Response to Reviewer 2

We greatly appreciate the time and effort the reviewer spent reviewing our manuscript. The comments are thoughtful and helpful in improving the quality of our paper. Below, we make a point-by-point response to these comments. The response to the reviewer is structured in the following sequence: (1) Comments from the reviewer in black color; (2) Our response in blue color; (3) Our changes in the revised manuscript in red color.

Li et al. have utilized Orbitrap mass spectrometry to examine the products from the ozonolysis of styrene in the presence vs. absence of ammonia. In the presence of ammonia, the authors report the formation of a peroxide amine, which they attribute to the reaction of ammonia with the styrene-derived 7-carbon Criegee intermediate. They observe a reduction in other products that they attribute to Criegee intermediate-driven SOA formation, such as benzoic acid. This study provides new mechanistic insights on the potential contribution for ozonolysis driven intermediates to contribute to the formation of tropospheric SOA, but requires significant edits for clarity and accuracy. Comments and recommended edits follow:

We thank the reviewer for providing valuable suggestions to enhance the quality of our paper. Following the reviewer's suggestion, we have added sufficient experimental and simulation details in the *Materials and methods* section to enhance the clarity of the manuscript, and have added contents of calculation and analysis in the *Results and discussion* section to enhance the accuracy of the manuscript.

Line 33: There have been several studies published on the reactions of Criegee intermediates with ammonia and amines that were conducted prior to the previous study by these authors which should be cited:

S. Jørgensen, A. Gross, Theoretical Investigation of the Reaction between Carbonyl Oxides and Ammonia, JPCA (2009).

Liu, C. Yin, M. C. Smith, S. Liu, M. Chen, X. Zhou, C. Xiao, D. Dai, J. J.-M. Lin, K. Takahashi, W. Dong, X. Yang, Kinetics of the reaction of the simplest Criegee intermediate with ammonia: a combination of experiment and theory, PCCP (2018).

J. P. Misiewicz, S. N. Elliott, K. B. Moore, H. F. Schaefer, Re-examining ammonia addition to the Criegee intermediate: converging to chemical accuracy, PCCP (2018).

W. Chao, C. Yin, K. Takahashi, J. J. M. Lin, Effects of water vapor on the reaction of CH_2OO with NH3, PCCP (2019).

R. Chhantyal-Pun, R. J. Shannon, D. P. Tew, R. L. Caravan, M. Duchi, C. Wong, A. Ingham, C. Feldman, M. R. McGillen, M. A. H. Khan, I. O. Antonov, B. Rotavera, K. Ramasesha, D. L. Osborn, C. A. Taatjes, C. J. Percival, D. E. Shallcross, A. J. Orr-Ewing, Experimental and computational studies of Criegee intermediate reactions with NH_3 and CH_3NH_2. PCCP (2019).

Thanks for the reviewer. These references are very helpful for our manuscript. According to the reviewer's advice, we have added these contents on Page 2, Lines 33-38:

Quantum calculations suggest that NH_3 may influence the SOA formation from styrene through reactions with stable Criegee intermediates (SCIs) (Ma et al., 2018; Banu et al., 2018). The reaction rate between NH_3 and C_1-Criegee intermediate (CH_2OO) has been determined by theoretical calculations (Jørgensen and Gross, 2009; Misiewicz et al., 2018) and experiments (Liu et al., 2018; Chao et al., 2019a, b; Chhantyal-Pun et al., 2019). Our recent study has shown new laboratory evidence that NH_3 can also react with isoprene-derived SCIs to form NOCs, thereby changing the chemical characteristics of SOA (Li et al., 2024).

Line 53 (and line 14 of the SM): define FEP.

We have defined FEP in the experiments section. Page 3, Line 60:

The chamber experiments were conducted in Fluorinated Ethylene Propylene (FEP, 200A, DuPont) reactors under dark conditions, with background air supplied by purified zero air.

Line 55: Please provide concentration ranges of styrene, O3, and NH3 used.

The reactants and their concentration ranges used in the exp.1-5 are: styrene (0.34~0.36 ppm), O_3 (1 ppm), and NH_3 (0~0.8 ppm), respectively. The concentration ranges used in the exp.6-10 are: styrene (0.4~0.7 ppm), O_3 (2 ppm), and NH_3 (0~10 ppm), respectively. The concentration used in the exp.11 is styrene (3 ppm), O_3 (10 ppm), and NH_3 (0.8 ppm), respectively. We have listed the initial concentrations used in each experiment in Table S1, and added the concentration ranges in the *Materials and methods* section on Page 3, Lines 63-64:

The reactants and their concentration ranges used in the experiment are styrene (0.3~3 ppm), O_3 (1~10 ppm), and NH_3 (0~10 ppm), respectively.

