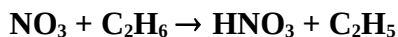


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet NO₃_VOC4

Website: <http://iupac.pole-ether.fr>. See website for latest evaluated data. Data sheets can be downloaded for personal use only and must not be retransmitted or disseminated either electronically or in hardcopy without explicit written permission.

This data sheet updated: 29th October 2007 (with no revisions of the preferred values).



$$\Delta H^\circ = -3.9 \text{ kJ}\cdot\text{mol}^{-1}$$

Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$\leq 4 \times 10^{-18}$	298 ± 2	Wallington et al., 1986	FP-A (a)
$5.7 \times 10^{-12} \exp[-(4426 \pm 337)/T]$	453-553	Bagley et al., 1990	DF-A
2.0×10^{-18}	298*		
$\leq (2.7 \pm 0.2) \times 10^{-17}$	302	Boyd et al., 1991	(b)

Comments

- (a) NO₃ radicals were generated by the flash photolysis of ClONO₂-He mixtures and detected by optical absorption at 662 nm.
- (b) Stopped-flow system with optical absorption detection of the NO₃ radical at 662 nm. Secondary reactions were expected to lead to a stoichiometry factor of ≥ 2 , leading to the upper limit to the rate coefficient cited in the table.

Preferred Values

$$k < 1 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

Comments on Preferred Values

Extrapolation of the absolute rate coefficients obtained by Bagley et al. (1990) over the temperature range 453-553 K to 298 K leads to a 298 K rate coefficient of $2 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, probably uncertain to at least a factor of 2 due to the long extrapolation and possible non-Arrhenius behaviour of the rate coefficient for this reaction. The preferred upper limit is based on the upper limit of Wallington et al. (1986) and extrapolation to 298 K of the elevated temperature rate coefficients of Bagley et al. (1990).

References

- Bagley, J. A., Canosa-Mas, C., Little, M. R., Parr, A. D., Smith, S. J., Waygood, S. J. and Wayne, R. P.: J. Chem. Soc. Faraday Trans., 86, 2109, 1990.
- Boyd, A. A., Canosa-Mas, C. E., King, A. D., Wayne, R. P. and Wilson, M. R.: J. Chem. Soc. Faraday Trans., 87, 2913, 1991.
- Wallington, T. J., Atkinson, R., Winer, A. M. and Pitts Jr., J. N.: J. Phys. Chem., 90, 4640, 1986.