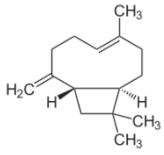
IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation - Data Sheet HOx_VOC92

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

OH +  **(β-caryophyllene) → products**

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/Comments
Relative Rate Coefficients			
$(2.0\ ^{+0.5}_{-0.9}) \times 10^{-10}$	296±2	Shu and Atkinson, 1995	RR (a)

β-caryophyllene is 4,11,11-trimethyl-8-methylene-bicyclo[7.2.0]undec-4-ene

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. β-caryophyllene and 2,3-dimethyl-2-butene (reference reactant) were monitored by GC-FID. Corrections for the dark decay of β-caryophyllene were made. The rate constant ratio, k(OH + β-caryophyllene) / k(OH + 2,3-dimethyl-2-butene) = 1.79 ± 0.22 is placed on an absolute basis using k(OH + 2,3-dimethyl-2-butene) = 1.1 × 10^{-10} cm^3 molecule^{-1} s^{-1} at 298 K (Atkinson and Arey, 2003).

Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	2.0 x 10^{-10}	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 reaction is expected to proceed predominantly by addition to both the exocyclic and endocyclic double bonds. A large yield (68%) of secondary organic aerosol was reported by Lee at al. (2006) along with gas phase organic species such as HCHO (42±10%), CH_3CHO (0.6±0.2%), HCOOH (6.2±2%), $CH_3C(O)CH_3$ (1.5±0.4%) and $CH_3C(O)OH$ (8.7±2%). Hydroxy-hydroperoxides, dihydroxy compounds and hydroketones are expected to be among the first generation products (Jenkin et al., 2012).

References

Atkinson, R., and Arey, J.:, Chem. Rev., 103, 4605-4638, 2003.

Jenkin, M. E., Wyche, K. P., Evans, C. J., Carr, T., Monks, P. S., Alfarra, M. R., Barley, M. H., McFiggans, G. B., Young, J. C., and Rickard, A. R.: Atmos. Chem. Phys., 12, 5275–5308, 2012.

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

Orlando, J. J., Nozière, B., Tyndall, G. S., Orzechowska, G. E., Paulson, S. E., and Rudich, Y.: J. Geophys. Res., 105, 11,561-11,572, 2000.

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