Line 72 (and SM Line 46): Which unimolecular and bimolecular reactions of the styrene-derived Criegee intermediates were included in the mechanism aside from the reaction with NH3?

In addition to the reaction with NH_3 we have added, this mechanism also includes the pre-existing unimolecular reactions of styrene-derived Criegee intermediates to generate benzoic acid, benzaldehyde, H_2O_2 and HCOOH. And the pre-existing bimolecular reactions of styrene-derived Criegee intermediates with CO, NO, NO_2 and SO_2. Based on the reviewer's suggestions, we have added these contents to the manuscript and the *supplementary materials*.

Page 4, Lines 91-94: Gas-phase reactions were simulated using the Master Chemical Mechanism (MCM v3.3.1, website: https://mcm.york.ac.uk/MCM). To evaluate the influence of NH_3-SCI reactions, we added four reactions to the MCM mechanism, including those between NH_3 and C_1-/C_7-SCIs (CH_2OO/PHCHOO) and the subsequent decomposition of $C_7H_9O_2N$ into C_7H_7N and C_7H_7ON.

Page 3-4, Lines 50-71 in *supplementary materials*: Gas-phase reactions were simulated using the Master Chemical Mechanism (MCM v3.3.1, website: https://mcm.york.ac.uk/MCM), the reaction between NH_3 and C_1-/C_7-SCIs

(CH_2OO/PHCHOO) and the subsequent decomposition of $C_7H_9O_2N$ into C_7H_7N and C_7H_7ON was introduced into MCM for simulation:

$CH_2OO+NH_3= CH_2OONH_3$

$PHCHOO+NH_3=PHCHOONH_3$

$PHCHOONH_3= PHCHNH$

$PHCHOONH_3= PHCONH_2$

In addition to the reaction with NH_3, MCM mechanism also includes the following unimolecular and bimolecular reactions of the styrene-derived Criegee intermediates:

$PHCHOO+SO_2=BENZAL+SO_3$

$CO+PHCHOO=BENZAL$

$NO+PHCHOO=BENZAL+NO_2$

$NO_2+PHCHOO=BENZAL+NO_3$

$PHCHOO=BENZAL+H_2O_2$

$PHCHOO=PHCOOH$

$CH_2OO=HCOOH$

$CH_2OO=H_2O_2+HCHO$

$CH_2OO+CO=HCHO$

$CH_2OO+NO=HCHO+NO_2$

$CH_2OO+NO_2=HCHO+NO_3$

$CH_2OO+SO_2=HCHO+SO_3$

Line 78: Do you use SOA yield to refer to SOA total mass, or number of particles?

The SOA yield mentioned refers to SOA mass yield, calculated based on the mass of reacted styrene and the total mass concentration of SOA. Based on the reviewer's suggestion, we have clarified SOA yields to SOA mass yields in the text and Figure 1 a.

Page 4, Lines 99-100: As NH_3 concentrations increased, SOA mass yields

decreased significantly from (4.9±0.3)% (0 ppm NH_3) to (1.0±0.1)% (0.8 ppm NH_3), showing an obvious inhibitory effect (Fig.1a).

Line 78: What are the uncertainties on your reported 4.9% yield of SOA?

According to the reviewer's suggestion, we have included the instrumental uncertainties in the manuscript. The uncertainty of the PTR-MS (for styrene measurement) is ±6%, and that of the SMPS (for aerosol mass concentration) is ±2%. Based on the theory of error propagation, the relative uncertainty of the SOA yield is calculated to be ±6.32%. The corresponding absolute uncertainty for the reported 4.9% yield is therefore ±0.3%. The manuscript has been revised accordingly at the relevant positions on Page 4, Lines 99-100:

As NH_3 concentrations increased, SOA mass yields decreased significantly from (4.9±0.3)% (0 ppm NH_3) to (1.0±0.1)% (0.8 ppm NH_3), showing an obvious inhibitory effect (Fig.1a).

Line 80: Provide the ranges of reported SOA yields for the studies cited to demonstrate that these are in line with the current work.

According to the reviewer's suggestion, we have added the ranges of SOA yields from the cited studies on Page 4, Lines 101-102:

The observed yields with 0 ppm NH_3 are within the range of those previously reported for styrene ozonolysis under no NH_3 conditions (2.7%~6.5%) (Bracco et al., 2019; Díaz-de-Mera et al., 2017; Yu et al., 2022, 2024b), which demonstrates the reasonability of our experiments.

