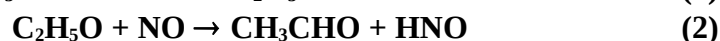


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet II.A5.111 RO_12

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This data sheet last evaluated: 4th June 2009. Last change in preferred values: 12th June 2003.



$$\Delta H^\circ(1) = -178.5 \text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta H^\circ(2) = -127.6 \text{ kJ}\cdot\text{mol}^{-1}$$

Low-pressure rate coefficients Rate coefficient data

$k_{01}/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$(2.2 \pm 1.2) \times 10^{-28} [\text{He}]$	298	Daële <i>et al.</i> , 1995 ¹	DF/LIF&MS (a)

Comments

- (a) $\text{C}_2\text{H}_5\text{O}$ radicals were generated by the reaction of F atoms with $\text{C}_2\text{H}_5\text{OH}$. Measurements were carried out at 0.7 mbar, 1.3 mbar and 2.6 mbar. The rate coefficient k_{01} was obtained from a Lindemann-Hinshelwood analysis, assuming identical intermediates in reactions (1) and (2); $k_2 = (1.1 \pm 0.5) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ was derived.

Preferred Values

$$k_{01} = 2.2 \times 10^{-28} [\text{N}_2] \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

$$k_2 = 1.1 \times 10^{-11} [\text{N}_2] \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

Reliability

$$\Delta \log k_{01} = \pm 0.3 \text{ at } 298 \text{ K.}$$

$$\Delta \log k_2 = \pm 0.5 \text{ at } 298 \text{ K.}$$

Comments on Preferred Values

The preferred values are from Daële *et al.*,¹ assuming that reactions (1) and (2) can be separated by Lindemann-Hinshelwood extrapolation and $k = k_1([\text{M}]) + k_2$. We assume equal values of k_{01} for He and N_2 as third bodies. In contrast to the simple Lindemann-Hinshelwood evaluation of ref. 1 corresponding to $F_c = 1$, we recommend to use $F_c = 0.6$ for a construction of the falloff curve for $k_1([\text{M}])$.

High-pressure rate coefficients Rate coefficient data

$k_{\infty 1}/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$(4.4 \pm 0.4) \times 10^{-11}$	298	Frost and Smith, 1990 ²	PLP-LIF (a)
$(3.1 \pm 0.8) \times 10^{-11}$	298	Daële <i>et al.</i> , 1995 ¹	DF/LIF&MS (b)
$(3.7 \pm 0.7) \times 10^{-11} (T/300)^{0.2}$	286-388	Fittschen <i>et al.</i> , 1999 ³	PLP-LIF (c)

Comments

- (a) The rate coefficient k_1 is found not to depend on the pressure between 20 mbar and 130 mbar of Ar.
- (b) See comment (a) for k_0 .
- (c) Measurements over the range 39-658 mbar of He. Results assumed to be in the high pressure range. Values taken from table of results, not abstract.

Preferred Values

$k_{\infty 1} = 4.4 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ over the temperature range 200 to 400 K.

Reliability

$\Delta \log k_{\infty 1} = \pm 0.3$ at 298 K.

$\Delta n = \pm 0.5$.

Comments on Preferred Values

The preferred value of $k_{\infty 1}$ is from ref. 2 in close agreement with ref. 3. For the falloff curve of reaction (1), $F_c = 0.6$ is chosen. The value of k_2 derived in ref. 1 with the preferred $k_{\infty 1}$ is in good agreement with the ratio $k_2/k_{\infty 1} = 0.3$ observed in ref. 4.

References

- ¹ V. Daële, A. Ray, I. Vassalli, G. Poulet, and G. LeBras, *Int. J. Chem. Kinet.* **27**, 1121 (1995).
- ² M. J. Frost and I. W. M. Smith, *J. Chem. Soc. Faraday Trans* **86**, 1757 (1990).
- ³ C. Fittschen, A. Frenzel, K. Imrik, and P. Devolder, *Int. J. Chem. Kinet.* **31**, 800 (1999).
- ⁴ G. Baker and R. Shaw, *J. Chem. Soc. A*, 6965 (1965).