Analysis of the third spectrum of iodine: I III

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The spectrum of iodine was photographed in the 300–2000-Å wavelength region on a 3-m normal-incidence spectrograph. The source used was a triggered spark. The previously reported analysis of I III was found to be completely erroneous. All levels of the ground state $5s^25p^3$ and all but three levels of the three excited configurations $5s5p^4$, $5s^25p^25d$, and $5s^25p^26s$ have been established. 117 lines have been classified in this spectrum. Configuration-interaction calculations involving the $5s5p^4$, $5s^25p^26s$, $5s^25p^25d$, and $5s^25p^26d$ configurations describe the observed spectrum quite satisfactorily.

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I. INTRODUCTION AND EXPERIMENTAL DETAILS

The ground state of the third spectrum of iodine (I III) is $5s^25p^3$ and it belongs to the Sb I isoelectronic sequence. The three lowest excited configurations are $5s5p^4$, $5s^25p^25d$, and $5s^25p^26s$. The earlier analyses reported by Seth [1] and Krishnamurty and Parthasardhy [2] were judged to be so unreliable by Moore that they were not included in *Atomic Energy Levels* (Vol. III) [3]. This spectrum has not been investigated since 1949. The principal reason for this was the fact that the three excited configurations interact strongly with each other and thus modify the observed spectrum. The configuration-interaction calculations [4] have become available for moderately powered computers quite recently. In a continuing program at our laboratory focusing on understanding the structure of the 4d open subshell ions of Sn I [5–8] and Sb I [9,10] isoelectronic sequences, we have investigated such interactions quite extensively. All I III lines also appeared on the plates obtained for the analyses of I IV [6], I V, and I VI [11] spectra. All these factors prompted us to study the I III spectrum.

The spectra of iodine were photographed in the 300–2000-Å region on a 3-m normal-incidence spectrograph (first-order plate factor 1.385 Å/mm). The source used was a triggered spark. Spectroscopically pure Li I powder was packed into the cavity of an aluminum electrode which was made a cathode. The anode was normally an aluminum electrode. The charging condenser bank consisted of a 14-μF low-inductance capacitor, charged to 4–8 kV. The discharge was initiated by a 30-kV pulse transformer connected to the third (triggering) electrode. The conditions of discharge plasma were varied either by changing the charging potential or by introducing different turns of an inductance coil in the discharge circuit. These variations helped to discriminate lines of different ionization stages. Experimental conditions were adjusted in such a way that I V and higher ionization lines could be eliminated. Since the spectrograph was almost stigmatic below 1220 Å ($i=9.5°$), the spectral lines exhibited polarities. The higher the ionization stage to which the line belonged, the more polar the line was. This latter criterion together with discharge conditions criteria helped to give us very reliable data on the ionization assignments to the lines. All exposures were taken on Kodak short-wave radiation (SWR) plates and the spectrograms were measured on a Gránt semiautomatic comparator. The internal standards of C, O, and Al [12] and of I II [13] were used to reduce the spectrograms. The accuracy of wavelength measurements for sharp lines is estimated to be ±0.005 Å.

II. RESULTS AND DISCUSSION

From our recent work on Xe IV [9] and Cs V [10] involving configuration-interaction calculations [4], we could extrapolate the scaling factors [the ratio of the least-squares-fitted (LSF) [4,14] and Hartree-Fock (HF) [15] parameter values] for I III. This allowed us to predict the $5s^25p^3$-$(5s5p^4+5s^25p^25d+5s^25p^26s)$ transition array of I III. Seth [1] studied $5s^25p^2(5d+6s)$-$5s^25p^26p$ transitions and reported ten even-parity levels. However, none of these levels agreed with our observed levels. Krishnamurty and Parthasardhy [2] did not publish any levels but reported three intervals, $5s^25p^26s(^4P_{3/2}$-$^4P_{1/2})$, $(^2D_{5/2}$-$^2D_{3/2})$, and $(^2P_{3/2}$-$^2P_{1/2})$, as 6313, 11 254, and 1609 cm^{-1}, respectively. However, these intervals neither correspond to the predicted intervals nor to the observed levels. This is another case [16] in the atomic spectral analysis where the previous work was completely incorrect. All lines used in our present analysis have been thoroughly checked against ionization assignments. 117 lines have been classified in this spectrum and they are given in Table I.

All five levels of the ground-state configuration have been established. They are given in Table II along with their calculated values and LS-percentage compositions. The agreement between the calculated and the experimental levels is very good. The LSF parameters used for the calculations and the corresponding Hartree-Fock parameters are given in Table III. There are 44 levels arising out of the three even-parity configurations, viz., $5s5p^4$, $5s^25p^25d$, and $5s^25p^26s$, of which two levels have J values of $\frac{9}{2}$ and give no electric dipole transitions to the ground-state levels. We have established 41 out of the

TABLE I. Classified lines of the I III spectrum.