Line 83: Suggest rephrasing "breaks up" with "competes with" or similar for clarity.

According to the reviewer's suggestion, we have replaced the "breaks up" on Page 4, Lines 104-106:

In the styrene-O_3 reaction system, SOA is primarily derived from SCI-related products. As the concentration of NH_3 increases, the SOA concentration decreases linearly. This indicates that the observed reduction of SOA is attributed to the competitive consumption of SCI by NH_3.

Line 89: Do you see any evidence in the mass spectra for the sequential insertion of the 1 and/or 7 carbon Criegee intermediates into the initial peroxide amine reaction product (e.g., oligomerization).

We have carefully reexamined the MS data of SOA from styrene-O_3-NH_3 systems, and did not find any products that formed by insertion of C_1 or C_7 Criegee intermediates into the initial peroxide amine.

Line 92: Please provide a reference for a study that demonstrates the formation of benzoic acid from the C7 Criegee intermediate with water.

According to the reviewer's suggestion, we have added corresponding references.

Page 4, Lines 115-116: Since benzoic acid is mainly formed from the reaction of C_7-SCI with H_2O (Na et al., 2006; Banu et al., 2018), the presence of NH_3 apparently competes with H_2O for SCIs and inhibits the formation of benzoic acid (Fig.1d).

Line 95: Do you see any evidence for the water-mediated enhancement of the Criegee intermediate reaction with ammonia in your experiments, as reported by the Lin group? (I imagine that the MCM mechanism you are using in your analysis doesn't include this process):

W. Chao, C. Yin, Y.-L. Li, K. Takahashi, J. J.-M. Lin, Synergy of Water and Ammonia Hydrogen Bonding in a Gas-Phase Reaction, JPCA (2019)

W. Chao, C. Yin, K. Takahashi, J. J.-M. Lin, Effects of water vapor on the reaction of CH2OO with NH3, PCCP (2019)

We thank the reviewer for pointing out these important findings from Chao et al.

2019). This research reveals that NH_3 and H_2O have a synergic effect on the reaction of CH_2OO. We have cited the work of Chao et al. in the introduction section. In the present study, our primary focus is on the reaction between C_7-SCI and NH_3. It should be noted that the Q-Exactive mass spectrometer used here can only detect ions with an m/z greater than 50. Since the reaction products of C_1-SCI with H_2O or NH_3 have molecular weights below 50 Da, we were unable to detect any of these products. Consequently, no synergic enhancement effect between H_2O and NH_3 was observed under our experimental conditions. Hence, the MCM mechanism did not include synergistic promotion effect in this study. According to the reviewer's suggestions, we have revised the following content on Page 2, Lines 33-39:

Quantum calculations suggest that NH_3 may influence the SOA formation from styrene through reactions with stable Criegee intermediates (SCIs) (Ma et al., 2018; Banu et al., 2018), and NH_3 and H_2O have a synergic effect on the reaction of C_1-Criegee intermediate (Chao et al., 2019a,b). The reaction rate between NH_3 and C_1-Criegee intermediate (CH_2OO) has been determined by theoretical calculations (Jørgensen and Gross, 2009; Misiewicz et al., 2018) and experiments (Liu et al., 2018; Chao et al., 2019; Chhantyal-Pun et al., 2019). Our recent study has shown new laboratory evidence that NH_3 can also react with isoprene-derived SCIs to form NOCs, thereby changing the chemical characteristics of SOA (Li et al., 2024).

Figure1 (upper): please add error bars.

According to the reviewer's suggestion, we have added error bars in Figure 1 a.

