

EXTENDED ANALYSIS OF THE $5s^25p7d$ AND $5s^25p8s$ CONFIGURATIONS OF SINGLY IONIZED ANTIMONY: SbII

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Abstract- Almost all the data used in the present work is based on the plates taken on a 3-m normal incidence vacuum spectrograph, at the Physics Department, St. Francis Xavier University, Antigonish, Nova Scotia, Canada. The analysis is considerably extended to complete the $5p7d$, and $5p8s$ configurations for the first time. Arcimowicz et al had classified 88 lines of Sb II for $5p^2 - (5s5p^3 + 5p5d + 5p6s + 5p7s)$ array while presently I have identified more lines and have added two more configurations namely $5p7d$, and $5p8s$. The Hartree- Fock calculations with relativistic corrections using Cowan Codes for SbII to get ab- initio energy parameters used in the level fitting calculations are used.

Keywords - Singly ionized antimony atoms, Isoelectronic Sequence, triggered Spark source, Fitted and HFR energy parameter, Least Squares Fitted levels.

I. INTRODUCTION

The ground state configuration of singly ionized antimony (Sb II) is $5s^2 5p^2$. The configurations of odd parity lying very close to each other and overlapping, therefore, strong interaction is seen in the entire sequence Te III - La VIII [1 - 6]. The leading multiplet of this spectrum was first reported by Lang and Vestine [7], followed by two more papers one by Krishnamurty [8] and the other by Murakawa and Suwa [9]. The three term lists were discordant, to provide a satisfactory array of energy levels. Charlotte E. Moore [10] used the line list published by Lang and Vestine in the region 691\AA to 7343\AA and unpublished measurements by W.F. Meggers (1272\AA - 8742\AA) to improve the level values of the published multiplets. The agreement was not good with the tolerance between the observed and calculated wave numbers. With a few more tentative revisions, she compiled the data in A.E.L (10). The limit was adapted from Murakawa and Suwa's paper at 133327.5 cm^{-1} . Arcimowicz, Joshi and Kaufman [11] published the $5p^2 - (5s5p^3 + 5p5d + 5p6s + 5p7s)$ transition array with theoretical support. Since Sb II sequence has been studied very well recently [1-6], therefore, once again Sb II was undertaken to present even better picture.

The light source used for exciting the antimony ions plasma was mainly a triggered spark. The charging potential is applied to the spark electrodes by a $14.5\text{ }\mu\text{F}$, Tobb Deutschman, low inductance (nano henry) capacitor bank. As the power supply was Sorensen (20kv, 30 milli amp) it had to be protected against back current in case of a misfire of the spark. Therefore, the condenser is charged to a requisite voltage, Due to the nature of the electrical circuit (capacitor discharge) the electrical energy is not imparted in a single voltage pulse and therefore this leads to high as well as low ionization stages being excited in each discharge. However, the major problem in experimental atomic

spectroscopy is to identify/discriminate lines of various ionization stages

The data obtained from the 3-m normal incidence vacuum Spectrograph were supplemented by line list from a hollow cathode source exposures taken at the 6.65m normal incidence spectrograph at the Zeeman Laboratory, University of Amsterdam, which existed at the Antigonish laboratory as well as NIST Plates.

The recorded plates at Zeeman lab Amsterdam using hollow cathode source, are the most suitable for singly ionized spectra as well as the plates recorded in Antigonish lab with triggered spark source using high inductance coil in the discharge circuit, also being quite good for Sb II lines.

The NIST hollow cathode plates were also available to us at the time of the analysis. This provided me very good data to analyze the spectrum of singly ionized antimony atoms.

All exposures were taken on Kodak SWR plates and the Spectrograms were measured on a grant comparator at the Antigonish laboratory in Canada and on an abbe comparator in Aligarh. The wavelengths were calculated by using internal standards of C, N, O, and Al [13]. The wavelength accuracy for the symmetric lines are $\pm 0.005\text{ }\mu$ in the wavelength region reported here.

Further experimental details can be found in our earlier publication [12].

RESULT AND DISCUSSION

Scaling the isoelectronic sequence members from Te III - La VIII [1-6] multi-configuration interaction calculations were performed to predict the $5p^2 - (5s5p^3 + 5p5d + 5p6d + 5p7d + 5p6s + 5p7s + 5p8s)$ transition array.

Independent analysis was performed for the resonance transitions without considering the published data [11]. All the ground levels reported by Arcimowicz [11] were confirmed.

