

## ***Interactive comment on “Highly oxygenated organic molecules (HOM) formation in the isoprene oxidation by NO<sub>3</sub> radical” by Defeng Zhao et al.***

### **Anonymous Referee #1**

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Isoprene is one of most critical biogenic VOCs precursor world widely towards forming secondary organic aerosols (SOA). This work investigated detailly the HOM formation from NO<sub>3</sub> oxidation of isoprene. Molecules of isoprene-HOM monomer, dimer, and trimer containing 1-5 nitrogen atoms were detected, and their detailed formation pathways were discussed. These HOMs can contribute to SOA significantly globally. I, therefore, recommend this manuscript can be published in ACP after some minor revision.

#### Specific comments

1. What's the definition of HOM in this work? Does it follow the definition in Bianchi

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et al., Chemical Reviews 2019, e.g. contains at least 6 oxygens formed from RO<sub>2</sub> auto-oxidation.

2. Did the authors find some molecules that can be identified from NO<sub>3</sub> oxidation but not contain any N atom?

3. Line 83-84: There was some discussion on NO<sub>3</sub> oxidation of monoterpene to form HOM, e.g. Yan et al., 2016; 2020.

4. Line 149-150: I may suggest adding more statements on how to rule out the reaction with O<sub>3</sub> and OH.

5. Line 158-150: may need to add the reference Jokinen et al., ACP, 2012.

6. The first panel of Table 1: why molecules with 1 N atom (one nitrate group) can be formed from isoprene+NO<sub>3</sub>+NO<sub>3</sub>.

7. The 2nd panel of Table 2: what is PN?

8. Figure 3: how C<sub>5</sub>H<sub>10</sub>N<sub>2</sub>O<sub>7</sub> formed? Besides the two nitrate groups, only one oxygen.

9. Scheme 2: Panel 1: -ONO<sub>2</sub> is missed from the 2nd molecule, RO radical (C<sub>5</sub>H<sub>9</sub>N<sub>2</sub>O<sub>9</sub>.) should not be detected. Panel 2: the 3rd reaction stop should not be H-shift.

10. Scheme 3: Panel 2: the structure of the final molecule maybe not correct.

11. How molecules with 7 H atoms formed? E.g. C<sub>5</sub>H<sub>7</sub>N<sub>2</sub>O<sub>9</sub>.

12. Is there any observational evidence on the formation of NO<sub>3</sub>-isoprene-HOM dimer and trimer in the real atmosphere?

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