

Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet NO₃_VOC51

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Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Relative Rate Coefficients</i>			
$(6.79 \pm 0.47) \times 10^{-13}$	296	Atkinson et al., 1990	RR (a)

longifolene is: (1R,2S,7S,9S)-3,3,7-trimethyl-8-methylenetricyclo-[5.4.0.0^{2,9}]undecane.

Comments

- (a) Relative rate of loss of longifolene and trans-2-butene (reference reactant) in a 6700 L Teflon chamber at 987 mbar (740 Torr) of air was monitored by GC-FID. NO₃ was generated by the thermal decomposition of N₂O₅. The rate constant ratio, $k(\text{NO}_3 + \text{longifolene}) / k(\text{NO}_3 + \text{trans-2-butene}) = 1.74 \pm 0.12$ is placed on an absolute basis using $k(\text{NO}_3 + \text{trans-2-butene}) = 3.9 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (IUPAC 2016, datasheet NO₃_VOC30).

Preferred Values

Parameter	Value	T/K
$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	6.8×10^{-13}	298
<i>Reliability</i>		
$\Delta \log k$	± 0.25	298

Comments on Preferred Values

The preferred value at 298 K is based on the relative rate study of Shu and Atkinson (1995). The error limits have been expanded to reflect the fact that this is the only study available. The rate coefficient is consistent with estimates based on the number of double bonds and the number and position of the alkyl substituents around them (Atkinson 1991).

There are no studies of the gas-phase products of this reaction, though it is expected to proceed predominantly via addition of NO₃ across the double bond to form a nitrooxyalkyl radical which can react with O₂ to form a nitrooxyalkyl peroxy radical.

References

- Atkinson, R., *J. Phys. Chem. Ref. Data*, 20, 459-507, 1991.
- IUPAC: Task Group on Atmospheric Chemical Kinetic Data Evaluation, (Ammann, M., Cox, R.A., Crowley, J.N., Herrmann, H., Jenkin, M.E., McNeill, V.F., Mellouki, A., Rossi, M. J., Troe, J. and Wallington, T. J.) <http://iupac.pole-ether.fr/index.html>, <http://iupac.pole-ether.fr/index.html>, 2016.
- Shu, Y. H., and Atkinson, R., *J. Geophys. Res. -Atmos.*, 100, 7275-7281, 1995.