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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Evaluated kinetic and photochemical data for atmospheric chemistry: Volume IV – gas phase reactions of organic halogen species" *by* R. Atkinson et al.

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IUPAC evaluations, published over the years, have proven to be of the highest quality. The presented manuscript provides the latest recommendations from the IUPAC panel on photochemical properties of organic halogenated compounds. It presents the results from original research papers followed by the values recommended by the IUPAC Data Panel. The recommendations seem reasonable and well justified. The cited literature appears to be complete for the listed reactions. The amount and quality of work that has been done is very impressive. There is always an element of subjectivity in any data evaluation. This is why the present evaluation performed by

the well recognized group of top experts in the field is especially important for potential customers.
In a number of cases the assigned uncertainties seem too conservative. However, this should be considered as a consensus of the IUPAC Data Panel.
This manuscript is a very important contribution to the atmospheric modeling and gas kinetic research community. The publication is highly recommended.

Based on the above, I give no comments on the recommended data and their uncertainties. Below are a few minor comments on data presentation including the introductory guide to the data sheets. Authors may consider them when doing the final corrections.

Table 1:
A footnote/endnote reference "a" appears in the column headings for $\Delta log k$ and $\Delta(E/R)$. However, it looks like the corresponding footnote/endnote does not exist in the manuscript.

Table 1 (page 16354 reactions 14, 19 and later on through the entire Table 1):
Three or four significant digits are shown for *E/R* in the fifth column ("Temp. dependence"). It does not look consistent with other recommended parameters: the variation of the last digit in *E/R*, i.e. $\Delta(E/R) = \pm$ 5 K, results in less than 1% variation of the recommended expression over the entire temperature range. Meantime only two significant digits are shown for both k_{298} (column 3) and *A*-factor (column 5).

Table 1 (page 16361 lines 117-119 and later on through the entire Table 1):
Only an upper limit of the reaction rate constant is recommended. Therefore, the single significant digit is reasonably shown for both k_{298} (column 3) and *A*-factor

ACPD
7, S8474–S8477, 2008

(column 5). Meantime three significant digits are shown for E/R in the fifth column ("Temp. dependence").

Page 16383, line 20 through page 16384, line 4:
Does this paragraph with four newly employed parameters - C, D, H, G instead of common log$k$, Δlog$k$, E/R, and $\Delta(E/R)$ - clarify anything? They are not used in the manuscript. (Actually, C and D are used later but with different meaning!)

Page 16383, lines 21, 24:
Parameters C and D are introduced as $k = D$ and log $k = C \pm D$. Meantime, both C and D were already introduced earlier in page 16372, line 3 and used in a number of Comments with different meaning in the three-parameter equation.

Page 16383, line 22:
A parameter F is introduced as an uncertainty factor. Meantime, it was already introduced earlier in page 16377, line 18 with different meaning to be used through page 16379.

Page 16383, lines 21-22:
$\log_{10} K$ and $\log_{10} F$ are used instead of log K and log F. The base 10 should be shown either everywhere through the entire manuscript or nowhere so as to not confuse a reader. I would correct it in this page.

Page 16383, line 21:
$\log_{10} K$=... It should be log k=....

ACPD
7, S8474–S8477, 2008

Interactive Comment

Page 16384, line 4:
K(T). It should be *k(T)*.

Page 16384, line 13:
"or even 90% confi-". Should it be "or even 95% confi-"?

Page 16386, line 24-27:
It would be reasonable to cite the latest JPL/NASA Evaluation Number 15 - JPL Publication 06-2, 2006.

Page 16410, lines 14-15 through page 16458, line 24-27:
I would suggest clarifying the procedure used to derive the preferred Arrhenius expression. Actually it is the tangent to the three-parameter fit at the middle point of *1/T* range, T_m. Parameters *A* and *B* were calculated as $A = Ce^2{T_m}^2$ and $B = D + 2T_m$ with the particular "middle"; temperature, T_m, not the variable *T* as it is written. I would also clarify the choice of this temperature, T_m.

Interactive comment on Atmos. Chem. Phys. Discuss., 7, 16349, 2007.

ACPD
7, S8474–S8477, 2008