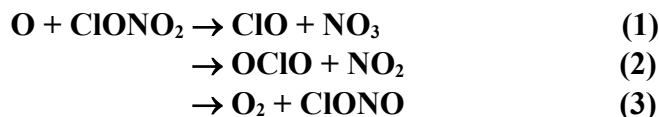


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet iClOx6

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 re-transmitted or disseminated either electronically or in hard copy without explicit written permission.

This data sheet updated: 23th July 2003.



$$\Delta H^\circ(1) = -96.7 \text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta H^\circ(2) = -144.3 \text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta H^\circ(3) = -216 \text{ kJ}\cdot\text{mol}^{-1}$$

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>			
$(2.0 \pm 0.2) \times 10^{-13}$	245	Ravishankara et al., 1977	FP-RF
$3.4 \times 10^{-12} \exp[-(840 \pm 60)/T]$	213-295	Molina et al., 1977	DF-CL
$(2.0 \pm 0.4) \times 10^{-13}$	295		
$1.9 \times 10^{-12} \exp[-(692 \pm 167)/T]$	225-273	Kurylo, 1977	FP-RF
1.8×10^{-13}	298*		
$(2.3 \pm 0.6) \times 10^{-13}$	298	Adler-Golden and Wiesenfeld, 1981	FP-RA
$(2.4 \pm 0.4) \times 10^{-13}$	298	Tyndall et al., 1997	PLP-RF
$4.5 \times 10^{-12} \exp[-(900 \pm 80)/T]$	202-325	Goldfarb et al., 1998	PLP-RF/A
$(2.2 \pm 0.2) \times 10^{-13}$	298		(a)

Comments

- (a) k was measured by two independent techniques: (1) pulsed laser photolysis with time-resolved resonance fluorescence detection of O-atom decay, and (2) pulsed laser photolysis with time-resolved long-path absorption at 662 nm by the product NO_3 radical. The yield of NO_3 radicals produced in the reaction was also measured in the long-path absorption apparatus.

Preferred Values

$$k = 2.2 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

$$k = 4.5 \times 10^{-12} \exp(-900/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ over the temperature range } 200 \text{ K to } 330 \text{ K.}$$

Reliability

$$\Delta \log k = \pm 0.08 \text{ at } 298 \text{ K.}$$

$$\Delta(E/R) = \pm 150 \text{ K.}$$

Comments on Preferred Values

The preferred values are based on the results of the study of Goldfarb et al. (1998). This study encompassed the broadest range of experimental conditions and used two completely different techniques. Results obtained by these two techniques were in complete agreement. Results of the earlier temperature dependent studies of Molina et al. (1977) and Kurylo (1977) and the room temperature studies of Adler-Golden and Wiesenfeld (1981) and Tyndall et al. (1997) are in good agreement with the preferred values.

Using the long-path absorption apparatus to monitor NO₃ radicals, Goldfarb et al. (1998) measured the yield of the NO₃ radical produced in this reaction to be approximately unity. Allowing for uncertainties in the measurements they concluded that NO₃ and ClO radicals are the primary products of this reaction and account for at least 70% of the reaction over the temperature range studied (248 K to 298 K) (Goldfarb et al., 1998).

References

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