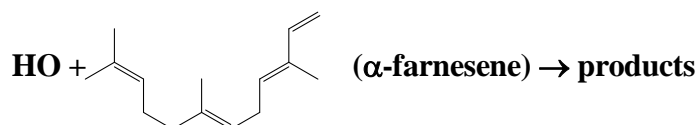


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HO_x_VOC107

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This datasheet last evaluated: December 2017; last change in preferred values: December 2017



Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Relative Rate Coefficients</i>			
$(2.19 \pm 0.11) \times 10^{-10}$	313-423	Kim et al., 2011	RR-MS (a)
α -farnesene is 3,7,11-trimethyl-dodeca-1,3,6,10-tetraene			

Comments

- (a) The concentrations of α -farnesene and 2-methylpropene (the reference compound) were monitored by MS during UV photolysis of H₂O₂ - α -farnesene - 2-methylpropene - He mixtures in a 160 cm³ volume quartz vessel at ~1 bar pressure. The measured rate coefficient ratios, $k(\text{HO} + \alpha\text{-farnesene})/k(\text{HO} + 2\text{-methylpropene})$, were placed on an absolute basis using $k(\text{HO} + 2\text{-methylpropene}) = 9.47 \times 10^{-12} \exp(504/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Atkinson, 1997), which agrees with the current IUPAC recommendation to within 0.5 % over the studied temperature range. The resultant values of k displayed no significant temperature dependence, and the reported rate coefficient was based on the mean of the measured values.

Preferred Values

Parameter	Value	T/K
$k / \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	2.2×10^{-10}	298
$k / \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	2.2×10^{-10}	298-430
<i>Reliability</i>		
$\Delta \log k$	± 0.3	298
$\Delta E/R$	± 200	

Comments on Preferred Values

The preferred temperature-independent value of k is based on the determination of Kim et al. (2011), with the lower bound of the temperature range extended to 298 K. This is the only reported investigation of

the reaction, and confirmatory studies are required.

There have been no reported product or mechanistic investigations, and such studies are also required. However, structure-activity methods (e.g. Vereecken and Peeters, 2001; Peeters et al., 2007) suggest that the reaction should proceed mainly by addition of HO to the C=C bonds (with contributions from all sites); but with a non-negligible contribution from H-atom abstraction, which results in formation of resonance-stabilized allyl and superallyl radicals from attack at all (saturated carbon) sites.

References

Atkinson, R.: Phys. Chem. Ref. Data, 26, 215, 1997.

Kim, D., Stevens, P. S. and Hites, R. A.: J. Phys. Chem. A, 115, 500, 2011.

Peeters, J., Boullart, W., Pultau, V., Vandenberg, S. and Vereecken, L.: J. Phys. Chem. A, 111, 1618, 2007.

Vereecken, L. and Peeters, J.: Chem. Phys. Lett., 333, 162, 2001.