λ (Å)	ν (cm⁻¹)	I	Odd level	Even level	Δ[a]
673.915	148 386.7	2	$5p^{3\,4}S_{3/2}$	$p^2d\ (^1D)^2D_{5/2}$	0.4
693.592	144 177.0	2	$5p^{3\,4}S_{3/2}$	$p^2\ (^3P)^2F_{5/2}$	−0.4
695.833	143 712.7	40	$5p^{3\,2}D_{3/2}$	$p^2d\ (^1S)^2D_{3/2}$	−0.9
709.262	140 991.6	54	$5p^{3\,2}D_{3/2}$	$p^2s\ (^1S)^2S_{1/2}$	−0.6
711.630	140 522.5	4	$5p^{3\,2}D_{5/2}$	$p^2d\ (^1S)^2D_{3/2}$	−0.4
713.751	140 104.9	45	$5p^{3\,4}S_{3/2}$	$sp^4\ (^3P)^2P_{3/2}$	−0.6
716.883	139 492.7	5	$5p^{3\,2}D_{3/2}$	$p^2d\ (^1D)^2P_{3/2}$	0.3
730.681	136 858.7	10	$5p^{3\,4}S_{3/2}$	$p^2s\ (^1D)^2D_{5/2}$	1.1
733.667	136 301.6	30	$5p^{3\,2}D_{5/2}$	$p^2d\ (^1D)^2P_{3/2}$	−0.1
735.865	135 894.5	45	$5p^{3\,2}D_{3/2}$	$sp^4\ (^3P)^2P_{1/2}$	−0.2
743.831	134 439.1	55	$5p^{3\,2}D_{3/2}$	$p^2d\ (^1D)^2D_{3/2}$	−0.5
748.174	133 658.8	65	$5p^{3\,4}S_{3/2}$	$p^2d\ (^3P)^4P_{1/2}$	0.0
749.148	133 484.9	50	$5p^{3\,2}D_{5/2}$	$p^2d\ (^1D)^2D_{5/2}$	0.4
753.934	132 637.6	68	$5p^{3\,4}S_{3/2}$	$p^2d\ (^3P)^4P_{3/2}$	−0.6
754.907	132 466.6	60	$5p^{3\,2}D_{3/2}$	$p^2d\ (^3P)^2F_{5/2}$	0.4
761.913	131 248.6	50	$5p^{3\,2}D_{5/2}$	$p^2d\ (^1D)^2D_{3/2}$	−0.3
762.625	131 126.0	50	$5p^{3\,2}P_{1/2}$	$p^2d\ (^1S)^2D_{3/2}$	0.5
765.613	130 614.3	68	$5p^{3\,4}S_{3/2}$	$p^2d\ (^3P)^4P_{5/2}$	−0.3
766.211	130 512.3	50	$5p^{3\,2}D_{3/2}$	$p^2d\ (^1D)^2P_{1/2}$	−0.2
773.545	129 274.9	60	$5p^{3\,2}D_{5/2}$	$p^2D\ (^3P)^2F_{5/2}$	−0.6
774.985	129 034.7	68	$5p^{3\,2}D_{5/2}$	$p^2d\ (^3P)^2F_{7/2}$	0.0
778.789	128 404.5	40	$5p^{3\,2}P_{1/2}$	$p^2S\ (^1S)^2S_{1/2}$	0.4
778.849	128 394.6	25	$5p^{3\,2}D_{3/2}$	$sp^4\ (^2P)^2P_{3/2}$	0.3
782.206	127 843.6	50	$5p^{3\,4}S_{3/2}$	$p^2s\ (^3P)^2P_{3/2}$	0.7
785.737	127 269.0	60	$5p^{3\,2}D_{3/2}$	$p^2s\ (^1D)^2D_{3/2}$	−0.1
787.104	127 048.0	16	$5p^{3\,4}S_{3/2}$	$sp^4\ (^1S)^2S_{1/2}$	0.3
787.997	126 904.0	48	$5p^{3\,2}P_{1/2}$	$p^2d\ (^1D)^2P_{3/2}$	−0.2
792.163	126 236.7	65	$5p^{3\,4}S_{3/2}$	$p^2s\ (^3P)^4P_{5/2}$	−0.6
794.984	125.788.7	35	$5p^{3\,2}P_{3/2}$	$p^2d\ (^1S)^2D_{3/2}$	0.7
