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| Journal Name: | [**Asian Journal of Applied Chemistry Research**](https://journalajacr.com/index.php/AJACR) |
| Manuscript Number: | **Ms\_AJACR\_139812** |
| Title of the Manuscript: | **Theoretical investigation on mechanism and kinetics of M2CAA initiated by Cl atom in the atmosphere** |
| Type of the Article | **Original Research Article** |

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| 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.** | The work is devoted to a comprehensive theoretical investigation was conducted to elucidate the mechanism, kinetics, and thermochemistry of the gas-phase reactions between Methyl 2-chloroacetoacetate (CH₃C(O)CHClC(O)OCH₃, M2CAA) and Chlorine atoms using the M06-2X functional, which has a wide range of applications and it is important to know its decay period. | Manuscript has been revised as per reviewer’s suggestion. |
| **Is the title of the article suitable?**  **(If not please suggest an alternative title)** | Yes | As per reviewer’s suggestion, we have used same title. |
| 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. | The annotation clearly indicates the features of the calculations performed and the novelty | No correction is needed. |
| Is the manuscript scientifically, correct? Please write here. | Yes. The work is devoted to the theoretical calculation of the mechanism, kinetics, and thermochemistry of the gas-phase reactions between Methyl 2-chloroacetoacetate (CH₃C(O)CHClC(O)OCH₃, M2CAA) and Chlorine atoms using the M06-2X functional and for the first time shows the reaction rate at temperatures up to 450 K, which is important when air is polluted by this substance. | No correction is needed. |
| **Are the references sufficient and recent? If you have suggestions of additional references, please mention them in the review form.** | The work contains an exhaustive list of references, but most of them are more than 10 years old. It is preferable to use more recent references. | Necessary correction is made as per reviewer’s suggestion. We have used the most relevant references as required. |
| Is the language/English quality of the article suitable for scholarly communications? | Yes | **No correction is needed.** |
| Optional/General comments | The work reveals a comprehensive theoretical study that combines quantum chemical calculations (DFT), kinetics (via CTST), thermodynamic parameters analysis, application to atmospheric chemistry and predicts the behavior of the specified compound in the atmosphere. Also, theoretical rate constants for the Cl• + M2CAA reaction were obtained for the first time, it was found that the reaction is not direct: each path passes through a pre-reaction complex, which indicates a multi-step mechanism, a structural basis for the differentiated reactivity of different hydrogens is proposed. This is important for modeling the fate of chemical pollutants in the atmosphere and understanding the role of Cl• radicals in the degradation of organic compounds.  But it is better to break long sentences into several simple ones, because sometimes the text is difficult to understand. | **No correction is needed.** |

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| **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 ethical issues has been reported in this manuscript. It has also included in revised manuscript. |