|  |  |
| --- | --- |
|  | |
| Journal Name: | [**Chemical Science International Journal**](https://journalcsij.com/index.php/CSIJ) |
| Manuscript Number: | **Ms\_CSIJ\_141604** |
| Title of the Manuscript: | **Unveiling the Atmospheric Oxidation of E2CAA initiated by Cl Radical: DFT Study** |
| Type of the Article | **Original Research Article** |

|  |  |  |
| --- | --- | --- |
| PART 1: Comments | | |
|  | Reviewer’s comment **Artificial Intelligence (AI) generated or assisted review comments are strictly prohibited during peer review.** | **Author’s Feedback** (It is mandatory that authors should write his/her feedback here) |
| **Please write a few sentences regarding the importance of this manuscript for the scientific community. A minimum of 3-4 sentences may be required for this part.** | **Ethyl 2-chloroacetoacetate is a clear, colorless liquid with a pungent odor that is used as an important intermediate in organic synthesis, including pharmaceuticals, food preservatives, wood preservatives, pesticides, and other organic compounds.** **This organic material contains chlorine, a corrosive and irritating chemical that is also found in the atmosphere. Chemical conversion of ethyl 2-chloroacetoacetate could be a promising approach to eliminate this environmental pollutant. Understanding the reaction mechanism, kinetics, and thermodynamics, and the effective factors, is essential to advance the goals of scientists in this direction.** | Thank you for your valuable comments and we appreciate for your time and efforts. |
| **Is the title of the article suitable?**  **(If not please suggest an alternative title)** | **Yes, but “Unveiling the Atmospheric Oxidation of E2CAA Initiated by Cl Radical: DFT Study” is better.** | Necessary correction is made in revised manuscript as per reviewer’s suggestion. |
| Is the abstract of the article comprehensive? Do you suggest the addition (or deletion) of some points in this section? Please write your suggestions here. | **Yes, but it has several grammatical errors. For example: Ethyl 2-chloroacetoacetate (CH₃C(O)CHClC(O)OCH2CH₃, E2CAA) is a class of volatile organic compounds that finds its place in the atmosphere from anthropogenic sources.** | We are thankful to the reviewer for suggestion. Necessary correction is made in revised manuscript as per reviewer’s suggestion. |
| Is the manuscript scientifically, correct? Please write here. | **The manuscript is scientifically correct.** | No correction is needed. |
| **Are the references sufficient and recent? If you have suggestions of additional references, please mention them in the review form.** | **Yes** | Thank you for your valuable comments. |
| Is the language/English quality of the article suitable for scholarly communications? | **Yes, but it contains numerous errors in writing.** | We have gone through the manuscript and made necessary corrections. |
| Optional/General comments | * **It is best not to present reactions 1-4 in the introduction section.** * **Usually, the end of the “introduction section” is a paragraph that briefly describes the purpose of the paper and the work done.** | I agree with the reviewer but in most of recent papers, in introduction section, it has been mentioned the outline of the work carried by authors. Therefore, we have presented reactions 1-4 in the introduction section. |

|  |  |  |
| --- | --- | --- |
| **PART 2:** | | |
|  | **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)* |
| **Are there ethical issues in this manuscript?** | *(If yes, Kindly please write down the ethical issues here in details)* | No any ethical issues have been reported in this manuscript. |