798.494	125 235.7	60	$5p^{3\,2}P_{3/2}$	$p^2d\ (^1S)^2D_{5/2}$	0.0
798.696	125 204.1	60	$5p^{3\,2}D_{5/2}$	$sp^4\ (^3P)^2P_{3/2}$	0.5
799.064	125 146.4	62	$5p^{3\,2}D_{3/2}$	$p^2s\ (^1D)^2D_{5/2}$	−0.1
801.775	124 723.2	3	$5p^{3\,4}S_{3/2}$	$p^2s\ (^3P)^2P_{1/2}$	0.4
805.932	124 080.0	62	$5p^{3\,2}D_{5/2}$	$p^2s\ (^1D)^2D_{3/2}$	1.6
809.193	123 579.9	60	$5p^{3\,2}D_{5/2}$	$p^2d\ (^3P)^2D_{5/2}$	0.1
810.991	123 306.0	58	$5p^{3\,2}P_{1/2}$	$sp^4\ (^3P)^2P_{1/2}$	−0.6
812.567	123 066.7	55	$5p^{3\,2}P_{3/2}$	$p^2s\ (^1S)^2S_{1/2}$	0.2
813.037	122 995.7	45	$5p^{3\,2}D_{3/2}$	$p^2d\ {}^3P)^2D_{3/2}$	−0.1
816.721	122 440.9	68	$5p^{3\,4}S_{3/2}$	$p^2s\ (^3P)^4P_{3/2}$	0.1
820.669	121 851.8	40	$5p^{3\,2}P_{1/2}$	$p^2d\ (^1D)^2D_{3/2}$	0.3
822.594	121 566.7	55	$5p^{3\,2}P_{3/2}$	$p^2d\ (^1D)^2P_{3/2}$	−0.0
823.859	121 380.0	60	$5p^{3\,4}S_{3/2}$	$p^2d\ {}^3P)^4D_{5/2}$	−0.6
826.937	120 928.2	9	$5p^{3\,2}D_{3/2}$	$p^2d\ (^3P)^4P_{3/2}$	1.1
834.688	119 805.3	52	$5p^{3\,2}D_{5/2}$	$p^2d\ (^3P)^2D_{3/2}$	0.2
835.771	119 650.0	15	$5p^{3\,4}S_{3/2}$	$p^2d\ (^3P)^4D_{1/2}$	0.3
841.019	118 903.4	25	$5p^{3\,2}D_{3/2}$	$p^2d\ (^3P)^4P_{5/2}$	−0.1
842.114	118 748.7	60	$5p^{3\,2}P_{3/2}$	$p^2d\ (^1D)^2D_{5/2}$	−0.8
847.674	117 969.9	5	$5p^{3\,2}P_{3/2}$	$sp^4\ (^3P)^2P_{1/2}$	0.8
847.999	117 924.6	35	$5p^{3\,2}P_{1/2}$	$p^2d\ (^3P)^2P_{1/2}$	0.2
849.356	117 736.3	50	$5p^{3\,2}D_{5/2}$	$p^2d\ (^3P)^4P_{3/2}$	−0.1
857.629	116 600.5	62	$5p^{3\,2}D_{5/2}$	$p^2d\ (^1D)^2G_{7/2}$	−0.0
857.954	116 556.3	65	$5p^{3\,4}S_{3/2}$	$p^2s\ (^3P)^4P_{1/2}$	−0.5
858.263	116 514.4	38	$5p^{3\,2}P_{3/2}$	$p^2d\ (^1D)^2D_{3/2}$	0.4
861.094	116 131.3	65	$5p^{3\,2}D_{3/2}$	$p^2s\ (^3P)^2P_{3/2}$	−0.5
861.102	116 130.3	65	$5p^{3\,4}S_{3/2}$	$p^2d\ (^1D)^2F_{5/2}$	0.6
863.511	115 806.3	40	$5p^{3\,2}P_{1/2}$	$sp^4\ (^3P)^2P_{3/2}$	0.1
864.206	115 713.2	60	$5p^{3\,2}D_{5/2}$	$p^2d\ (^3P)^4P_{5/2}$	0.4
867.025	115 336.9	35	$5p^{3\,2}D_{3/2}$	$sp^4\ (^1S)^2S_{1/2}$	0.4
