IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet V.A5.5 HNDT5

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HNO_3 + NAT

Experimental data

Parameter	Temp./K	*Reference*	Technique/ Comments
Experimental uptake coefficients: γ, γ_0			
$\gamma_0 > 0.3$	191.5	Hanson, 1992	CWFT-CIMS a)
$\gamma_0 > 0.2$	200		
$\gamma_0 > 0.4$	197	Middlebrook et al., 1992	Knud (b)
γ = 0.165 HNO_3•3H_2O (NAT) 0.145 HNO_3•2H_2O (NAD) 0.13 HNO_3•H_2O (NAM)	160-170	Reinhardt, Fida and Zellner, 2003	(c)
Partition coefficients: K(cm)			
No reversible adsorption			

Comments

(a) HNO_3 deposited on ice condensed from the vapor phase onto the cold flow tube. γ corrected for gas diffusion using estimated diffusion coefficients. Pressure = 0.6 mbar He. Rapid uptake observed, but with increasing surface coverage of HNO_3 the rate of uptake decreased. The steady-state partial pressure of HNO_3 over an ice surface with a coverage of approximately 1 monolayer of HNO_3 was about a factor of five higher than the vapor pressure over NAT, showing that new hydrate was not formed.

(b) Static chamber with time-dependent FTIR monitoring of depositing NAT film. The thickness of the deposited NAT film was measured by optical interference in the range 4000 cm^{-1} to 7000 cm^{-1} assuming a refractive index of 1.45 for NAT. p_{H2O} = 2 x 10^{-4} mbar and p_{HNO3} = (5.3-13.3) x 10^{-7} mbar. A doubling of the H_2O left the uptake coefficient unchanged.

(c) Slow flow reaction cell with DRIFTS for detection of adsorbed species and downstream FTIR for gas phase HNO_3. Total pressure 10-30 mbar. At 170K and $[HNO_3]$= (2-5) x 10^{14} molecule cm^{-2} continuous uptake was observed with formation of crystalline HNO_3•3H_2O (NAT). Monohydrates and dihydrates formed at higher p_{HNO3}. Uptake coefficient independent of p_{HNO3}.

Preferred Values

Parameter	Value	T/K
α_s	>0.2	190 - 240
Reliability		
$\Delta \log (\alpha_s)$	± 0.3	190 - 200

Comments on Preferred Values

There have been few experimental studies of nitric acid interaction with specifically prepared HNO_3-hydrate surfaces at temperatures and concentrations corresponding to hydrate thermodynamically stability regions. Under these conditions at T< 210 K uptake is continuous and irreversible.

References

Hanson, D. R.: J. Geophys. Res. Lett. 19, 2063 1992.
Middlebrook, A.M., Koehler, B.G., McNeill, L.S. and Tolbert, M.A.: Geophys. Res. Lett. 19, 2417 (1992).
Reinhardt, H.; Fida, M. and Zellner, R.: J. Mol. Struct. 661-662, 567-577 (2003).