IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation - Data Sheet HOx_VOC88

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

OH + (β-phellandrene) → products

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/Comments
Relative Rate Coefficients			
$(1.66 \pm 0.41) \times 10^{-10}$	297±2	Shorees et al., 1991	RR (a)

β-phellandrene is 3-isopropyl-6-methylene-cyclohexene.

Comments

(a) 6400 L Teflon chamber at 980 mbar (735 Torr) of air. OH radical was generated by the photolysis of CH_3ONO at wavelengths > 300 nm. β-phellandrene and 2,3-dimethyl-2-butene (reference reactant) were monitored by GC-FID. Correction made to the β-phellandrene loss rate due to reaction with NO_2 was <32 % (typically 10-20%). β-phellandrene concentrations were corrected to account for the presence of a co-eluting limonene impurity, initially present at 9.8 % of the β-phellandrene concentration. The rate constant ratio, k(OH + β-phellandrene) / k(OH + 2,3-dimethyl-2-butene) = 1.51 ± 0.20 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}	1.7 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 Shorees et al. (1991) with increased uncertainties reflecting the difficulties of the experiment and the single measurement.

The reaction proceeds by initial addition of the OH radical to the carbon atoms of the C=C bonds and by H-atom abstraction from the various C-H bonds with the OH radical addition channel being expected to be the dominant. Hakola et al. (1999) have identified 4-isopropyl-2-cyclohexen-1-one as a product of the reaction with a formation yield of (29±7%). 4-Isopropyl-2-cyclohexen-1-one is expected to be produced through the initial OH addition at the acyclic >C=C< bond as shown below:
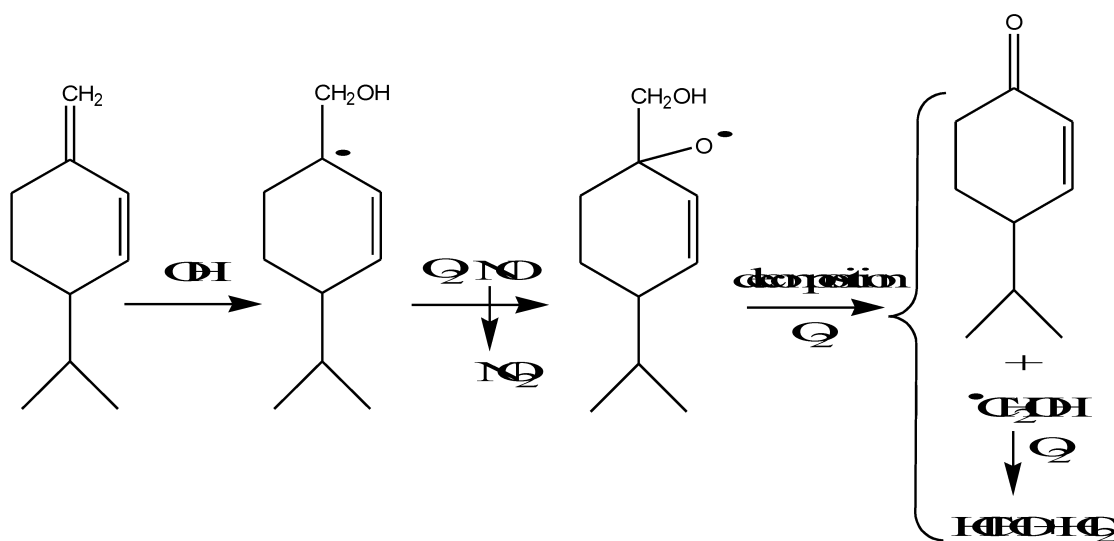
References

Atkinson, R., and Arey, J.: Chem. Rev., 103, 4605-4638, 2003.
Hakola, H., Shorees, B., Arey, J., and Atkinson R.: Environ. Sci. Technol. 27, 278-283, 1993.
Shorees, B., Atkinson, R. and Arey, J.: Int. J. Chem. Kinet., 23, 897-906, 1991.