

IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation - Data Sheet HO_x_VOC85

Datasheets can be downloaded for personal use only and must not be retransmitted or disseminated either electronically or in hardcopy without explicit written permission. The citation for this datasheet is: IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation, <http://iupac.pole-ether.fr>.

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



Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Relative Rate Coefficients</i>			
$(1.73 \pm 0.18) \times 10^{-10}$	294 \pm 1	Atkinson et al., 1986	RR (a)

γ -terpinene is 1-isopropyl-4-methyl-cyclohexa-1,4-diene.

Comments

- (a) 6400 L Teflon chamber at 980 mbar (735 Torr) of air. OH radical was generated by the photolysis of CH₃ONO at wavelengths > 300 nm. γ -terpinene and 2,3-dimethyl-2-butene (reference reactant) were monitored by GC-FID. The rate constant ratio, $k(\text{OH} + \gamma\text{-terpinene}) / k(\text{OH} + 2,3\text{-dimethyl-2-butene}) = 1.57 \pm 0.16$ is placed on an absolute basis using $k(\text{OH} + 2,3\text{-dimethyl-2-butene}) = 1.1 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson and Arey, 2003).

Preferred Values

Parameter	Value	T/K
$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	1.7×10^{-10}	298
<i>Reliability</i>		
$\Delta \log k$	0.10	298

Comments on Preferred Values

The preferred value of the room temperature rate coefficient is based on the relative rate study of Atkinson et al. (1986).

The reaction proceeds by addition of the OH radical to the >C=C< double bonds and by H-atom abstraction from the various C-H bonds with the addition channel being expected to be dominant. Rio et

al. (2010) reported a branching ratio of (31±9%) for the H-atom abstraction channel. Reissell et al. (1999) observed acetone as a reaction product (10±3% molar yield) but could not ascribe the reaction pathways leading to its formation; OH-addition and H-abstraction could both be involved. Aschmann et al. (2011) observed p-cymene [1-methyl-4-(1-methylethyl)benzene or 4-isopropyltoluene] as a product from the reaction of OH with γ -terpinene with a molar yield of 13.6±2.5%. They suggested that p-cymene is formed after H-abstraction from the two ring CH₂ groups. Lee et al. (2006) observed γ -terpinaldehyde (57±6%), HCHO (17±2%), CH₃CHO (1.2±0.2%), HCOOH (8.3±0.8%), CH₃C(O)CH₃ (5.3±0.5%) and CH₃C(O)OH (4.5±0.5%) as products of HO- radical initiated oxidation of γ -terpinene in the presence of NO_x.

References

- Aschmann, S. M., Arey, J., and Atkinson, R.: *Atmos. Environ.*, 45, 4408-4411, 2011.
- Atkinson, R., Aschmann, S. M., and Pitts, J. N.: *Int. J. Chem. Kinet.*, 18, 287-299, 1986.
- Atkinson, R., and Arey, J.: *Chem. Rev.*, 103, 4605-4638, 2003.
- Lee, A., Goldstein, A. H., Kroll, J. H., Ng, N. L., Varutbangkul, V., Flagan, R. C., and Seinfeld, J. H.: *J. Geophys. Res.*, 111, D17305, 2006.
- Reissell, A., Harry, C., Aschmann, S. M., Atkinson, R., and Arey, J.: *J. Geophys. Res.*, 104, 13869-13879, 1999.
- Rio, C., Flaud, P-M., Loison, J-C., and Villenave, E. : *Chem. Phys. Chem.*, 11, 3962-3970, 2010.