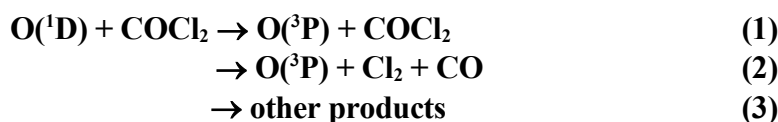


## IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet IV.A2.87 oClOx13

Website: <http://iupac.pole-ether.fr>. See website for latest evaluated data. Data sheets can be downloaded for personal use only and must not be retransmitted or disseminated either electronically or in hardcopy without explicit written permission. The citation for this data sheet is: Atkinson, R., Baulch, D. L., Cox, R. A., Crowley, J. N., Hampson, R. F., Hynes, R. G., Jenkin, M. E., Rossi, M. J., Troe, J., and Wallington, T. J.: Atmos. Chem. Phys., 8, 4141, 2008; IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation, <http://iupac.pole-ether.fr>. This data sheet last evaluated: June 2015; last change in preferred values: November 2003.



$$\Delta H^\circ(1) = -190 \text{ kJ mol}^{-1}$$

$$\Delta H^\circ(2) = -80 \text{ kJ mol}^{-1}$$

### Rate coefficient data ( $k = k_1 + k_2 + k_3$ )

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$(2.6 \pm 0.5) \times 10^{-10}$	298	Chichinin, 1997	PLP-LMR
$2.04 \times 10^{-10} \exp[(27 \pm 10/T)]$	194-429	Strekowski et al., 2000	PLP-RF
$(2.22 \pm 0.33) \times 10^{-10}$	298		
<i>Branching Ratios</i>			
$(k_1 + k_2)/k = 0.20 \pm 0.04$	194-429	Strekowski et al., 2000	PLP-RF (a)

### Comments

- (a) Branching ratio for conversion of O(<sup>1</sup>D) to O(<sup>3</sup>P), i.e.  $(k_1 + k_2)/k$  was determined by comparison of the O(<sup>3</sup>P) yield from O(<sup>1</sup>D) + COCl<sub>2</sub> relative to that for O(<sup>1</sup>D) + N<sub>2</sub>.

### Preferred Values

Parameter	Value	T/K
$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	$2.2 \times 10^{-10}$	298
$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	$2.0 \times 10^{-10} \exp(25/T)$	190-430
$(k_1 + k_2)/k$	0.20	298
<i>Reliability</i>		
$\Delta \log k$	$\pm 0.1$	298
$\Delta(E/R)$	$\pm 25$	298
$\Delta(k_1 + k_2)/k$	$\pm 0.1$	298

### Comments on Preferred Values

The preferred values of  $k$  are based on the results reported by Strekowski et al. (2000). The room temperature value reported by Chichinin et al. (1997) is 17% higher than the preferred value. The branching ratio  $(k_1 + k_2)/k$  is taken from Strekowski et al. (2000). Jayanty et al. (1976) present

evidence, based on high yields of CO, that the reaction channel to produce ClO + ClCO is very important.

### References

Chichinin, A. I.: J. Chem. Phys. 106, 1057, 1997.

Jayanty, R. K. M., Simonaitis, R. and Heicklen, J.: J. Photochem., 5, 217, 1976.

Strekowski, R. S., Nicovich, J. M. and Wine, P. H.: Chem. Phys. Lett. 330, 354, 2000.