

**IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation**  
**Data Sheet HI26; V.A1.26**

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This datasheet last evaluated: June 2014; last change in preferred values: December 2007

**CH<sub>3</sub>C(O)OONO<sub>2</sub> + Ice → products**

**Experimental data**

<i>Parameter</i>	Temp./K	Reference	Technique/ Comments
<i>K<sub>linC</sub> (cm)</i>			
1.49×10 <sup>-9</sup> exp(3608/T)	160-180K	Bartels-Rausch et al., 2002	PBFT-RC (a)

**Comments**

- (c) Peroxyacetylnitrate (PAN) – ice partitioning coefficients derived from packed ice bed (PBFT) experiments using radioactively labelled PAN at concentrations of 3 ppbv and below. PAN was produced from NO<sub>2</sub> through photolysis of acetone. Ice was prepared from freezing water drops in liquid N<sub>2</sub> and then annealing at 258 K during at least 12 hours. The technique involves observation of migration of the radioactively labelled PAN molecules along the temperature gradient established along the flow tube. The adsorption enthalpy of -30 ± 7 kJ/mol was derived by solving a migration model of linear gas chromatography, and assuming a value of the adsorption entropy of -45 Jmol<sup>-1</sup>K<sup>-1</sup> (based on A<sub>0</sub> = 6.7 x 10<sup>6</sup> m<sup>2</sup>) based on theoretical arguments. The tabulated *K<sub>linC</sub>* was derived from these values. Due to the low partitioning coefficient of PAN, adsorption could only be observed at temperatures below 180 K. No decomposition products (NO<sub>2</sub> or NO) were observed).

**Preferred Values**

<b>Parameter</b>	<b>Value</b>	<b>T/K</b>
<i>K<sub>linC</sub> /cm</i>	1.49×10 <sup>-9</sup> exp(3608/T)	160 – 180
<i>Reliability</i>		
Δ(E/R) / K	± 100	160 – 180

*Comments on Preferred Values*

Due to the low interaction energy, the adsorption kinetics or equilibrium of PAN can only be observed at very low temperature. The partitioning derived from Bartels-Rausch et al. (2002) is tied to the observation at about 170 K. Therefore the extrapolation to higher temperature is somewhat problematic and should be treated with caution as the properties of the ice surface may change towards higher temperatures.

## References

Bartels-Rausch, T., Eichler, B., Zimmermann, P., Gaggeler, H. W., Ammann, M.: Atmos. Chem. Phys. 2, 235-247, 2002.