



**SDI Review Form 1.6**

Journal Name:	<a href="#">Asian Journal of Physical and Chemical Sciences</a>
Manuscript Number:	Ms_AJOPACS_38092
Title of the Manuscript:	A theoretical study of aniline and nitrobenzene by computational overview
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>)

**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)
<b><u>Compulsory</u></b> REVISION comments	The article is related to a theoretical study of aniline and nitrobenzene by 3 computational overview Molecular mechanic studies are extensively used for structural characterization of huge molecules like proteins. These methods assume that atoms are charged particles, so it has low accuracy for relatively smaller metal complexes. If authors think a computational study, all of the metal complexes and the ligand should be studied by DFT or HF methods.	For all of the metal complexes and the ligand should not be studied by DFT or HF methods. For more accuracy, these molecules are optimized by Molecular Mechanics basis set such as Mm+or MP3. The structure of nitrobenzene and aniline are not so large like proteins. So the DFT or HF methods are more suitable methods for calculations of nitrobenzene and aniline.
<b><u>Minor</u></b> REVISION comments		
<b><u>Optional/General</u></b> comments		