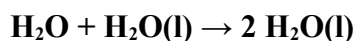


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet VIA1.18 HET_H2OL_18

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Experimental data

Parameter	Temp./K	Reference	Technique/ Comments
<i>Accommodation coefficients: α_b, α_t</i>			
$\alpha_b > 0.5$	263-298	Eames et al., 1997	(a)
$\alpha_b > 0.1$ (dynamic conditions) $\alpha_b < 0.1$ (stagnant conditions)	255-372	Marek and Straub, 2001	(b)
$\alpha_b = 0.17 \pm 0.03$ (H_2^{17}O on liquid)	280	Li et al., 2001	DT (c)
$\alpha_b = 0.32 \pm 0.04$	258		
$\alpha_t = 1.0 \pm 0.1$ (D_2O H/D exchange)	265-280		
$\alpha_b = 1.0$ (Ag-seeded μm -size droplets)	250-290	Winkler et al., 2004	(d)
$\alpha_b = 0.3$	295	Cappa et al., 2005	LJ-MS (e)
$\alpha_b = 0.62 \pm 0.09$	295	Smith et al., 2006	(f)
$\alpha_b = 0.18 \pm 0.08$	273	Zientara et al., 2008	(g)
$\alpha_b = 0.13 \pm 0.02$	293		
$\alpha_t = 1.0 \pm 0.1$	273-293		
$\alpha_b = 0.57 \pm 0.06$ (D_2O)	295	Drisdell et al., 2008	(h)

Comments

- Literature review in which most of the early experimental results on the evaporation coefficient (ϵ) of H_2O from liquid water surfaces were evaluated.
- Review of literature for liquid H_2O up until 2001..
- Droplet diameters 70–130 μm or 150–300 μm . Experiments conducted at various carrier gas pressures and for different carrier gases.
- Cloud expansion chamber study. Experimental water droplet growth curves monitored by Mie scattering of laser light.
- Measurement of the evaporation rate from a 2.5 μm radius H_2O microjet. The conditions were chosen so as to avoid recondensation of water vapour.
- The change in volume-averaged temperature of an evaporating train of microdroplets of 6-8 μm radius was measured using Raman emission excited at 514.5 nm to obtain evaporation rates. The numerical fit used a model explicitly taking into account the T-gradient of the droplet.

- (g) The temporal droplet radius evolution of a levitated water droplet of around 8 μ m diameter was observed in an electrostatic balance using angle-resolved Mie scattering at atmospheric pressure of N₂ or air on evaporation.
- (h) Same as (f), but for D₂O.

Preferred Values

Parameter	Value	T/K
α_b	$3.6 \times 10^{-5} \exp(2370/T)$	258-298
<i>Reliability</i>		
$\Delta \log(\alpha_b)$	± 0.3	258-298

Comments on Preferred Values

The uptake of gas phase water to liquid water has seen a long history of experiment, theory and debate due to its significance in cloud droplet and aerosol particle growth. The most recent evaluation of experimental and theoretical results within the atmospheric science community on this subject has been compiled by Davidovits et al. (2006), Garrett et al. (2006) and updated by Kolb et al. (2010) and Davidovits et al. (2011). This debate has been initiated by the conflicting results between H₂O uptake experiments to a train of droplets (Li et al., 2001) and cloud droplet growth experiments (Winkler et al., 2004) and involved consideration of mass transfer aspects in the gas phase but also questions around energy dissipation in the condensed phase. We are not reiterating a detailed discussion here.

The preferred values refer to pure water and to experimental conditions that only marginally depart from equilibrium and where the growth rates due to condensation of water vapor are accordingly low. H/D isotope exchange experiments on a train of liquid water droplets essentially yield $\alpha_s = 1.0$, when we do not differentiate between surface accommodation and thermal accommodation. The differing kinetic behaviour of oxygen isotope exchange vs. H/D exchange reported by Li et al. (2001) provides convincing evidence for precursor mediated bulk accommodation as proposed by Davidovits (1991) that is consistent with the negative temperature dependence of α_b observed in the droplet train experiments. Davidovits et al. (2004) in their comparison between Li et al. (2001) and Winkler et al. (2004) point out the agreement on the measured value of the thermal accommodation coefficient ($0.85 \leq \alpha_t \leq 1.0$) but state the disagreement of the results on α_b . A potential reason may lie in the vastly differing growth rates applied in the two experiments. We allow for sufficient uncertainty in the absolute value of α_b to take into account possible systematic errors in the analysis of the experiments discussed in the above mentioned reviews. Similar negative temperature dependence of α_b and values between 0.1 and 1 have also been found for other highly soluble trace gases to liquid substrates as well as for the uptake of H₂O on ice (see datasheet V.A1.6, Crowley et al., 2010).

