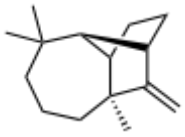
IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation - Data Sheet HOx_VOC90

This datasheet last evaluated: June 2014; last change in preferred values: June 2014.

OH +  **(longifolene) → products**

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/Comments
Relative Rate Coefficients			
$(4.7 \pm 1.0) \times 10^{-11}$	296±2	Shu and Atkinson, 1995	RR (a)

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

Comments

(a) 6400 L Teflon chamber at 987 mbar (740 Torr) of air. OH radical was generated by the photolysis of CH_3ONO at wavelengths > 300 nm. Longifolene and trans-2-butene (reference reactant) were monitored by GC-FID. The rate constant ratio, k(OH + longifolene) / k(OH + trans-2-butene) = 0.729 ± 0.025 is placed on an absolute basis using k(OH + trans-2-butene) = 6.4×10^{-11} cm^3 molecule^{-1} s^{-1} at 298 K (IUPAC, current recommendation).

Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	4.7 x 10^{-11}	298
Reliability		
$\Delta \log k$	0.15	298

Comments on Preferred Values

The preferred value of the rate coefficient at 298 K is based on the relative rate coefficient determination of Shu and Atkinson (1995). The uncertainties were expanded to reflect the existence of a single measurement. The reaction is expected to proceed predominantly by addition to the >C=C< double bond. The OH-initiated oxidation mechanism of longifolene is complex with many different pathways that produce a large number of organic compounds. Lee et al. (2006) reported molar product yields for

HCHO (25±3%), CH_3CHO (3.7±0.4%), HCOOH (31±3%), $CH_3C(O)CH_3$ (3.8±0.3%) and $CH_3C(O)OH$ (15±1%).

References

Atkinson, R., Cox, R. A., Crowley, J. N., Hynes, R. G., Jenkin, M. E., Mellouki, A., Rossi, M. J., Troe, J. and Wallington, T. J.: Evaluated kinetic data: http://iupac.pole-ether.fr, 2013.

Lee, A. Allen H. Goldstein, A. H., Kroll, J. H., Ng, N. L., Varutbangkul, V., Flagan, R. C., and Seinfeld, J. H.: J. Geophys. Res., 111, D17305, 2006.

Shu, Y., and Atkinson, R.: J. Geophys. Res., 100, 7275-7281, 1995.