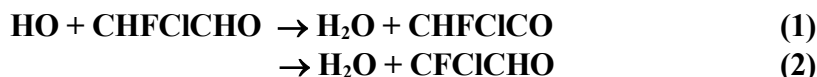


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oClOx65

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This data sheet last evaluated: June 2015; last change in preferred values: November 2003.



Rate coefficient data ($k = k_1 + k_2$)

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$(2.2 \pm 0.2) \times 10^{-12}$	298 ± 2	Scollard et al., 1993	PLP-RF
<i>Relative Rate Coefficients</i>			
$(1.9 \pm 0.3) \times 10^{-12}$	298 ± 2	Scollard et al., 1993	RR (a)

Comments

- (a) HO radicals were generated by the photolysis of CH_3ONO or $\text{C}_2\text{H}_5\text{ONO}$ in CH_3ONO (or $\text{C}_2\text{H}_5\text{ONO}$)-CHFCICHO-toluene-air mixtures at 987 ± 13 mbar pressure. The concentrations of CHFCICHO and toluene were measured by GC and/or FTIR spectroscopy. Scollard et al. (1993) did not report a value for the rate coefficient ratio $k(\text{HO} + \text{CHFCICHO})/k(\text{HO} + \text{toluene})$. Dividing the reported value of $k(\text{HO} + \text{CHFCICHO})$ by the value of $k(\text{HO} + \text{toluene})$ used by Scollard et al. (1993) gives $k(\text{HO} + \text{CHFCICHO})/k(\text{HO} + \text{toluene}) = 0.336 \pm 0.050$ which is placed on an absolute basis in the table above using $k(\text{HO} + \text{toluene}) = 5.63 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Calvert et al., 2002).

Preferred Values

Parameter	Value	T/K
$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	2.1×10^{-12}	298
<i>Reliability</i>		
$\Delta \log k$	± 0.15	298

Comments on Preferred Values

The preferred value is an average of the absolute and relative rate coefficients of Scollard et al. (1993), which are in good agreement. The reaction is expected to proceed by channel (1) at room temperature (Scollard et al., 1993).

References

Calvert, J. G., Atkinson, R., Becker, K. H., Kamens, R. M., Seinfeld, J. H., Wallington, T. J.

and Yarwood, G.: *The Mechanism of Atmospheric Oxidation of Aromatic Hydrocarbons*, Oxford University Press, New York, NY, 2002.

Scollard, D. J., Treacy, J. J., Sidebottom, H. W., Balestra-Garcia, C., Laverdet, G., LeBras, G., MacLeod, H. and Téton, S.: *J. Phys. Chem.*, 97, 4683, 1993.