

We thank the reviewers for their thoughtful comments. Our response (in blue text) to the specific comments made by the reviewers and changes to the manuscript (in red text) is given below.

Reviewer 1

This manuscript constitutes Volume IX of the series Evaluated kinetic and photochemical data for atmospheric chemistry. The authors present data sheets in Volume IX for the gas-phase and photochemical reactions of halogenated organic species that have been added since the publication of Volume IV. It covers the extension of the gas-phase and photochemical reactions of halogenated alkanes, alkenes, and oxygenated organic compounds, as implemented on the IUPAC website since 2008. This is excellent work that will be very useful for modelers and experimental kineticists.

Thank you.

The manuscript consists of a summary table of the recommended kinetic parameters for the evaluated reactions and a supplement containing the data sheets that provide the information on which the recommendations are based. This structure is well designed: the overall organization is clear, and the data presentation is intuitive, allowing readers to efficiently search for and compare kinetic and photochemical parameters across different reaction systems. I recommend publication after the authors address the following minor comments.

1. The data sheet table in the Supporting Information (Pages 2-4) currently lacks page numbers for reactions, which may hinder data navigation. It is recommended that the authors add this information.

We have added page numbers as suggested.

Page numbers added to table.

2. On Page 94 of the Supporting Information, there is a typo in the unit of the reported rate coefficient ($\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$).

Typo corrected.

Typo corrected.

Reviewer 2

(1). In Section 2.3, the reactions $A + B + M \rightarrow AB + M$ and $AB + M \rightarrow A + B + M$ are presented in the text. Assigning equation numbers to these reactions would increase the clarity. In other words, all equations need to carry equation numbers for clarity.

We have numbered all reactions and equations.

Reactions and equations numbered.

(2). If this study focuses on a series of halogenated oxygenated VOCs, why were esters not included in the selected compounds?

We focused our attention on the currently more commercially significant and environmentally important compounds. We will consider halogenated esters in future work.

No changes made to manuscript.

(3). In your previous work (Volume IV), theoretical data were referenced for branching ratio calculations of C_3 molecules. In the present study, the system involves molecules larger than C_3 , yet no theoretical data are provided for the branching ratio. The authors may include these data for completion purposes.

We have not strived to consistently list all theoretical studies in the past. We generally mention theoretical work only when theory helps resolve experimental differences (or e.g., confirms unexpected results).

No changes made to manuscript.

Reviewer 3

1) General Comments

This manuscript presents the ninth volume of a series of IUPAC evaluations of atmospheric chemical kinetic and photochemical data. It provides updated and newly assessed gas-phase and photochemical reactions for halogenated alkanes, alkenes, and oxygenated organic compounds, reflecting developments since the 2008 Volume IV publication. These kinds of evaluations/compilations are greatly appreciated not only for atmospheric chemists but also for policy makers and modelers. Thus, the article highlights the expanding environmental and regulatory relevance of halogenated species—particularly HFCs and their industrial replacements—and emphasizes the need for accurate kinetic data to support atmospheric modeling and policy.

Thank you.

The evaluation of kinetic data focuses mainly on OH reactions, but Cl, NO₃ and O₃ reactions are also included for some halogenated species. However, since the last evaluation in 2008, the literature on gas-phase reaction kinetic studies on halogenated species has notably increased. Despite that, new results have not been incorporated in the present evaluation, and it would be worth including them, in my opinion.

As the reviewer notes, there is great interest in halogenated species and the kinetic database for their atmospheric reactions has increased notably. It was not possible to include all reactions for which data have become available. We have tried to focus on atmospherically important reactions for the most commercially significant and environmentally important compounds. We will be continuing to expand our coverage in the future and look forward to providing more evaluated data.

No changes made to manuscript.

Regarding the photochemical data, this assessment is only focused on fluorinated aldehydes as these species (slightly) absorb in the solar actinic region. It is likely that iodine species can also present some UV absorption in that spectral region. In fact, UV absorption cross sections for the iodine species included in the kinetic data evaluation were already published (Roehl et al. 1997 Journal of Geophysical Research, 102, 12,819-12,829). Authors have to consider if it is worth including them or not.

We thank the reviewer for suggesting that we broaden the coverage of photochemical reactions of iodine containing species. We will consider this in our future work.

No changes made to manuscript.

Overall, the manuscript provides a highly valuable update of the kinetic and photochemical data that complements the interactive online IUPAC database.

Thank you.

2) Specific Comments on the manuscript

Unify “gas phase reactions” or “gas-phase reactions”. Generally, the second one is used.

We have harmonized the text throughout to “gas-phase reactions” when used as an adjective before a noun.

Text has been made consistent.

