

Rate Data for Inelastic Collision Processes in the Diatomic Halogen Molecules. 1986 Supplement.

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The previously published compilation of rate data for inelastic collision processes involving the homonuclear and heteronuclear diatomic halogen molecules [J. Phys. Chem. Ref. Data **13**, 445 (1984)] has been updated through June, 1986. Additional data on collision processes involving the interhalogens, and on processes at very low kinetic temperatures, are presented; in addition, several previously accepted rate data have been corrected.

Key words: energy transfer; halogens; inelastic collisions; quenching; radiative lifetimes; rotational relaxation; vibrational relaxation.

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1. Introduction

In 1984, we published a survey¹ of rate data for inelastic collision processes in diatomic halogen molecules, including both homonuclear ($X_2 = Br_2, Cl_2, F_2, I_2$) and heteronuclear ($XY = BrCl, BrF, BrI, ClF, ClI, and FI$) species. Processes reviewed in the survey included electronic quenching, electronic \leftrightarrow vibrational energy transfer, vibrational relaxation, rotational relaxation, dephasing, depolarization, line broadening, and radiative decay. Theoretical treatments of these processes were also noted. The survey was based on literature published through April, 1983.

During the past several years, sufficient additional data

have been published to warrant this supplement (see Tables 1.1 and 1.4–1.10). In particular, much more data are available on the interhalogens, particularly FI, and on collision processes at low relative kinetic energies in supersonic molecular beams. In addition, some previously reported data have been corrected, such as the I^*-Cl_2 reaction rate and the BrI radiative lifetime. Other conclusions based on the original survey, particularly the applicability of angular-momentum based scaling laws,² have been borne out by additional measurements.

The supplementary literature references are based on material sent to us by scientists active in the field who have seen the original survey, and on searches of the Molecular Spectroscopy Newsletter published by Physics and Astronomy Departments of the University of California at Berkeley (1983–1986), and the Lockheed Dialog[®] data base. For further discussion of the methodology, including definitions of collision processes, experimental techniques, and units, please consult Ref. 1.

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Table 1.1. Inelastic Collision Data for Bromine

Experimental Data for Bromine														
State		Collision		Temp	Meth	v_i	j_i	v_f	j_f	Quant	Data	Units	Est.	Ref
I	F	Process	Partner											
B		quench	Br ₂		LIF	7,11,14	<15			k	4.2E-10	cm ³ s ⁻¹	12%	3
B		quench	He		LIF	7,11,14	<15			k	<2E-12	cm ³ s ⁻¹	12%	3
B	B	R-T	Br ₂		LIF	7,11,14	<15			k	6E-10	cm ³ s ⁻¹	30%	3
X		E-V?	N ₂ [*] (A ³ Σ)	300 K						k	12E-11	cm ³ s ⁻¹	17%	4
X	X	V-T	CCl ₄ (liq.)	298 K	FP(ps)					θ_{vib}	8E-11	s		5

Theoretical Data for Bromine

Theoretical Data for Bromine					
State		Collision		Method, Comments	Ref
I	F	Process	Partners		
X		V-T+R-T	H, Li ⁺	VRI/OSA calc'n, 0.08-1.2 eV relative kinetic energy	6
X		T-V	Li ⁺	Cross sections for 0 → 1, 0 → 2 using BSA	7
X		V-T	Ar, Br	Classical trajectory calc'n @ T=2000-3500 K	8
X		dissoc	Ar, Br	Use results of preceding to calc dissoc rates	9

Radiative Lifetimes for Bromine

Radiative Lifetimes for Bromine				
State		Meth	Data (s)	Ref
I	F			
A'		FP	5.5E-9	5

Table 1.4. Inelastic Collision Data for Bromine Iodide

Experimental Data for Bromine Iodide														
State		Collision		Temp	Meth	v_i	j_i	v_f	j_f	Quant	Data	Units	Est.	Ref
I	F	Process	Partner											
D		quench	N ₂		MEF					k	5E-10	cm ³ s ⁻¹	20%	10
D		quench	O ₂		MEF					k	2.1E-10	cm ³ s ⁻¹	15%	10
D		quench	CH ₄		MEF					k	9.4E-10	cm ³ s ⁻¹	11%	10

Radiative Lifetimes for Bromine Iodide

Radiative Lifetimes for Bromine Iodide						
State		Meth	v_i	j_i	Data (s)	Ref
I	F					
D	X	MEF			27±4E-9	10
B	X	LIF	2	8-33	0.29-0.07E-6	11 (a)
B	X	LIF	3	4-31	0.72-0.28E-7	11 (a)

(a) Supersedes previous data of Wright & Havey [J. Chem. Phys. **68**, 864 (1978)].

