39 eV as cathodic inhibitor (Table2). Cathodic and anodic (Back donation).	OK

6. All adsorption processes are spontaneous with a negative sign to ΔG . But on P.7 ΔG is shown with a positive sign.	No, we did not say that. We said that all compounds show positive Gibbs free energy except Mesembrenone (page7).	Ok.
7. P.6: Statement "Al atoms can accept electrons from inhibitor molecule to form a coordinated bond" (anodic inhibitor). How to support the statement?	Table 2 shows clearly the strong interaction between the HOMO of the inhibitor and LUMO of Al and also the HOMO of Al and LUMO of inhibitor especially for Mesembrenone.	Without the statement on the mode of interaction the paper appears to be incomplete.
8. P 6:Explanation /mode of action for donation and back-donation processes strengthen the adsorption of Mesembrenone onto the aluminum surface and increase the inhibition efficiency is required Authors have given some theoretical foundation for the experimentalists to probe further before and either to approve or disapprove the fact. Theoretical materials scientists will really appreciate the content. However, the manuscript can be considered for publication as a note in the journal only after getting satisfactory explanation for above queries.	Again see table 2 to compare the interactions between four compounds.	It is not the data in a table could answer the question. Explanation for the mode of action is needed and without it the manuscript becomes incomplete.

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