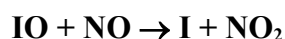


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet iIOx18

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.



$$\Delta H^\circ = -66 \text{ kJ}\cdot\text{mol}^{-1}$$

Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$(1.67 \pm 0.16) \times 10^{-11}$	298	Ray and Watson, 1981 ¹	DF-MS (a)
$(2.8 \pm 0.2) \times 10^{-11}$	298	Inoue <i>et al.</i> , 1983 ²	PLP-LIF (b)
$6.9 \times 10^{-12} \exp[(328 \pm 71)/T]$	242-359	Daykin and Wine, 1990 ³	PLP-AS (c)
$(2.17 \pm 0.22) \times 10^{-11}$	298		
$1.02 \times 10^{-11} \exp[(185 \pm 70)/T]$	237-346	Turnipseed <i>et al.</i> , 1995 ⁴	PLP-LIF (d)
$(1.92 \pm 0.07) \times 10^{-11}$	298		
$(1.9 \pm 0.5) \times 10^{-11}$	295	Atkinson, Hudgens, and Orr-Ewing, 1999 ⁵	PLP-AS (e)
$8.3 \times 10^{-12} \exp[(269 \pm 85)/T]$	273-353	Knight and Crowley, 2001 ⁶	DF-MS (f)
$2.17 \pm 0.2 \times 10^{-11}$	298		
$4.3 \times 10^{-12} \exp[(397 \pm 65)/T]$	233-346	Hölscher and Zellner, 2002 ⁷	PLP-LIF (g)
$(1.68 \pm 0.11) \times 10^{-11}$	296		
$(1.82 \pm 0.1) \times 10^{-11}$	294	Dillon and Heard, 2003 ⁸	PLP-LIF (h)
<i>Relative Rate Coefficients</i>			
$7.2 \times 10^{-12} \exp[(330 \pm 160)/T]$	293-366	Buben <i>et al.</i> , 1996 ⁹	DF-RF (i)
2.18×10^{-11}	298*		

Comments

- IO radicals were produced by the reaction $\text{I} + \text{O}_3$ and monitored by MS in an excess of NO. Pressure varied between 1.33 and 2.8 mbar He.
- IO formed from laser photolysis of HI-N₂O at 193 nm, or HI-O₃ at 248 nm. Total pressure was 1.33 mbar He.
- Pulsed laser photolysis of NO₂-I₂ mixtures at 351 nm. IO radical concentrations were monitored by longpath absorption spectroscopy in an excess of NO. k was found to be independent of pressure over the range 50 mbar to 260 mbar of N₂.
- Pulsed laser photolysis of N₂O-I₂ mixtures at 193 nm. IO radical concentrations were monitored by LIF in an excess of NO. k was found to be independent of pressure over the range 6.5 mbar to 130 mbar of N₂.
- Pulsed laser photolysis of N₂O-CF₃I-NO-Ar mixtures at 193 nm. IO radicals were monitored by cavity ring-down spectroscopy at 445.04 nm. k was found to be independent of pressure over the range 12.5 mbar to 40 mbar of Ar.
- IO radicals made by $\text{O} + \text{I}_2$ and detected by MS.

- (g) IO made by laser photolysis of N₂O-CF₃I at 193 nm. Pressure varied between 13 and 130 mbar synthetic air.
- (h) IO made by laser photolysis of N₂O-CF₃I at 193 nm. Pressure varied between 88 and 173 mbar N₂ or synthetic air.
- (i) IO made in photolysis of CH₃I-O₂-O₃ mixtures. Steady state I atom signals were monitored by resonance fluorescence and shown to depend on the relative concentration of O₃ and NO, and the relative rate coefficients for I + O₃ and IO + NO, i.e. $k/k(I + O_3)$ was derived. The expression for $k(T)$ was derived using the temperature dependent, recommended value for $k(I + O_3)$.¹⁰

Preferred Values

$k = 1.95 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K.

$k = 7.15 \times 10^{-12} \exp(300/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ over the temperature range 240 K to 370 K.

Reliability

$\Delta \log k = \pm 0.15$ at 298 K.

$\Delta(E/R) = \pm 100$ K.

Comments on Preferred Values

Most of the available rate coefficient data for this reaction¹⁻⁹ are in good agreement, only the result of Inoue *et al.*² is anomalously high. The preferred value of $k = 1.95 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K is the mean of all other values.

The preferred expression for $k(T)$ is obtained by taking the mean of the values of E/R of Daykin and Wine,³ Turnipseed *et al.*,⁴ Knight and Crowley,⁶ Hölscher and Zellner,⁷ and Buben *et al.*,⁹ and combining it with a pre-exponential factor adjusted to give the preferred value of k at 298 K.

References

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