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APPROXIMATE TRANSITION PROBABILITIES AND LIFETIME OF SOME OF THE EXCITED STATES OF NEUTRAL IODINE

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REPORT 1093-43

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ABSTRACT

Approximate transition probabilities and lifetime of some of the 5d, 6p, and 6s states of neutral iodine is given with the assumption that the states are purely pair coupled.

APPROXIMATE TRANSITION PROBABILITIES AND LIFETIME OF SOME OF THE EXCITED STATES OF NEUTRAL IODINE

Approximate transition probabilities for some of the excited levels of neutral iodine have been calculated. These data are useful in the approximate determination of line strength and prediction of possible new laser lines. The states are assumed to be pair coupled[1] and transition probabilities for $5p^4$-$5d \rightarrow 5p^4$-$6p$, $5p^4$-$6p \rightarrow 5p^4$-$6s$ and $5p^4$-$6s \rightarrow 5p^5$ configurations are given in Tables Ia through Ic, based upon the assumption that the states are not mixed. Table II gives the radials integrals

$$\int r\,\mathcal{F}_{n\ell}(r)\,\mathcal{F}_{n\ell'}(r)\,dr$$

which have been used in the calculations of the transition probabilities. Table III gives the exchange, direct and spin orbit interaction integrals for the three configurations $5p^4$-$5d$, $5p^4$-$6p$ and $5p^4$-$6s$ of iodine I. The above radial integrals were calculated using wavefunctions obtained from a computer program given by Herman and Skilman[2] for the solution of the self-consistent Hartree Fock equation in the Slater approximation. Finally in Table IV we have the lifetimes of some of the upper states.

In the calculations of the transition probabilities from the $5p^4$-$6s$ and $5p^4$-$5d$ states to the ground $5p^5\ {}^2P_J$ state one has first to express the ground $|5p^5\ {}^2P_J>$ state in terms of its parents, i.e.,

$$|\ell^5 LSJM> = \sum_{\overline{L}\,\overline{S}} (\ell^5\ LS\ \ |\ell^4 \overline{L}\,\overline{S})\{|\ell^4\ \overline{L}\ \overline{S};\ell_s, LSJM>$$

or

$$= \sum_{\overline{L}\,\overline{S}} \sum_{\overline{J}K} (-1)^{2\overline{S}+\overline{L}+\ell+\frac{1}{2}+K+L+J}\ (\ell^5\ LS\{|\ell^4\overline{L}\ \overline{S})\ \times$$

$$\{[\overline{J}]\ [L]\ [K]\ [S]\}^{\frac{1}{2}} \times$$

$$\begin{Bmatrix} \overline{S} & \overline{L} & \overline{J} \\ \ell & K & L \end{Bmatrix} \begin{Bmatrix} L & \overline{S} & K \\ s & J & S \end{Bmatrix} \quad |\ell^4\ \overline{L}\ \overline{S}\ \overline{J}, \ell;K, s\ , JM>$$

where $\ell = 1$ and L S J stands for the ${}^2P_J$ ground state of iodine I. The symbol $(\ell^5\ LS\ \{|{}^4\ell\ LS)$ is the coefficient of fractional parentage[3] and $[x] = 2x + 1$.

CONCLUSIONS:

The results, although approximate, are more or less in agreement with the experimentally observed laser lines[4] with the exception of the 2056 cm^{-1} line which according to these calculations must have a strength much lower than that indicated by experiment. Experimentally, the $[^3P_0]\ 5d[2]_{5/2} \rightarrow [^3P_0]\ 6p[1]_{3/2}$ at 1818.61 cm^{-1} has a relative intensity of 5 and a transition probability of $0.23 \times 10^{+6}\ sec^{-1}$. The $[^3P_2]\ 5d[4]_{7/2} \rightarrow [^3P_2]\ 6p[3]_{5/2}$ at 2915 cm^{-1} has a relative intensity of 10 and a transition probability of $0.91 \times 10^6\ sec^{-1}$ but the $[3P_2]\ 5d[4]_{9/2} \rightarrow [^3P_2]\ 6p\,[3]_{7/2}$ at 2056 cm^{-1} has a relative intensity of 100 and a transition probability of $0.33 \times 10^6\ sec^{-1}$. However there are two other upper levels which have transitions at the same wavelength, namely

$$[3P_2] - 6f\,[3]_{7/2} \rightarrow [3P_2] - 7d\,[4]_{9/2}$$

and

$$[3P_2] - 9f\ [4]_{7/2} \rightarrow [3P_2] - 8d[4]_{7/2}$$

and the laser action could originate from these. This is somewhat unlikely since these two levels are lying far above the ground state. Other explanations such as cascade filling of the $[3P_2] - 5d\,[4]_{9/2}$ could be considered to explain the high intensity of the 2056 cm^{-1} transition.

