IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet PCl32

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

$CFCl_2CHO + h\nu \rightarrow$ products

Primary photochemical transitions

Reaction		$\Delta H°$/kJ·mol^{-1}	$\lambda_{threshold}$/nm
$CFCl_2CHO + h\nu \rightarrow CFCl_2 + HCO$	(1)		
$\rightarrow CFCl_2CO + H$	(2)		
$\rightarrow CHFCl_2 + CO$	(3)		

Absorption cross-section data

Wavelength range/nm	References	Comments
235-370	Rattigan et al., 1998	(a)

Quantum yield data

There are no reported quantum yield data.

Comments

(a) Absolute absorption cross-sections were measured using a dual-beam diode array spectrometer over the temperature range 243-298 K. The UV spectrum of dichlorofluoroacetaldehyde shows a broad band, centered at 295 nm and extending out to 365 nm. Values of σ were given at 5 nm intervals at 298 K together with the values of B in the expression $\ln \sigma(T) = \ln \sigma(298\ K) + B(T\text{-}298)$.

Preferred Values

Absorption cross-sections of $CFCl_2CHO$ at 298 K and their temperature dependence

Wavelength/nm	10^{20} σ (298 K)/cm^2	10^4 B/K^{-1} [a]
235	0.402	136.0
240	0.502	87.0
245	1.080	30.6
250	1.597	6.41
255	2.391	1.24

260	3.483	-6.12
265	4.869	-7.55
270	6.527	-8.11
275	8.351	-8.28
280	10.1	-8.04
285	11.8	-7.82
290	13.0	-6.89
295	13.7	-6.41
300	13.6	-4.50
305	12.9	-2.93
310	11.6	1.73
315	9.80	2.70
320	7.93	6.97
325	5.61	12.2
330	3.89	15.6
335	2.46	24.6
340	1.26	36.5
345	0.628	58.1
350	0.254	84.9
355	0.052	92.8
360	0.017	93.2
365	0.007	103.2
370	0.002	138.3

[a)] $\ln \sigma(T) = \ln \sigma(298\ \mathrm{K}) + B(T\text{-}298)$.

Quantum yields of $CFCl_2CHO$

No recommendation.

Comments on Preferred Values

The preferred values for the cross-sections are those reported by Rattigan et al. (1998). There are no data on the quantum yields but, by analogy with acetaldehyde which shows a similar absorption spectrum, photodissociation is expected to be predominantly by channel (1).

References

Rattigan, O. V., Wild, O. and Cox, R. A.: J. Photochem. Photobiol. A: Chem., 112, 1, 1998.