IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oClOx66

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This data sheet last evaluated: June 2015; last change in preferred values: November 2004.

$$HO + CHCl_2CHO \rightarrow H_2O + CHCl_2CO \quad (1)$$
$$\rightarrow H_2O + CCl_2CHO \quad (2)$$

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

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$(2.4 \pm 0.5) \times 10^{-12}$	298	Balestra-Garcia et al., 1992	PLP-RF
Relative Rate Coefficients			
$(2.4 \pm 0.1) \times 10^{-12}$	298 ± 2	Scollard et al., 1993	RR (a)

Comments

(a) HO radicals were generated by the photolysis of CH_3ONO or C_2H_5ONO in CH_3ONO (or C_2H_5ONO)-NO-$CHCl_2CHO$-$CH_3C(O)CH_2CH_3$-air mixtures at 987 ± 13 mbar pressure. The concentrations of $CHCl_2CHO$ and 2-butanone were measured by GC and/or FTIR spectroscopy. The measured rate coefficient ratio of k(HO + $CHCl_2CHO$)/k(HO + 2-butanone) is placed on an absolute basis by use of a rate coefficient of k(HO + 2-butanone) = 1.2×10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K (Atkinson et al., 2006).

Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	2.4×10^{-12}	298
Reliability		
$\Delta \log k$	± 0.15	298

Comments on Preferred Values

The preferred 298 K rate coefficient is the average of those of Balestra-Garcia et al. (1992) and Scollard et al. (1993), which are in excellent agreement. The reaction is expected to proceed essentially totally by channel (1) at 298 K (Scollard et al., 1993).

References

Atkinson, R., Baulch, D. L., Cox, R. A., Crowley, J. N., Hampson, R. F., Hynes, R. G., Jenkin, M. E., Rossi, M. J., and Troe, J.: Atmos. Chem. Phys., 6, 3625, 2006; IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation, http://iupac.pole-ether.fr

Balestra-Garcia, C., Le Bras, G. and Mac Leod, H., : J. Phys. Chem., 96, 3312, 1992.

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.