Atmos. Chem. Phys. Discuss., 12, C4733–C4735, 2012
www.atmos-chem-phys-discuss.net/12/C4733/2012/

Atmospheric Chemistry and Physics Discussions

Interactive comment on "Cyclobutyl methyl ketone as a model compound for pinonic acid to elucidate oxidation mechanisms" *by* A. P. Praplan et al.

Anonymous Referee #3

Received and published: 15 July 2012

This manuscript describes an excellent study attempting to elucidate the OH oxidation chemistry chemistry of oxidized organic compounds associated with organic-aerosol formation and aging. The idea is to use a simplified surrogate compound containing key structural elements. In this case, cyclobutyl methyl ketone (CMK) is the surrogate for the important a-pinene oxidation product cis pinonic acid. CMK has two important structural elements in close enough proximity to influence each other – the ketone and the cyclobutyl ring. However, CMK is much more volatile than pinonic acid as well as being structurally simpler. Thus, CMK can be used to explore the hypothesis that interactions of just these two elements in purely gas-phase oxidation can explain the fairly puzzling observation of tricarboxylic acid formation from a single generation of pinonic acid oxidation.

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More broadly, the work has the potential to clearly illustrate a straightforward but important point: the oxidation chemistry of oxidized organic compounds containing multiple interacting structural elements can rapidly deviate from canonical intuition. Because the chemistry described here is unambiguously in the gas phase, and because the CMK is a fairly simple compound, this work serves as a potentially outstanding probe of these important issues.

That being said, the manuscript as currently written fails to make these points clearly. Instead, it plunges into the mechanistic details in the very first sentence of the abstract and for all practical purposes never surfaces. Consequently, while the work and the interpretation appear to be sound and significant, the manuscript requires extensive revision before it is suitable for any but the most dedicated readers.

Here are some specific suggestions.

1. The abstract should be completely rewritten, starting from scratch. Something more along the lines of the big-picture assessment I present above would work well. At present the abstract is a succinct summary of the work, but as such it is even more densely packed with detail than the body of the paper. No non-specialist could possibly read the abstract and have any idea why the work is important.

2. To me, the big-picture important point of this work is that "non-traditional" chemistry can quickly dominate over "traditional" chemistry even in situations where there is no doubt that the chemistry is occurring in the gas phase. This strongly supports the conclusions of Muller et al that the triacid MBTCA is formed in a single generation of gas-phase oxidation from pinonic acid, but significantly refines the constraints on the mechanism. The authors should be aware that the mechanistic detail pervading the manuscript will be off putting to many readers, and so the writing should surface from those details from time to time to emphasize the big-picture implications of the work.

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3. I don't think Fig. 2 serves much of a purpose – it shows that different OH sources produced different absolute amounts of OH. That is not a surprise.

4. There are a few points where it is obvious the authors are not native speakers of English. For example:

   (a) "are increasing" on p 10659 (hereafter 59) line 4 should be "increase".

   (b) "mechanisms . . . needs" on lines 21-23 of the abstract should be "mechanisms . . . need"

etc

Interactive comment on Atmos. Chem. Phys. Discuss., 12, 10651, 2012.