



**SDI Review Form 1.6**

Journal Name:	<a href="#">Asian Journal of Chemical Sciences</a>
Manuscript Number:	Ms_AJOCS_41128
Title of the Manuscript:	Theoretical Study of High-nitrogen Salts Composed of Amine Cations and Pyrazole-based Anions
Type of the 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 (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>Compulsory</b> REVISION comments	<ol style="list-style-type: none"> <li>1. Used molecule is not direct Pyrazole. It is derivative of pyrazole. Am I right? If yes, need to change the title of the part pyrazole based Anions.</li> <li>2. In line 10, the "NH<sub>3</sub>OH<sup>+</sup>" is not correct.</li> <li>3. In line 12, mistake the –NO<sub>2</sub> front.</li> <li>4. The fig . 1 and 2 are not clear.</li> <li>5. Need working flow chart.</li> <li>6. Must add the screen shots of working and optimization process in methodology.</li> <li>7. The language of this paper is very poor.</li> <li>8. In table 2, Ref. Needs for each vale of (<math>\Delta H_{of}</math>(literature) in a column not in line 179 and 180.</li> <li>9. In line 59, Gaussian G09 is the correct form as Gaussian 09. Am I right?</li> <li>10. Add the standard value of heats of formation acts as sensitivity.</li> </ol>	<ol style="list-style-type: none"> <li>1. We changed the name of "pyrazole" to "pyrazole derived".</li> <li>2. We changed the position of cation sign on nitrogen as "<sup>+</sup>NH<sub>3</sub>OH".</li> <li>3. We have adjusted the format of the " –NO<sub>2</sub>".</li> <li>4. The fig.1 and 2 have been clarified.</li> <li>5-6. All involved pictures of optimized molecule structures were attached as supporting information in the document of opt.zip.</li> <li>7. We have improved the language.</li> <li>8. The standard values of heats of formation were listed in Table 2 and the references of these values are denoted below the table.</li> <li>9. We corrected it accordingly.</li> <li>10. The standard value of heats of formation of some small molecules and ions were listed in Table 2.</li> </ol>
<b>Minor</b> REVISION comments	<ol style="list-style-type: none"> <li>1. The term of "ionic salts" are known as ionic liquids, Author can use it as ionic liquids for specific use.</li> <li>2. The no. Of equation 3, 4, 5, 6, 7 are not in same format.</li> <li>3. All fig. Need clear image.</li> <li>4. Scheme needs clearness.</li> <li>5. Methodology is to write up more specific of Gaussian basis set.</li> <li>6. Author did not mention that why use five member ring not six member?</li> </ol>	<ol style="list-style-type: none"> <li>1. Yes, we change it to "salts".</li> <li>2. The format of equations and schemes were adjusted.</li> <li>3. All figures were redrawn.</li> <li>4. Schemes were redrawn.</li> <li>5. Gaussian basic set have been more specific.</li> <li>6. Our purpose of this paper is to probe the potential use of pyrazole-derived salts instead of comparing the five member rings with six member rings.</li> </ol>
<b>Optional/General</b> comments	<ol style="list-style-type: none"> <li>1. It is excellent and interesting work with simple example.</li> </ol>	