**Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oClOx27**

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

**Cl + CH3CF3 (HFC-143a)  HCl + CH2CF3**

*H* = 18.0 kJ mol-1

**Rate coefficient data**

|  |  |  |  |
| --- | --- | --- | --- |
| *k*/cm3 molecule-1 s-1  | Temp./K | Reference | Technique/ Comments |
| *Absolute Rate Coefficients* |  |  |  |
| < 1 x 10-14 | 298 | Hitsuda et al., 2001 | PLP-LIF (a) |  |
| *Relative Rate Coefficients* |  |  |  |  |
| 6.9 x 10-12 exp(-3720/*T*) | 281-368 | Tschuikow-Roux et al., 1985 | RR (b) |  |
| 2.6 x 10-17 | 298 |  |  |  |
| (3.85 ± 0.25) x 10-17 | 296 | Nielsen et al. (1994) | RR (c) |  |

**Comments**

1. Laser photolysis of HCl at 193 nm as Cl atom source. Both Cl(2P3/2) and Cl(2P1/2) detected by VUV-LIF.
2. Cl atoms were generated by the photolysis of Cl2. Product yield ratios were determined by GC and the the measured rate coefficient *k*(Cl+CH3CF3)/*k*(CH4) = 1.05 exp(-2479/T) is 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).
3. Cl atoms were generated by the photolysis of Cl2 in the UV irradiation of CH3CF3 –CH3CF2Cl – Cl2 in 920 mbar of N2, or air, diluent. The measured rate coefficient ratio of *k*(Cl + CH3CF3)/*k*(Cl + CH3CF2Cl) = 0.094  0.006 was placed on an absolute basis using *k*(Cl + CH3CF2Cl) = 4.1 x 10-16 cm3 molecule-1 s-1 (Atkinson et al., 2006).

**Preferred Values**

|  |  |  |
| --- | --- | --- |
| **Parameter** | **Value** | ***T*/K** |
|  |  |  |
| *k* /cm3 molecule-1 s-1 | 3.2 x 10-17 | 298 |
| *k* /cm3 molecule-1 s-1 | 8.4 x 10-12 exp(-3720/*T*) | 280-370 |

*Reliability*

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

*Comments on Preferred Values*

The recommended rate coefficient at room temperature is an average of the results of the relative rate studies of Tschuikow-Roux et al. (1985) and Nielsen et al. (1994). The temperature dependence is based upon the work by Tschuikow-Roux et al. (1985). The room temperature upper limit to *k* of Hitsuda et al. (2001) is consistent with the recommendation.

# 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 Atmosoheric Chemical Kinetic Data Evaluation, [http://iupac.pole-ether.fr](http://iupac.pole-ether.fr/)

Hitsuda, K., Takahashi, K., Matsumi, Y. and Wallington, T. J.: J. Phys. Chem. A, 105, 5131, 2001.

Nielsen, O. J., Gamborg, E., Sehested, J.,Wallington, T. J. and Hurley, M. D.: J. Phys. Chem., 98, 9518, 1994.

Tschuikow-Roux, E., Yano, T. and Niedzielski, J.: J. Chem. Phys., 82, 65, 1985.

