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| JournalName: | [**AsianJournalofChemicalSciences**](https://journalajocs.com/index.php/AJOCS) |
| ManuscriptNumber: | **Ms\_AJOCS\_142108** |
| TitleoftheManuscript: | **TheoreticalinsightonmechanismandkineticsofgasphasereactionofE2CAAwithOHradicalintheatmosphere** |
| TypeoftheArticle | **OriginalResearchArticle** |

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| **PART1:Comments** | | |
|  | **Reviewer’scomment**  **ArtificialIntelligence(AI)generatedorassistedreviewcommentsarestrictlyprohibitedduringpeerreview.** | **Author’sFeedback**(Itismandatorythatauthorsshouldwritehis/her feedback here) |
| **Pleasewriteafewsentencesregardingtheimportance 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 ourunderstandingofchlorinatedVOCoxidationpathways.Bycombininghigh-levelDFTcalculationswithcanonical 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. Theseresults will enable more accurate modeling of OVOC lifetimes and secondary pollutant formation, with direct implications for air‐quality forecasting and regulatory assessments. | We are thankful to the learned reviewer for his/her valuable comments. |
| **Isthetitleofthearticlesuitable?**  **(Ifnotpleasesuggestanalternativetitle)** | 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” | We have modified the title of the manuscript as per reviewer’s suggestion. |
| **Is the abstract of the article comprehensive? Do you suggesttheaddition(ordeletion)ofsomepointsinthis 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 methodologicalrigor 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” | We have incorporated the necessary corrections in revised manuscript. |
| **Isthemanuscriptscientifically,correct?Pleasewrite here.** | The manuscript is scientifically sound and technically robust. |  |
| **Arethereferencessufficientandrecent?Ifyouhave 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 VolatileOrganic 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 M06-2XandOtherDensityFunctionalsfor   Hydrogen‐AbstractionReactions,”J.Chem.TheoryComput.,2018,14(3),1766–1775.   * Nguyen,H.H.;Nguyen,T.T.;VanDoren,E.;Truhlar,D.G.:“QuantifyingTunnelingEffectsin 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 etal. (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). | Necessary corrections are made in revised manuscript.  We have added more references to strengthen the manuscript.  However, we could not find the marked references as suggested by learned reviewer. It is better to provide link of the references or DOI of the manuscripts. |

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| **Isthelanguage/Englishqualityofthearticlesuitable for scholarly communications?** | Themanuscript’sEnglishisgenerallyofhighscholarlyquality,withclearandprecisetechnicalterminology  appropriatefora journal.Sentencesarewell-structured,andthescientificnarrativeflowslogically.  However,afew minor issues should be addressed:   * Standardizespacingaroundendashes(e.g.,“250–450K”ratherthan“250 –450K”)andensureuniform 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. * Somesentencescouldbetightened.Forexample,compress“pre-andpost-reactioncomplexes”to “reaction complexes” where context permits. * Reviewinstancesofmissingarticles(e.g.,“performedIRCanalysis”→“performedanIRCanalysis”). | | | Necessary corrections are incorporated in the revised manuscript. | |
| **Optional/General**comments | 1. Pleaseverifythatallrateconstants,energies,andlifetimesuseconsistentunitsthroughout(e.g.,cm³   molecule⁻¹s⁻¹,kJmol⁻¹)anddefineanynon-standardunitsatfirstuse.   1. Where feasible, estimate uncertainties or error bars for key computed parameters (e.g., rate constants)arising from methodological approximations. 2. Brieflymentioncomputationalresources(e.g.,CPUhours,softwareversions)usedfortheDFTand 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 namesandabbreviations(e.g., E2CAA, OVOC) are definedonce andused consistently to avoid reader confusion. 5. Brieflyoutlinehowthiscomputationalframeworkcouldbeextendedtostudymulti-oxidantscenarios   (e.g.,Cl,NO₃radicals)infuture work. | | | Necessary corrections are incorporated in the revised manuscript. | |
| **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 have been reported in this manuscript. | |