Table 1.5. Inelastic Collision Data for Chlorine

Experimental Data for Chlorine														
State		Collision		Temp	Meth	v_i	j_i	v_f	j_f	Quant Data		Units	Est.	
I	F	Process	Partner							Rept	Entry		Error	Ref
X	X	E-V	I*	300 K	IRF					k	<8E-15	cm ³ s ⁻¹		12
X		E-V?	N ₂ *(A ³ Σ)	300 K						k	7.8E-11	cm ³ s ⁻¹	20%	4
X	X	E-V	I*	300 K	IRF					k	2.0E-14	cm ³ s ⁻¹	5%	13 (a)
X	X	E-V	I*	300 K	IRF					k	1.7E-14	cm ³ s ⁻¹	30%	14 (a)

(a) Actual rate probably <8E-15 cm³s⁻¹, fast I*-Cl atom quenching observed. [12]

Table 1.6. Inelastic Collision Data for Chlorine Fluoride

Experimental Data for Chlorine Fluoride														
State		Collision		Temp	Meth	v_i	j_i	v_f	j_f	Quant Data		Units	Est.	
I	F	Process	Partner							Rept	Entry		Error	Ref
X		(a)	I*	298 K	LIF					k	1.1E-13	cm ³ s ⁻¹	30%	15

(a) Assumed to be reactive, I* + XY → IX + Y, rather than E-V transfer.

Table 1.7. Inelastic Collision Data for Chlorine Iodide

Experimental Data for Chlorine Iodide														
State		Collision		Temp	Meth	v_i	j_i	v_f	j_f	Quant Data		Units	Est.	
I	F	Process	Partner							Rept	Entry		Error	Ref
B		quench	He		LIF	1	14			σ	0.005E-16	cm ²	40%	16
B		quench	O ₂		LIF	1	14			σ	0.6E-16	cm ²	17%	16
B		quench	Kr		LIF	1	14			σ	0.8E-16	cm ²	25%	16
B		quench	CCl ₄		LIF	1	14			σ	4.5E-16	cm ²	12%	16
B		quench	CH ₂ Cl ₂		LIF	1	14			σ	5.5E-16	cm ²	8%	16
B		quench	CHCl ₃		LIF	1	14			σ	6.3E-16	cm ²	10%	16
B		quench	t-C ₂ H ₂ Cl ₂		LIF	1	14			σ	3.8E-16	cm ²	10%	16
B		quench	g-C ₂ H ₂ Cl ₂		LIF	1	14			σ	6.5E-16	cm ²	10%	16
B		quench	c-C ₂ H ₂ Cl ₂		LIF	1	14			σ	8.2E-16	cm ²	12%	16
B		quench	C ₆ H ₆		LIF	1	14			σ	33E-16	cm ²	17%	16
B		quench	He		LIF	2	15			σ	0.11E-16	cm ²	20%	16
B		quench	O ₂		LIF	2	15			σ	8.0E-16	cm ²	12%	16
B		quench	Kr		LIF	2	15			σ	19E-16	cm ²	20%	16
B		quench	CCl ₄		LIF	2	15			σ	35E-16	cm ²	17%	16
B		quench	CH ₂ Cl ₂		LIF	2	15			σ	38E-16	cm ²	12%	16
B		quench	CHCl ₃		LIF	2	15			σ	40E-16	cm ²	12%	16
B		quench	t-C ₂ H ₂ Cl ₂		LIF	2	15			σ	41E-16	cm ²	10%	16
B		quench	g-C ₂ H ₂ Cl ₂		LIF	2	15			σ	51E-16	cm ²	10%	16
B		quench	c-C ₂ H ₂ Cl ₂		LIF	2	15			σ	57E-16	cm ²	10%	16
B		quench	C ₆ H ₆		LIF	2	15			σ	79E-16	cm ²	10%	16
X	X	E-V	I*	300 K	IRF					k	1.5E-11	cm ³ s ⁻¹	30%	14
X	X	E-V	I*	300 K	IRF					k	3.3E-11	cm ³ s ⁻¹	12%	13
X		E-V?	N ₂ *(A ³ Σ)	300 K						k	8.0E-11	cm ³ s ⁻¹	20%	4
B		quench	ICl ₃		LIF	3	5-52			k	8.7E-10	cm ³ s ⁻¹	10%	17

