

Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet NO₃_VOC52

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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>			
$(3.89 \pm 0.41) \times 10^{-12}$	298 ± 2	Canosa-Mas et al., 1999	RR (a)

isolongifolene is: 2,2,7,7-Tetramethyltricyclo[6.2.1.0^{1,6}]undec-5-ene.

Comments

- (a) Relative rate of loss of isolongifolene and α -pinene (reference reactant) in a 56 L Teflon bag at 1013 mbar (760 Torr) of N₂ was monitored by GC-FID. NO₃ was generated by the thermal decomposition of N₂O₅. The rate constant ratio, $k(\text{NO}_3 + \text{isolongifolene}) / k(\text{NO}_3 + \alpha\text{-pinene}) = 0.627 \pm 0.066$ is placed on an absolute basis using $k(\text{NO}_3 + \alpha\text{-pinene}) = 6.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (IUPAC 2016, datasheet NO₃_VOC9).

Preferred Values

Parameter	Value	T/K
$k / \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	3.9×10^{-12}	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 Canosa-Mas et al. (1999). The error limits have been expanded to reflect the fact that this is the only study available.

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

Canosa-Mas, C. E., King, M. D., Scarr, P. J., Thompson, K. C., and Wayne, R. P., *Phys. Chem. Chem. Phys.*, 1, 2929-2933, 1999.

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.