

Interactive comment on “Technical Note: Relating functional group measurements to carbon types for improved model-measurement comparisons of organic aerosol composition” by Satoshi Takahama and Giulia Ruggeri

Anonymous Referee #1

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General Comments

In this paper the authors report further on a framework they have been developing to extend the utility of functional group analysis of organic aerosol to obtain more accurate information on possible missing chemical components, organic mass/organic carbon ratio, elemental composition (O/C ratio), and carbon oxidation state. A thorough discussion of the conceptual and analytical aspects of the methods are presented and discussed, and software is made available that can be downloaded by others wishing to use these methods. The methods were applied to a data set of SOA composition

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predicted for α -pinene photooxidation using the MCM coupled with gas-particle partitioning, and for which FTIR functional group data were also available. A variety of useful results are extracted from the analysis. The paper is technically very dense and beyond my ability to fully understand without a much greater investment of time and effort, and so I am unable to evaluate many of the details that are presented. Nonetheless, the approach seems reasonable to me.

Overall, I think this is likely to be a useful paper as more people begin to adapt these methods for analysis of functional group data. Not many group conduct functional group analysis, but there are reasons to think this could increase in the future because of its unique value compared with molecular and AMS analysis. I'm very pleased to see that the authors have made the software needed to conduct the analysis freely available. I recommend the paper be published after these very minor comments are addressed.

Specific Comments

Page 5, line 7: I have never heard it said that FTIR measures the total abundance of bonds. The spectrum depends on vibrations and bending of molecules, but I don't see how this translates directly into bond abundance. This should be clarified.

Page 13, lines 4–5: Baltensperger and co-workers (AMT) measured a peroxide lifetime of a few hours in chamber SOA generated from α -pinene + ozone.

Technical Comments

Page 1, line 17: Insert “a” before “framework”.

Page 3, line 1: Should “metric” be inserted after “carbon-centric”?

Page 4, line 8: Delete “a” after “specific”.

Page 5, line 10 or 11. Delete “weighted” on one line or the other.

Page 6, line 1: Can probably delete “expressed”.

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Page 6, line 2: Should be “below” not “blow”.

Page 7, line 4: Should “atoms” be inserted after “carbon”?

Page 7, line 11: Should a comma be added after “eCH”?

Interactive comment on Atmos. Chem. Phys. Discuss., doi:10.5194/acp-2016-926, 2016.