Since condensation and evaporation rates are equal at equilibrium, information about α_b can also be retrieved from evaporation rate measurements. These were therefore also considered a source of relevant data. Eames et al. (1997) propose that the most probable value of the evaporation coefficient ε (numerically equal to α_b) is unity across all experimental conditions. In contrast, Marek and Straub (2001) conclude in their review that the condensation and evaporation coefficients are different from each other, and a decline of both coefficients with increasing temperature and pressure is derived, at variance with theoretical predictions. The data of Zientara et al. (2008) obtained on a stationary droplet are consistent with a negative T dependence of α_b and $\alpha_t = 1$. Other evaporation rate measurements were inconclusive about the temperature dependence (Smith et al., 2006; Drisdell et al., 2008). Although the emphasis of the work of Cappa et al. (2005) was placed on obtaining (H/D) isotope fractionation ratios, the cooling of the microjet along the axis was used to derive $E_a = 55$ kJ/Mol for the evaporation rate of H₂O which is approximately 10 kJ/Mol larger than ΔH_{vap} . Supporting TST (transition

state) calculations by Cappa et al. (2007) were also consistent with a negative T dependence of the evaporation coefficient but with a different slope than in the experiments. They noted a temperature dependence of the pre-exponential factor, though. Therefore, most evaporation rate measurements are also in reasonable agreement with our recommended uptake parameters.

References

- Cappa, C.D.; Drisdell, W.S.; Smith, J.D.; Saykally, R.J., Cohen, R.C.: *J. Phys. Chem. B*, 109, 24391-24400, 2005.
- Cappa, C. D., Smith, J. D., Drisdell, W. S., Saykally, R. J., and Cohen, R. C.: *The Journal of Physical Chemistry C*, 111, 7011-7020, 2007.
- Davidovits, P.; Jayne, J.T.; Duan, S.X.; Worsnop, D.R.; Zahniser, M.S., Kolb, C.E.: *J. Phys. Chem.*, 95, 6337-6340, 1991.
- Davidovits, P.; Worsnop, D.R.; Jayne, J.T.; Kolb, C.E.; Winkler, P.; Vrtala, A.; Wagner, P.E.; Kulmala, M.; Lehtinen, K.E.J.; Vesala, T.; Mozurkewich, M.: *Geophys. Res. Lett.*, 31, art no. L22111, doi:10.1029/2004GL020835, 2004.
- Davidovits, P., Kolb, C. E., Williams, L. R., Jayne, J. T., and Worsnop, D. R.: *Chem. Rev.*, 106, 1323-1354, 2006.
- Davidovits, P., Kolb, C. E., Williams, L. R., Jayne, J. T., and Worsnop, D. R.: *Chem. Rev.*, 111, doi: 10.1021/cr100360b, 2011.
- Drisdell, W.S.; Cappa, C.D.; Smith, J.D.; Saykally, R.J.; Cohen, R.C.: *Atmos. Chem. Phys.*, 8, 6699-6706, 2008.
- Eames, I.W.; Marr, N.J. and Sabir, H.: *Int. J. Heat Mass Transfer*, 40, 2963-2973, 1997.
- Garrett, B. C., Schenter, G. K., and Morita, A.: *Chem. Rev.*, 106, 1355-1374, 2006.
- Li, Y.Q.; Davidovits, P.; Shi, Q.; Jayne, J.T.; Kolb, C.E., Worsnop, D.R.: *J. Phys. Chem. A*, 105, 10627-10634, 2001.
- Kolb, C.E., Cox, R.A., Abbatt, J.P.D., Ammann, M., Davis, E.J., Donaldson, D.J., Garrett, B.C., George, C., Griffiths, P.T., Hanson, D.R., Kulmala, M., McFiggans, G., Pöschl, U., Riipinen, I., Rossi, M.J., Rudich, Y., Wagner, P.E., Winkler, P.M., Worsnop, D.R., O'Dowd, C.D.: *Atmos. Chem. Phys.*, 10, 10561-10605, 2010.
- Marek, R., Straub, J.: *Int. J. Heat Mass Transfer*, 44, 39-53, 2001.
- Smith, J.D.; Cappa, C.D.; Drisdell, W.S.; Cohen, R.C., Saykally, R.J.: *J. Amer. Chem. Soc.*, 128, 12892-12898, 2006.
- Wei, X., Miranda, P.B., Shen, Y.R.: *Phys. Rev. Lett.*, 86, 1554-1557, 2001.
- Winkler, P.M.; Vrtala, A.; Wagner, P.E.; Kulmala, M.; Lehtinen, K.E.J., Vesala, T.: *Phys. Rev. Lett.*, 93, art. no. 075701, 10.1103/PhysRevLett.93.075701, 2004.
- Zientara, M., Jakubczyk, D., Kolwas, K., Kolwas, M.: *J. Phys. Chem. A*, 112, 5152-5158, 2008.