**Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oClOx25**

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

**Cl + CH3CHF2 (HFC-152a)  HCl + CH3CF2 (1)**

** HCl + CH2CHF2 (2)**

*H*(1) = -4.9 kJ mol-1

*H*(2) = 11.1 kJ mol-1

**Rate coefficient data (*k* = *k*1 + *k*2)**

|  |  |  |  |
| --- | --- | --- | --- |
| *k*/cm3 molecule-1 s-1 | Temp./K | Reference | Technique/ Comments |
| *Absolute Rate Coefficients* |  |  |  |
| (2.54  0.25) x 10-13 | 295 | Taketani et al. (2005) | PLP-LIF (a) |
| *Relative Rate Coefficients* |  |  |  |
| *k*1 = 7.0 x 10-12 exp(-965/*T*) | 280-360 | Yano and Tschuikow-Roux, 1986 | RR (b) |
| *k*1 = 2.7 x 10-13 | 298 |  |  |
| *k*2 = 7.8 x 10-12 exp(-2399/*T*) | 280-360 |  |  |
| *k*2 = 2.5 x 10-15 | 298 |  |  |
| (2.4  0.7) x 10-13 | 295 | Wallington and Hurley, 1992 | RR (c) |
| (2.4  0.5) x 10-13 | 298 | Tuazon, et al., 1992 | RR (d) |
| *k*1 = (2.35  0.31) x 10-13 | 295 | Taketani et al. (2005) | RR (e) |
| *k*2 = (1.92  0.30) x 10-15 | 295 |  |  |

**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 ratios of *k*1/*k*(Cl + C2H6) = 0.0835 exp(866/T) and *k*2/*k*(Cl + C2H6) = 0.0932 exp(2299/T) were placed on an absolute basis using *k*(Cl + C2H6) = 8.3 x 10-11 exp(-100/*T*) cm3 molecule-1 s-1 (Atkinson et al., 2006).

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

(d) Cl atoms were generated by the photolysis of Cl2 in the presence of CH3CHF2 and CH4 in 986 mbar of air. The decays of CH3CHF2 and CH4 were measured by FTIR spectroscopy. The measured rate coefficient ratio *k*(Cl + CH3CHF2)/*k*(Cl +CH4) = 2.36  0.02 is placed on an absolute basis using *k*(Cl + CH4) = 1.0 x 10-13 cm3 molecule-1 s-1 (Atkinson et al., 2006).

(e) Cl atoms were generated by the photolysis of Cl2 in the UV irradiation of CH3CHF2 – CH4 – Cl2 and CH3CHF2 – CH3Cl – Cl2 in 920 mbar of N2, or air, diluent. Ratios of *k*(Cl + CH3CHF2)/*k*(Cl +CH4) = 2.39  0.15 and *k*(Cl + CH3CHF2)/*k*(Cl + CH3Cl) = 0.49  0.01 were placed on an absolute basis using rate coefficients of *k*(Cl + CH4) = 1.0 x 10-13 and *k*(Cl + CH3Cl) = 4.8 x 10-13 cm3 molecule-1 s-1 (Atkinson et al., 2006) leading to a value of *k*(Cl + CH3CHF2) = (2.37  0.31) x 10-13 cm3 molecule-1 s-1. The UV irradiation of CH3CHF2 – Cl2 – N2 mixtures led to the formation of CH3CF2Cl and CH2ClCHF2 in molar yields of 99  4 % and 0.81  0.07 %, respectively. Rate coefficients in the table above were derived from the measured value of *k*(Cl + CH3CHF2) = (2.37  0.31) x 10-13 cm3 molecule-1 s-1, the yield of CH2ClCHF2  = *k2*/*k* = 0.0081  0.0007, and the assumption that *k1*/*k* + *k2*/*k*. = 1.

**Preferred Values**

|  |  |  |
| --- | --- | --- |
| **Parameter** | **Value** | ***T*/K** |
|  |  |  |
| *k*1 /cm3 molecule-1 s-1 | 2.5 x 10-13 | 298 |
| *k*1/cm3 molecule-1 s-1 | 6.3 x 10-12 exp(-965/*T*) | 280-360 |
| *k*2/cm3 molecule-1 s-1 | 2.3 x 10-15 | 298 |
| *k*2/cm3 molecule-1 s-1 | 7.0 x 10-12 exp(-2400/*T*) | 280-360 |

*Reliability*

|  |  |  |
| --- | --- | --- |
|  log *k*1 | ± 0.15 | 298 |
| Δlog *k*2 | ± 0.15 | 298 |
| Δ(*E*1/*R*) | ± 500 |  |
| Δ(*E*2/*R*) | ± 500 |  |

*Comments on Preferred Values*

The recommended value of the overall rate constant at room temperature is an average of the absolute rate and all four relative rate studies, which show good agreement. The temperature dependence of *k*, *k*1 and *k*2 are taken from work of Yano and Tschuikow-Roux, (1986), which supersedes their previous data (Tschuikow-Roux et al. 1985).

**References**

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