Table 1.7. Inelastic Collision Data for Chlorine Iodide (continued)

Radiative Lifetimes for Chlorine Iodide						
State					Data	Est.
I	F	Meth	v_i	j_i	(s)	Error Ref
B	X	LIF	3	5-52	0.5-1.0E-9	17
B	X	LIF	1	7-55	4.1E-6	5% 18
B	X	LIF	2	7-54	(3.3 to 0.07)E-6 function of j	18

Table 1.8. Inelastic Collision Data for Fluorine

Experimental Data for Fluorine												
State		Collision		Temp	Meth	v_i	j_i	v_f	j_f	Quant Data	Units	Est.
I	F	Process	Partner							Rept Entry		Error Ref
X		(a)	I*	298 K	LIF					k <8.7E-14	cm ³ s ⁻¹	15

(a) Assumed to be reactive, I* + XY → IX + Y, rather than E-V transfer.

Table 1.9. Inelastic Collision Data for Fluorine Iodide

Experimental Data for Fluorine Iodide												
State		Collision		Temp	Meth	v_i	j_i	v_f	j_f	Quant Data	Units	Est.
I	F	Process	Partner							Rept Entry		Error Ref
B		quench	He	298 K	LIF	all	v'			k <1.0E-14	cm ³ s ⁻¹	19
B		quench	N ₂	298 K	LIF	all	v'			k <1.0E-14	cm ³ s ⁻¹	19
B		quench	SF ₆	298 K	LIF	all	v'			k <1.0E-14	cm ³ s ⁻¹	19
B		quench	F ₂	298 K	LIF	all	v'			k 4E-12	cm ³ s ⁻¹	25% 19
B		quench	He	298 K	LIF	3-8				σ <7.9E-20	cm ²	20
B		quench	Ne	298 K	LIF	3-8				σ <1.6E-19	cm ²	20
B		quench	Ar	298 K	LIF	3-8				σ <2.2E-19	cm ²	20
B		quench	Kr	298 K	LIF	3-8				σ <2.9E-19	cm ²	20
B		quench	Xe	298 K	LIF	3-8				σ <3.1E-19	cm ²	20
B		quench	F ₂	298 K	LIF	3				k 3.4E-12	cm ³ s ⁻¹	15% 20
B		quench	F ₂	298 K	LIF	3				σ 7.4E-17	cm ²	15% 20
B		quench	F ₂	298 K	LIF	6				k 4.5E-12	cm ³ s ⁻¹	15% 20
B		quench	F ₂	298 K	LIF	6				σ 9.9E-17	cm ²	15% 20
B		quench	F ₂	298 K	LIF	7				k 5.2E-12	cm ³ s ⁻¹	8% 20
B		quench	F ₂	298 K	LIF	7				σ 1.1E-16	cm ²	8% 20
B		quench	I ₂	298 K	LIF	3-7				σ 9.2E-15	cm ²	20
B		quench	N ₂	298 K	LIF	3-8				σ <1.9E-19	cm ²	20
B		quench	H ₂ O	298 K	LIF	3-6				σ 3.8E-15	cm ²	30% 20
B		quench	H ₂ O	298 K	LIF	4				σ 2.8E-17	cm ²	20% 20
B		quench	H ₂ O	298 K	LIF	5				σ 6.2E-17	cm ²	25% 20
B		quench	H ₂ O	298 K	LIF	6				σ 1.2E-16	cm ²	25% 20
B		quench	O ₂	298 K	LIF	3-8				σ 1.2E-16	cm ²	20% 20
B		quench	O ₂	298 K	LIF	3-8				σ 2.1E-17	cm ²	15% 20
B	B	V-T	He	298 K	LIF	4	3			k 6.9E-12	cm ³ s ⁻¹	10% 19
B	B	V-T	N ₂	298 K	LIF	4	3			k 3.5E-12	cm ³ s ⁻¹	10% 19
B	B	V-T	He	298 K	LIF	3	2			k 5.4E-12	cm ³ s ⁻¹	10% 19
B	B	V-T	N ₂	298 K	LIF	3	2			k 2.5E-12	cm ³ s ⁻¹	10% 19
B		V-T	Ar/N ₂	300 K		1				k 0.6E-12	cm ³ s ⁻¹	30% 21
B		V-T	Ar/N ₂	300 K		2				k 1.6E-12	cm ³ s ⁻¹	30% 21
B		V-T	Ar/N ₂	300 K		3				k 2.6E-12	cm ³ s ⁻¹	30% 21
B		V-T	Ar/N ₂	300 K		4				k 3.5E-12	cm ³ s ⁻¹	30% 21
B		V-T	Ar/N ₂	300 K		5				k 2.6E-12	cm ³ s ⁻¹	30% 21
B		V-T	Ar/N ₂	300 K		6				k 4.1E-12	cm ³ s ⁻¹	30% 21
D		V-T	Ar/N ₂	300 K		7				k 4.0E-12	cm ³ s ⁻¹	30% 21
B		V-T	Ar/N ₂	300 K		8				k 2.9E-12	cm ³ s ⁻¹	30% 21
B		quench	I ₂ ⁺	300 K		3-6				k 3.5E-10	cm ³ s ⁻¹	6% 22
X	B	V-E	HF ⁺	900-2000 K	CL					k 3.6E-14	cm ³ s ⁻¹	23
X	B	E-E	N ₂ [*]	300 K				3-6		k 2.0E-10	cm ³ s ⁻¹	21
X		(a)	I*	400 K	AA					k 1.3E-11	cm ³ s ⁻¹	50% 15

