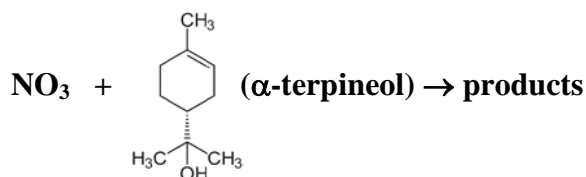


Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet NO₃_VOC56

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This datasheet last evaluated: June 2018; last change in preferred values: June 2018



Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Relative Rate Coefficients</i>			
$(1.9 \pm 0.2) \times 10^{-11}$	297 ± 3	Jones and Ham, 2008.	RR (a)
$(1.6 \pm 0.2) \times 10^{-11}$			RR (b)

(α -terpineol is: (2-(4-methyl-1-cyclohex-3-enyl)propan-2-ol).

Comments

- (a) Relative rate of loss of α -terpineol and either 2-carene or 3-carene (reference reactants) in a ≈ 65 L Teflon bag at atmospheric pressure of air was monitored by GC-MS. NO_3 was generated by the thermal decomposition of N_2O_5 . $k(\alpha\text{-terpineol}) / k(2\text{-carene}) = 0.95 \pm 0.02$ was put on an absolute basis using $k(2\text{-carene}) = 2.0 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (IUPAC, 2018).
- (b) See note (a). $k(\alpha\text{-terpineol}) / k(3\text{-carene}) = 1.76 \pm 0.02$ was put on an absolute basis using $k(3\text{-carene}) = 9.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (IUPAC, 2018).

Preferred Values

Parameter	Value	T/K
$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	1.7×10^{-11}	298
<i>Reliability</i>		
$\Delta \log k$	± 0.15	298

Comments on Preferred Values

The preferred value at 298 K is an average of the relative rate studies of Jones and Ham, (2008). The error limits have been expanded to reflect the fact that this is the only study available.

Jones and Ham (2008) identified carbonyls, dicarbonyls and hydroxy-nitrates as the products of the reaction between NO_3 and terpineol, concluding that both addition of NO_3

to the double bond as well as abstraction of the tertiary H-atom take place. Yields were not reported.

References

Jones, B.T., and Ham, J. E., *Atmos. Env.*, 42, 6689-6698, 2008.
IUPAC: Task Group on Atmospheric Chemical Kinetic Data Evaluation, (Ammann, M., Cox, R.A., Crowley, J.N., Herrmann, H., Jenkin, M.E., McNeill, V.F., Mellouki, A., Rossi, M. J., Troe, J. and Wallington, T. J.) <http://iupac.pole-ether.fr/index.html>., <http://iupac.pole-ether.fr/index.html>., 2018.