TABLE 1a

TRANSITION PROBABILITIES FOR SOME OF THE $5p^4$-$5d \rightarrow 5p^4$-$6p$ STATES OF IODINE I

$[^3P]$ Core

Upper J_c K J	Lower J_c K J	$A \times 10^{-6}$ 1/sec	wavelength cm^{-1}
0 [2] 3/2	- 0 [1] 1/2	0.1939	1825.36
	- 0 [1] 3/2	0.0231	1662.54
0 [2] 5/2	- 0 [1] 3/2	0.2302	1818.61
1 [1] 1/2	- 1 [0] 1/2	0.1640	1975.77
	- 1 [1] 1/2	0.000008	90.09
	- 1 [1] 3/2	0.0004	422.70
	- 1 [2] 3/2	0.0003	670.11
1 [1] 3/2	- 1 [0] 1/2	0.6248	3085.95
	- 1 [1] 1/2	0.0046	1200.27
	- 1 [1] 3/2	0.0478	1532.88
	- 1 [2] 3/2	0.0006	1780.29
	- 1 [2] 5/2	0.0083	2058.26
1 [2] 3/2	- 1 [1] 1/2	0.3461	2436.78
	- 1 [1] 3/2	0.1016	2769.39
	- 1 [2] 3/2	0.2364	3016.80
	- 1 [2] 5/2	0.0342	3294.77
1 [2] 5/2	- 1 [1] 3/2	0.6605	2844.37
	- 1 [2] 3/2	0.0188	3091.78
	- 1 [2] 5/2	0.3417	3369.75
1 [3] 5/2	- 1 [2] 3/2	0.4755	2370.11
	- 1 [2] 5/2	0.0474	2648.08
1 [3] 7/2	- 1 [2] 5/2	0.1163	1448.54
2 [0] 1/2	- 2 [1] 1/2	0.2678	2758.79
	- 2 [1] 3/2	0.0957	1553.66
2 [1] 1/2	- 2 [1] 1/2	0.0573	1441.37
	- 2 [1] 3/2	0.0001	236.24
	- 2 [2] 3/2	0.1177	2308.33
2 [1] 3/2	- 2 [1] 1/2	0.0006	498.14
	- 2 [2] 3/2	0.0024	1365.10
	- 2 [2] 5/2	0.0262	1448.79
2 [2] 3/2	- 2 [1] 1/2	1.0157	4497.91
	- 2 [1] 3/2	0.0797	3292.78
	- 2 [2] 3/2	3.1022	5364.87
	- 2 [2] 5/2	0.3611	5448.56
	- 2 [3] 5/2	0.2666	4710.38

TABLE 1a (Cont.)

Upper J_c K J	Lower J_c K J	$A \times 10^{-6}$ 1/sec	wavelength cm^{-1}
2 [2] 5/2	- 2 [1] 3/2	0.3948	3089.12
	- 2 [2] 3/2	0.2046	5161.21
	- 2 [2] 5/2	3.0060	5244.90
	- 2 [3] 5/2	0.0111	4506.72
	- 2 [3] 7/2	0.2186	4481.22
2 [3] 5/2	- 2 [2] 3/2	0.0261	1030.48
	- 2 [2] 5/2	0.0024	1114.17
	- 2 [3] 5/2	0.0006	375.99
	- 2 [3] 7/2	0.00003	350.49
2 [3] 7/2	- 2 [2] 5/2	0.0348	1108.70
	- 2 [3] 5/2	0.00002	370.52
	- 2 [3] 7/2	0.0005	345.02
2 [4] 7/2	- 2 [3] 5/2	0.9140	2915.02
	- 2 [3] 7/2	0.0330	2889.52
2 [4] 9/2	- 2 [3] 7/2	0.3328	2056.38

TABLE 1b

TRANSITION PROBABILITIES OF SOME OF THE $5p^4$-$6p \rightarrow 5p^4$-$6s$ STATES OF IODINE I

