

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

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

NO₃ + 3-methylfuran → products

Rate coefficient data

| $k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ | Temp./K | Reference | Technique/ Comments |
|--|---------|-----------------------|---------------------|
| <i>Relative Rate Coefficients</i> | | | |
| $(1.31 \pm 0.02) \times 10^{-11}$ | 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) NO₃ radicals were generated by thermal decomposition of N₂O₅ 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 $k(\text{NO}_3 + 3\text{-methylfuran})/k(\text{NO}_3 + 2\text{-methyl-2-butene}) = 1.40 \pm 0.02$ is placed on an absolute basis by use of a rate coefficient of $k(\text{NO}_3 + 2\text{-methyl-2-butene}) = 9.37 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Atkinson, 1997).
- (b) Carried out in a flow system at a total pressure of 6.8 mbar of N₂. NO₃ radicals were generated by thermal decomposition of N₂O₅. The concentrations of 3-methylfuran and 2,3-dimethyl-2-butene (the reference compound) were measured by GC. The measured rate coefficient ratio of $k(\text{NO}_3 + 3\text{-methylfuran})/k(\text{NO}_3 + 2,3\text{-dimethyl-2-butene}) = 0.50 \pm 0.01$ is placed on an absolute basis by use of a rate coefficient of $k(\text{NO}_3 + 2,3\text{-dimethyl-2-butene}) = 5.72 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Atkinson, 1997). In the same study, the measured rate coefficient for the reaction of NO₃ radicals with furan was shown to be independent of total pressure (of N₂ diluent) over the range 6.8-200 mbar.

Preferred Values

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

Reliability

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

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 NO₃ radicals with 3-methylfuran proceeds by initial addition of the NO₃ 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.