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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Technical Note: Development of chemoinformatic tools to enumerate functional groups in molecules for organic aerosol characterization" *by* G. Ruggeri and S. Takahama

Anonymous Referee #1

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General Comments:

In this manuscript the authors report on the use of chemoinformatic methods to classify organic molecules according to their functional groups, using compounds from the SIMPOL.1 database, FTIR measureable groups, products predicted by the Master Chemical Mechanism for the oxidation of an aromatic compound and a-pinene, and bonds needed to determine compound oxidation state. The types of information that is extractable using this approach is then demonstrated for the products predicted for the oxidation of a-pinene by the Master Chemical Mechanism and GC-MS and FTIR

analyses of wood smoke. I suspect that this topic will be new and challenging to most readers (as it is to me), and that the authors will need to present more applications in the future to demonstrate the clear value of this approach, and exactly what its benefits are. Nonetheless, I think this brief Technical Note is a useful way to introduce the topic to the atmospheric science community. The paper is concise, well organized and clearly written, and I think is suitable for publication in ACP after the following very minor comments are addressed.

Specific Comments:

1. P. 33642: Usually one uses the term low-NOx reaction to mean that organic peroxy radicals have reacted with HO2 or other RO2 radicals, or perhaps by autooxidation. If an organic nitrate contributes 26% of the gas-phase mass of products then this does not seem to qualify. The authors should make clear what they mean by low-NOx.

2. My understanding is that the present classification method does not separate positional isomers. Is this correct?

3. P. 33643: In the Conclusions it would be useful to summarize the value of this approach and clarify its advantages over getting this information other ways.

Technical Comments:

None.

Interactive comment on Atmos. Chem. Phys. Discuss., 15, 33631, 2015.