IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet PCl28

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

HC(O)Cl + hν → products

Primary photochemical processes

Reaction	$\Delta H°$/kJ·mol^{-1}	$\lambda_{threshold}$/nm
HC(O)Cl + hν → HCO + Cl	340 (est)	350

Preferred Values

Absorption cross-sections of HC(O)Cl at the band maxima (298 K, 1013 mbar of N_2, spectral resolution 0.7 nm)

λ/nm	10^{20} σ/cm^2	λ/nm	10^{20} σ/cm^2
236.1	3.8	280.2	2.4
241.5	4.9	282.7	2.3
247.3	5.6	285.3	1.64
251.4	5.4	286.8	1.04
253.7	6.0	288.0	0.86
256.1	5.6	289.4	0.97
258.2	5.8	292.2	0.81
260.2	6.0	294.9	0.46
263.5	5.1	296.7	0.32
265.7	5.3	298.1	0.22
267.9	5.2	299.5	0.25
269.1	3.9	302.3	0.172
270.2	3.5	305.2	0.080
271.4	4.0	308.1	0.027
273.8	4.1	309.3	0.021
276.3	3.4	311.1	0.020
277.7	2.4	314.1	0.013
278.9	2.1	316.7	0.008
		318.7	0.007

Comments on Preferred Values

The preferred values of the absorption cross-sections at 298 K are those reported by Libuda et al. (1990) These are the values of the absorption cross-sections at the absorption maxima and were measured at a spectral resolution of 0.7 nm. The absorption bands for λ >265 nm became distinctly sharper when the spectral resolution was improved to 0.4 nm. The spectrum of HC(O)Cl is similar to that of HCHO but is shifted to shorter wavelengths by 45 nm. Although there have been no quantum yield studies of HC(O)Cl photolysis, it is reasonable to assume by analogy with the photolysis of $C(O)Cl_2$ that the primary photolysis pathway proceeds by breaking of the C-Cl bond to yield HCO + Cl.

References

Libuda, H. G., Zabel, F., Fink, E. H. and Becker, K. H.: J. Phys. Chem. 94, 5860, 1990.