**Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oClOx22**

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

**Cl + CHFCl2 (HCFC-21)  HCl + CFCl2**

*H* = -17.8 kJ mol-1

# Rate coefficient data

|  |  |  |  |
| --- | --- | --- | --- |
| *k*/cm3 molecule-1 s-1 | Temp./K | Reference | Technique/Comments |
| *Absolute Rate Coefficients* |  |  |  |
| 5.2 x 10-12 exp[-(1675  60)/*T*] | 298-430 | Talhaoui et al., 1996 | DF-MS |
| (1.9  0.3) x 10-14 | 296 |  |  |
| *Relative Rate Coefficients* |  |  |  |
| (1.0  0.2) x 10-14 | 294 | Glavas and Heicklen, 1985 | RR (a) |
| (2.1  0.4) x 10-14 | 298 | Tuazon et al., 1992 | RR (b) |

**Comments**

(a) Steady-state photolysis of Cl2-CHFCl2-O2-NO-NO2-N2 mixtures. The measured rate coefficient ratio is placed on absolute basis using a rate coefficient of *k*(Cl + NO + M) = 1.0 x 10-31 cm6 molecule-2 s-1.

(b) Cl atoms were generated by the photolysis of Cl2. The decays of the reactant and reference organic were measured by FTIR spectroscopy. The measured rate coefficient was placed on absolute basis using a rate coefficient of *k*(Cl + CH4) = 1.0 x 10-13 cm3 molecule-1 s-1 (Atkinson et al., 2006).

**Preferred Values**

|  |  |  |
| --- | --- | --- |
| **Parameter** | **Value** | ***T*/K** |
|  |  |  |
| *k* /cm3 molecule-1 s-1 | 2.0 x 10-14 | 298 |
| *k* /cm3 molecule-1 s-1 | 5.5 x 10-12 exp(-1675/*T*) | 290-430 |

*Reliability*

|  |  |  |
| --- | --- | --- |
|  log *k* | ± 0.2 | 298 |
|  E/R | ± 400 |  |

*Comments on Preferred Values*

The preferred value at 298 K is based on the absolute study of Talhaoui et al. (1996) and the relative rate study of Tuazon et al. (1992). These results are preferred over the earlier, less direct results of Glavas and Heicklen (1985). The recommended temperature dependence is based on the results of Talhaoui et al. (1996), with expanded error limits to reflect the fact that this is the only study of *k*(T). The A-factor has been adjusted to reproduce the recommended value of *k* at 298 K.

**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/)

Glavas, S. and Heicklen, J.: J. Photochem., 31, 21, 1985.

Talhaoui, A., Louis, F., Meriaux, B., Devolder, P. and Sawerysyn, J. P.: J. Phys. Chem., 100, 2107, 1996.

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