

IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet PCI31

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

CF₂ClCHO + hv → products

Primary photochemical transitions

Reaction	$\Delta H^\circ/\text{kJ}\cdot\text{mol}^{-1}$	$\lambda_{\text{threshold}}/\text{nm}$
CF ₂ ClCHO + hv → CF ₂ Cl + HCO	(1)	
→ CF ₂ ClCO + H	(2)	
→ CHF ₂ Cl + 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) Absorption cross-sections were measured using a dual-beam diode array spectrometer over the temperature range 243-298 K. The UV spectrum of difluorochloroacetaldehyde shows a broad band, centered at 300 nm and extending out to 365 nm. Values of σ were given at 5 nm intervals at 298 K together with values of B in the expression $\ln \sigma(T) = \ln \sigma(298 \text{ K}) + B(T-298)$.

Preferred Values

Absorption cross-sections of CF₂ClCHO at 298 K and their temperature dependence

Wavelength/nm	$10^{20} \sigma(298 \text{ K})/\text{cm}^2$	$10^4 B/\text{K}^{-1 \text{ a}}$
235	0.192	-29.0
240	0.408	-17.9
245	0.736	-13.5
250	1.25	-11.8
255	1.99	-10.7

260	3.02	-10.5
265	4.36	-10.4
270	6.05	-10.5
275	8.00	-9.96
280	10.1	-10.6
285	12.1	-10.2
290	14.0	-10.6
295	15.4	-9.54
300	16.3	-10.4
305	15.9	-7.09
310	15.4	-9.73
315	13.4	-8.32
320	11.7	-7.71
325	9.24	-5.02
330	6.51	-3.03
335	4.76	-2.83
340	2.84	-2.84
345	1.52	14.0
350	0.711	37.3
355	0.148	68.1
360	0.036	75.8
365	0.012	52.9
370	0.003	63.1

^{a)} $\ln \sigma(T) = \ln \sigma(298 \text{ K}) + B(T-298)$

Quantum yields for CF₂CICHO

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.