

# ***Interactive comment on* “Estimation of rate coefficients and branching ratios for gas-phase reactions of OH with aliphatic organic compounds for use in automated mechanism construction” by Michael E. Jenkin et al.**

## **Anonymous Referee #1**

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### General Comments

This paper describes structure-activity relationship (SAR) methods for the gas-phase reactions of the OH radical with a large number of aliphatic hydrocarbons and oxygenated organic compounds. The approach involves determination of a partial rate coefficient for each reactive site in the compounds, thus enabling overall rate coefficients and branching ratios to be obtained. It successfully builds on previous efforts in the area by updating existing parameters for common compounds, while also extending the approach to new groups of compounds. The scope of the paper is wide-ranging and

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considers virtually all types of aliphatic hydrocarbons, monofunctional and bifunctional oxygenated organic compounds. This paper is part of a series by the same authors - SAR methods for the reactions of aromatic organic compounds are considered in a companion paper, with the reactions of peroxy radicals being covered in another.

Overall, this paper is very carefully written and remarkably error-free. The large amounts of information contained in it are presented in a logical and neat fashion. In particular, the supplementary information will be a very valuable resource for the atmospheric chemistry community. The research is well within the scope of Atmospheric Chemistry and Physics: I recommend publication after the authors have addressed the comments below.

#### Specific Comments:

1. Figures 1-7: There are a number of significant outliers in the log-log correlation plots. It would be useful to mention which compounds these are and if possible discuss why they are outliers.
2. Page 8, lines 22-24: Here, I think it would be worth referring to the work of Porter et al. (1997) who first highlighted the inability of Kwok and Atkinson's SAR to predict the reactivity of diethers and proposed that some type of Hydrogen-bonding like interaction between OH and the ethers is taking place. This idea was further discussed by Smith and Ravishankara (2002), who also considered hydrogen bonding for OH reactions with a wider range of oxygenated organic compounds.
3. Page 19, Section 6: Up until this point in the paper, the emphasis has been solely on estimation of rate coefficients and branching ratios for OH attack at different sites in molecules. It therefore seems a little strange to include this section on the reactions of alkyl radicals (other than reaction with molecular oxygen to produce organic peroxy radicals). I think the authors should either justify the inclusion of this material here or leave it out and consider incorporating it into another of the planned papers in the series.

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4. Page 24, Section 7: It might be useful to briefly comment on whether developing SARs for other organic compounds, e.g. halocarbons, Sulfur- and Nitrogen-containing compounds etc., would be worthwhile.

#### Technical Corrections:

1. Page 5, line 1, the rate coefficient symbol should be in italics.
2. Page 7, lines 6-8, the authors should refer to Figure 2 here.
3. Page 10, line 34: Nielsen et al. (1989) is not included in the list of references.
4. Page 11, line 1: Liu et al. (1990) is not included in the list of references.
5. Page 16, line 3: Typo – should be Table 10.
6. Page 18, line 28: Boodaghians et al. (1989) is not included in the list of references.
7. Page 31-38: The following phrase contained in the figure captions of the log-log plots “ the  $\pm$  a factor of 2 range” is a bit awkward and should be reworded.

#### References:

Porter, E., Wenger, J., Treacy, J., Sidebottom, H., Mellouki, A., Téton S., and LeBras, G.: Kinetic Studies on the Reaction of Hydroxyl Radicals with Diethers and Hydroxy Ethers, *J. Phys. Chem. A*, 101, 5770-5775, 1997.

Smith, I.W.M., and Ravishankara, A.R.: Role of Hydrogen-Bonded Intermediates in the Bimolecular Reactions of the Hydroxyl Radical, *J. Phys. Chem. A*, 106, 4798–4807, 2002.

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