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

Website: [http://iupac.pole-ether.fr](http://iupac.pole-ether.fr/). See website for latest evaluated data. Data sheets can be downloaded for personal use only and must not be retransmitted or disseminated either electronically or in hardcopy without explicit written permission.

The citation for this data sheet is: Atkinson, R., Baulch, D. L., Cox, R. A., Crowley, J. N., Hampson, R. F., Hynes, R. G., Jenkin, M. E., Rossi, M. J., Troe, J., and Wallington, T. J.: Atmos. Chem. Phys., 9, 4141, 2008; IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation, [http://iupac.pole-ether.fr](http://iupac.pole-ether.fr/).

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.

