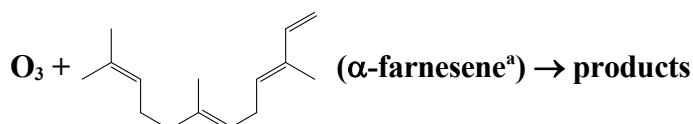


Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet O_x_VOC35

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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>			
$3.50 \times 10^{-12} \exp[-(2590 \pm 393)/T]$	298-318	Kim et al., 2011	RR-MS (b)
$(5.88^{+1.78}_{-1.37}) \times 10^{-16}$	298		

Comments

- (a) 3,7,11-trimethyl-dodeca-1,3,6,10-tetraene.
- (b) The concentrations of α -farnesene and *trans*-but-2-ene (the reference compound) were monitored by MS in reacting O₃ - α -farnesene - *trans*-but-2-ene - acetaldehyde - He mixtures in a 160 cm³ volume quartz vessel at ~1 bar pressure, with acetaldehyde being present to scavenge HO radicals. The measured rate coefficient ratios, $k(\text{O}_3 + \alpha\text{-farnesene})/k(\text{O}_3 + \textit{trans}\text{-but-2-ene})$, are placed on an absolute basis using $k(\text{O}_3 + \textit{trans}\text{-but-2-ene}) = 6.6 \times 10^{-15} \exp(-1060/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (IUPAC, current recommendation).

Preferred Values

Parameter	Value	T/K
$k / \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	5.9×10^{-16}	298
$k / \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	$3.5 \times 10^{-12} \exp(-2590/T)$	290-320
<i>Reliability</i>		
$\Delta \log k$	± 0.3	298
$\Delta E/R$	± 500	290-320

Comments on Preferred Values

The preferred values of k are based on the temperature dependence expression of Kim et al. (2011), the only reported investigation of the reaction. Confirmatory studies are required.

There have currently been no reported product or mechanistic investigations, and such studies are also required. However, structure-activity methods based on a summation of the rate coefficients for simple alkene and diene structures (e.g. Calvert et al., 2000) suggest that the reaction should proceed mainly via O_3 addition to the two non-conjugated methyl-substituted $C=C$ bonds with about equal probability at 298 K, as has been reported for the structurally similar sesquiterpene, β -farnesene, by Kourtchev et al. (2009) (see datasheet for the reaction of O_3 with β -farnesene).

References

- Calvert, J. G., Atkinson, R., Kerr, J. A., Madronich, S., Moortgat, G. K., Wallington, T. J., and Yarwood, G.: The mechanisms of atmospheric oxidation of alkenes, Oxford University Press, New York, ISBN 0-19-513177-0, 2000.
- Kim, D., Stevens, P. S. and Hites, R. A.: J. Phys. Chem. A, 115, 500, 2011.
- Kourtchev, I., Bejan, I., Sodeau, J. R., and Wenger, J. C: Atmos. Environ., 43, 3182, 2009.