IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet PCl19

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CH_3CFCl_2 (HCFC-141b) + hν → products

Primary photochemical processes

Reaction	$\Delta H°$/kJ·mol^{-1}	$\lambda_{threshold}$/nm
$CH_3CFCl_2 + h\nu \rightarrow CH_3CFCl + Cl$	335 (est)	360
$\rightarrow CH_2CFCl_2 + H$	400 (est)	300

Preferred Values

Absorption cross-sections for CH_3CFCl_2 at 298 K and 210 K

λ/nm	10^{20} σ/cm^2		λ/nm	10^{20} σ/cm^2	
	298 K	210 K		298 K	210 K
190	83.8	80.1	210	2.1	1.6
192	64.1	59.5	212	1.4	1.0
194	47.4	42.8	214	0.88	0.65
196	34.0	30.0	216	0.57	0.41
198	23.8	20.6	218	0.37	0.26
200	16.4	13.8	220	0.24	0.16
202	11.1	9.2	222	0.16	0.10
204	7.4	6.0	224	0.10	0.06
206	4.9	3.9	226	0.07	0.04
208	3.2	2.5	228	0.04	0.03

Comments on Preferred Values

The preferred values of the absorption cross sections at 298 K are the values reported by Fahr et al. (1993). In this study (Fahr et al., 1993), measurements were made in the gas phase (190–260 nm) and the liquid phase (230–260 nm) at 298 K. Correction factors were used to convert these liquid-phase values into accurate gas-phase values at the long wavelengths. Results reported in this study (Fahr et al., 1993) are in very good agreement with those reported by Gillotay and Simon (1991). The results of Talukdar et al. (1991) are lower at shorter wavelengths
and higher at longer wavelengths. Gillotay and Simon (1991) and Talukdar et al. (1991) report the temperature dependence down to 210 K. The low temperature values of Gillotay and Simon (1991) are preferred, and their 210 K values are given in the table. Photolysis is expected to occur with unit quantum efficiency. At 193 nm Melchior et al. (1997) have shown that C-Cl bond fission to give $CH_3CFCl + Cl$ is the main channel, but that C-H bond cleavage also occurs with a branching ratio of about 15%. H atom formation is also observed at 205-209 nm using the photofragment velocity map imaging technique (Mashino et al., 2005).

References

Fahr, A., Braun, W. and Kurylo, M. J.: J. Geophys. Res. 98, 20467, 1993.

Gillotay, D. and Simon, P. C.: J. Atmos. Chem. 12, 269, 1991.

Mashino, M., Yamada, H., Sugita, A. and Kawasaki, M.: J. Photochem. Photobiol. A: Chem.,176, 78, 2005.

Melchior, A., Bar, I. and Rosenwaks, S.: J. Chem. Phys. 107, 8476, 1997.

Talukdar, R., Mellouki, A., Gierczak, T., Burkholder, J. B., McKeen, S. A. and Ravishankara,A. R.: J. Phys. Chem. 95, 5815, 1991.