

IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data sheet Hox_VOC49

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This data sheet updated: 29th October 2007 (with no revisions of the preferred values).

HO + HCN → products

Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$1.2 \times 10^{-13} \exp(-400/T)$	296-433	Fritz et al., 1984	FP-RA (a)
$(3 \pm 1) \times 10^{-14}$	298		

Comments

- (a) The measured rate coefficients were observed to be pressure dependent over the range ~13-600 mbar (~10-450 Torr) of N₂ diluent. The cited rate coefficients are those extrapolated to the high-pressure limit (k_∞) using a simple Lindemann extrapolation.

Preferred Values

$k = 3 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K and 1 bar.

$k = 1.2 \times 10^{-13} \exp(-400/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ over the temperature range 290-440 K at 1 bar.

Reliability

$\Delta \log k = \pm 0.5$ at 298 K.

$\Delta(E/R) = \pm 300$ K.

Comments on Preferred Values

The preferred values are those of Fritz et al. (1984) with wider error limits. The rate coefficient increases with increasing pressure over this temperature range, and the rate coefficients cited are those extrapolated by Fritz et al. (1984) to the high-pressure limit.

The reaction proceeds by HO radical addition over this temperature range. At higher temperatures the available rate coefficient data indicate a direct abstraction reaction (Atkinson, 1989).

References

- Atkinson, R.: J. Phys. Chem. Ref. Data, Monograph 1, 1, 1989.
Fritz, B., Lorenz, K., Steinert, W. and Zellner, R.: Oxid. Comm., 6, 363, 1984.