871.986	114 680.7	35	$5p^{3\,2}P_{1/2}$	$p^2s\ (^1D)^2D_{3/2}$	−0.3
873.048	114 541.2	10	$5p^{3\,2}P_{3/2}$	$p^2d\ (^3P)^2F_{5/2}$	0.6
873.157	114 526.9	9	$5p^{3\,2}D_{3/2}$	$p^2s\ (^3P)^4P_{5/2}$	0.7
882.433	113 323.0	38	$5p^{3\,4}S_{3/2}$	$p^2d\ (^3P)^2P_{1/2}$	0.3
884.869	113 011.1	65	$5p^{3\,2}D_{3/2}$	$p^2s\ (^3P)^2P_{1/2}$	−0.5
893.059	111 974.7	60	$5p^{3\,2}D_{5/2}$	$p^2d\ (^3P)^4D_{7/2}$	−0.0
894.403	111 806.4	62	$5p^{3\,4}S_{3/2}$	$p^2d\ (^3P)^4F_{5/2}$	0.3
898.188	111 335.3	60	$5p^{3\,2}D_{5/2}$	$p^2s\ (^3P)^4P_{5/2}$	−0.1
903.099	110 729.8	50	$5p^{3\,2}D_{3/2}$	$p^2s\ (^3P)^4P_{3/2}$	0.1
905.235	110 468.5	20	$5p^{3\,2}P_{3/2}$	$sp^4\ (^3P)^2P_{3/2}$	−0.2
905.733	110 407.8	55	$5p^{3\,2}P_{1/2}$	$p^2d\ (^3P)^2D_{3/2}$	0.1
908.010	110 130.9	52	$5p^{3\,4}S_{3/2}$	$p^2d\ (^3P)^4F_{3/2}$	0.5
911.824	109 670.3	52	$5p^{3\,3}D_{3/2}$	$p^2d\ (^3P)^4D_{5/2}$	0.8
914.560	109 342.2	45	$5p^{3\,2}P_{3/2}$	$p^2s\ (^1D)^2D_{3/2}$	−1.3
918.739	108 844.8	12	$5p^{3\,2}P_{3/2}$	$p^2d\ (^3P)^2D_{5/2}$	−0.1
926.453	107 938.5	25	$5p^{3\,2}D_{3/2}$	$p^2d\ (^3P)^4D_{1/2}$	−0.0
929.900	107 538.5	42	$5p^{3\,2}D_{5/2}$	$p^2s\ (^3P)^4P_{3/2}$	−0.5
932.663	107 219.9	3	$5p^{3\,2}P_{3/2}$	$p^2s\ (^1D)^2D_{5/2}$	−1.0
937.921	106 618.8	38	$5P^{3\,4}S_{3/2}$	$sp^4\ (^1D)^2D_{5/2}$	−0.2
939.156	106 478.6	50	$5p^{3\,2}D_{5/2}$	$p^2d\ (^3P)^4D_{5/2}$	−0.2
951.746	105 070.0	25	$5p^{3\,2}P_{3/2}$	$p^2d\ (^3P)^2D_{3/2}$	−0.2
953.783	104 845.6	60	$5p^{3\,2}D_{3/2}$	$p^2s\ (^3P)^4P_{1/2}$	−0.1
954.046	104 816.7	26	$5p^{3\,2}D_{5/2}$	$p^2d\ (^3P)^4D_{3/2}$	−0.0
957.690	104 417.9	50	$5p^{3\,2}D_{3/2}$	$p^2d\ (^1D)^2F_{5/2}$	−0.6
964.134	103 720.0	30	$5p^{3\,2}D_{5/2}$	$p^2d\ (^1D)^2F_{7/2}$	−0.0
965.774	103 543.9	22	$5p^{3\,2}P_{1/2}$	$p^2s\ (^3P)^2P_{3/2}$	0.2
970.863	103 001.1	6	$5p^{3\,2}P_{3/2}$	$p^2d\ (^3P)^4P_{3/2}$	−0.4
973.256	102 747.9	55	$5p^{3\,2}P_{1/2}$	$sp^4\ (^1S)^2S_{1/2}$	−0.5
984.143	101 611.2	3	$5p^{3\,2}D_{3/2}$	$p^2d\ (^3P)^2P_{1/2}$	−0.3
994.751	100 527.7	55	$5p^{3\,2}D_{5/2}$	$p^2d\ (^3P)^4F_{7/2}$	−0.0
