

IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet PCI22

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CF₃CHCl₂ (HCFC-123) + hv → products

Primary photochemical processes

Reaction	$\Delta H^\circ/\text{kJ}\cdot\text{mol}^{-1}$	$\lambda_{\text{threshold}}/\text{nm}$
CF ₃ CHCl ₂ + hv → CF ₃ CHCl + Cl	335 (est)	360

Preferred Values

Absorption cross-sections for CF₃CHCl₂ at 298 K and 220 K

λ/nm	$10^{20} \sigma/\text{cm}^2$		λ/nm	$10^{20} \sigma/\text{cm}^2$	
	298 K	220 K		298 K	220 K
190	61.5	54.3	210	1.8	1.2
192	46.2	39.7	212	1.3	0.82
194	33.9	28.1	214	0.84	0.55
196	24.1	19.2	216	0.57	0.38
198	17.2	13.4	218	0.38	0.27
200	12.0	9.1	220	0.26	0.18
202	8.3	6.1	222	0.18	0.13
204	5.7	4.1	224	0.12	0.09
206	3.9	2.7	226	0.09	0.06
208	2.7	1.8	228	0.06	0.04

Comments on Preferred Values

The preferred values of the absorption cross-sections at 298 K are the mean of the values reported by Gillotay and Simon (1991), Orlando et al. (1991) and Nayak et al. (1996). The agreement

between these studies over the wavelength range of preferred values is very good. The temperature dependence down to about 220 K has been reported by Gillotay and Simon (1991), Orlando et al. (1991) and Nayak et al. (1996). The preferred values at 220 K for the wavelength range 190 nm to 220 nm are the mean of the values reported by Gillotay and Simon (1991), Orlando et al. (1991) and Nayak et al. (1996). Because Nayak et al. (1996) did not report values for $\lambda > 220$ nm at their lowest temperature of 223 K, and the values of Orlando et al. (1991) at wavelengths greater than approximately 220 nm have been questioned (Gillotay and Simon, 1991; Nayak et al., 1996), the preferred values at 220 K and $\lambda > 220$ nm are the values reported by Gillotay and Simon (1991). Photolysis is expected to occur with unit quantum efficiency by breaking of the C-Cl bond to yield $\text{CF}_3\text{CHCl} + \text{Cl}$.

References

- Gillotay, D. and Simon, P. C.: J. Atmos. Chem. 12, 269, 1991.
Nayak, A. K., Buckley, T. J., Kurylo, M. J. and Fahr, N.: J. Geophys. Res. 101, 9055, 1996.
Orlando, J. J., Burkholder, J. B., McKeen, S. A. and Ravishankara, A. R.: J. Geophys. Res. 96, 5013, 1991.