Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet Ox_VOC12

 This data sheet updated : 12th December 2007 (with no revision of the preferred values).

O_3 + 3-methyl furan → products

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Relative Rate Coefficients (2.04 ± 0.08) x 10^{-17}	296 ± 2	Alvarado et al., 1996	RR (a)

Comments

(a) Relative rate method carried out at atmospheric pressure of air. The concentrations of 3-methylfuran and propene (the reference compound) were measured by GC, and cyclohexane was added to the reactant mixtures to scavenge the HO radicals formed. The measured rate coefficient ratio of $k(O_3$ + 3-methylfuran$)/k(O_3$ + propene$) = 2.12 \pm 0.08$ is placed on an absolute basis by use of a rate coefficient of $k(O_3$ + propene$) = 9.6 \times 10^{-18}$ cm^3 molecule^{-1} s^{-1} at 296 K (IUPAC, current recommendation).

Preferred Values

$k = 2.0 \times 10^{-17}$ cm^3 molecule^{-1} s^{-1} at 298 K.

Reliability

$\Delta \log k = \pm 0.3$ at 298 K.

Comments on Preferred Values

The preferred value is based on the sole study of this reaction by Alvarado et al. (1996). The reaction proceeds by initial addition of O_3 to the C=C bonds. HO radicals were observed to be formed from the reaction of O_3 with 3-methylfuran in ~ 60% yield (Alvarado et al., 1996).

References

Alvarado, A., Atkinson, R. and Arey, J.: Int. J. Chem. Kinet., 28, 905, 1996.
IUPAC,: http://iupac.pole-ether.fr, 2013.