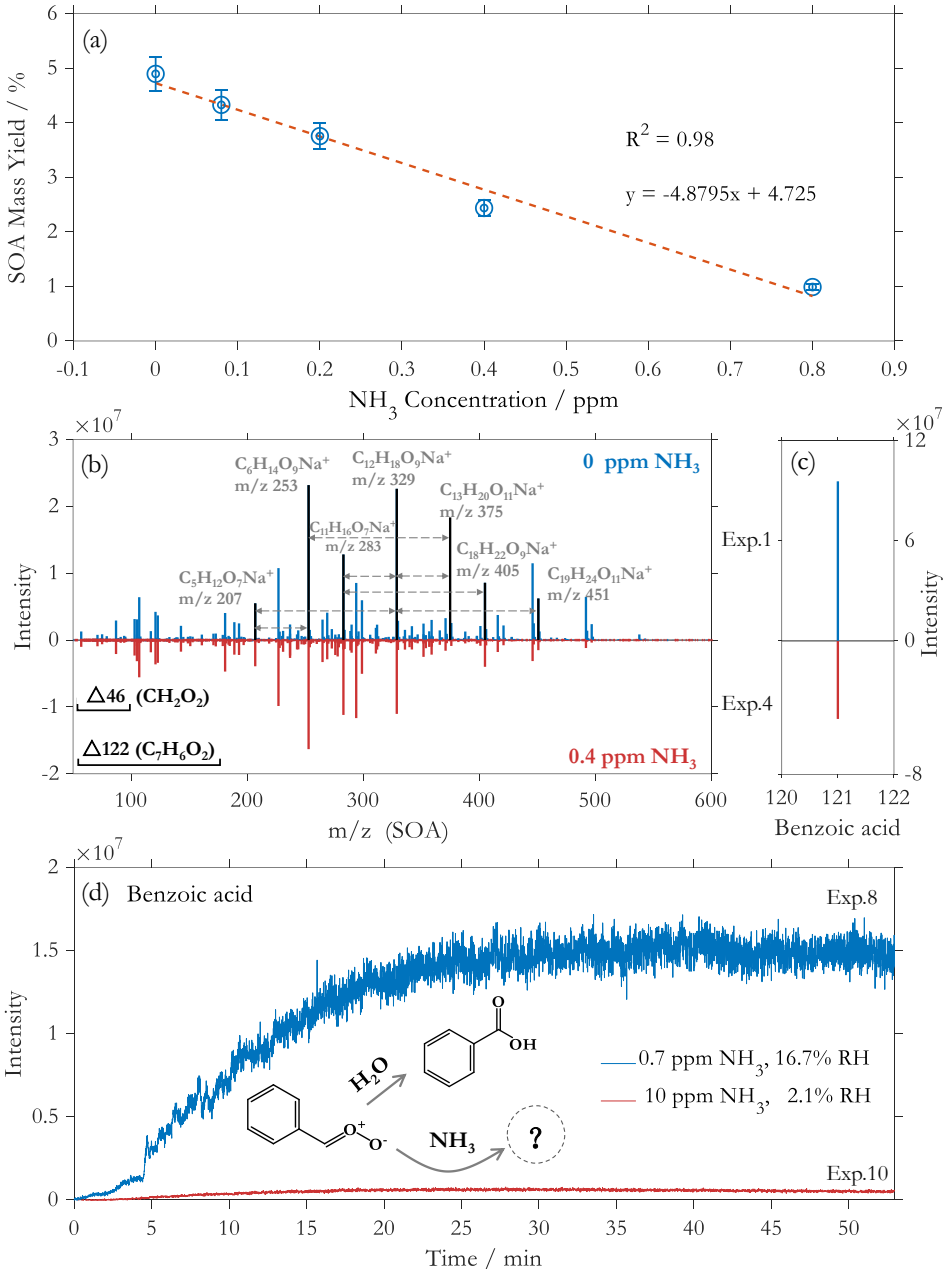

Figure 1: SOA mass yields from styrene ozonolysis under different NH_3 concentrations (a); Positive mode mass spectra of SOA from styrene ozonolysis systems with 0 ppm (blue) and 0.4 ppm NH_3 (red) (b), several top ion peaks assigned to SCI-derived oligomer are marked in black; The mass spectra of benzoic acid from styrene ozonolysis systems with 0 ppm (blue) and 0.4 ppm NH_3 (red) (c); Online observation of benzoic acid in the experiments with low concentration NH_3 with normal humidity (Ex.8, blue) and high concentration NH_3 with low humidity (Ex.10, red) (d).

Figure 1 (middle): Are there any mass peaks which do not have changes in intensity in the presence vs absence of ammonia?

Yes, there are some peaks whose intensity remain almost unchanged. These primarily correspond to some species not directly involved in the SCI or NH_3 reaction pathways. For example, the intensity of benzaldehyde (C_7H_6O, m/z=107.049) are 5.6×10^6 and 6.4×10^6 in the presence vs absence of ammonia, respectively, whose difference is within the uncertainty of ±15% in MS measurement.

Figure 1(lower): Please can you explain the rationale for changing the concentration of both ammonia and water in the red vs. blue datasets, rather than keeping one of the co-reactant concentrations the same.

