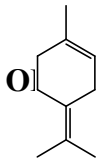
IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation - Data Sheet HOx_VOC86

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



(terpinolene) → products

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	***Reference***	Technique/ Comments
Relative Rate Coefficients			
$(2.21 \pm 0.56) \times 10^{-10}$	295 ± 2	Corchnoy and Atkinson, 1990	RR-GC (a)

4-isopropylidene-1-methyl-cyclohexene

Comments

(a) 6400 L Teflon chamber at 735 Torr (980 mbar) of air. OH was generated using the photolysis of CH_3ONO at wavelengths of >300 nm. Terpinolene and isoprene (reference reactant) were monitored by GC-FID. The rate constant ratio k(OH + terpinolene) / (k(OH + isoprene) = 2.21 ± 0.09 is placed on an absolute basis by k(OH + isoprene) = 1.0×10^{-10} cm^3 molecule^{-1} s^{-1} (IUPAC, current recommendation).

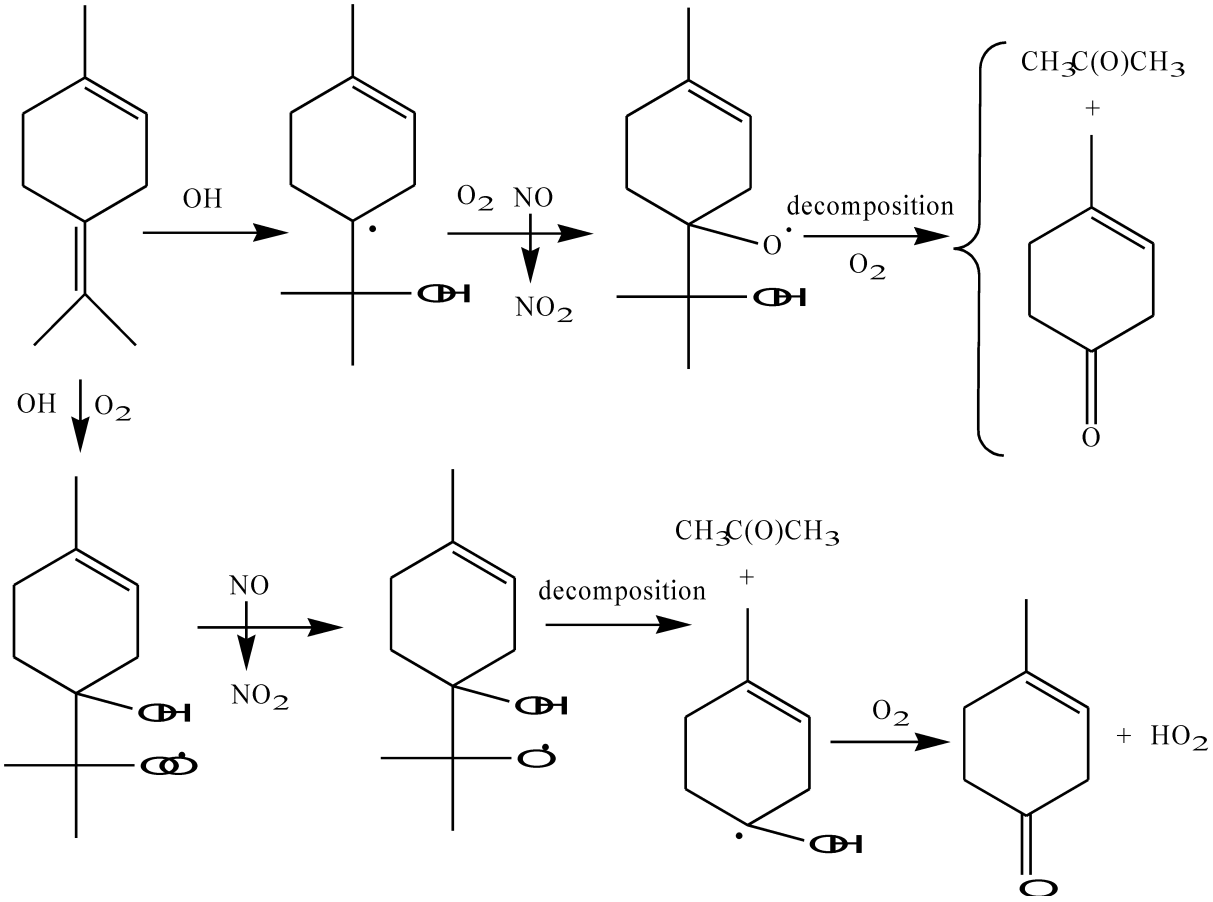
Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	2.2×10^{-10}	298
Reliability		
$\Delta \log k$	0.15	298

Comments on Preferred Values

The preferred value of the room temperature rate coefficient is based on the single relative rate study of Corchnoy and Atkinson (1990). The error limits are expanded to reflect the single measurement. The reaction proceeds almost entirely by OH radical addition to the C=C bonds in terpinolene. Hakola et al. (1994) identified 4-methyl-3-cyclohexen-1-one as a major product from the reaction of OH

radical with terpinolene in presence of NOx with a yield of (26±6) %. Acetone has been reported to be formed with a yield of 32-39 % (Reissell et al., 1999, Orlando et al., 2000) which is similar to the measured yield of the co-product 4-methyl-3-cyclohexen-1-one (reaction scheme given below). Hakola et al. (1994) observed another product with a minor yield of (8±2) % which was tentatively identified as a keto-aldehyde compound ($(CH_3)_2C=C(CH_2CHO)CH_2CH_2C(O)CH_3$) arising from the addition of OH to the endocyclic C=C bond (Hakola et al., 1994). Orlando et al. (2000) identified formaldehyde and formic acid as reaction products with yields of (29±6%) and (8±2%), respectively. Lee at al. (2006) reported a yield of 31% for secondary organic aerosol (SOA) formation along with organic compounds such as HCHO (23±3%), CH_3CHO (0.7±0.1%), HCOOH (3.5±0.7%), $CH_3C(O)CH_3$ (20±2%) and $CH_3C(O)OH$ (1±0.2%).



References

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