(a) Process assumed to be reactive, I* + XY → IX + Y, rather than E-V transfer.

Table 1.10. Inelastic Collision Data for Iodine

Experimental Data for Iodine														
State		Collision		Temp	Meth	v _i	j _i	v _f	j _f	Quant Data		Units	Est. Error	Ref
I	F	Process	Partner							Rept	Entry			
B		quench	Kr		LIF	8-49				σ	5-12E-16	cm ²	15%	24
B		quench	t-C ₂ H ₂ Cl ₂		LIF	8-49				σ	30-60E-16	cm ²	10%	24
B	B	V-T	He	19 K	LIF	43	12+16	44 to 33		k [equation]		cm ³ s ⁻¹		25 (a)
B	B	V-T	H ₂	30 K	LIF	43	12+16	44 to 33		k [equation]		cm ³ s ⁻¹		25 (a)
X		E-V?	N ₂ ⁺ (A ³ Σ)	300 K						k	23E-11	cm ³ s ⁻¹	20%	4
X	D'	E-E	N ₂ ⁺ (A ³ Σ)	300 K						k	4E-14	cm ³ s ⁻¹		4
X	X	E-V	I [*]	300 K	IRF					k	3.0E-11	cm ³ s ⁻¹	3%	13
X	A'?	E-E	O ₂ [*] (benzene solution)	300 K	FP					k	2.3E-18	cm ³ s ⁻¹	15%	26
X	X	V-T	He	E _T =0-500 meV	BS	0		1,2,3		σ [graph]		cm ²		27 (b)
X	X	V-T	H ₂ , D ₂	E _T =0-500 meV	BS	0		1,2,3		σ [graph]		cm ²		28 (b)
B	B	V-T+R-T	He	300 K	LIF	13	41	12	39	k	526E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				41	k	556E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				43	k	526E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				45	k	512E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				47	k	470E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				49	k	439E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				51	k	400E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				53	k	357E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				55	k	319E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				57	k	289E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				59	k	258E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				61	k	211E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				63	k	186E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				65	k	170E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				67	k	139E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				69	k	115E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				71	k	95E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				73	k	74E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				75	k	61E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				77	k	45E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				79	k	37E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				81	k	31E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				83	k	31E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				85	k	21E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				87	k	23E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				89	k	18E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				91	k	12E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				93	k	14E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				95	k	11E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				97	k	4E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				99	k	9E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				101	k	8E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				103	k	7E-14	cm ³ s ⁻¹	10-20%	29

