**Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oClOx24**

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 + CH3CH2F (HFC-161)  HCl + CH3CHF (1)**

** HCl + CH2CH2F (2)**

Δ*H*(1) = -9.6 kJ mol-1

Δ*H*(2) = 5.3 kJ mol-1

**Rate coefficient data**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| *k*/cm3 molecule-1 s-1 | Temp./K | Reference | Technique/ Comments | |
| *Absolute Rate Coefficients* |  |  |  | |
| (6.8  0.5) x 10-12 | 298 | Hitsuda et al., 2001 | PLP-LIF (a) |  |
| Relative Rate Coefficients |  |  |  |  |
| *k*1 = 1.0 x 10-11 exp(-130/*T*) | 281-368 | Tschuikow-Roux et al., 1985 |  |  |
| *k*1 = 6.5 x 10-12 | 298 |  | RR (b) |  |
| *k*2 = 8.3 x 10-12 exp(-720/*T*) | 281-368 |  |  |  |
| *k*2 = 7.4 x 10-13 | 298 |  |  |  |

**Comments**

(a) Laser photolysis of HCl at 193 nm as Cl atom source. Both Cl(2P3/2) and Cl(2P1/2) detected by VUV-LIF.

(b) Cl atoms were generated by the photolysis of Cl2. Product yield ratios were determined by GC and the measured rate coefficient ratios of *k*1/*k*(Cl + CH4) = 1.60 exp(1113/T) and *k*2/*k*(Cl + CH4) = 1.26 exp(515/T) 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).

**Preferred Values**

|  |  |  |
| --- | --- | --- |
| **Parameter** | **Value** | ***T*/K** |
|  |  |  |
| *k*1 /cm3 molecule-1 s-1 | 6.5 x 10-12 | 298 |
| *k*1/cm3 molecule-1 s-1 | 1.0 x 10-11 exp(-130/*T*) | 280-370 |
| *k*2/cm3 molecule-1 s-1 | 7.4 x 10-13 | 298 |
| *k*2/cm3 molecule-1 s-1 | 8.3 x 10-12 exp(-720/*T*) | 280-370 |

*Reliability*

|  |  |  |
| --- | --- | --- |
|  log *k*1= Δlog *k*2 | ± 0.3 | 298 |
| Δ(*E*1/*R*) = Δ(*E*2/*R*) | ± 500 |  |

*Comments on Preferred Values*

The recommended values are based on the results of the relative rate study of Tschuikow-Roux et al. (1985). The overall rate constant *k* at room temperature, (*k* = *k*1 + *k*2) of Hitsuda et al. (2001) is consistent with this 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 Atmospheric 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.

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