[^{3}P] Core

Upper J_c K J		Lower J_c K J	$A \times 10^{-8}$ 1/sec	wavelength cm^{-1}
0 [1] 1/2	-	0 [0] 1/2	0.4155	10917.67
0 [1] 3/2	-	0 [0] 1/2	0.4344	11080.49
1 [0] 1/2	-	1 [1] 1/2	0.0612	8314.72
	-	1 [1] 3/2	0.1932	9681.71
1 [1] 1/2	-	1 [1] 1/2	0.2259	10200.40
	-	1 [1] 3/2	0.1647	11567.39
1 [1] 3/2	-	1 [1] 1/2	0.0511	9867.79
	-	1 [1] 3/2	0.3773	11234.78
1 [2] 3/2	-	1 [1] 1/2	0.2369	9626.38
	-	1 [1] 3/2	0.0706	10987.37
1 [2] 5/2	-	1 [1] 3/2	0.3922	10709.40
2 [1] 1/2	-	2 [2] 3/2	0.2972	9764.08
2 [1] 3/2	-	2 [2] 3/2	0.0421	10969.21
	-	2 [2] 5/2	0.5517	12428.63
2 [2] 3/2	-	2 [2] 3/2	0.2024	8897.12
	-	2 [2] 5/2	0.0355	10356.54
2 [2] 5/2	-	2 [2] 3/2	0.0146	8813.43
	-	2 [2] 5/2	0.3231	10272.85
2 [3] 5/2	-	2 [2] 3/2	0.2597	9551.61
	-	2 [2] 5/2	0.0284	11011.03
2 [3] 7/2	-	2 [2] 5/2	0.4292	11036.53

[^{1}D] core

	-	2 [2] 5/2	0.3608×10^8	10415.74
2 [2] 5/2	-	2 [2] 5/2	0.0213×10^8	10004.68
	-	2 [2] 3/2	0.2929×10^8	9942.80
2 [2] 5/2	-	2 [2] 5/2	0.4577×10^8	11537.58
	-	2 [2] 3/2	0.0322×10^8	11475.70
2 [2] 3/2	-	2 [2] 5/2	0.0480×10^8	11451.95
	-	2 [2] 3/2	0.4246×10^8	11390.07
2 [1] 3/2	-	2 [2] 5/2	0.2727×10^8	9827.38
	-	2 [2] 3/2	0.0297×10^8	9765.50
2 [1] 1/2	-	2 [2] 3/2	0.4310×10^8	11051.84

TABLE 1c

TRANSITION PROBABILITIES OF SOME OF THE $5p^4$-$6s \to 5p^5$ STATES OF IODINE I

^{3}P Core

J_c K J	J_c K J	A × 10^{-8} 1/sec	wavelength cm^{-1}
0 [0] 1/2	- $^2P_{1/2}$	0.1117	53293.08
	- $^2P_{3/2}$	0.0833	60896.23
1 [1] 1/2	- $^2P_{1/2}$	0.4747	55583.60
	- $^2P_{3/2}$	0.4187	63186.75
1 [1] 3/2	- $^2P_{1/2}$	0.1323	54216.61
	- $^2P_{3/2}$	0.7346	61819.76
2 [2] 3/2	- $^2P_{1/2}$	0.0526	48489.73
	- $^2P_{3/2}$	0.2604	56092.88
2 [2] 5/2	- $^2P_{3/2}$	0.0902	54633.46

^{1}D Core

2 [2] 5/2	- $^2P_{3/2}$	0.3570	68587.87
2 [2] 3/2	- $^2P_{1/2}$	0.2098	61046.60
	- $^2P_{3/2}$	0.0597	68649.75

TABLE 1d
TRANSITION PROBABILITIES OF SOME OF THE $5p^4$-$5d \rightarrow 5p^5$ STATES OF IODINE I

Upper $J_c K$	J	Ground state	$A \times 10^{-8}$ 1/sec	wavelength cm^{-1}
0 [2]	1/2	- $^2P_{1/2}$	0.7530	66036.11
		- $^2P_{3/2}$	0.0522	73637.26
0 [2]	5/2	- $^2P_{3/2}$	0.3153	73795.33
1 [1]	1/2	- $^2P_{1/2}$	1.6818	65874.09
1 [1]	3/2	- $^2P_{1/2}$	0.4421	66984.27
		- $^2P_{3/2}$	0.1221	74587.42
1 [2]	3/2	- $^2P_{1/2}$	0.4670	68220.78
		- $^2P_{3/2}$	0.1282	75823.93
1 [2]	5/2	- $^2P_{3/2}$	0.3430	75898.91
1 [3]	5/2	- $^2P_{3/2}$	1.1666	75177.24
2 [0]	1/2	- $^2P_{1/2}$	0.2970	61012.60
		- $^2P_{3/2}$	0.2112	68615.75
2 [1]	1/2	- $^2P_{1/2}$	0.4172	59695.18
		- $^2P_{3/2}$	1.1955	67298.33
		- $^2P_{1/2}$	0.0944	58751.95
		- $^2P_{3/2}$	0.0286	66355.10
2 [2]	3/2	- $^2P_{1/2}$	0.2827	62751.72
		- $^2P_{3/2}$	1.9920	70354.87
2 [3]	5/2	- $^2P_{3/2}$	1.5802	66020.48

