IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet NOx9

This data sheet last evaluated: 28th July 2007; no revision of preferred values.

HO + HONO → H_2O + NO_2

ΔH° = -166.3 kJ mol^{-1}

Rate coefficient data

k/cm^3 $molecule^{-1}$ s^{-1}	Temp./K	**Reference**	Technique/ Comments
Absolute Rate Coefficients			
$1.80 \times 10^{-11} \exp[-(390 \pm 80)/T]$	278-342	Jenkin and Cox, 1987	MM-RA
$(4.9 \pm 0.5) \times 10^{-12}$	298		
$2.8 \times 10^{-12} \exp[(260 \pm 140)/T]$	298-373	Burkholder et al., 1992	PLP-LIF (a)
$(7.05 \pm 1.41) \times 10^{-12}$	298		
Relative Rate Coefficients			
$(6.0 \pm 0.4) \times 10^{-12}$	296	Cox et al., 1976	(b)

Comments

(a) HO radicals were monitored by LIF with HONO in excess. [HONO] and [NO_2] were also monitored using *in situ* diode-array spectroscopy.

(b) Photolysis of HONO-NO and HONO-H_2 mixtures at a total pressure of 1 bar of N_2 or N_2-O_2 diluent. A value of $k/k(HO + H_2) = 945 \pm 48$ was obtained. The value of k given in the table is calculated using $k(HO + H_2) = 6.4 \times 10^{-15}$ cm^3 $molecule^{-1}$ s^{-1} at 296 K (IUPAC, 2007).

Preferred Values

$k = 6.0 \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1} at 298 K.
$k = 2.5 \times 10^{-12} \exp(260/T)$ cm^3 $molecule^{-1}$ s^{-1} over the temperature range 290-380 K.

Reliability

$\Delta \log k = \pm 0.15$ at 298 K.
$\Delta(E/R) = \pm 260$ K.

Comments on Preferred Values

There are significant differences between the two direct studies of Jenkin and Cox (1987) and Burkholder et al. (1992), particularly with respect to the temperature dependence of k. The work of Burkholder et al. (1992) has substantially better precision than that of Jenkin and Cox (1987). Furthermore, the small negative temperature dependence of k found by Burkholder et al. (1992) is consistent with that observed for the analogous reaction of HO radicals with $HONO_2$.

The preferred value of k at 298 K is an average of the room temperature rate coefficients of Jenkin and Cox (1987), Burkholder et al. (1992) and Cox et al. (1976). The temperature dependence of k is that

given by Burkholder et al. (1992), with the pre-exponential factor being adjusted to fit the preferred value of k at 298 K.

References

Burkholder, J. B., Mellouki, A., Talukdar, R. and Ravishankara, A. R.: Int. J. Chem. Kinet. 24, 711, 1992.
Cox, R. A., Derwent, R. G. and Holt, P. M.: J. Chem. Soc. Faraday Trans. 1, 72, 2031, 1976.
IUPAC: http://iupac.pole-ether.fr, 2007.
Jenkin, M. E. and Cox, R. A.: Chem. Phys. Lett. 137, 548, 1987.