

IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet PCI26

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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., 9, 4141, 2008; IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation, <http://iupac.pole-ether.fr>.

This datasheet last evaluated: June 2015; last change in preferred values: December 2005.

CF₃CF₂CHCl₂ (HCFC-225ca) + hv → products

Primary photochemical processes

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

Preferred Values

Absorption cross-sections for CF₃CF₂CHCl₂ at 298 K

λ/nm	$10^{20} \sigma/\text{cm}^2$	λ/nm	$10^{20} \sigma/\text{cm}^2$
160	269	200	16
165	197	205	6.9
170	183	210	2.9
175	191	215	1.2
180	177	220	0.46
185	129	225	0.17
190	74	230	0.065
195	37	240	0.011

Comments on Preferred Values

The preferred values of the absorption cross-sections at 298 K are the values reported by Braun et al. (1991). In the same study, absorption cross-section measurements in the liquid phase were made over the wavelength range 205-270 nm. Correction factors were used to convert these liquid-phase values into gas-phase values. The combined set of gas-phase values for the wavelength range 170-270 nm were fitted with the expression:

$$\log_{10}\sigma = -17.966 + 4.542 \times 10^{-2} X - 2.036 \times 10^{-3} X^2 + 1.042 \times 10^{-5} X^3 \text{ where } X = (\lambda - 160 \text{ nm})$$

Photolysis is expected to occur with unit quantum efficiency by breaking of the C-Cl bond to yield CF₃CF₂CHCl + Cl.

Reference

Braun, W., Fahr, A., Klein, R., Kurylo, M.J. and Huie, R.E.: J. Geophys. Res., 96, 13009, 1991.