995.782	100 423.6	62	$5p^{3\,2}P_{1/2}$	$p^2s\ (^3P)^2P_{1/2}$	0.1
999.050	100 095.1	58	$5p^{3\,2}D_{3/2}$	$p^2d\ (^3P)^4F_{5/2}$	0.2
1003.464	99 654.8	50	$5p^{3\,2}D_{3/2}$	$p^2d\ (^3P)^2P_{3/2}$	0.5
1016.067	98 418.7	55	$5p^{3\,2}D_{3/2}$	$p^2d\ (^3P)^4F_{3/2}$	−0.6
1018.271	98 205.7	30	$5p^{3\,2}P_{3/2}$	$p^2s\ (^3P)^2P_{3/2}$	−0.4
1026.582	97 410.6	1	$5p^{3\,2}P_{3/2}$	$sp^4\ (^1S)^2S_{1/2}$	−0.3
1031.957	96 903.3	10	$5p^{3\,2}D_{5/2}$	$p^2d\ (^3P)^4F_{5/2}$	−0.9
1036.666	96 463.1	12	$5p^{3\,2}D_{5/2}$	$p^2d\ (^3P)^2P_{3/2}$	−0.5
1048.767	95 350.1	3	$5p^{3\,2}P_{1/2}$	$p^2d\ (^3P)^4D_{1/2}$	−0.3
1053.651	94 908.1	10	$5p^{3\,2}D_{3/2}$	$sp^4\ (^1D)^2D_{5/2}$	0.2
1076.401	92 902.2	60	$5p^{3\,4}S_{3/2}$	$sp^4\ (^3P)^4P_{1/2}$	−0.4
1077.535	92 804.4	5	$5p^{3\,2}P_{3/2}$	$p^2s\ (^3P)^4P_{3/2}$	0.3
1089.807	91 759.4	55	$5p^{3\,2}D_{3/2}$	$sp^4\ (^1D)^2D_{3/2}$	−0.2
1090.313	91 716.8	55	$5p^{3\,2}D_{5/2}$	$sp^4\ (^1D)^2D_{5/2}$	−0.4
1099.344	90 963.3	60	$5p^{3\,4}S_{3/2}$	$sp^4\ (^3P)^4P_{3/2}$	−0.6
1129.057	88 569.5	14	$5p^{3\,2}D_{5/2}$	$sp^4\ (^1D)^2D_{3/2}$	0.6
1150.474	86 920.7	2	$5p^{3\,2}P_{3/2}$	$p^2s\ (^3P)^4P_{1/2}$	0.6
1165.078	85 831.2	16	$5p^{3\,2}P_{1/2}$	$p^2d\ (^3P)^4F_{3/2}$	0.1
1168.840	85 554.9	65	$5p^{3\,4}S_{3/2}$	$sp^4\ (^3P)^4P_{5/2}$	−0.0
1216.992	82 169.8	6	$5p^{3\,2}P_{3/2}$	$p^2d\ (^3P)^4F_{5/2}$	0.5
1261.779	79 253.2	5	$5p^{3\,2}D_{3/2}$	$sp^4\ (^3P)^4P_{3/2}$	0.4
1263.089	79 171.0	2	$5p^{3\,2}P_{1/2}$	$sp^4\ (^1D)^2D_{3/2}$	−0.5
1298.993	76 982.7	32	$5p^{3\,2}P_{3/2}$	$sp^4\ (^1D)^2D_{5/2}$	0.4
1314.708	76 062.5	28	$5p^{3\,2}D_{5/2}$	$sp^4\ (^3P)^4P_{3/2}$	0.4
1354.208	73 843.9	40	$5p^{3\,2}D_{3/2}$	$sp^4\ (^3P)^4P_{5/2}$	0.1
1415.370	70 652.9	60	$5p^{3\,2}D_{5/2}$	$sp^4\ (^3P)^4P_{5/2}$	−0.1
1457.649	68 603.6	10	$5p^{3\,2}P_{1/2}$	$sp^4\ (^3P)^4P_{1/2}$	0.3
1580.630	63 265.9	6	$5p^{3\,2}P_{3/2}$	$sp^4\ (^3P)^4P_{1/2}$	0.1
1630.606	61 326.9	16	$5p^{3\,2}P_{3/2}$	$sp^4\ (^3P)^4P_{3/2}$	−0.2

