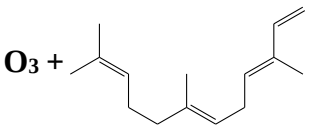
Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet Ox_VOC35

The citation for this data sheet is: IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation, (http://iupac.pole-ether.fr)
This datasheet last evaluated: August 2018; last change in preferred values: June 2015



Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Relative Rate Coefficients			
3.50×10^{-12} exp[-(2590 ± 393)/T]	298-318	Kim et al., 2011	RR-MS (a)
$(5.88\ ^{+1.78}_{-1.37}) \times 10^{-16}$	298		

α-farnesene is 3,7,11-trimethyl-dodeca-1,3,6,10-tetraene

Comments

(a) The concentrations of α-farnesene and *trans*-but-2-ene (the reference compound) were monitored by MS in reacting O_3 - α-farnesene - *trans*-but-2-ene - acetaldehyde - He mixtures in a 160 cm^3 volume quartz vessel at ~1 bar pressure, with acetaldehyde being present to scavenge HO radicals. The measured rate coefficient ratios, $k(O_3$ + α-farnesene)/$k(O_3$ + *trans*-but-2-ene), are placed on an absolute basis using $k(O_3$ + *trans*-but-2-ene) = 6.6×10^{-15} exp(-1060/T) cm^3 molecule^{-1} s^{-1} (IUPAC, current recommendation).

Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	5.9×10^{-16}	298
k /cm^3 molecule^{-1} s^{-1}	3.5×10^{-12} exp(-2590/T)	290-320
Reliability		
Δ log k	± 0.3	298
Δ 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 data sheet Ox_VOC36).

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.