**Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oClOx21**

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., 8, 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 + CHF2Cl (HCFC-22)  HCl + CF2Cl**

*H* = -9.0 kJ mol-1

**Rate coefficient data**

|  |  |  |  |
| --- | --- | --- | --- |
| *k*/cm3 molecule-1 s-1  | Temp./K | Reference | Technique/ Comments |
| *Absolute Rate Coefficients* |  |  |  |
| (1.4  0.2) x 10-15 | 298 | Jourdain et al., 1977 | DF-MS |
| (1.7  0.2) x 10-15 | 297 | Sawerysyn et al., 1992 | DF-MS |
| 5.3 x 10-12 exp[-(2430  90)/*T*] | 298-430 | Talhaoui et al., 1996 | DF-MS |
| (1.4  0.3) x 10-15 | 296 |  |  |
| *Relative Rate Coefficients* |  |  |  |
| (2.0  0.4) x 10-15 | 298 | Tuazon, et al., 1992 | RR (a) |
| (1.7  0.1) x 10-15 | 296 | Sokolov et al., 1998 | RR (b) |

# Comments

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

1. Photolysis of Cl2 in presence of CHF2Cl and CD4 in 920 mbar N2 bath gas. The rate constant ratio obtained, *k*(CHF2Cl)/*k*(CD4) = 0.28  0.02 was placed on an absolute value using *k*(CD4) = 6.1  10-15 cm3 molecule-1 s-1.

**Preferred Values**

|  |  |  |
| --- | --- | --- |
| **Parameter** | **Value** | ***T*/K** |
|  |  |  |
| *k* /cm3 molecule-1 s-1 | 1.6 x 10-15 | 298 |
| *k* /cm3 molecule-1 s-1 | 4.2 x 10-12 exp(-2345/*T*) | 290-430 |

*Reliability*

|  |  |  |
| --- | --- | --- |
|  log *k* | ± 0.15 | 298 |
|  E/R | ± 400 |  |

*Comments on Preferred Values*

The rate constants reported at room temperature from the absolute rate studies by Jourdain et al. (1977), Sawerysyn et al. (1992), and Talhaoui et al. (1996) and the relative rate studies by Tuazon et al. (1992) and Sokolov et al. (1998) are in good agreement. The recommended Arrhenius expression was derived from a fit to the combined data set from all studies.

**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/)

Jourdain, G. L.; Poulet, G.; Barassin, J.; Lebras, G. et Combourieu, J.: J. Pollut. Atmos. 75, 256, 1977.

Sawerysyn, J. P., Talhaoui, A., Meriaux, B. and Devolder, P.: Chem. Phys. Lett., 198, 197, 1992.

Sokolov, O., Hurley, M. D., Wallington, T. J., Kaiser, E. W., Platz, J., Nielsen, O. J., Berho, F., Rayez, M.-T., and Lesclaux, R.: J. Phys. Chem. A, 102, 10671, 1998.

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

Tuazon, E. C., Atkinson, R. and Corchnoy, S. B.: Int. J. Chem. Kinet., 24, 639, 1992.

