



SDI Review Form 1.6

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| Journal Name: | Asian Journal of Chemical Sciences |
| Manuscript Number: | Ms_AJOCS_47995 |
| Title of the Manuscript: | Comparitive study of calculated and expermintal Pka values for fluoro-acetoxy derivative |
| Type of the Article | <u>Original Research Article</u> |

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) |
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| Compulsory REVISION comments | <p>1. Editorial comments. a. This manuscript has substantial spelling, sentence structure, syntax and grammatical errors which are too numerous to list here. I have provided a partially annotated manuscript (through page 4) which highlights many of these errors as well as suggested corrections to be made.</p> <p>2. Content comments. Following are review observations and recommendations that would make this article much stronger. a. Article title. The title suggests that the fluorinated compounds in the study will receive special emphasis and analysis. Given that no such emphasis was given to F-acetates examined in the manuscript, the title is misleading and should be adjusted. b. The authors refer to "cis" and "trans" molecules. This is a stereochemical designation that is incorrectly applied in the paper. Given that the acetate derivatives have sp³ hybridized carbons around the carbon atom of interest, the correct terminology should be syn-periplanar ("cis") with respect to the carbonyl and antiperiplanar ("trans") with respect to the carbonyl. A figure that clearly shows the appropriate conformations prior to Table 1 would be most helpful to the reader to visualize the molecular geometry discussed. c. The authors have alluded to "good agreement" between experimental and calculated pK_a values. However, in the case of the "cis" molecules, a 20% or greater deviation in exp vs calc values is recorded; a much larger deviation is found in the "trans" data. Yet, there is no discussion for why this is the case. This is an important finding if the authors' contention is that the CBS-Q method is acceptable to estimate important molecular values. d. Within the data presented (Tables 2 & 3), there are several interesting trends that bear discussion. For example: (1) Why are the fluorinated derivatives substantially lower in overall energy than the nonfluorinated examples? (2) How do the authors rationalize the small differences in overall energies between the "cis" and "trans" compounds examined in light of the large differences in the pK_a values? Recommend that the authors address these issues in a revised manuscript.</p> | <p>It had been given for English improvement.</p> <p>Had been changed.</p> <p>Had been changed.</p> <p>Need to calculate pka of the same molecule by other methods.</p> |
| Minor REVISION comments | <p>1. Article title. The title contains misspelled words and must be corrected. Additionally, it is not descriptive of the work presented. Recommend changing it to include something about use of the CBS-Q method: Determination of pK_a values for substituted acetate derivatives by the CBS-Q method</p> <p>2. References. Of the 20 references cited, only 4 are published within the last 10 years. Recommend the authors consider conducting a more thorough literature review with an eye to including additional recent citations.</p> <p>3. Table and figure formatting. The Table and figure titles are inconsistently formatted. The first word of the title should be capitalized and a period should be placed at the end of the title. In addition, tables and figures should have legends that explain acronyms or terms that are not explained in the body of the manuscript.</p> | <p>Comparative study of CBS-Q calculated pka and experimental Pka values for fluoro-acetoxy derivative.</p> <p>It had been done.</p> <p>It had been done.</p> |



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| Optional/General comments | The body of work the authors have presented represents a small contribution to further understanding of ab initio calculations of pK_a values and other molecular properties for a limited series of acetates. While the work has merit, serious editorial and content-related shortcomings in the manuscript should require a revision and, in my opinion, a resubmission for another round of reviews. | |
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PART 2:

| | 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> |
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| Are there ethical issues in this manuscript? | <i>(If yes, Kindly please write down the ethical issues here in details)</i> | No, there is no ethical issues in this manuscript. |