IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet NO3_VOC19

This data sheet updated: 10th December 2007 (with no revision of the preferred values).

NO_3 + 3-methylfuran → products

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Relative Rate Coefficients			
$(1.31 \pm 0.02) \times 10^{-11}$	296 ± 2	Alvarado et al., 1996	RR (a)
$(2.86 \pm 0.06) \times 10^{-11}$	295 ± 2	Kind et al., 1996	RR (b)

Comments

(a) NO_3 radicals were generated by thermal decomposition of N_2O_5 in air at atmospheric pressure. The concentrations of 3-methylfuran and 2-methyl-2-butene (the reference compound) were measured by GC. The measured rate coefficient ratio of $k(NO_3$ + 3-methylfuran$)/k(NO_3$ + 2-methyl-2-butene$) = 1.40 \pm 0.02$ is placed on an absolute basis by use of a rate coefficient of $k(NO_3$ + 2-methyl-2-butene$) = 9.37 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} (Atkinson, 1997).

(b) Carried out in a flow system at a total pressure of 6.8 mbar of N_2. NO_3 radicals were generated by thermal decomposition of N_2O_5. The concentrations of 3-methylfuran and 2,3-dimethyl-2-butene (the reference compound) were measured by GC. The measured rate coefficient ratio of $k(NO_3$ + 3-methylfuran$)/k(NO_3$ + 2,3-dimethyl-2-butene$) = 0.50 \pm 0.01$ is placed on an absolute basis by use of a rate coefficient of $k(NO_3$ + 2,3-dimethyl-2-butene$) = 5.72 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} (Atkinson, 1997) In the same study, the measured rate coefficient for the reaction of NO_3 radicals with furan was shown to be independent of total pressure (of N_2 diluent) over the range 6.8-200 mbar.

Preferred Values

$k = 1.9 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 298 K.

Reliability

$\Delta \log k = \pm 0.5$ at 298 K.

Comments on Preferred Values

The rate coefficients measured in the relative rate studies of Alvarado et al. (1996) and Kind et al. (1996) disagree by a factor of 2.2, for unknown reasons. The preferred value is a simple average of the rate coefficients from these two studies of Alvarado et al. (1996) and Kind et al. (1996), with a large uncertainty limit. The reaction of NO_3 radicals with 3-methylfuran proceeds by initial addition of the NO_3 radical to the C=C bonds (Alvarado et al., 1996).

References

Alvarado, A., Atkinson, R. and Arey, J.: Int. J. Chem. Kinet., 28, 905, 1996.
Atkinson, R.: J. Phys. Chem. Ref. Data, 26, 215, 1997.
Kind, I., Berndt, T., Böge, O. and Rolle, W.: Chem. Phys. Lett., 256, 679, 1996.