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ACPD 11, C1012–C1013, 2011

> Interactive Comment

## Interactive comment on "Rate coefficients for the gas-phase reaction of OH with $(\vec{Z})$ -3-hexen-1-ol, 1-penten-3-ol, $(\vec{E})$ -2-penten-1-ol, and $(\vec{E})$ -2-hexen-1-ol between 243 and 404 K" by M. E. Davis and J. B. Burkholder

## Anonymous Referee #2

Received and published: 21 March 2011

The authors provide a useful set of data describing the temperature dependence of the title reactions. As is typical for this research group, the study has been carried out in a careful manner and is very thorough, with experiments having been carried out (for example) using different OH sources, at different pressures, with addition of O2, with on-line concentration measurements, and with OD as the reactant. I have a couple of minor comments (detailed below), mostly regarding the structure-reactivity discussion; otherwise, it is my opinion that the paper is essentially publishable in its current form.

For (E)-2-penten-1-ol and (E)-2-hexen-1-ol, it doesn't appear that any tests for OH





regeneration were conducted at high temperature? Can this process be entirely ruled out in these cases? (Regeneration might be most favorable at elevated temperature?)

The observation of different reactivity for the E- and Z- isomers is an interesting and valuable one, and I have just a few suggestions to help clarify the discussion. First, the 2001 Papagni et al. paper presents evidence that the enhancement factor for –OH substituents is closer to a factor of two, rather than the value of 1.6 given by Kwok and Atkinson, and I would suggest using this updated value in the calculations performed and discussed. Further, I don't think the SAR calculation for (Z)-3-hexen-1-ol currently includes an effect for the presence of the OH functionality. Given the discussion in Papagni et al. (and confirmed here), that the position of the OH group relative to the double bond is not critical, would it not make sense to include the enhancement for the (Z)-3-hexen-1-ol SAR calculation as well?

Minor editorial comments:

pg. 2378, line 2 – there is a period after the structure of 3-hexen-1-ol that should be deleted.

- Pg. 2379, line 18 please insert a comma after 'onion'.
- Pg. 2383 'determined' would be better than 'performed'.
- Pg. 2387, line 1 should be 'obey' rather than 'obeys', I think.
- Pg. 2387, line 22 should be "(E)-2-hexen-1-ol" (also line 4 on following page).
- Pg. 2392, line 11 Lifetimes between about 2.5 to 5 hrs. might be more accurate, for the OH concentration given?

Table 6 – last compound listed in the table title should be (E)-2-hexen-1-ol.

Interactive comment on Atmos. Chem. Phys. Discuss., 11, 2377, 2011.

Interactive Comment

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