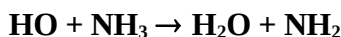


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet NOx8

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 retransmitted or disseminated either electronically or in hardcopy without explicit written permission.

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



$$\Delta H^\circ = -44.4 \text{ kJ mol}^{-1}$$

Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$(1.5 \pm 0.4) \times 10^{-13}$	298	Stuhl, 1973	FP-RF
$2.3 \times 10^{-12} \exp(-805/T)$	228-472	Zellner and Smith, 1974; Smith and Zellner, 1975	FP-RA
1.58×10^{-13}	298		
$2.93 \times 10^{-12} \exp[-(861 \pm 151)/T]$	298-427	Perry et al., 1979	FP-RF
$(1.64 \pm 0.16) \times 10^{-13}$	298		
$5.41 \times 10^{-12} \exp[-(1067 \pm 72)/T]$	294-1075	Silver and Kolb, 1980	DF-RF
$(1.44 \pm 0.29) \times 10^{-13}$	294		
$4.55 \times 10^{-12} \exp[-(973 \pm 78)/T]$	297-364	Stephens, 1984	DF-RF
$(1.73 \pm 0.11) \times 10^{-13}$	297		
$3.29 \times 10^{-12} \exp[-(922 \pm 100)/T]$	273-433	Diau et al., 1990	FP/PLP-LIF (a)
$(1.47 \pm 0.07) \times 10^{-13}$	297		

Comments

- (a) Pulsed laser photolysis and conventional flash photolysis of H₂O and H₂O₂ were used as the sources of HO radicals. The total pressure was varied over the range 0.091-0.672 bar (68-504 Torr).

Preferred Values

$$k = 1.6 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

$$k = 3.5 \times 10^{-12} \exp(-925/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ over the temperature range } 230\text{-}450 \text{ K.}$$

Reliability

$$\Delta \log k = \pm 0.1 \text{ at } 298 \text{ K.}$$

$$\Delta(E/R) = \pm 200 \text{ K.}$$

Comments on Preferred Values

The preferred values are obtained from a least-squares fit to the data of Stuhl (1974), Zellner and Smith (1974), Smith and Zellner (1975), Perry et al. (1976), Stephens (1984), Diau et al. (1990), and the data of Silver and Kolb (1980) below 450 K. The relative rate measurement of $k/k(\text{HO} + \text{HONO})$ by Cox

et al. (1975) at 296 ± 2 K is in good agreement with the preferred value when the value of $k(\text{HO} + \text{HONO})$ from this review is used (IUPAC, 2007). Results from other low temperature studies (Kurylo, 1973; Hack et al., 1974; Pagsberg et al., 1979) are well outside the error limits obtained from the direct studies cited in the table above (Stuhl, 1973; Zellner and Smith, 1974; Smith and Zellner, 1975; Perry et al., 1976; Silver and Kolb, 1980; Stephens, 1984; Diau et al., 1990) and are not used in this evaluation.

There are numerous high temperature studies which, together with the studies cited here, indicate a distinct curvature on the Arrhenius plot (Jeffries and Smith, 1986). However, the simple Arrhenius expression given here as the preferred expression for k is sufficiently precise over the temperature range cited.

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