

## Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet NO<sub>3</sub>\_VOC55

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### Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Relative Rate Coefficients</i>			
$(7.9 \pm 0.2) \times 10^{-12}$	$298 \pm 2$	Ham, 2013.	RR (a)

valencene is: (2*R*)-8,8, 8*a*-trimethyl-2-prop-1-en-2-yl- 1,2,3,4,6,7-hexahydronaphthalene.

### Comments

- (a) Relative rate of loss of valencene and 3-carene or limonene (reference reactants) in a  $\approx 100$  L Teflon bag at atmospheric pressure of air was monitored by GC-MS. NO<sub>3</sub> was generated by the thermal decomposition of N<sub>2</sub>O<sub>5</sub>. Individual, relative loss rates for the two experiments were not reported, however. Ham (2013) used rate coefficients for NO<sub>3</sub> + 3-carene ( $9.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ) and NO<sub>3</sub> + limonene ( $1.22 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ) that agree with present IUPAC recommendations (IUPAC, 2016., datasheets: NO<sub>3</sub>\_VOC33 and NO<sub>3</sub>\_VOC35).

### Preferred Values

Parameter	Value	T/K
$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	$7.9 \times 10^{-12}$	298
<i>Reliability</i>		
$\Delta \log k$	$\pm 0.25$	298

### Comments on Preferred Values

The preferred value at 298 K is based on the relative rate study of Ham, (2016). The error limits have been expanded to reflect the fact that this is the only study available.

There are no studies of the gas-phase products of this reaction, though it is expected to proceed predominantly via addition of NO<sub>3</sub> across the double bond to form a nitrooxyalkyl radical which can react with O<sub>2</sub> to form a nitrooxyalkyl peroxy radical.

### References

Ham, J. E., *Int. J. Chem. Kinet.*, 45, 508-514, 2013.  
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>, 2016.