 (a) For He-I₂⁺(v),

$$k(v, v') = (1.70 \pm 0.05 \text{ cm}^3 \text{ s}^{-1}) \times (0.0065)^{|\Delta v - 1|} v(v-1)(v-2) \dots (v+\Delta v+1)$$

 For H₂-I₂⁺(v),

$$k(v, v') = (3.2 \pm 0.1 \text{ cm}^3 \text{ s}^{-1}) \times (0.009)^{|\Delta v - 1|} v(v-1)(v-2) \dots (v+\Delta v+1)$$

 (b) Cross section σ varies between 0.0 and 0.02E-16 cm², energy- and v_f- dependent.

Table 1.10. Inelastic Collision Data for Iodine (continued)

Experimental Data for Iodine														
State		Collision		Temp	Meth	v_i	j_i	v_f	j_f	Quant	Data	Units	Est.	Ref
I	F	Process	Partner											
B	B	V-T+R-T	He	300 K	LIF	13	91	12	49	k	78E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				53	k	83E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				55	k	60E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				57	k	87E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				59	k	72E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				61	k	106E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				63	k	103E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				73	k	203E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				75	k	237E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				77	k	281E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				79	k	297E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				81	k	324E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				83	k	340E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				85	k	391E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				87	k	416E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				89	k	421E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				91	k	464E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				93	k	472E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				95	k	451E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				99	k	409E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				101	k	357E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				105	k	307E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				107	k	292E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	He	300 K	LIF				109	k	277E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF	13	41	12	39	k	107E-14	cm ³ s ⁻¹	10-20%	29
D	D	V-T+R-T	Xe	300 K	LIF				41	k	109E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF				47	k	115E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF				49	k	104E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF				51	k	112E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF				53	k	113E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF				55	k	113E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF				57	k	120E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF				59	k	119E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF				61	k	118E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF				63	k	116E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF				65	k	120E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF				67	k	118E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF				73	k	113E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF				75	k	119E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF				77	k	110E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF				79	k	103E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF				81	k	110E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF				83	k	108E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF				85	k	95E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF				87	k	108E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF				89	k	88E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF				91	k	94E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF				93	k	81E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF				95	k	88E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF				97	k	84E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF				99	k	86E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF				101	k	77E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF	13	91	12	51	k	50E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF				53	k	60E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF				55	k	59E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF				57	k	69E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF				59	k	65E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF				61	k	71E-14	cm ³ s ⁻¹	10-20%	29

Table 1.10. Inelastic Collision Data for Iodine (continued)

