IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet PI6

This data sheet updated: 15th December 2000.

IBr + hν → products

Primary Photochemical Transitions

Reaction	ΔH°/kJ mol^{-1}	$\lambda_{threshold}$/nm
IBr+ hν → I + Br	178	672
→ Br($^2P_{1/2}$) + I	222	539
→ Br + I($^2P_{1/2}$)	269	445

Absorption cross-section data

Wavelength range/nm	Reference	Comments
220-600	Seery and Britton, 1964[1]	(a)

Quantum yield data

Wavelength/nm	Quantum yield	Reference	Comments
267	Φ(Br*) = 0.35	Kim *et al.*, 1993[2]	(b)
267	Φ(I*) = 0.42		
	Φ(I) = 0.23		
500	Φ(Br*) = 0.73	Haugen *et al.*, 1985[3]	(c)

Comments

(a) Four measurements of the UV/Vis absorption spectrum have been performed in a 10 cm long quartz cell and the pressure was measured using a Pyrex spiral manometer. Runs with added Br_2 indicated the disproportionation reaction to be unimportant under the prevailing experimental conditions. The uncertainty in the absorption cross section was $\pm 0.95 \times 10^{-20}$ throughout the wavelength range.

(b) The stated relative quantum yields are derived from the following measured concentration ratio observed in the diffusive molecular beam photodissociation experiment with REMPI detection of [Br*] and [Br], respectively, within the same laser pulse: [Br*]/[Br] = 0.54 at 267 nm. Center-stripe analysis of velocity profiles affords the stated quantum yields for the channels yielding ground-state Br (Φ(I) = 0.23, Φ(I*)= 0.42)).

(c) Approximate value resulting from a time-resolved laser gain vs. absorption spectroscopy technique.

Preferred Values

Absorption Cross Sections at 298K

λ/nm	10^{20} σ/cm^2	λ/nm	10^{20} σ/cm^2
220	3.59	420	31.73
230	5.70	430	44.77
240	10.21	440	58.69
250	16.71	450	71.92
260	21.45	460	85.18
270	23.09	470	98.49
280	21.10	480	111.10
290	16.82	490	119.86
300	12.43	500	121.66
310	7.95	510	115.92
320	5.39	520	103.08
330	3.36	530	85.83
340	2.14	540	67.52
350	1.45	550	52.34
360	1.53	560	36.63
370	2.37	570	27.22
380	4.17	580	19.88
390	6.96	590	14.57
400	12.04	600	11.32
410	20.46		

Comments on Preferred Value

The listed values are the only ones available.

References

1 D. J. Seery and D. Britton, J. Phys. Chem. **68**, 2263 (1964).
2 Y. S. Kim, Y.-J. Jung, and K.-H. Jung, J. Chem. Phys. **107**, 3805 (1997).
3 H. K. Haugen, E. Weitz, and S. R.Leone, J. Chem.Phys. **83**, 3402 (1985).