These experiments were designed to maximally reveal the potential of NH_3 and H_2O to compete for C_7-SCI under extreme conditions. By contrasting the two very different conditions of low NH_3/normal humidity vs. high NH_3/extremely low humidity, the strong suppression on the formation of benzoic acid can be most clearly demonstrated when the concentration of NH_3 is much higher than that of H_2O. This is not to directly compare rates, but to qualitatively verify the existence of competition mechanisms. According to the reviewer's comment, we have revised the following sentence on Page 5, Line 117-119.

To maximize the potential of NH_3 and H_2O to compete for C_7-SCI under extreme conditions, we further conducted two experiments with low NH_3/normal humidity vs. high NH_3/extremely low humidity. The strong suppression on the formation of benzoic acid can be most clearly demonstrated when the concentration of NH_3 is much higher than that of H_2O.

Line 112: Please cite the (aforementioned) papers prior to the 2024 Li et al. work where the reaction mechanism for the reaction of Criegee intermediates with ammonia has been deduced.

According to the reviewer's advice, we have added the citation and the contents on Page 7, Lines 138-140:

Referring to the reaction mechanism between C_1-SCI and NH_3 (Jørgensen and Gross, 2009; Misiewicz et al., 2018; Liu et al., 2018; Chao et al., 2019a,b; Chhantyal-Pun et al., 2019), and the reaction mechanism between C_4-SCI and NH_3 from isoprene (Li et al., 2024), C_7-SCI should react with NH_3 to produce a molecule $C_7H_9O_2N$.

Line 127: Please provide details of the iodometry kinetics measurements in Section 2.

According to the reviewer's advice, we have moved the details of the iodometry kinetics measurements from the *supplementary material* to the *Materials and methods* of the manuscript on Page 3, Lines 81-87:

To detect peroxides in the sample, experiment 11 was conducted in the 1.2 m^3 chamber. The collected sample was immediately extracted by 400μL acetonitrile (ACN) before being injected into HPLC-HRMS. Using ACN as extraction solvent to minimize other unwanted decomposition processes such as hydrolysis. Half of the liquid (180 μL) from the combined extract mixed with 10 μL acetic acid (600 mM in ACN) in a vial, followed by the addition of 10 μL KI (99.5%, Sigma-Aldrich) (400 mM in H_2O) to trigger the iodometry reaction; another 180 μL aliquot was treated in a same way by adding 10 μL acetic acid (600 mM in ACN) and 10 μL H_2O, instead of KI. These two SOA samples are designated as KI-treated and non-treated respectively, which were injected into HPLC-HRMS (Li et al., 2025).

Figure 2 (a-g): Changing between labelling the (detected) protonated m/z and the (actual) product m/z in these figures is confusing. Perhaps the labelling can be made clearer, for example in (g) by providing both the actual molecular mass, and the mass at which the molecule was detected.

According to the reviewer's advice, we have revised a clearer labeling by providing both the actual molecular mass, and the mass at which the molecule was

detected in Figure 2.

