

Interactive comment on “Does acetone react with HO₂ in the upper-troposphere?” by T. J. Dillon et al.

Anonymous Referee #2

Received and published: 29 August 2010

This paper describes a laboratory study of the HO₂ + acetone reaction at low temperatures. The results from this study are used as input to an atmospheric model to evaluate the significance of this chemistry with regards to acetone loss and acetic acid production. This is a rather difficult reaction to study directly and the authors have used an indirect method to extract kinetic data using modeling of experimentally measured OH profiles. The subject of this paper is definitely suitable for publication in ACP, however, I have an issue with the clarity of the paper in its present form and the thoroughness of the data analysis/interpretation.

The description of the data analysis and determination of the rate constants and equilibrium constant in the text is difficult to follow. The data analysis requires fitting of OH temporal profiles using an extensive reaction mechanism (provided in a table), but the

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sensitivity of the obtained k_1 and K_{eq} values to the model parameters is not clearly established. The kinetic results are given in Table 2, but the reader pretty much has to take these values on faith. Another complication to the clarity of the text is the interwoven discussion of the kinetic parameters reported from previous theoretical studies. I would much prefer to know what the experimental data “says” independent of the theoretical calculations. The experimental results should then be compared with the theoretical predictions. If the experimental data can't be interpreted independently of the theoretical calculations that should be made more clear in the text. In the present form, I get an impression that the kinetic data for this reaction is still not well determined, i.e., I do not get a clear answer to the title of the manuscript.

The atmospheric model calculations presented are reasonable, but a clearer definition of the experimental data is needed before these calculations are meaningful. Figure 5 does not really provide much useful information related to the present study. It is useful to show the model sensitivity but a comparison to field measurements of CH₃C(O)OH with the model calculations is almost meaningless until better quality measurements become available.

A few comments and typos:

Page 16748, line 8: “provide evidence” should be “provide indirect evidence” ?

Page 16748, line 12: “larger” should be “greater”

Page 16749, line 4: provide units for E in the given Arrhenius expression, it would be better yet to just use E/R values throughout.

Page 16750, lines 5-10: It is not clear or true that the agreement of theoretical calculations for other reaction systems should give you confidence in the Hermans et al. (2004) calculations. The reason for giving the text following these statements is also not clearly stated.

Page 16751, line 13: Referring to an interference filter is rather vague, what are the

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optical properties?

The discussion of the data in figures 1 and 2 given on pages 16754 and 16755 is vague and unclear. For example, on page 16755 the phrase “were in roughly inverse” is given, but then the results are referred to as “robust”.

Page 16755, lines 6 and 24: exponent should be “-12”

Figure 2, caption: is the k -1 value of 30000 s-1 right? The numbers in Table 2 are not in line with such a large value.

Figure 4: narrow down the range on the x-axis to reduce the amount of empty white space.

Table 3: The text font is too small.

Interactive comment on Atmos. Chem. Phys. Discuss., 10, 16747, 2010.