Experimental Data for Iodine														
State		Collision		Temp	Meth	v _i	j _i	v _f	j _f	Quant Rept	Data Entry	Units	Est. Error	Ref
I	F	Process	Partner											
B	B	V-T+R-T	Xe	300 K	LIF	13	91	12	63	k	67E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF				75	k	78E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF				77	k	83E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF				79	k	94E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF				81	k	94E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF				83	k	66E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF				85	k	90E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF				87	k	85E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF				89	k	75E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF				91	k	98E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF				93	k	99E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF				95	k	91E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF				99	k	72E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF				101	k	100E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T+R-T	Xe	300 K	LIF				105	k	96E-14	cm ³ s ⁻¹	10-20%	29
B	B	V-T	He(?)	300 K?		15	14			σ	3.1E-16	cm ²	10%	30
B	B	V-T	He(?)	300 K?		15	13			σ	0.78E-16	cm ²	10%	30
B	B	dephase	I ₂	300 K?	CT	[589.7nm]				σ	590E-16	cm ²	15%	31
B	B	e-loss	I ₂	300 K?	CT	[589.7nm]				σ	227E-16	cm ²	10%	31
X		dissoc	MgO(100)	548 K	BS(TOF)									32 (c)
A'		quen	He	300 K	FP					k	9.4E-15	cm ³ s ⁻¹	10%	33 (d)
A'		quen	Ar	300 K	FP					k	2.8E-14	cm ³ s ⁻¹	35%	33 (d)
A'		quen	N ₂	300 K	FP					k	3.5E-14	cm ³ s ⁻¹	30%	33 (d)
A'		quen	SF ₆	300 K	FP					k	2.4E-13	cm ³ s ⁻¹	5%	33 (d)
A'		quen	I ₂	300 K	FP					k	5.5E-11	cm ³ s ⁻¹	15%	33 (d)
B		quen	He	298 K	CT	2	59	15	60	σ	1.16E-16	cm ²	6%	34,35,36
B		quen	Ne	298 K	CT	2	59	15	60	σ	3.58E-16	cm ²	6%	34,35,36
B		quen	Ar	298 K	CT	2	59	15	60	σ	10.4E-16	cm ²	5%	34,35,36
B		quen	Kr	298 K	CT	2	59	15	60	σ	22.2E-16	cm ²	2%	34,35,36
B		quen	Xe	298 K	CT	2	59	15	60	σ	48.7E-16	cm ²	2%	34,35,36
B		quen	I ₂	298 K	CT	2	59	15	60	σ	115E-16	cm ²	20%	34,35,36
B		V-T+R-T	He	298 K	CT	2	59	15	60	σ	54.3E-16	cm ²	2%	34,35,36
B		V-T+R-T	Ne	298 K	CT	2	59	15	60	σ	89.5E-16	cm ²	3%	34,35,36
B		V-T+R-T	Ar	298 K	CT	2	59	15	60	σ	136E-16	cm ²	3%	34,35,36
B		V-T+R-T	Kr	298 K	CT	2	59	15	60	σ	154E-16	cm ²	2%	34,35,36
B		V-T+R-T	Xe	298 K	CT	2	59	15	60	σ	150E-16	cm ²	2%	34,35,36
B		V-T+R-T	I ₂	298 K	CT	2	59	15	60	σ	110E-16	cm ²	40%	34,35,36
B		dephas	He	298 K	CT	2	59	15	60	σ	66E-16	cm ²	10%	34,35,36
B		dephas	Ne	298 K	CT	2	59	15	60	σ	110E-16	cm ²	10%	34,35,36
B		dephas	Ar	298 K	CT	2	59	15	60	σ	160E-16	cm ²	10%	34,35,36
B		dephas	Kr	298 K	CT	2	59	15	60	σ	207E-16	cm ²	10%	34,35,36
B		dephas	Xe	298 K	CT	2	59	15	60	σ	270E-16	cm ²	10%	34,35,36
B		quen	I ₂	243-273 K	LIF	14	0-8			σ	190E-16	cm ²	7%	37
B		quen	H ₂	243-273 K	LIF	14	0-8			σ	2.5E-16	cm ²	12%	37
B		quen	CO	243-273 K	LIF	14	0-8			σ	15.1E-16	cm ²	4%	37
B		quen	CH ₄	243-273 K	LIF	14	0-8			σ	18.0E-16	cm ²	4%	37
B		quen	He	9.4 K	LIF	11				σ	0.33E-16	cm ²	25%	38

+SSE

(c) Dissociation measured on collision of I₂ with heated MgO surface.

(d) Temperature dependence of quenching rate measured, 330 K > T > 280 K.

Table 1.10. Inelastic Collision Data for Iodine (continued)

Theoretical Data for Iodine					
State	Process	Collision Partners	Method, Comments		Ref
I					
B	V-T	He	Resonance analysis, T = 0 to 5 K		39
	V-V	I ₂	Quantum calculation		40
B	R-T	He	Quasi-classical, collision energy < 0.5 cm ⁻¹		41
X	V-T	He, Ar	Scaling law for vibrational energy transfer		42
B	R-T	He	620 K	(formula)	43
B	R-T	Xe	550 K	(formula)	43
X	V-V+V-T	I ₂	Quantum calculation		44
X	V-V+V-T	I ₂	Quantum calculation		45
X	V-T	He	VEDW/IOS calculation		46
X	V-T	He	VCC/IOS calculation, cf. to Hall et al. expts. [27]		47
	V-T	He	Semiclassical calculation at low relative K.E.		48
X	V-T	(Ne) _n clusters n=4,8,16	Theoretical calculation, classical dynamics		49
X	V-T	He	Theoretical calculation at very low temperatures using VCC-RIOS		50

Radiative Lifetimes for Iodine						
State	I	F	Meth	v _i	j _i	Ref
B	X	43	12,16	(formula) with $\Gamma_{\text{rad}} = 0.314 \pm 0.018E+6 \text{ s}^{-1}$		51

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