

Interactive comment on “Database for the kinetics of the gas-phase atmospheric reactions of organic compounds” by Max R. McGillen et al.

Anonymous Referee #4

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General comments:

The article entitled “Database for the kinetics of the gas-phase atmospheric reactions of organic compounds” by McGillen et al., is a very good collection of the rate coefficients for the reactions occurring in gas phase with OH and NO₃ radicals, ozone and chlorine atoms. The article is very well written and concise.

One general comment regarding the database behind the article is related to the rate coefficients presentation and the link with the initial article which published the kinetic results. The database is fully functional and it is a perfect collection for the researchers working on SAR methods and chemical models. However, the database is constructed on the results provided by many articles which deserve as well the citations as the database itself. I suggest to link in a more visible manner the references which are

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providing the rate coefficients values for the database. Please find a way to add in Excel spreadsheet for the recommended kinetic parameters a hidden comment easily visible by selecting the value including the reference articles which are linked with that rate coefficient value.

Specific comments:

I do not agree with the sentence from line 99. The relative rate studies rely on the rate coefficient values for reference reactions whose rate coefficient is already established. It should be not specified that such reference rate coefficients it is obtained by an absolute method or a relative method. I agree with the fact that for the first time, first reaction rate coefficient obtained by relative techniques requires a reference reaction whose rate constant is measured with an absolute method but for later cases is not true.

The paragraph from 159 to 164 I consider to be revisited. Firstly there you should avoid to refer to “long chain hydrocarbons” only when you present the rate coefficients at 298 K as discussed in the present compilation which span the range from the gas kinetic limit for the reactions of chlorine atoms. However in the data base you have a rate constant for 1-ethenoxy butane with chlorine atom with the value of $9.9\text{E}-10 \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ to give just an example out of “long chain hydrocarbons”. Secondly, I suggest expanding this discussion about gas kinetic limit for each type of reactions involving those four oxidants. Would be great adding in the text a limit value (or range) for each of the four oxidants. Please explain the reason why you include in the database such high rate coefficients as that one presented above.

Line 104: please consider other techniques as well (e.g. PTR, monitors) and not exclusively GC and FTIR.

Line 104: Please mention that should be there a “near zero intercept” for the slope.

Line 123: I would write there “standard Arrhenius equation” if later you formulate the

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“extended” one

Eq.2: line 124, please describe E for the equation since you described A (pre-exponential factor)

Line 331: I suggest replace “daughter” with “secondary”

Technical corrections:

Entire text: please be consistent with the space between the temperature values and K units. (e.g. “298K” vs “298 K”)

Interactive comment on Earth Syst. Sci. Data Discuss., <https://doi.org/10.5194/essd-2019-236>, 2020.

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