

Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet V.A5.5 HNNT5

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HNNT₃ + NAT

Experimental data

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

Comments

- HNNT₃ 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 HNNT₃ the rate of uptake decreased. The steady-state partial pressure of HNNT₃ over an ice surface with a coverage of approximately 1 monolayer of HNNT₃ was about a factor of five higher than the vapor pressure over NAT, showing that new hydrate was not formed.
- 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. $p_{H_2O} = 2 \times 10^{-4}$ mbar and $p_{HNNT_3} = (5.3-13.3) \times 10^{-7}$ mbar. A doubling of the H₂O left the uptake coefficient unchanged.
- Slow flow reaction cell with DRIFTS for detection of adsorbed species and downstream FTIR for gas phase HNNT₃. Total pressure 10-30 mbar. At 170K and $[HNNT_3] = (2-5) \times 10^{14}$ molecule cm⁻² continuous uptake was observed with formation of crystalline HNNT₃•3H₂O

(NAT). Monohydrates and dihydrates formed at higher p_{HNO_3} . Uptake coefficient independent of p_{HNO_3}

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

Comments on Preferred Values

There have been few experimental studies of nitric acid interaction with specifically prepared HNO₃-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).