

IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet PCI18

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CH₃CF₂Cl (HCFC-142b) + hv → products

Primary photochemical processes

Reaction	$\Delta H^\circ/\text{kJ}\cdot\text{mol}^{-1}$	$\lambda_{\text{threshold}}/\text{nm}$
CH ₃ CF ₂ Cl + hv → CH ₃ CF ₂ + Cl	335 (est)	360
→ CH ₂ CF ₂ Cl + H	400 (est)	300

Preferred Values

Absorption cross-sections for CH₃CF₂Cl 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	1.01	0.75	210	0.017	0.010
2	0.69	0.51	2	0.010	0.006
4	0.49	0.34	4	0.007	0.003
6	0.33	0.22	6	0.004	0.002
8	0.22	0.15	8	0.003	0.001
200	0.14	0.091	220	0.002	0.0007
2	0.09	0.057	2	0.0009	0.0004
4	0.061	0.037	4	0.0005	0.0002
6	0.039	0.024	6	0.0003	0.0001
8	0.026	0.015	8	0.0002	0.0001

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 Simon¹, Orlando *et al.*² and (for 190-210 nm) Nayak *et al.*⁴ The agreement between these studies over the wavelength range of preferred values is good. The results of Hubrich and Stuhl³ are in reasonable agreement. The temperature dependence down to about 220 K has been reported by Gillotay and Simon,¹ Orlando *et al.*² and Nayak *et al.*⁴ The preferred values at 220 K for the wavelength range 190 nm to 210 nm are the mean of the values reported

by Gillotay and Simon,¹ Orlando *et al.*² and Nayak *et al.*⁴ Because Nayak *et al.*⁴ did not report values for $\lambda > 210$ nm at their lowest temperature of 223 K, and the values of Orlando *et al.*² at wavelengths greater than approximately 210 nm have been questioned^{1,4}, the preferred values at 220 K and $\lambda > 210$ nm are the values reported by Gillotay and Simon.¹ Photolysis is expected to occur with unit quantum efficiency. At 193 nm Melchior *et al.*⁵ have shown that C-Cl bond fission to give $\text{CH}_3\text{CF}_2 + \text{Cl}$ is the main channel, but that C-H bond cleavage also occurs with a branching ratio of about 40%.

References

- ¹ D. Gillotay and P. C. Simon, *J. Atmos. Chem.* **12**, 269 (1991).
- ² J. J. Orlando, J. B. Burkholder, S. A. McKeen, and A. R. Ravishankara, *J. Geophys. Res.* **96**, 5013 (1991).
- ³ C. Hubrich and F. Stuhl, *J. Photochem.* **12**, 93 (1980).
- ⁴ A.K. Nayak, T. J. Buckley, M. J. Kurylo, and A. Fahr, *J. Geophys. Res.* **101**, 9055 (1996).
- ⁵ A. Melchior, I. Bar, and S. Rosenwaks, *J. Chem. Phys.* **107**, 8476 (1997).