IUPAC Subcommittee on Gas Kinetic Data Evaluation – Data Sheet Ox_VOC11
Website: http://www.iupac-kinetic.ch.cam.ac.uk/. See website for latest evaluated data.
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$O_3 + CH_2=C(CH_3)C(O)OONO_2$ (MPAN) → products

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients $(8.2 \pm 2.0) \times 10^{-18}$	295 ± 5	Grosjean, Williams, and Grosjean, 1993[1]	(a)

Comments

(a) Experiments were carried out at atmospheric pressure of air, by monitoring the decay rates of $CH_2=C(CH_3)C(O)OONO_2$ (MPAN) in the presence of known excess concentrations of O_3. Cyclohexane was added to the reactant mixtures to scavenge any OH radicals present. MPAN concentrations were measured by GC with electron capture detection.

Preferred Values

$k = 8.2 \times 10^{-18}$ 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 Grosjean *et al*.[1] The rate coefficient for this reaction is similar in magnitude to those for the reactions of O_3 with propene[2,3] and 2-methylpropene,[3] and a factor of 5 higher than that for the reaction of O_3 with ethene.[2,3] This reactivity of MPAN towards O_3 is consistent with the recommended rate coefficient for the reaction of MPAN with HO radicals.[2] The reaction of O_3 with MPAN proceeds by initial addition of O_3 to the C=C bond, and formaldehyde has been observed as a reaction product with a formation yield of 60 ± 10%.[1]

References

1 D. Grosjean, E. Grosjean, and E. L. Williams II, Environ. Sci. Technol. **27**, 2548 (1993).
2 IUPAC, http://iupac-kinetic.ch.cam.ac.uk/ (2002).
3 R. Atkinson, J. Phys. Chem. Ref. Data **26**, 215 (1997).