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

This data sheet updated: 23th July 2003.

$IO + NO \rightarrow I + NO_2$

$\Delta H° = -66$ kJ·mol^{-1}

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$(1.67 \pm 0.16) \times 10^{-11}$	298	Ray and Watson, 1981[1]	DF-MS (a)
$(2.8 \pm 0.2) \times 10^{-11}$	298	Inoue *et al*., 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 *et al*., 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)
Relative Rate Coefficients			
$7.2 \times 10^{-12} \exp[(330 \pm 160)/T]$	293-366	Buben *et al*., 1996[9]	DF-RF (i)
2.18×10^{-11}	298*		

Comments

(a) IO radicals were produced by the reaction I + O_3 and monitored by MS in an excess of NO. Pressure varied between 1.33 and 2.8 mbar He.

(b) IO formed from laser photolysis of HI-N_2O at 193 nm, or HI-O_3 at 248 nm. Total pressure was 1.33 mbar He.

(c) Pulsed laser photolysis of NO_2-I_2 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 N_2.

(d) Pulsed laser photolysis of N_2O-I_2 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 N_2.

(e) Pulsed laser photolysis of N_2O-CF_3I-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.

(f) IO radicals made by O + I_2 and detected by MS.

(g) IO made by laser photolysis of N_2O-CF_3I at 193 nm. Pressure varied between 13 and 130 mbar synthetic air.
(h) IO made by laser photolysis of N_2O-CF_3I at 193 nm. Pressure varied between 88 and 173 mbar N_2 or synthetic air.
(i) IO made in photolysis of CH_3I-O_2-O_3 mixtures. Steady state I atom signals were monitored by resonance fluorescence and shown to depend on the relative concentration of O_3 and NO, and the relative rate coefficients for I + O_3 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

$k = 1.95 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 298 K.
$k = 7.15 \times 10^{-12} \exp(300/T)$ cm^3 molecule^{-1} 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 reaction[1-9] are in good agreement, only the result of Inoue *et al*.[2] is anomalously high. The preferred value of $k = 1.95 \times 10^{-11}$ cm^3 molecule^{-1} 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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