TABLE 2

THE RADIAL INTEGRAL USED IN THE CALCULATIONS OF THE TRANSITION PROBABILITIES IS GIVEN BELOW IN ATOMIC UNITS

$$\int_0^\infty r f_{5d}(r)\ f_{6p}(r)\, dr = 46.44$$

$$\int_0^\infty r f_{6p}(r)\ f_{6s}(rr)\, dr = 46.5$$

$$\int_0^\infty r f_{6s}(r)\ f_{5p}(r)\, dr = 0.8976$$

$$\int_0^\infty r f_{5d}(r)\ f_{5p}(r)\, dr = 1.69$$

TABLE 3

SOME OF THE RADIAL INTEGRALS OF p^4-$n\ell$ OF I. FROM DEFINITIONS OF Yamanachi et al[4] WE HAVE

$$G_{\ell-1} = 3G^{\ell-1}/2(2\ell+1)(2\ell-1)^2$$

$$G_{\ell+1} = 3G^{\ell+1}/2(2\ell+1)(2\ell+3)^2$$

and

$$F_2 = F^2/5(2\ell-1)(2\ell+1)\ .$$

$F^2(5p^4 - 5d) = 14957.2\ \text{cm}^{-1}$

$G^1(5p^4 - 5d) = 14155.8\ \text{cm}^{-1}$

$G^3(5p^4 - 5d) = 8485.6\ \text{cm}^{-1}$

$\zeta_{5p} = 2678.4\ \text{cm}^{-1}$

$\zeta_{5d} = 46.4\ \text{cm}^{-1}$

$F^2(5p^4 - 6p) = 9474.\ \text{cm}^{-1}$

$G^0(5p^4 - 6p) = 847\ \text{cm}^{-1}$

$G^2(5p^4 - 6p) = 1046\ \text{cm}^{-1}$

$\zeta_{5p} = 2739\ \text{cm}^{-1}$

$\zeta_{6p} = 124\ \text{cm}^{-1}$

$G^1(5p^4 - 6s) = 2292.9\ \text{cm}^{-1}$

TABLE 4
LIFE TIMES OF SOME OF THE
EXCITED IODINE I LEVELS

$5p^4[^3P_{J_c}]\,5d\,[K]\ J$

J_c K J	Energy level cm^{-1}	Lifetime (nsec)
0 [2] 3/2	73639.26	12.38
0 [2] 5/2	73795.33	31.49
1 [1] 1/2	73477.24	5.94
1 [1] 3/2	74587.42	17.52
1 [2] 3/2	75823.93	16.60
1 [2] 5/2	75898.91	28.31
1 [3] 5/2	75177.24	8.53
1 [3] 7/2	73977.70	8620.7
2 [0] 1/2	68615.75	19.54
2 [1] 1/2	67298.38	6.19
2 [1] 3/2	66355.10	77.94
2 [2] 3/2	70354.87	4.30
2 [2] 5/2	70151.21	261.1
2 [3] 5/2	66020.48	6.33
2 [3] 7/2	66015.01	28735.6
2 [4] 7/2	68559.51	1063.8
2 [4] 9/2	67726.37	3030.3

$5p^4\text{-}[^3P_{J_c}]\,6p\,[K]\ J$

0 [1] 1/2	71813.90	24.1
0 [1] 3/2	71976.72	23.0
1 [0] 1/2	71501.47	39.4
1 [1] 1/2	73387.15	25.6
1 [1] 3/2	73054.54	23.3
1 [2] 3/2	72807.13	32.6
1 [2] 5/2	72529.16	25.5
2 [1] 1/2	65856.96	33.7
2 [1] 3/2	67062.09	16.7
2 [2] 3/2	64990.00	42.1
2 [2] 5/2	64906.31	29.6
2 [3] 5/2	65644.49	34.7
2 [3] 7/2	65669.99	23.3

TABLE 4 (Cont.)

$5p^4 [^3P_{J_c}] 6s[K]$ J

J_c K J	Energy level cm^{-1}	Lifetimes (nsec)
0 [0] 1/2	60896.23	51.3
1 [1] 1/2	63186.75	23.9
1 [1] 3/2	61819.76	75.6
2 [2] 3/2	56092.88	32.0
2 [2] 5/2	54633.46	111.0

$5p^4 - [^1D_2] - 6p [K]$ J

[1] 1/2	79701.59	23.2
[1] 3/2	78415.25	33.1
[2] 3/2	80039.82	21.2
[2] 5/2	80125.45	20.2
[3] 5/2	78592.55	31.8
[3] 7/2	77003.61	27.7

$5p^4 [^1D_2] 6s [K]$ J

[2] 3/2	68549.75	37.2
[2] 5/2	68587.87	28.0

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