



SDI Review Form 1.6

Journal Name:	Physical Science International Journal
Manuscript Number:	Ms_PSIJ_36555
Title of the Manuscript:	Structural and solvent dependence of the electronic properties and corrosion inhibitive potentials of 1,3,4-thiadiazole and its substituted derivatives- a theoretical investigation.
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:

(<http://www.sciencedomain.org/page.php?id=sdi-general-editorial-policy#Peer-Review-Guideline>)



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PART 1: Review Comments

	Reviewer's comment	Author's comment <i>(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)</i>
<u>Compulsory</u> REVISION comments	<p>HOMO means Highest occupied molecular orbital, LUMO is Lowest unoccupied molecular orbital. It is written HOMO LUMO orbital energies.Delete orbital.</p> <p>The molecules are small. They should use larger basis sets for example 6-311++G(2d,2p).</p> <p>The sentence "The electronegativities of –CH₃ and –NH₂ are lower than that of unsubstituted 1,3,4-thidiazole" should be written again</p> <p>In Table 2 oscillator strength and excitation energies are not given. Relationship between electronic properties of molecules and experimental value should be given in more detail.</p> <p>Are there any experimental results as corrosion inhibitors for these substances.</p>	<ul style="list-style-type: none"> • Issue with "orbital" resolved, • "The electronegativities of –CH₃ and –NH₂ are lower than that of unsubstituted 1,3,4-thidiazole" also resolved, • Oscillator strength and excitation energies were mistakenly added, they have been replaced with hyperpolarizabilities on table 2, • Experimental value is only available for the UV absorption of one of the derivatives, the corrosion inhibitive potentials were investigated based on what some researchers did, theoretically in literature.
<u>Minor</u> REVISION comments		
<u>Optional/General</u> comments		