

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 Rept	Data Entry	Units	Est. Error	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 RSA	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'		(CCl ₄ , 298 K)	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 Rept	Data Entry	Units	Est. Error	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. Error Ref
I	F	Process	Partner							Rept	Entry		
X	X	E-V	I*	300 K	IRF					k	<8E-15	cm ³ s ⁻¹	12
X	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. Error Ref
I	F	Process	Partner							Rept	Entry		
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. Error Ref
I	F	Process	Partner							Rept	Entry		
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	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 Rept	Data Entry	Units	Est. 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 Rept	Data Entry	Units	Est. 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
B		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 Rept	Data Entry	Units	Est. Error Ref
I	F	Process	Partner										
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	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)

State		Experimental Data for Iodine												
I	F	Process	Collision Partner	Temp	Meth	v_i	j_i	v_f	j_f	Quant Rept	Data Entry	Units	Est. Error	Ref
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
B	B	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 Partner	Temp	Meth	v_i	j_i	v_f	j_f	Quant Rept	Data Entry	Units	Est. Error	Ref
I	F												
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'		quench He	300 K	FP					k	9.4E-15	cm ³ s ⁻¹	10%	33 (d)
A'		quench Ar	300 K	FP					k	2.8E-14	cm ³ s ⁻¹	35%	33 (d)
A'		quench N ₂	300 K	FP					k	3.5E-14	cm ³ s ⁻¹	30%	33 (d)
A'		quench SF ₆	300 K	FP					k	2.4E-13	cm ³ s ⁻¹	5%	33 (d)
A'		quench I ₂	300 K	FP					k	5.5E-11	cm ³ s ⁻¹	15%	33 (d)
B		quench He	298 K	CT	2	59	15	60	σ	1.16E-16	cm ²	6%	34, 35, 36
B		quench Ne	298 K	CT	2	59	15	60	σ	3.58E-16	cm ²	6%	34, 35, 36
B		quench Ar	298 K	CT	2	59	15	60	σ	10.4E-16	cm ²	5%	34, 35, 36
B		quench Kr	298 K	CT	2	59	15	60	σ	22.2E-16	cm ²	2%	34, 35, 36
B		quench Xe	298 K	CT	2	59	15	60	σ	48.7E-16	cm ²	2%	34, 35, 36
B		quench 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		quench I ₂	243-273 K	LIF	14	0-8			σ	190E-16	cm ²	7%	37
B		quench H ₂	243-273 K	LIF	14	0-8			σ	2.5E-16	cm ²	12%	37
B		quench CO	243-273 K	LIF	14	0-8			σ	15.1E-16	cm ²	4%	37
B		quench CH ₄	243-273 K	LIF	14	0-8			σ	18.0E-16	cm ²	4%	37
B		quench 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
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 $\Gamma_{\text{rad}} = 0.314 \pm 0.018\text{E}+6 \text{ s}^{-1}$		51

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