Unify “high (or low)-pressure limit” or “high (or low) pressure limit”

We have harmonized the text throughout to “high (or low)-pressure limit”.

Text has been made consistent.

Unify “cross-section” or “cross sections”

We have harmonized the text throughout to “cross sections”.

Text has been made consistent.

Some reactions in sections 2.2 and 2.3 are not numbered.

All reactions are now numbered.

Reaction numbers have been added.

Although Section 3.2 is of great interest from the theoretical background point of view, maybe this section on the treatment of termolecular reactions could be shortened. Only two termolecular reactions are evaluated here: oFOx162 and oFOx163.

Although there are only two termolecular reactions, for completeness we prefer to retain the complete theoretical background.

No changes made to manuscript.

Line 621: Authors state that “Rate coefficients are also known as rate constants, both terms are used here”. Perhaps this statement should be placed at the beginning of the manuscript, if authors consider the use of both terms. I would prefer to unify it. In fact, “rate constant” is only used only in section 3.2.

We have added the statement to the beginning of the manuscript following the reviewer's suggestion.

Text has been moved as suggested.

3) Specific Comments on the Supplementary Information

Although I did not make a large scrutiny, I noticed that **some reactions are not properly updated**. Is there any reason for not including them? For example:

oFOx143: The evaluation of this reaction was made in June 2025 with the newest data from 2011. However, a more recent article was published (Blázquez et al. 2022, <https://doi.org/10.1039/D2CP00160H>).

We have added the recent article by Blázquez et al. 2022 to the datasheet.

The article by Blázquez et al. 2022 has been added and is discussed in the datasheet.

oFOx149: The evaluation of the HO+sevoflurane reaction was made in September 2025 and a paper on published in June 2025 (Espinosa et al. 2025. <https://doi.org/10.1039/D5EM00061K>).

We have added the recent article by Espinosa et al. 2025 to the datasheet.

The article by Espinosa et al. 2025 has been added and is discussed in the datasheet

oFOx150: The HO+desflurane reaction was evaluated. What about isoflurane ($\text{CF}_3\text{CHClOCHF}_2$)? There are some papers on this reaction (see below).

The OH + isoflurane reaction was added to the database prior to 2008 (see Atkinson et al. 2008) and is not included in the current extension.

No changes made to manuscript.

I miss more recent results on some OH- and Cl-reactions which are not included in the evaluation. I am giving here *some examples*:

Halogenated alkanes

HO+CH₃CHBrCH₂CH₃ (**2025**, <https://doi.org/10.1039/d5cp00961h>)

Halogenated alkenes

HO+CH₂=CHCH₂OCF₂CHF₂ (**2024**, <https://doi.org/10.1007/s11356-024-35536-4>)

HO+CF₃(CF₂)₂CH=CH₂ (HFC-1447fz) (**2016**, <https://doi.org/10.1021/acs.est.5b04379>)

HO+ CF₃CH=CH₂ (HFO-1243zf) (**2015**, <https://doi.org/10.1007/s11356-014-3426-2>)

$\text{Cl} + \text{CH}_2 = \text{CHCH}_2\text{OCF}_2\text{CHF}_2$ (**2024**, <https://doi.org/10.1007/s11356-024-35536-4>)

$\text{Cl} + \text{C}_x\text{F}_{2x+1}\text{CH} = \text{CH}_2$ ($x=1-6$) (**2017**, <https://doi.org/10.1016/j.chemosphere.2016.09.156>)

$\text{O}_3 + \text{C}_x\text{F}_{2x+1}\text{CH} = \text{CH}_2$ ($x=1-6$) (**2018**, <https://doi.org/10.1016/j.chemosphere.2018.02.183>)

Halogenated ethers

$\text{HO} + \text{CHF}_2\text{CF}_2\text{CH}_2\text{OCH}_3$ (HFE-374pcf), and $\text{CF}_3\text{CF}_2\text{CH}_2\text{OCH}_3$ (HFE-365mcf3): **2022**, <https://doi.org/10.1039/D2CP00160H>.

$\text{HO} + \text{isoflurane}$ ($\text{CF}_3\text{CHClOCHF}_2$): Latest **2011**: <https://doi.org/10.1021/jp2077598>; **2025**: <https://doi.org/10.1039/D5EM00061K>.

We thank the reviewer for providing these citations. The goal of the present extension was to broaden the coverage of commercially important compounds, not to include all compounds for which kinetic data are available. The OH + isoflurane reaction was included prior to 2008, see Atkinson et al. (2008). We will continue to expand the coverage of the database and will consider adding these reactions.

No changes made to manuscript.

Revise the special characters and/or spelling of the last name of some authors. For example, Sellevag (instead of Sellevåg), Sulbæk (instead of Sulbaek), Antiñolo (instead of Antinolo) among others are misspelled in several ways and places.

