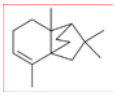
This datasheet last evaluated: Nov. 2016; last change in preferred values: Nov. 2016

NO_3 +  (α-neoclovene) → products

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Relative Rate Coefficients			
$(8.25 \pm 2.1) \times 10^{-12}$	298 ± 2	Canosa-Mas et al., 1999	RR (a)

α-neoclovene is: (1S,7aS)-1,2,3,6,7,7a-Hexahydro-2,2,4,7a-tetramethyl-1,3a-ethano-3aH-indene.

Comments

(a) Relative rate of loss of α-neoclovene and α-pinene (reference reactant) in a 56 L Teflon bag at 1013 mbar (760 Torr) of N_2 was monitored by GC-FID. NO_3 was generated by the thermal decomposition of N_2O_5. Significant loss of α-neoclovene was observed in the absence of NO_3 and correction was applied. The resulting rate constant ratio, $k(NO_3 + \alpha\text{-neoclovene}) / k(NO_3 + \alpha\text{-pinene}) = 1.33 \pm 0.34$ is placed on an absolute basis using $k(NO_3 + \alpha\text{-pinene}) = 6.2 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K (IUPAC 2016, datasheet NO_3_VOC9).

Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	8.25×10^{-12}	298
Reliability		
$\Delta \log k$	± 0.25	298

Comments on Preferred Values

The preferred value at 298 K is based on the relative rate study of Canosa-Mas et al. (1999). 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_3 across the double bond to form a nitrooxyalkyl radical which can react with O_2 to form a nitrooxyalkyl peroxy radical.

References

Canosa-Mas, C. E., King, M. D., Scarr, P. J., Thompson, K. C., and Wayne, R. P., Phys. Chem. Chem. Phys., 1, 2929-2933, 1999.
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.