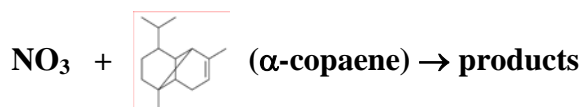


## Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet NO3\_VOC50

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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>			
$(1.61 \pm 0.07) \times 10^{-11}$	296	Atkinson et al., 1990	RR (a)

$\alpha$ -copaene is: (1R,2S,6S,7S,8S)-8-isopropyl-1,3-dimethyltricyclo[4.4.0.0<sup>2,7</sup>]dec-3-ene.

### Comments

- (a) Relative rate of loss of  $\alpha$ -copaene and 2-methyl-2-butene (reference reactant) in a 6700 L Teflon chamber at 987 mbar (740 Torr) of air was monitored by GC-FID.  $\text{NO}_3$  was generated by the thermal decomposition of  $\text{N}_2\text{O}_5$ . The rate constant ratio,  $k(\text{NO}_3 + \alpha\text{-copaene}) / k(\text{NO}_3 + 2\text{-methyl-2-butene}) = 1.72 \pm 0.08$  is placed on an absolute basis using  $k(\text{NO}_3 + 2\text{-methyl-2-butene}) = 9.37 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (Atkinson and Arey, 2003).

### Preferred Values

Parameter	Value	T/K
$k / \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	$1.6 \times 10^{-11}$	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 Shu and Atkinson (1995). The error limits have been expanded to reflect the fact that this is the only study available. The rate coefficient is consistent with estimates based on the number of double bonds and the number and position of the alkyl substituents around them (Atkinson 1991).

There are no studies of the gas-phase products of this reaction, though it is expected to proceed predominantly via addition of  $\text{NO}_3$  across the double bond to form a nitrooxyalkyl radical which can react with  $\text{O}_2$  to form a nitrooxyalkyl peroxy radical.

## References

- Atkinson, R., *J. Phys. Chem. Ref. Data*, 20, 459-507, 1991.  
Atkinson, R., and Arey, J., *Chem. Rev.*, 103, 4605-4638, 2003.  
Shu, Y. H., and Atkinson, R., *J. Geophys. Res. -Atmos.*, 100, 7275-7281, 1995.