We have revised the special characters to reflect the author names as they appeared in the publications cited (e.g., Sellevåg, Antiñolo, Jiménez, Martínez, Blázquez). We retain “Sulbaek Andersen” as it is the spelling used by this author.

The special characters have been added to the manuscript.

Format of the plot in **oFOx161** datasheet is not the same as the rest.

Different graphic software is used by different members of the Task Group. For simplicity we have not redrawn figures in the supporting information using a common software.

No changes made to manuscript.

Page 234: Some absorption cross sections of $n\text{-C}_4\text{F}_9\text{CHO}$ are negative. Can these values be substituted by ~ 0 ? Usually, a negative value means that there is no absorption at that wavelength. On the other hand, the presented absorption cross sections do not include uncertainties.

We have added a statement that the negative numbers (at wavelengths longer than 370 nm) reflect instrumental noise and that we are dealing with measurements at the detection

limit of the apparatus used. We decided to remove the preferred data below 240 nm because of the limited data at these wavelengths.

A statement that negative numbers (at wavelengths longer than 370 nm) reflect instrumental noise and that we are dealing with measurements at the detection limit of the apparatus used has been added.

Page 232 and 239: Dashed lines in the figure are not visible in the legend.

Thank you for pointing this out. This was a problem with converting the original Word file into a pdf file. We have resolved this problem.

We have replaced dotted lines with solid lines in the figure.

4) Suggestions/ Typographical errors

Line 96: Change “If the temperature coefficient has been measured...” by “If the temperature **dependence of the rate** coefficient...”

Thanks, suggestion adopted.

Text modified as suggested.

Line 98: Change “...the normal Arrhenius form” by “the **conventional** Arrhenius form”

Thanks, suggestion adopted.

Text modified as suggested.

Line 99: Replace E by E_a (activation energy) to avoid any confusion with E parameter in $k = E T^2 \exp(-F/T)$. I suggest using E_a/R instead of E/R throughout the paper.

We choose to retain “E” for simplicity as we feel there is little danger of confusion with the parameter in the modified Arrhenius expression.

No changes made to manuscript.

Line 120: Please, delete “spectroscopy” from CIMS – chemical ionization mass spectroscopy/spectrometry. It is not an spectroscopic technique.

We agree it is mass *spectrometry* and have made this correction.

Text modified as suggested.

Line 408: The **next table** lists the preferred absorption cross section data and the preferred quantum yields at appropriate wavelength intervals. What table?

We have added “in each datasheet” for clarification.

Text modified for clarity.

Line 425: I_0 is defined as the incident light intensity, however it should be defined as the transmitted light intensity in the absence of absorber. Experimentally, the incident light intensity can be higher than the transmitted light intensity in the absence of absorber.

Thanks, suggestion adopted.

Text modified as suggested.

Reviewer 4

This kinetic and photochemical data evaluation is important and timely. Some of my comments overlap with those of other reviewers, so I won't repeat them here. I only have a few questions and suggestions in addition to what has already been said.

For the perfluorinated acids - Hurley 2004 reported for $n=2-4$, $k(\text{OH} + \text{F}(\text{CF}_2)_n\text{COOH})$ has a rate coefficient of $(1.69 (0.22) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K. I wonder why two k_{296} values were listed in the evaluation for the same technique, neither of them the reported value, and then a preferred value of $1.5 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ was chosen.

The two values listed are based on the results obtained in separate experiments using two different reference compounds (C_2H_2 and C_2H_4) in the relative rate experiments. For consistency across the database, wherever possible, we have used preferred values from the database for reference rate coefficients to place the measured rate constant ratios on an absolute basis. The reference rate coefficients that we used are different from those used by Hurley et al. (2004). The final preferred value is the average of the two determinations ($1.54\text{E-}13$ and $1.56\text{E-}13$). We agree with the reviewer that it is confusing that the average of $1.54\text{E-}13$ and $1.56\text{E-}13$ is $1.55\text{E-}13$, but instead we rounded the result to $1.5\text{E-}13$. We now quote $1.55\text{E-}13$ to remove this confusion.

Text modified for clarity.

When evaluating the OH reaction with photolabile molecules such as CHF_2CHO (PF5), the authors should also comment on how, or if, a correction for photolysis at the wavelengths used to generate OH radicals in experiments (e.g., 248 nm and 310 nm in oFOx97) has been made and how that infers their preferred values.

The fluence of the laser used to generate OH radicals was varied with no discernable effect on the measured rate constant indicating the absence of complications from photolysis of photolabile compounds such as CHF_2CHO . Comment have been added to datasheet oFOx97.

A comment has been added to datasheet oFOx97.