

Interactive comment on “Investigation of the oxidation of methyl vinyl ketone (MVK) by OH radicals in the atmospheric simulation chamber SAPHIR” by Hendrik Fuchs et al.

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We thank the reviewer for the helpful comments.

Comment: The authors should examine the tenses used in the paper. It is usual to use the past tense for experiments (e.g. p9 l1, should be “MVK...was injected...”) and the present tense for results etc.

Response: The manuscript was checked and tenses are corrected.

Comment: P4, l9. Change to “...prevents ambient air entering...” and P4, l21. change to “...detection limit of the instruments.”

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Response: This is changed as suggested.

Comment: Either square brackets or the word concentrations should be inserted. i.e. “...OH concentrations agree...”. This error occurs on a number of occasions (e.g. later on the same line)

Response: This was checked and is corrected for the entire manuscript.

Comment: The sentence beginning “The predicted rate constant... ” would be helped by inserting a diagram into the SI – I presume the term “limited protruding section” means that part of the forward barrier that lies above the reactant energy, but it is not obvious. The comment on the reversibility of the alkoxy decomposition is not very clear – again this would be helped by a diagram of the PES and some additional comment in the SI.

Response: The paragraph is rephrased to explain more clearly what was meant, i.e. a barrier protruding less than 2 kcal/mol above the products, and hence a low barrier for the reverse H-migration. SAR-derived energy barriers for the alkoxy product decomposition (≥ 4 kcal/mol) are also mentioned now to further emphasize the potential competition on the product fate. Table 2 was found to contain a typo which added to the confusion. (a reaction energy of 2.40 which should have read 20.4). Finally, we show an energy diagram in the supporting information.

Comment: P11, R7. The mechanism would be clearer if the underlined phrase below were inserted: “...HMKAO2 1,4 H migration ...-OH group, followed by H abstraction at the -OH site by O2 forming HO2...” Also the O2 in reaction R7 is not involved in the rate determining step and so + O2 should be placed in brackets. Generally speaking, it is necessary to have the MCM site open on reading the paper to appreciate the details of the reactions being discussed. While this is OK, it does slow reading down – the authors might consider putting the structures, with MCM names, in the SI.

Response: The phrase is added as suggested. Structures of all molecules relevant for

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the discussion are given together with their names in the MCM in Figure 1. We have the feeling that this is sufficient for the reader to follow the discussion.

Comment: P13, l4. The first sentence needs rephrasing – the word rates should be inserted and a reference made to the steady state (the reaction rates are equal – they are not genuinely in equilibrium.) I suggest “OH is in steady state because of its short lifetime, so that its rates of production and destruction are equal.”

Response: The sentence is changed accordingly.

Interactive comment on Atmos. Chem. Phys. Discuss., <https://doi.org/10.5194/acp-2018-265>, 2018.