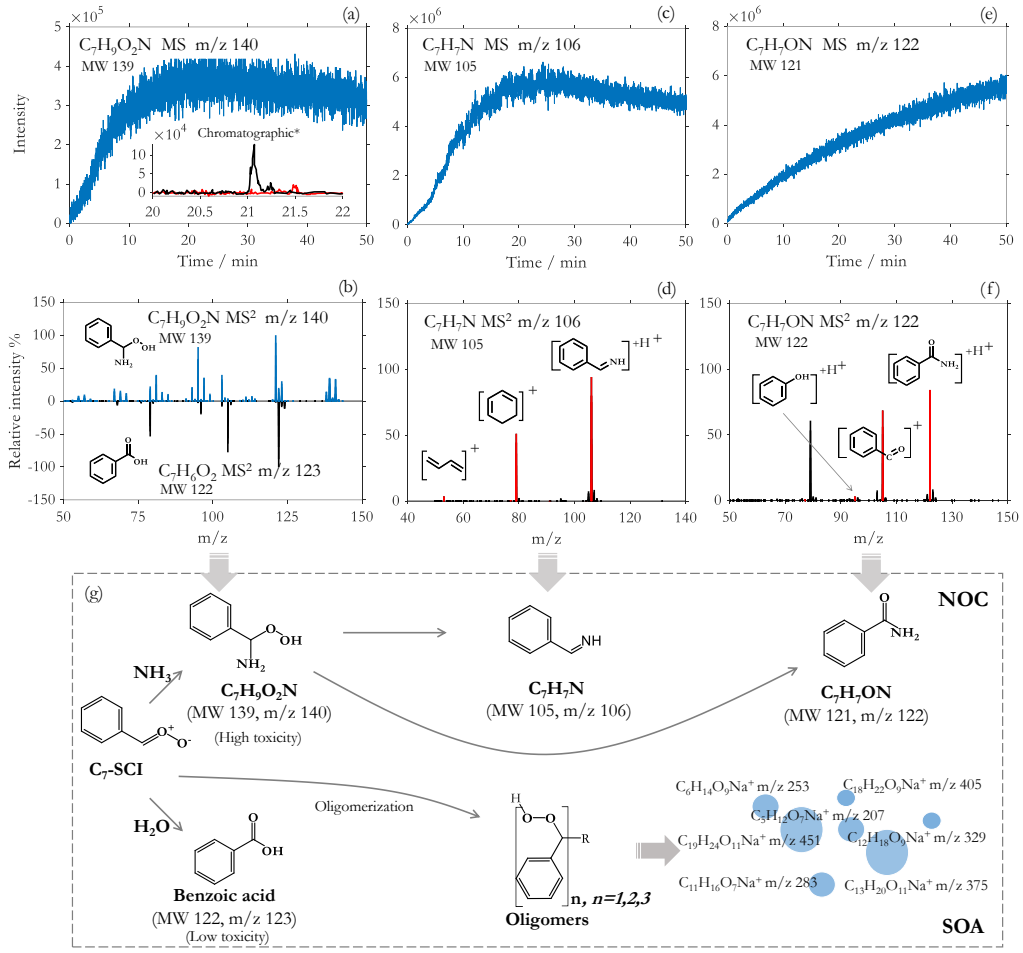

Figure 2: Time series of online observation (a) and the chromatograms of molecule $C_7H_9O_2N$ (MW 139, m/z 140.071) are shown as an inset with the initial non-KI-treated sample (black) and KI-treated sample (red). MS^2 spectra of $C_7H_9O_2N$ (MW 139, m/z 140.071, blue) and $C_7H_6O_2$ (MW 122, m/z 123.044, black) in positive modes (b). Time series of online observation of C_7H_7N and C_7H_7ON (c, e). The comparison of the ion peaks in the MS^2 spectra of $C_7H_8N^+$ and $C_7H_8ON^+$ (black bars) with the major simulated product ions of C_7H_7N and C_7H_7ON (red bars) (d, f). The mechanism of NH_3 effects on SOA from styrene ozonolysis in this study (g).

Figure 2(g): Oligomers in the context of Criegee intermediates typically mean products that result from the insertion of several Criegee intermediate molecules into a

single co-reactant molecule, via sequential reactions. I believe that you are here referring to products resulting from the self-reaction(s) of Criegee intermediates, and so this distinction should be clearly made.

Thanks for the reviewer's comments. The structure we drew in Figure 2(g) did not clearly represent the oligomers we originally intended to explain. According to the reviewer's advice, we have revised the structure in Figure 2(g).

Line 139: Peroxides have been detected in both laboratory studies and in the field in the gas phase. Why do you think that this peroxide amine (which you detect here) would not survive under atmospherically relevant conditions? Please provide references for your proposed decomposition mechanism for this peroxide under atmospherically relevant conditions.

The $C_7H_9O_2N$ molecule contains an unstable peroxide bond (-O-O-), which makes it highly reactive. Our experimental observations have confirmed its rapid decomposition into C_7H_7N and C_7H_7ON. As stated in our response to the first reviewer, based on the experimental measurements and theoretical calculations in the reference, we have determined the rate constants for the decomposition of $C_7H_9O_2N$ into C_7H_7N and C_7H_7ON are $(3.0\pm0.4)\times10^{-5}$ s^{-1} and $(5.1\pm0.6)\times10^{-5}$ s^{-1}, respectively (Page 9, Lines 177-196). In the actual atmosphere, in addition to self-decomposition, $C_7H_9O_2N$ may also react with OH radicals and undergo photolysis. After considering these 3 consumption pathways, the atmospheric lifetime of $C_7H_9O_2N$ was estimated to be 2.1 hours. According to the reviewer's comments, we have provided a detailed analysis and explanation on Lines 199-210 of Page 10, and added references on Page 9, Line 168-172.

