

# IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet P13

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This data sheet updated: 16<sup>th</sup> May 2002.

## HOCH<sub>2</sub>OOH + hv → products

### Primary photochemical transitions

Reaction	$\Delta H_{298}^{\circ}/\text{kJ}\cdot\text{mol}^{-1}$	$\lambda_{\text{threshold}}/\text{nm}$
HOCH <sub>2</sub> OOH + hv → HOCH <sub>2</sub> O + HO	~188	~637

### Absorption cross-section data

Wavelength range/nm	Reference	Comments
205-360	Bauerle and Moortgat, 1999 <sup>1</sup>	(a)

### Quantum yield data

No data

### Comments

- (a) HOCH<sub>2</sub>OOH prepared by liquid phase reaction of HCHO with excess H<sub>2</sub>O<sub>2</sub>. A diode-array spectrometer was used to make relative absorption measurements over the whole wavelength range. The HOCH<sub>2</sub>OOH concentration measured *in situ* by FTIR using a peak IR absorption coefficient of  $\sigma = 7.4 \times 10^{-19} \text{ cm}^2 \text{ molecule}^{-1}$  at 1049 cm<sup>-1</sup>. This cross section was determined in the same system by quantitative measurement of the decomposition products of HOCH<sub>2</sub>OOH (HCOOH and HCHO) using the yields of these products. The decomposition channels were previously established by Neeb *et al.*<sup>3</sup>

### Preferred Values Absorption cross-sections at 298 K

$\lambda/\text{nm}$	$10^{20} \sigma/\text{cm}^2$	$\lambda/\text{nm}$	$10^{20} \sigma/\text{cm}^2$
205	26.91	290	0.63
210	22.56	295	0.51
215	18.75	300	0.40
220	15.46	305	0.29
225	12.47	310	0.22
230	10.06	315	0.18
235	7.89	320	0.13
240	5.98	325	0.10

245	4.68	330	0.073
250	3.78	335	0.059
255	3.88	340	0.045
260	2.31	345	0.036
265	1.81	350	0.028
270	1.48	355	0.022
275	1.21	360	0.017
280	0.93	365	0.012
285	0.75		

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### *Quantum Yields*

$\phi_1 = 1.0$  for  $\lambda > 290$  nm.

### *Comments on Preferred Values*

The preferred absorption cross-section data are those of Bauerle and Moortgat, 1999<sup>1</sup> which are the only data reported for the absorption spectrum of HOCH<sub>2</sub>OOH. The values are close to those recommended for CH<sub>3</sub>OOH based on the measurements of Vaghjiani and Ravishankara.<sup>2</sup> The recommended quantum yields are based on an analogy with methyl hydroperoxide. Other channels may occur in photolysis at shorter wavelengths.

### **References**

- <sup>1</sup> S. Bauerle and G. K. Moortgat, Chem. Phys. Lett. **309**, 43 (1999).
- <sup>2</sup> G. L. Vaghjiani and A. R. Ravishankara, J. Chem. Phys. **92**, 996 (1990).
- <sup>3</sup> P. Neeb, F. Sauer, O. Horie, G. K. Moortgat, Atmos. Environ., **31**, 1417, (1997).