[a]Δ = difference between the experimental and the calculated (from Tables II and IV) values (cm⁻¹) of the transition.

TABLE II. Energy levels and their *LS*: percentage compositions of the ground-state configuration $5s^25p^3$ of I III.

Designation	Energy (cm^{-1}) Expt.	Calc.	Δ^a	*LS* composition
$^4S_{3/2}$	0.0	0.4	−0.4	$87\%\ ^4S+9\%\ ^2P+2\%\ ^2D$
$^2D_{3/2}$	11 711.2	11 706.7	4.5	$78\%\ ^2D+15\%\ ^2P+7\%\ ^4S$
$^2D_{5/2}$	14 901.9	14 905.8	−3.9	$100\%\ ^2D$
$^2P_{1/2}$	24 299.3	24 301.3	−2.0	$100\%\ ^2P$
$^2P_{3/2}$	29 636.8	29 635.0	1.8	$76\%\ ^2P+19\%\ ^2D+4\%\ ^4S$

$^a\Delta$ = experimental value minus calculated value (cm^{-1}).

TABLE III. Energy levels of the $5sp^4$, $5s^25p^25d$, and $5s^25p^26s$ configurations of I III and their *LS*-percentage composition.

Configuration	Designation	*J*	Level (cm^{-1}) Expt.	Calc.	Δ^a	*LS* composition^b
$5s5p^4$	$sp^4(^3P)^4P$	$\frac{1}{2}$	92 902.6	92 940.8	−38.2	$82\%+13\%\ p^2d(^3P)^4P+3\%\ sp^4(^1S)^2S$
$5p^25d$	$p^2d(^3P)^2P$	$\frac{1}{2}$	113 322.7	113 254.2	68.5	$48\%+16\%\ p^2d(^3P)^4D+15\%\ sp^4(^5P)^2P$
$5p^26s$	$p^2s(^3P)^4P$	$\frac{1}{2}$	116 556.8	116 510.1	46.7	$69\%+10\%\ p^2s(^3P)^2P+10\%\ p^2d(^3P)^4D$
$5p^25d$	$p^2d(^3P)^4D$	$\frac{1}{2}$	119 649.7	119 634.6	15.1	$70\%+9\%\ p^2d(^3P)^2P+7\%\ p^2s(^3P)^4P$
$5p^26s$	$p^2s(^3P)^2P$	$\frac{1}{2}$	124 722.8	124 764.7	−41.9	$66\%+11\%\ p^2s(^3P)^4P+11\%\ sp^4(^1S)^2S$
$5s5p^4$	$sp^4(^1S)^2S$	$\frac{1}{2}$	127 047.7	126 970.0	77.7	$43\%+23\%\ p^2d(^1D)^2S+14\%\ p^2d(^3P)^2P$
$5p^25d$	$p^2d(^3P)^4P$	$\frac{1}{2}$	133 658.8	133 686.6	−27.8	$73\%+11\%\ sp^4(^3P)^4P+8\%\ p^2d(^1D)^2P$
$5p^25d$	$p^2d(^1D)^2P$	$\frac{1}{2}$	142 223.7	142 036.5	187.2	$83\%+8\%\ p^2d(^3P)^4P+4\%\ sp^4(^3P)^2P$
$5s5p^4$	$sp^4(^3P)^2P$	$\frac{1}{2}$	147 605.9	148 130.0	−524.1	$17\%+44\%\ sp^4(^3P)^2P+21\%\ p^2d(^1D)^2S$
$5p^26s$	$p^2s(^1S)^2S$	$\frac{1}{2}$	152 703.9	152 679.5	23.8	$71\%+12\%\ sp^4(^3P)^2P+5\%\ sp^4(^1S)^2S$
$5p^25d$	$p^2d(^1D)^2S$	$\frac{1}{2}$		[15 8105]		$40\%+22\%\ sp^4(^1S)^2S+15\%\ p^2s(^1S)^2S$
$5s5p^4$	$sp^4(^3P)^4P$	$\frac{3}{2}$	90 963.9	90 906.7	57.2	$83\%+13\%\ p^2D(^3P)^4P+2\%\ sp^4(^1D)^2D$
$5s5p^4$	$sp^4(^1D)^2D$	$\frac{3}{2}$	103 470.7	103 660.8	−190.1	$43\%+16\%\ p^2d(^1D)^2D+14\%\ p^2d(^3P)^2P$
$5p^25d$	$p^2d(^3P)^4F$	$\frac{3}{2}$	110 130.4	110 027.1	103.3	$60\%+17\%\ sp^4(^1D)^2D+10\%\ p^2d(^3P)^4D$
$5p^25d$	$p^2d(^3P)^2P$	$\frac{3}{2}$	111 365.5	111 318.8	46.7	$47\%+19\%\ p^2d(^3P)^4F+13\%\ sp^4(^3P)^2P$
$5p^25d$	$p^2d(^3P)^4D$	$\frac{3}{2}$	119 718.6	119 727.7	−9.1	$81\%+6\%\ p^2d(^3P)^4F+4\%\ p^2d(^3P)^2P$