Pages 9-10, Lines 197-205: The $C_7H_9O_2N$ molecule contains an unstable peroxide bond (-O-O-), which makes it highly reactive and short-lived in the atmosphere (Smith and March, 2020). Our experimental observations have confirmed its rapid decomposition into more stable imines (C_7H_7N) and amides (C_7H_7ON). To quantify the expected atmospheric lifetime of $C_7H_9O_2N$, we have considered 3 primary removal

pathways: (1) Reaction with OH radicals, the reaction rate constant between $C_7H_9O_2N$ and OH was estimated to be 4.77×10^{-11} cm^3 $molecule^{-1}$ s^{-1} using a tool of AOPWIN (Atmospheric Oxidation Program for Microsoft Windows) in EPI (Estimation Program Interface). Using an average OH radical concentration of 1.0×10^6 molecules cm^{-3}, the atmospheric lifetime of τ_{OH} = 5.8 hours; (2) Photolysis: Based on the general photolysis rates of peroxides 1.3×10^{-6} s^{-1} (Roehl et al., 2007), the photolytic lifetime τ_{hv} = 214 hours; (3) Thermal decomposition: Based on our results, the decomposition rate of $C_7H_9O_2N$ is 8.1×10^{-5} s^{-1}, and its self-decomposition lifetime τ_{decomp}= 3.4 hours. The total atmospheric lifetime was calculated to be 2.1 hours based on $1/\tau=1/\tau_{OH}+1/\tau_{hv}+1/\tau_{decom}$. This suggests that $C_7H_9O_2N$ predominantly exists in the atmosphere as its more stable transformation products, namely the imine C_7H_7N and the amide C_7H_7ON.

Page 9, line 168-170: Due to the high reactivity of peroxide bonds, the peroxide amine $C_7H_9O_2N$ is expected to be highly unstable and easily decomposed by removing one H_2O_2 or H_2O (Smith and March, 2020), and may further decompose into imines and amides based on theoretical calculation (Banu et al., 2018; Ma et al., 2018).

Lines 149-150: Please provide supporting references that the C7 Criegee intermediates definitively lead to the formation of SOA via benzoic acid and oligomers, or adjust your statement accordingly.

According to the reviewer's suggestions, we have added citations supporting the contribution of C_7- Criegee intermediates to SOA through oligomerization, such as Yu et al., 2022 and Yu et al., 2025, and revised the following sentence on Page 10, Lines 207-208:

Styrene reacts with O_3 to form C_7-SCI, which then generates benzoic acid and forms SOA through oligomerization (Yu et al., 2022; Yu et al., 2025).

Line 151: You state that the peroxide amine will 'rapidly' decompose to an imine and amide, but you detect the peroxide amine in the present work. Given your experimental conditions, can you determine a lower limit of the lifetime of the peroxide

amine?

The $C_7H_9O_2N$ molecule contains an unstable peroxide bond (-O-O-), which makes it highly reactive. Our experimental observations have confirmed its rapid decomposition into C_7H_7N and C_7H_7ON. As stated in our response to the first reviewer, based on the experimental measurements and theoretical calculations in the reference, we have determined the rate constants for the decomposition of $C_7H_9O_2N$ into C_7H_7N and C_7H_7ON are $(3.0\pm0.4) \times 10^{-5}$ s^{-1} and $(5.1\pm0.6) \times 10^{-5}$ s^{-1}, respectively (Page 9, Lines 177-196). In the actual atmosphere, in addition to self-decomposition, $C_7H_9O_2N$ may also react with OH radicals and undergo photolysis. After considering these 3 pathways, the atmospheric lifetime of $C_7H_9O_2N$ was estimated to be 2.1 hours. We have provided a detailed analysis and explanation on Lines 197-205 of Page 10.

Line 163: Does your analysis account for the nucleation of peroxide amines onto existing particles, or just for new particle formation?

We did not add any additional seeds to the experimental system. In our previous research (Yu et al., 2022), we have found that styrene ozonolysis can produce extremely low-volatility compounds responding to nucleation. The molecular weight of the species $C_7H_9O_2N$ in this study is too small, mainly entering the particle phase through gas-particle distribution.

General comment: it is unclear in the manuscript which species were detected in the gas or particle phase.

