# IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet VI.A1.1 HET_H2OL_1



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**$O_3 + H_2O(liq) \rightarrow$ products**

## Experimental data

| *Parameter* | Temp./K | Reference | Technique/ Comments |
|---|---|---|---|
| *Accommodation coefficients: $\alpha_b$* | | | |
| $\alpha_b > 2\times10^{-3}$ (± 20 %) | 276 | Utter et al., 1992 | WWFT-CLD(a) |
| $\alpha_b > 2\times10^{-3}$ (2.89 M >[$I^-$] > 0.36 M) | 282 | Magi et al., 1997 | DT-MS (b) |
| $> 2.0\times10^{-2}$ | 298 | Schütze and Herrmann, 2002 | (c) |

## Comments

(a) Wetted-wall flow reactor with flowing film of liquid water (0.2 mm thick). The ozone concentration was $10^{11}$ molecule $cm^{-3}$. No uptake of $O_3$ was observed into pure deionized water, but $\gamma$ increased as a function of the concentration of the trapping agent (*e.g.*, $Na_2SO_3$) to values in the $10^{-2}$ range. A conservative lower limit for the accommodation coefficient of $2 \times 10^{-3}$was obtained.

(b) Uptake on a train of aqueous drops (80 to 150 μm) in a laminar flow tube coupled to an ion trap MS with [$O_3$] monitored at m/e 46 ($NO_2^+$) after titration by NO to $NO_2$. . No measurable uptake of $O_3$ on pure water. The lower limit for $\alpha_b$ was found from the intercept of a plot of $1/\gamma$ vs. $1/(a_{I-})^{½}$ when NaI was used as scavenger.

(c) Uptake onto static single drop (2-3 mm in diameter) containing NaI as scavenger. The product $I_3^-$ was monitored by time-resolved UV/Vis absorption spectroscopy. Absorbance-time profiles at two different wavelengths (288, 353 nm) were used to derive uptake coefficients. The tabulated value of $\alpha_b$ results from the intercept of $1/\gamma$ vs. $1/(a_{I^-})$ plots.

## Preferred Values

| **Parameter** | **Value** | **T/K** |
|---|---|---|
| $\alpha_b$ | $> 10^{-3}$ | 298 |
| $D_l$ ($cm^{-2}$ $s^{-1}$) | $1.85 \times 10^{-5}$ | |
| $H$ (M $atm^{-1}$) | $1.15\times 10^{-2}$ exp (2560/T-8.6) | 298 |

*Reliability*

| | | |
|---|---|---|
| $\Delta$ log ($\alpha$) | ± 0.3 | 298 |
| $\Delta$ log ($k^{II}$) | ± 0.5 | |

*Comments on Preferred Values*

In the absence of fast loss processes, the uptake of $O_3$ on pure water is reversible (Staehelin and Hoigné, 1982). The low solubility of $O_3$ means that uptake rapidly saturates and net $O_3$ uptake is observable under conditions of the work of Utter et al. (1992). Therefore, the studies which derived an estimate for the bulk accommodation coefficient $\alpha_b$ used a scavenger ($SO_3^{2-}$ or $I^-$) to obtain $\alpha_b$ from the intercept of $1/\gamma$ vs. $1/(a_{I-})^{½}$ plots. We prefer the

lower limit obtained by Magi et al. (1997) from a relatively large data set. The data by Schütze and Herrmann (2002) are more strongly affected by diffusion, and the model to take that into account required several simplifications. In addition, Schütze and Herrmann found evidence for limitation of product formation via $HOI + 2I^- \rightarrow I_3^- + OH^-$ , while Magi et al. directly determined the net loss of $O_3$ from the gas phase. Note that for more concentrated iodide solutions, we prefer a value of $\alpha_b > 0.1$. Since halogenide ions may play a role in the bulk accommodation of ozone, we refrain from transferring the high bulk accommodation coefficient to dilute solutions.
The preferred solubility is the expression compiled by Chameides (1984). The room temperature value of the diffusion coefficient is from Matrozov et al. (1976).

## References

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