$5p^26s$	$p^2s(^3P)^4P$	$\frac{3}{2}$	122 440.8	122 525.2	−84.4	$93\%+6\%\ p^2s(^3P)^2P+1\ \ p^2d(^3P)^4D$
$5p^26s$	$p^2s(^3P)^2P$	$\frac{3}{2}$	127 842.9	127 868.1	−25.1	$50\%+34\%\ p^2s(^1D)^2P+6\%\ p^2d(^1D)^2P$
$5p^25d$	$p^2d(^3P)^4P$	$\frac{3}{2}$	132 638.2	132 520.5	117.7	$68\%+10\%\ sp^4(^3P)^4P+8\ \ p^2d(^1D)^2P$
$5p^25d$	$p^2d(^3P)^2D$	$\frac{3}{2}$	134 707.0	134 487.4	219.6	$53\%+18\%\ p^2d(^1S)^2D+17\%\ p^2s(^3P)^2P$
$5p^26s$	$p^2s(^1D)^2D$	$\frac{3}{2}$	138 980.2	139 071.2	−91.0	$52\%+19\%\ p^2s(^3P)^2P+9\%\ p^2d(^3P)^2D$
$5s5p^4$	$sp^4(^3P)^2P$	$\frac{3}{2}$	140 105.5	139 767.0	338.5	$47\%+33\%\ p^2d(^1D)^2P+9\%\ p^2d(^1D)^2D$
$5p^25d$	$p^2d(^1D)^2D$	$\frac{3}{2}$	146 150.7	146 088.7	62.0	$49\%+17\%\ p^2d(^1D)^2P+15\%\ sp^4(^1D)^2D$
$5p^25d$	$p^2d(^1D)^2P$	$\frac{3}{2}$	151 203.5	150 984.7	218.8	$24\%+23\%\ p^2d(^3P)^2P+22\%\ sp^4(^3P)^2P$
$5p^25d$	$p^2d(^1S)^2D$	$\frac{3}{2}$	155 424.7	155 528.5	−103.8	$67\%+24\%\ p^2d(^3P)^2D+4\%\ p^2d(^3P)^2D$
$5s5p^4$	$sp^4(^3P)^4P$	$\frac{5}{2}$	85 554.9	85 585.4	−30.5	$84\%+12\%\ p^2d(^3P)^4P+3\%\ sp^4(^1D)^2D$
$5s5p^4$	$sp^4(^1D)^2D$	$\frac{5}{2}$	106 619.0	106 574.6	44.4	$63\%+24\%\ p^2d(^1D)^2D+4\%\ sp^4(^3P)^4P$
$5p^25d$	$p^2d(^3P)^4F$	$\frac{5}{2}$	111 806.1	111 853.3	−47.2	$73\%+18\%\ p^2d(^3P)^4D+3\%\ sp^4(^1D)^2D$
$5p^25d$	$p^2d(^1D)^2F$	$\frac{5}{2}$	116 129.7	116 134.5	−4.8	$39\%+35\%\ p^2d(^3P)^2F+13\%\ p^2d(^3P)^4D$
$5p^25d$	$p^2d(^3P)^4D$	$\frac{5}{2}$	121 380.6	121 475.5	−94.9	$58\%+13\%\ p^2d(^3P)2F+10\%\ p^2d(^1D)^2F$
$5p^26s$	$p^2s(^3P)^4P$	$\frac{5}{2}$	126 237.3	126 206.9	30.4	$72\%+26\%\ p^2s(^1D)^2D+1\%\ p^2d(^3P)^4D$
$5p^25d$	$p^2d(^3P)^4P$	$\frac{5}{2}$	130 614.6	130 573.9	40.7	$73\%+8\%\ sp^4(^3P)^4P+8\%\ p^2d(^3P)^4D$
$5p^26s$	$p^2s(^1D)^2D$	$\frac{5}{2}$	136 857.6	136 697.6	160.0	$37\%+30\%\ p^2d(^3P)^2D+19\%\ p^2s(^3P)^4P$
$5p^25d$	$p^2d(^3P)^2D$	$\frac{5}{2}$	138 481.7	138 555.6	−73.9	$26\%+30\%\ p^2s(^1D)^2D+13\%\ p^2d(^3P)^2F$
$5p^25d$	$p^2d(^3P)^2F$	$\frac{5}{2}$	144 177.4	144 043.9	133.5	$19\%+27\%\ p^2d(^1D)^2F+14\%\ p^2d(^3P)^2D$
$5p^25d$	$p^2d(^1D)^2D$	$\frac{5}{2}$	148 386.3	148 502.2	115.9	$50\%+21\%\ p^2d(^1S)^2D+10\%\ p^2d(^3P)^2D$
$5p^25d$	$p^2d(^1S)^2D$	$\frac{5}{2}$	154 872.5	154 793.7	78.8	$57\%+14\%\ p^2d(^3P)^2D+10\%\ p^2d(^3P)^2F$
$5p^25d$	$p^2d(^3P)^4F$	$\frac{7}{2}$	115 429.6	115 437.6	−8.0	$86\%+12\%\ p^2d(^3P)^4D+2\%\ p^2d(^1D)^2G$
$5p^25d$	$p^2d(^1D)^2F$	$\frac{7}{2}$	118 621.9	118 665.9	−44.0	$33\%+40\%\ p^2d(^3P)^4D+19\%\ p^2d(^3P)^2F$
$5p^25d$	$p^2d(^3P)^4D$	$\frac{7}{2}$	126 876.6	126 963.1	−86.5	$44\%+23\%\ p^2d(^3P)^2F+13\%\ (^1D)^2G$