Styrene was measured online using a proton transfer reaction-mass spectrometer in the gas phase. O_3 was measured with an O_3 analyzer in the gas phase. The collected particles were extracted for composition analysis in the particle phase. The species $C_7H_9O_2N$, C_7H_7N and C_7H_7ON were online ionized by a gas aerosol in-situ ionization source (GAIS), and then measured by Orbitrap MS in the gas phase. According to the reviewer's suggestions, we have revised the following sentence on Page 3, Lines 67-80:

During these experiments, styrene was measured online using a proton transfer reaction-mass spectrometer (PTR-MS P1000-L-AI, Anhui Province Key Laboratory of Medical Physics and Technology) with a time resolution of 20 s in the gas phase. O_3 was measured every 0.5 hours lasting for 5 minutes with an O_3 analyzer (Model 49C, Thermo Scientific) with a time resolution of 10 s in the gas phase. The particle concentrations and size distributions were determined by a scanning mobility particle sizer (SMPS, Model 3936, DMA-3080, CPC-3776, TSI) with a time resolution of 5 minutes. The online measurements covered the entire experimental process (4~5h). Particles were collected on a 25 mm polytetrafluoroethylene (PTFE) membrane with a pore size of 0.45 μm at the 4^{th} hour, and the sample flow rate was 6 L/min and lasted for 40 min. The collected particles were extracted with methanol for composition analysis in the particle phase, which were injected by a high-performance liquid chromatography (HPLC, Thermo Scientific), ionized by a heated electrospray ionization source (ESI), and then the molecular composition was measured by a high-resolution Orbitrap mass spectrometer (Orbitrap MS, Q-Exactive, Thermo Scientific) with a resolution R= 70,000 at m/z 200. To determine the kinetics and mechanism of the reaction between C_7-SCI and NH_3, experiments 6-10 were performed with higher concentrations in a 150 L chamber. During these experiments, the products were online ionized by a gas aerosol in-situ ionization source (GAIS), and then measured by Orbitrap MS in the gas phase. The time resolution of GAIS-Orbitrap MS measurement is about 0.5 s, and all the experiments lasted about 1 h.

SM Line 22: Please provide concentration of n-hexane used for OH scavenging.

According to the reviewer's suggestion, we have added the sentence on Page 3, Lines 64-65:

Because ozonolysis of styrene can form OH radicals, n-Hexane was used as an OH radical scavenger (>100ppm with a removal efficiency >90%). Detailed experimental conditions are provided in Table S1.

References:

Banu, T., Sen, K., and Das, A. K.: Atmospheric Fate of Criegee Intermediate Formed During Ozonolysis of Styrene in the Presence of H2O and NH3 : The Crucial Role of Stereochemistry, J. Phys. Chem. A, 122, 8377–8389, https://doi.org/10.1021/acs.jpca.8b06835, 2018.

Bracco, L. L. B., Tucceri, M. E., Escalona, A., Díaz-de-Mera, Y., Aranda, A., Rodríguez, A. M., and Rodríguez, D.: New particle formation from the reactions of ozone with indene and styrene, Phys. Chem. Chem. Phys., 21, 11214–11225, https://doi.org/10.1039/C9CP00912D, 2019.

Chao, W., Yin, C., Takahashi, K., and Lin, J. J.-M.: Effects of water vapor on the reaction of CH2OO with NH3, Phys. Chem. Chem. Phys., 21, 22589–22597, https://doi.org/10.1039/C9CP04682H, 2019a.

Chao, W., Yin, C., Takahashi, K., and Lin, J. J.-M.: Hydrogen-Bonding Mediated Reactions of Criegee Intermediates in the Gas Phase: Competition between Bimolecular and Termolecular Reactions and the Catalytic Role of Water, J. Phys. Chem. A, 123, 8336–8348, https://doi.org/10.1021/acs.jpca.9b07117, 2019b.

Chen, Y., Zhou, X., Liu, Y., Jin, Y., Dong, W., and Yang, X.: Kinetics of the simplest criegee intermediate CH2OO reacting with CF3CF=CF2, Chinese Journal of Chemical Physics, 33, 234–238, https://doi.org/10.1063/1674-0068/cjcp2002025, 2020.

Chhantyal-Pun, R., Shannon, R. J., Tew, D. P., Caravan, R. L., Duchi, M., Wong, C., Ingham, A., Feldman, C., McGillen, M. R., Khan, M. A. H., Antonov, I. O., Rotavera, B., Ramasesha, K., Osborn, D. L., Taatjes, C. A., Percival, C. J., Shallcross, D. E., and Orr-Ewing, A. J.: Experimental and computational studies of Criegee intermediate reactions with NH3 and CH3 NH2, Phys. Chem. Chem. Phys., 21, 14042–14052, https://doi.org/10.1039/C8CP06810K, 2019.

Díaz-de-Mera, Y., Aranda, A., Martínez, E., Rodríguez, A. A., Rodríguez, D., and Rodríguez, A.: Formation of secondary aerosols from the ozonolysis of styrene: Effect of SO2 and H2O, Atmos. Environ., 171, 25–31, https://doi.org/10.1016/j.atmosenv.2017.10.011, 2017.

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