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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Estimation of rate coefficients for the reactions of O_3 with unsaturated organic compounds for use in automated mechanism construction" *by* Michael E. Jenkin et al.

Anonymous Referee #2

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The authors present a useful and detailed structure-reactivity based system for the prediction of rate coefficients for reactions of ozone with unsaturated hydrocarbons, including oxygenated species. The new SAR, created from an up-to-date set of more than 200 measured rate coefficients, will be very useful for the development of detailed chemical mechanisms used in atmospheric modeling, and potentially other applications. The authors have done a good job of acknowledging and dealing with the many challenges associated with these ozonolysis reactions, including substituent and steric effects, molecular size, etc.

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Discussion paper

While I think this is clearly a publishable body of work, I do have some comments that I would like to see addressed prior to publication. These are listed below.

Line 80: Are the averages referred to here obtained from averages of A-factors and E/R values, or is a different process used? (Also, there are a couple of A-factors in the Supplementary Table for the 1-enes that look incorrect).

Line 160: While some examples are given, it is not totally clear to me what the 30 compounds referred to here are, and what distinguishes them from those discussed previously. Can more explanation be given, or can these compounds be highlighted somehow in the supplemental tables?

Line 180 or so: It was not immediately obvious to me what was being called an a,b-unsaturated compound – e.g. CH2=CH-CH2-CH(=O) and CH2=CH-CH2-OH are both in this category but with different numbers of C-atoms. Maybe a couple of explicit examples can be given here to clarify?

Line 206: There is a CH2 group missing in the structure shown.

Line 270 or so: It seems appropriate to reference some of the work done by Moortgat and co-workers on sesquiterpene ozonolysis, where I believe some relative reactivity of different sites within a molecule are discussed/quantified.

While I realize that data are limited, and assumptions must be made, the discussion or presentation of the temperature dependence of the rate coefficients is too limited in my opinion, and often buried in figure captions, etc. I think that this information needs to be presented more fully in the main text. For example, I think the only mention of T-dependent parametrization for non-oxygenates occurs in the captions to Tables 2-5. Further discussion of temperature dependence and its uncertainties could also be given at the end of Section 3 (where a summary of non-oxygenated species is given), and/or in Section 6.

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