TABLE III. (*Continued*).

Configuration	Designation	J	Level (cm^{-1}) Expt.	Calc.	Δ[a]	LS composition[b]
$5p^25d$	$p^2d(^1D)^2G$	$\frac{7}{2}$	131 502.4	131 636.6	−134.2	75%+20% $p^2d(^1D)^2F$+4% $p^2d(^3P)^4D$
$5p^25d$	$p^2d(^3P)^2F$	$\frac{7}{2}$	143 936.6	144 247.2	−310.6	55%+34% $p^{2d}(^1D)^2F$+6% $p^2d(^1D)^2G$
$5p^25d$	$p^2d(^3P)^4F$	$\frac{9}{2}$		118 931.3		88%+12% $p^2d(^1D)^2G$
$5p^25d$	$p^2d(^1D)^2G$	$\frac{9}{2}$		133 687.9		88%+12% $p^2d(^3P)$ ^4F

[a]Δ = experimental level value minus calculated level value.
[b]Only three largest components given. The first percentage corresponds to the level designation.

TABLE IV. Least-squares-fitted and HF parameter values (cm^{-1}) for $5s^25p^3$ configuration of I III.

Parameter	LSF	HFR[b]	LSF-to-HFR ratio
E_{av}	15 170±3		
F^2	37 311±22	48 372	0.771
α	−110±1		
ζ_{5p}	6 633±6	6228	1.065
σ[a]	7		

[a] σ = mean error

$$= \left[\frac{\sum(\text{obs. value} - \text{calc. value})^2}{n-m} \right]^{1/2},$$

where n = number of known levels and m = number of free parameters.
[b]HFR = relativistic Hartree-Fock.

TABLE V. Energy parameter values (cm^{-1}) of the $5s5p^4$, $5p^25d$, $5p^26s$, and $5p^26d$ configurations of I III.

Parameter	Value LSF	HFR	LSF-to-HFR ratio
$E_{av}(5s5p^4)$	114 742±185	116 328	0.986
$F^2(5p,5p)$	41 913±1032	48 425	0.866
α	−333±80		
ζ_{5p}	6 348±259	6 214	1.022
$G^1(5s,5p)$	43 382±416	63 900	0.679
$E_{av}(5p^25d)$	129 745±61	129 867	0.999
$F^2(5p,5p)$	37 768±552	49 473	0.763
α	−68		
ζ_{5p}	6 795±138	6 587	1.032
ζ_{5d}	445±83	273	1.630
$F^2(5p,5d)$	27 283±560	32 038	0.852
$G^1(5p,5d)$	25 677±242	34 727	0.739
$G^3(5p,5d)$	15 711±566	21 641	0.726
$E_{av}(5p^26s)$	131 168±110	131 472	0.998
$F^2(5p,5p)$	37 522±953	50 040	0.750
α	−240±95		
ζ_{5p}	7 156±202	6 777	1.056
$G^1(5p,6s)$	3 628±323	4 934	0.735
$E_{av}(5p^26d)$	188 458[a]	188 628	1.000
$F^2(5p,5p)$	42 941[a]	50 519	0.850
α	−100[a]		
ζ_{5p}	6 868[a]	6 868	1.000
ζ_{6d}	89[a]		1.000
$F^2(5p,6d)$	7 475[a]	8 794	0.850

TABLE V. (*Continued*).

Parameter	Value LSF	HFR	LSF-to-HFR ratio
$G^1(5p,6d)$	5 005[a]	6 674	0.750
$G^3(5p,6d)$	3 377	4 504	0.750
$R^1(5p5p,5s6s)^b$	−10 76±10	−1 560	0.690
$R^1(5p5p,5s5d)^b$	30 805±297	44 659	0.690
$R^2(5p5d,5p6s)^c$	−9 035±858	12 165	0.743
$R^1(5p5d,5p6s)^c$	−3 587±341	4 830	0.743
$R^1(5p5p,5s6d)$	16 891[a]	19 871	0.850
$R^2(5p6s,5p6d)$	1 162[a]	1 366	0.850
$R^1(5p6s,5p6d)$	−601[a]	−706	0.850
$R^0(5p5d,5p6d)$	0[a]	0	
$R^2(5p5d,5p6d)$	9 147[a]	10 760	0.850
$R^1(5p5d,5p6d)$	12 38[a]	14 570	0.850
$R^3(5p5d,5p6d)$	7 991[a]	9 401	0.850
σ^d	196		

[a]Parameter value fixed at a predetermined value in the iteration process.
[b,c]The ratio of two parameters were fixed to that of the HFR (relativistic HF) values in the iteration process.
[d]σ = standard deviation (see Table IV).

remaining 42 levels. All even-parity levels (experimental and calculated) and their *LS*-percentages are given in Table IV. The *LS* designations for 85% of the levels are quite unambiguous. Two $J=\frac{5}{2}$ levels at 138 478 and 144 174 cm^{-1} correspond to the second largest composition. The agreement between the calculated and the experimental level values is good ($\sigma=196$ cm^{-1}). The level at 147 606 cm^{-1} gives two strong transitions at 735.85 Å (45) and 811.00 Å (58) and a weak transition 847.69 Å (5) to the ground-state levels $^2D_{3/2}$, $^2P_{1/2}$, and $^2P_{3/2}$, respectively. Since the transition to $^2D_{5/2}$ is missing it can be assigned as either $J=\frac{3}{2}$ or $\frac{1}{2}$. Since all $J=\frac{3}{2}$ levels were known, this level was finally assigned the value $J=\frac{1}{2}$. However, it deviates from its predicted value by 524 cm^{-1} (the largest deviation for any level). When this level was excluded from the LSF calculations the mean error σ changed to 108 cm^{-1} and only one level showed a deviation of over 200 cm^{-1}. However, we could not find any alternative for the level at 147 606 cm^{-1}. It should be pointed out that this level does not show large deviations in Xe IV [9] or in Cs V [10] analyses. It needs confirmation through transitions to the $5s^25p6p$ configuration levels.

In the parametric configuration-interaction calculations we also included the $5s^25p^26d$ configuration whose Slater-Condon and interaction parameters were fixed at predetermined values as determined from the sequence [9,10]. The least-squares-fitted parameters and their corresponding HF parameters values and the scaling factors are given in Table V.

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