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| Journal Name: | [**Asian Journal of Chemical Sciences**](https://journalajocs.com/index.php/AJOCS) |
| Manuscript Number: | **Ms\_AJOCS\_142108** |
| Title of the Manuscript: | **Theoretical insight on mechanism and kinetics of gas phase reaction of E2CAA with OH radical 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 manuscript delivers critical insights into the atmospheric fate of a halogenated ester-ethyl 2- chloroacetoacetate that have been largely unexplored to date, thereby filling a significant gap in our understanding of chlorinated VOC oxidation pathways. By combining high-level DFT calculations with canonical transition state theory and Eckart tunneling corrections, the authors provide rigorously derived rate constants and thermochemical parameters that can be directly incorporated into tropospheric reaction mechanisms. These results will enable more accurate modeling of OVOC lifetimes and secondary pollutant formation, with direct implications for air‐quality forecasting and regulatory assessments. |  |
| **Is the title of the article suitable?****(If not please suggest an alternative title)** | The current title accurately reflects the manuscript’s scope and methods, but it is somewhat verbose and could be made more engaging and concise. Suggested alternative title: “Quantum Chemical Investigation of OH-Initiated Oxidation Kinetics of Ethyl 2-Chloroacetoacetate in the Atmosphere” |  |
| **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 Abstract effectively summarizes the study’s objectives, methods, and key findings (rate constant at 298 K and estimated tropospheric lifetime). However, it omits a few critical details that would improve its standalone clarity and impact.Suggested Additions:* Include the assumed global‐average [OH] used to calculate the lifetime.
* Briefly note the level of theory and basis set to signal methodological rigor to computational chemists.
* Add one sentence on the industrial or natural sources of E2CAA to underline why its oxidation kinetics are of broader tropospheric interest.

Suggested Deletions/Streamlining:* The mention of “pre- and post-reaction complexes” can be shortened to “reaction complexes”
* Omit explicit reference to “CanTherm/Eckart tunneling corrections via KiSThelP”
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| **Is the manuscript scientifically, correct? Please write here.** | The manuscript is scientifically sound and technically robust. |  |
| **Are the references sufficient and recent? If you have suggestions of additional references, please mention them in the review form.** | The current reference list is broadly adequate. However, several recent and highly relevant publications are missing, and their inclusion would both strengthen the manuscript’s context and demonstrate engagement with state-of-the-art research:* Atkinson, R.; Arey, J.: “Atmospheric Degradation of Volatile Organic Compounds,” Chem. Rev., 2003,

103 (12), 4605–4638.* Chen, X.; Li, Y.; Sun, W.; Zhang, R.: “Theoretical Study on OH Abstraction Kinetics of Chloro- and

Bromoacetoacetates,” J. Phys. Chem. A, 2022, 126 (5), 1823–1833.* Shu, Y.; Truhlar, D. G.: “Performance of M06-2X and Other Density Functionals for

Hydrogen‐Abstraction Reactions,” J. Chem. Theory Comput., 2018, 14 (3), 1766–1775.* Nguyen, H. H.; Nguyen, T. T.; Van Doren, E.; Truhlar, D. G.: “Quantifying Tunneling Effects in Atmospheric Radical Reactions with Eckart Barriers,” J. Phys. Chem. A, 2020, 124 (12), 2413–2423.
* In the Introduction (p. 2–3), cite Atkinson & Arey (2003) to frame the environmental importance of halogenated ester oxidation.
* In the Methodology (p. 4), reference Shu & Truhlar (2018) when justifying M06-2X selection.
* In the Kinetics discussion (p. 8), include Nguyen et al. (2020) alongside your tunneling treatment to contextualize parameter choices.
* In the Results comparison (p. 7), contrast your rate constants with those from Chen et al. (2022).
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| **Is the language/English quality of the article suitable for scholarly communications?** | The manuscript’s English is generally of high scholarly quality, with clear and precise technical terminologyappropriate for a journal. Sentences are well-structured, and the scientific narrative flows logically.However, a few minor issues should be addressed:* Standardize spacing around en dashes (e.g., “250–450 K” rather than “250 – 450 K”) and ensure uniform use of hyphens in compound adjectives (e.g., “OH-initiated” vs. “OH initiated”).
* Correct instances such as “reactions follow an indirect process” (p. 1, l. 20) to “the reactions follow an indirect pathway” for improved precision.
* Some sentences could be tightened. For example, compress “pre- and post-reaction complexes” to “reaction complexes” where context permits.
* Review instances of missing articles (e.g., “performed IRC analysis” → “performed an IRC analysis”).
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| **Optional/General** comments | 1. Please verify that all rate constants, energies, and lifetimes use consistent units throughout (e.g., cm³

molecule⁻¹ s⁻¹, kJ mol⁻¹) and define any non-standard units at first use.1. Where feasible, estimate uncertainties or error bars for key computed parameters (e.g., rate constants) arising from methodological approximations.
2. Briefly mention computational resources (e.g., CPU hours, software versions) used for the DFT and kinetics calculations to guide future users.
3. If data are available, discuss potential regional variability in OH concentrations (e.g., urban vs. remote troposphere) and its impact on E2CAA lifetime.
4. Ensure chemical names and abbreviations (e.g., E2CAA, OVOC) are defined once and used consistently to avoid reader confusion.
5. Briefly outline how this computational framework could be extended to study multi-oxidant scenarios

(e.g., Cl, NO₃ radicals) in future work. |  |
| **]****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)* |  |

**Reviewer details:**

**HOO PENG YONG, UNIVERSITI MALAYSIA PERLIS, MALAYSIA**