## Response to reviewers

We gratefully appreciate the reviewers for the valuable time and insightful comments. The manuscript has been greatly improved based on these comments and suggestions. All the comments have been addressed point by point in the revised manuscript, and the revisions are marked in red colour. The responses to the specific comments are listed as follows.

## Response to the Comments from Reviewer #1:

**Reviewer #1:** The clarification of the formation mechanism of HOMs/OOMs is of great importance for atmospheric chemistry. In this study, the authors investigated the elaborate oxidation mechanisms of terpinolene initiated by OH and NO<sub>3</sub>, elucidating the new formation mechanism of OOMs, the molecular structures of the products, and their time-dependent yields and volatility. These findings contribute to the molecular structure identification of OOMs in atmospheric monitoring and the refinement of atmospheric chemical models. Overall, the work is well-presented and innovative. I recommend publication after the following issues are addressed:

**Response:** Response: Thank you for the positive and valuable comments. We have revised the manuscript carefully according to the comments and suggestions, and marked them in red in the manuscript.

**Comment #1:** Line 21-21, the logic flow of the context is not smooth and should be revised.

**Response to Comment #1**: Thank you for the valuable comment. We have revised this description in the manuscript, specifically as follows:

Measurements in forested areas revealed that monoterpene oxidation products played a dominant role in driving new particle growth (Mohr et al., 2019; Huang et al., 2016), while the atmospheric oxidation mechanisms of monoterpenes, especially the formation of OOMs, have not been fully elucidated.

**Comment #2:** *Line 162, here "dominant reaction" or "rate-determining step"?* 

**Response to Comment #2**: Thank you for pointing out. "Rate-determining step" is more accurate herein, and we have revised this expression and marked the change in red in the manuscript.

Comment #3: Line 203, how do free radical centers migrate? It should be specified in the manuscript for better understanding.

**Response to Comment #3**: Thank you for the valuable comment. The radical center of 2-IM3b migrates from the oxygen atom to the carbon atom, due to the cleavage of the C-C bond. The revision is supplemented in the manuscript, as detailed below:

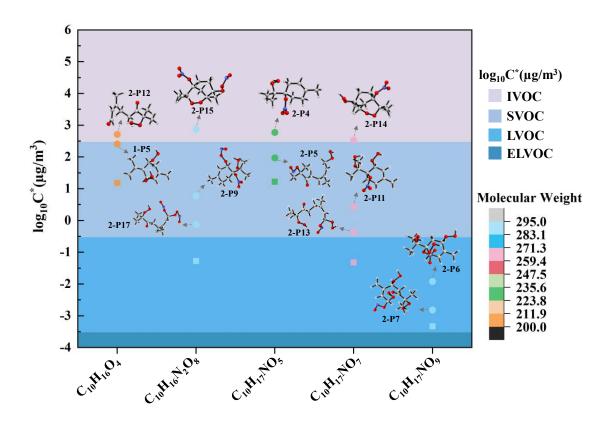
Besides, Fig.4(c) indicates that the radical center of 2-IM3b migrates from the oxygen atom to the

<u>Comment #4:</u> Why was the NO<sub>3</sub>-Terpinolene-R• (2-IM3) chosen for subsequent oxidation mechanism research? A justification should be provided.

**Response to Comment #4**: Thank you for the valuable comment. Since the formation reaction of the NO<sub>3</sub>-Terpinolene-R• (2-IM3) is barrierless and releases more heat, being the dominant intermediate, 2-IM3 is selected for the investigation of subsequent oxidation mechanisms.

<u>Comment #5:</u> In Figure 8, the values of  $C^*$  for different isomers are difficult to distinguish. The figure format should be modified for better readability.

**Response to Comment #5**: Thank you for pointing out this problem. We have modified Figure 8 for clarity in the manuscript.



**Figure 8.** The molecular weight ranges and volatility classifications of C10-OOMs isomers. (Volatility prediction methods:  $(\bigcirc)$  the functional group contribution method(SIMPOL.1),  $(\square)$  the molecular formula parameterization method)

<u>Comment #6:</u> Language: The manuscript should be carefully revised for grammar and style. Several sentences contain errors, such as verb tense errors.

**Response to Comment #6**: Thank you for the valuable comment. We have checked the whole manuscript carefully and modified formatting problems and grammatical errors.