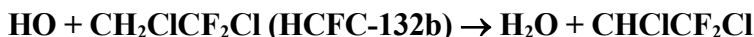


## IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oClOx52

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



### Rate coefficient data

| $k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$   | Temp./K | Reference           | Technique/ Comments |
|--|---------|---------------------|---------------------|
| <i>Absolute Rate Coefficients</i>                      |         |                     |                     |
| $1.87 \times 10^{-12} \exp[-(1351 \pm 78)/T]$          | 250-350 | Watson et al., 1979 | FP-RF (a)           |
| $(1.9 \pm 0.2) \times 10^{-14}$                        | 298     |                     |                     |
| $5.54 \times 10^{-26} T^{4.58} \exp[(252 \pm 377)/T]$  | 249-473 | Jeong et al., 1984  | DF-RF               |
| $(2.42 \pm 0.16) \times 10^{-14}$                      | 297     |                     |                     |
| $8.53 \times 10^{-19} T^{2.28} \exp[-(937 \pm 296)/T]$ | 295-788 | Fang et al., 1999   | PLP-LIF             |
| $(1.84 \pm 0.07) \times 10^{-14}$                      | 295     |                     |                     |

### Comments

- (a) The sample of  $\text{CH}_2\text{ClCF}_2\text{Cl}$  used was shown by GC to contain  $\sim 0.045\%$  of  $\text{C}_2$  halogenated alkenes. After correction for possible contributions to the observed OH radical decays from these measured impurities, assuming a rate coefficient for reaction of the  $\text{C}_2$  halogenated alkene impurities with HO radicals of  $5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  independent of temperature, then the rate coefficient was estimated to be  $3 \times 10^{-12} \exp(-1578/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  over the temperature range of 250-350 K, with a rate coefficient at 298 K of  $1.67 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ .

### Preferred Values

| Parameter  | Value                               | T/K     |
|--|-------------------------------------|---------|
| $k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ | $1.7 \times 10^{-14}$               | 298     |
| $k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ | $3.5 \times 10^{-12} \exp(-1585/T)$ | 250-350 |
| <i>Reliability</i>                                   |                                     |         |
| $\Delta \log k$                                      | $\pm 0.15$                          | 298     |
| $\Delta(E/R)$  | $\pm 300$                           | 250-350 |

### Comments on Preferred Values

The rate coefficients of Jeong et al. (1984) are higher than those of Watson et al. (1979) and Fang et al. (1999), especially at  $<300$  K, suggesting the presence of reactive impurities in the  $\text{CH}_2\text{ClCF}_2\text{Cl}$  sample used. The rate coefficients of Jeong et al. (1984) are therefore not used in

the evaluation. The rate coefficients of Fang et al. (1999) at 295 K and 347 K are in good agreement with the corrected data of Watson et al. (1979) at 298 K and 350 K (see Comment (a) above). Accordingly, the absolute rate coefficients of Watson et al. (1979) [corrected for the impurity observed; see Comment (a)] and Fang et al. (1999) have been fitted to the three parameter equation  $k = CT^2 \exp(-D/T)$ , resulting in  $k = 5.72 \times 10^{-18} T^2 \exp(-1006/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  over the temperature range 250-788 K. The preferred Arrhenius expression,  $k = A \exp(-B/T)$ , is centered at 290 K and is obtained from the three parameter equation with  $A = C e^2 T^2$  and  $B = D + 2T$ .

### References

- Fang, T. D., Taylor, P. H. and Berry, R. J.: J. Phys. Chem. A, 103, 2700, 1999.  
 Jeong, K.-M. Hsu, K.-J., Jeffries, J. B. and Kaufman, F.: J. Phys. Chem., 88, 1222, 1984.  
 Watson, R. T., Ravishankara, A. R., Machado, G., Wagner, S. and Davis, D. D.: Int. J. Chem. Kinet., 11, 187, 1979.

