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

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

$$C_2H_5O + NO + M \rightarrow C_2H_5ONO + M \quad (1)$$
$$C_2H_5O + NO \rightarrow CH_3CHO + HNO \quad (2)$$

$\Delta H°(1) = -178.5$ kJ·mol^{-1}
$\Delta H°(2) = -127.6$ kJ·mol^{-1}

Low-pressure rate coefficients
Rate coefficient data

k_{01}/cm^3 molecule^{-1} s^{-1}	Temp./K	**Reference**	Technique/ Comments
Absolute Rate Coefficients			
(2.2 ± 1.2) x 10^{-28} [He]	298	Daële *et al*., 1995[1]	DF/LIF&MS (a)

Comments

(a) C_2H_5O radicals were generated by the reaction of F atoms with C_2H_5OH. 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); $k_2 = (1.1 \pm 0.5) \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} was derived.

Preferred Values

$k_{01} = 2.2 \times 10^{-28}$ [N_2] cm^3 molecule^{-1} s^{-1} at 298 K.
$k_2 = 1.1 \times 10^{-11}$ [N_2] cm^3 molecule^{-1} s^{-1} at 298 K.

Reliability

$\Delta \log k_{01} = \pm 0.3$ at 298 K.
$\Delta \log k_2 = \pm 0.5$ at 298 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 $k = k_1([M]) + k_2$. 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 $k_1([M])$.

High-pressure rate coefficients
Rate coefficient data

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