**Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet IV.A2.93**

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This data sheet last evaluated: June 2014; last change in preferred values: December 2007.

**Cl + CH2FCl (HCFC-31)  HCl + CHFCl**

**Rate coefficient data**

|  |  |  |  |
| --- | --- | --- | --- |
| *k*/cm3 molecule-1 s-1  | Temp./K | Reference | Technique/ Comments |
| *Relative Rate Coefficients* |  |  |  |
| 1.2 x 10-11 exp(-1230/*T*) | 273-368 | Tschuikow-Roux et al., 1988 | RR (a) |
| 1.9 x 10-13 | 298 |  |  |
| (1.10  0.25) x 10-13 | 298 | Tuazon et al., 1992 | RR (b) |

**Comments**

(a) Cl atoms were generated by the photolysis of Cl2. Product yield ratios were measured by GC. Kinetic data were derived by measuring the formation of CHFCl2 and CH3Cl following UV irradiation at 424 nm of CH4-CH2FCl-Cl2 mixtures at a total pressure of about 28 mbar. Derived values of *A*/*A*CH4 = (1.92  0.01) and (*E*-*E*CH4)/R = (-8  2) K were placed on an absolute basis using *k*(Cl + CH4) = 6.6 x 10-12 exp(-1240/*T*) cm3 molecule-1 s-1 (Atkinson et al., 2006).

1. Photolysis of Cl2 in presence of CH2FCl and CH4 in 986 mbar (740 Torr) air bath gas. The loss of CH2FCl and CH4 were measured by FTIR spectroscopy. The rate constant ratio obtained, *k*(Cl+CH2FCl)/*k*(Cl+CH4) = 1.10  0.02 was placed on an absolute value using *k*(CH4) = 1.0  10-13 cm3 molecule-1 s‑1 (Atkinson et al., 2006).

**Preferred Values**

|  |  |  |
| --- | --- | --- |
| **Parameter** | **Value** | ***T*/K** |
|  |  |  |
| *k* /cm3 molecule-1 s-1 | 1.1 x 10-13 | 298 |
| *k* /cm3 molecule-1 s-1 | 6.8 x 10-12 exp(-1230/*T*) | 270-370 |

*Reliability*

|  |  |  |
| --- | --- | --- |
|  log *k* | ± 0.3 | 298 |
|  E/R | ± 500 |  |

*Comments on Preferred Values*

 In the relative rate study by Tuazon et al. (1992) the rate constant ratio *k*(Cl+CH2FCl)/*k*(Cl+CH4) was measured by monitoring the loss of CH2FCl and CH4 following UV irradiation of CH2FCl–CH4–Cl2–air mixtures. The loss of CH2FCl and CH4 were monitored directly using in-situ FTIR spectroscopy. In the relative rate study by Tschuikow-Roux et al. (1988) the rate coefficient ratio *k*(Cl+CH2FCl)/*k*(Cl+CH4) was measured by monitoring the formation of CHFCl2 and CH3Cl following UV irradiation of CH2FCl–CH4–Cl2 mixtures. The formation of CHFCl2 and CH3Cl were measured by GC-FID and used to infer the loss of CH2FCl and CH4. Tschuikow-Roux et al. (1988) applied a large (5.089) correction factor to account for the response of the GC-FID to CHFCl2. In light of the less direct approach and large correction made in the work of Tschuikow-Roux et al. (1988) the room temperature result of Tuazon et al. (1992) is preferred. The recommended value is based on the room temperature results of Tuazon et al. (1992) and the temperature dependence reported by Tschuikow-Roux et al. (1988).

**References**

Atkinson, R., Baulch, D. L., Cox, R. A., Crowley, J. N., Hampson, R. F., Hynes, R. G., Jenkin, M. E., Rossi, M. J., and Troe, J.: Atmos. Chem. Phys., 6, 3625, 2006; IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation, [http://iupac.pole-ether.fr](http://iupac.pole-ether.fr/)

Tschuikow-Roux, E., Faraji, F., Paddison, S., Niedzielski, J. and Miyokawa, K.: J. Phys. Chem., 92, 1488, 1988.

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