IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet IV.A2.86 oClOx12

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

$$O(^1D) + COFCl \rightarrow O(^3P) + COFCl \qquad (1)$$

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$(3.7 \pm 0.4) \times 10^{-10}$	298	Fletcher and Husain, 1978	FP-RA (a)

Comments

(a) Flow system used, with O(^{1}D) atoms being monitored by time-resolved resonance absorption at 115 nm. The data analysis used a modified Beer-Lambert law.

Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	1.9×10^{-10}	298
Reliability		
$\Delta \log k$	± 0.3	200-350

Preferred Values

$k = 1.9 \times 10^{-10}$ cm^3 molecule^{-1} s^{-1} at 298 K.

Reliability

$\Delta \log k = \pm 0.3$ at 298 K.

Comments on Preferred Values

The preferred value is derived from the data of Fletcher and Husain (1978) by use of a scaling factor of 0.5. The weight of evidence from many O(^{1}D) rate studies suggests that O(^{1}D) rates reported by Husain and co-workers contain a systematic error, and that these results can be made consistent with other O(^{1}D) recommended values in this evaluation by use of this scaling factor, as has been done in previous evaluations by the IUPAC Subcommittee on Gas Kinetic Data Evaluation for Atmospheric Chemistry and by the NASA Panel for Data Evaluation. See also the discussion of this topic in Davidson et al. (1978).

References

Davidson, J. A., Schiff, H. I., Brown, T. J. and Howard, C. J.: J. Chem. Phys., 69, 4277, 1978.
Fletcher, I. S. and Husain, D.: J. Photochem. 8, 355, 1978.