IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet P5

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This data sheet updated: 16th May 2002.

$HOCH_2CHO + h\upsilon \rightarrow$ products

Primary photochemical transitions

Reaction		$\Delta H°_{298}$/kJ·mol^{-1}	$\lambda_{threshold}$/nm
$HOCH_2CHO + h\upsilon \rightarrow CH_3OH + CO$	(1)	-19.5	
$\rightarrow HOCH_2 + HCO$	(2)	355.3	337
$\rightarrow HOCH_2CO + H$	(3)	373.8	320

Absorption cross-sections

Wavelength range/nm	Reference	Comments
205-335	Bacher, Tyndall and Orlando, 2001[1]	(a)

Quantum yield data ($\phi = \phi_1 + \phi_2 + \phi_3$)

Measurement	Wavelength range/nm	Reference	Comments
$0.5 < \phi < 1.0$	285±25	Bacher, Tyndall and Orlando, 2001[1]	(b)

Comments

(a) Diode array spectrophotometric measurements with 90 cm pathlength. Data obtained with 1 nm resolution. Beer-Lambert plot linear over range of glycolaldehyde pressure of 0.04-0.6 mbar. Cross-sections tabulated at 1 nm intervals. Peak cross section at 277 nm was 5.49×10^{-20} $cm^2 molecule^{-1}$ with an error of ±15%.

(b) Overall quantum yields for the photolysis of ~100 ppm of $HOCH_2CHO$ in air at a total pressure of 1 bar, determined relative to a value of 0.3 determined for acetone in the same equipment. Products and mechanism of the steady state photolysis was deduced, which suggested that reaction (2) was the main channel but with a significant contribution from reaction (1).

Preferred Values

Absorption cross-sections at 298 K

λ/nm	$10^{20}\sigma/cm^2$	λ/nm	$10^{20}\sigma/cm^2$	λ/nm	$10^{20}\sigma/cm^2$
205	39.1	250	2.36	295	3.59
206	33.7	251	2.50	296	3.46
207	28.7	252	2.65	297	3.29
208	24.6	253	2.82	298	3.17
209	21.2	254	2.97	299	3.02
210	18.1	255	3.09	300	2.90
211	15.3	256	3.21	301	2.74
212	13.0	257	3.39	302	2.51
213	11.2	258	3.59	303	2.26
214	9.40	259	3.75	304	2.07
215	7.84	260	3.89	305	1.91
216	6.49	261	4.02	306	1.77
217	5.30	262	4.13	307	1.64
218	4.26	263	4.24	308	1.50
219	3.37	264	4.40	309	1.36
220	2.65	265	4.60	310	1.25
221	2.13	266	4.75	311	1.15
222	1.65	267	4.85	312	1.03
223	1.36	268	4.92	313	0.884
224	1.12	269	4.99	314	0.771
225	0.933	270	5.05	315	0.689
226	0.783	271	5.14	316	0.597
227	0.691	272	5.23	317	0.516
228	0.637	273	5.36	318	0.455
229	0.637	274	5.40	319	0.396
230	0.649	275	5.41	320	0.329
231	0.644	276	5.39	321	0.285
232	0.680	277	5.42	322	0.249
233	0.723	278	5.37	323	0.213
234	0.785	279	5.34	324	0.185
235	0.833	280	5.34	325	0.147
236	0.880	281	5.37	326	0.128
237	0.939	282	5.37	327	0.105
238	1.03	283	5.25	328	0.087
239	1.11	284	5.12	329	0.084
240	1.20	285	5.01	330	0.068
241	1.28	286	4.93	331	0.058
242	1.38	287	4.80	332	0.043
243	1.50	288	4.67	333	0.040
244	1.59	289	4.58	334	0.040
245	1.71	290	4.50	335	0.039
246	1.83	291	4.41		
247	1.95	292	4.19		
248	2.09	293	3.96		
249	2.22	294	3.76		

Quantum Yield

$\phi = 0.75 \pm 0.25$

Comments on Preferred Values

The preferred absorption cross-sections are from the study of Bacher *et al*.[1] which are the only measurments reported and appear to be reliable. The preferred value for the overall quantum yield is based on the work of Bacher *et al*.[1] The value was determined relative to $\phi(CH_3COCH_3) = 0.3$ in 1 bar air for the wavelength region 260-310 nm, which is consistent with the work of Gierczak *et al*.[2] which forms the basis of the current IUPAC evaluation. The most likely decomposition channel was shown to be HCO production in channel (2), but there is insufficient information to recommend a branching ratio.

References

1 C. Bacher, G. S. Tyndall and J. J. Orlando, J. Atm. Chem, **39**, 171, 2001.

2 T. Gierczak, J. B. Burkholder, S. Bauerle, and A. R. Ravishankara, Chem. Phys., **231** 229 (1998).