IUPAC Subcommittee on Gas Kinetic Data Evaluation – Data Sheet NO3_VOC17
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NO_3 + [-$CH_2CHC(CH_3)CH_2O$-] (3-methyl furan) → products

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Relative Rate Coefficients			
(1.31 ± 0.02) x 10^{-11}	296 ± 2	Alvarado, Atkinson, and Arey, 1996[1]	RR (a)
(2.86 ± 0.06) x 10^{-11}	295 ± 2	Kind *et al*., 1996[2]	RR (b)

Comments

(a) Relative rate method carried out at one atmosphere of air. NO_3 radicals were generated by thermal decomposition of N_2O_5. 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 ± 0.02 is placed on an absolute basis by use of a rate coefficient of $k(NO_3$ + 2-methyl-2-butene) = 9.37 x 10^{-12} cm^3 molecule^{-1} s^{-1}.[3]

(b) Relative rate method 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 ± 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 x 10^{-11} cm^3 molecule^{-1} s^{-1}.[3] 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 x 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*.[1] and Kind *et al*.[2] 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,[1,2] 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.[1]

References

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