Publication History

Manuscript Received : 25 April 2014
Manuscript Accepted : 28 April 2014
Revision Received : 29 April 2014
Manuscript Published : 30 April 2014

Table :1 continued

1576.114	63447.2	99	5s ² 5p ² 3P ₁ -sp ³ 3D ₂	0.004
1581.365	63236.5	99	5s ² 5p ² 3P ₁ -sp ³ 3D ₁	0.011
1584.578	63108.3	75	5s ² 5p ² 1D ₂ -5p6s 1P ₁	0.009
1600.405	62484.2	72	5s ² 5p ² 1D ₂ -5p5d 1D ₂	0.016
1606.973	62228.8	99	5s ² 5p ² 3P ₂ -sp ³ 3D ₃	0.003
1634.297	61188.4	56	5s ² 5p ² 1S ₀ -5p5d 3D ₁	0.001
1643.550	60843.9	99	5s ² 5p ² 3P ₂ -sp ³ 3D ₂	-0.003
1649.270	60632.9	99	5s ² 5p ² 3P ₂ -sp ³ 3D ₁	0.014
1677.847	59600.2	64	5s ² 5p ² 1D ₂ -5p5d 1D ₂	-0.005
1762.236	56746.1	75	5s ² 5p ² 1D ₂ -5p6s 3P ₁	-0.008
1814.964	55097.5	99	5s ² 5p ² 1D ₂ -sp ³ 3D ₃	-0.003
1861.771	53712.3	64	5s ² 5p ² 1D ₂ -sp ³ 3D ₂	0.000
1869.086	53502.1	33	5s ² 5p ² 1D ₂ -sp ³ 3D ₁	-0.008
1878.513	53233.6	54	5s ² 5p ² 1S ₀ -sp ³ 3P ₁	0.003
1923.325	51993.3	66	5s ² 5p ² 1S ₀ -5p6s 3P ₁	-0.009
2054.717	48668.5	99	5s ² 5p ² 3P ₁ -sp ³ 5S ²	-0.017
2170.860	46064.7	99	5s ² 5p ² 3P ₂ -sp ³ 5S ²	-0.007
2191.526	45630.3	99	5s ² 5p ² 1S ₀ -5p6s 3P ₁	-0.003
2359.258	42386.2	10	5s ² 5p ² 1S ₀ -sp ³ 3D ₁	0.004
2568.528	38932.8	15	5s ² 5p ² 1D ₂ -sp ³ 5S ²	0.016

Table 2: Fitted and HFR energy parameteric values (cm⁻¹) and scaling factors for the odd parity configurations of Sb II

Parameter	LSF	Accu.	HF	LSF/HF	
E _{av} (5s5p ³)	80053	213	78656	1.021	
F ² (5p,5p)	32038	1074	40013	0.801	
α _{sp}	-233	-78			
ζ _{sp}	3660	464	3526	1.038	
G1(5s,5p)	34147	316	53006	0.644	
Eav(5s25p5d)	82787	140	83232	0.995	
ζ _{5p}	4145	268	3899	1.063	
ζ _{5d}	94	(fixed)	93	1.013	
F2(5p,5d)	18802	1611	21218	0.886	
G1(5p,5d)	14980	493	20851	0.718	
G3(5p,5d)	10815	1362	12859	0.841	
Eav(5s25p6d)	109466	110	109909	0.997	
ζ _{5p}	4403	157	4071	1.082	
ζ _{6d}	34	(fixed)	34	1.000	
F2(5p,6d)	5422	1051	5953	0.911	
G1(5p,6d)	3165	679	4975	0.636	
G3(5p,6d)	2261	1103	3237	0.699	
Eav(5s25p7d)	120264	91	12078	0.996	
ζ _{5p}	4743	139	4102	1.156	
ζ _{7d}	17	(fixed)	17	1.000	
F2(5p,7d)	2202	901	2634	0.836	
G1(5p,7d)	1653	615	2141	0.772	
G3(5p,7d)	922	(fixed)	1418	0.650	
Eav(5s25p6s)	73944	187	74464	0.994	
ζ _{5p}	4220	233	3978	1.061	
G1(5p,6s)	2745	881	4141	0.663	
Eav(5s25p7s)	105787	145	106310	0.996	
ζ _{5p}	4331	195	4082	1.061	
G1(5p,7s)	877	758	1101	0.797	
Eav(5s25p8s)	117893	14	119000	0.991	
ζ _{5p}	3949	185	4106	0.962	
G1(5p,8s)	362	(fixed)	482	0.750	
Configuration	Parameter	LSF	Accu.	HF	LSF/HF
5s5p ³ -5s ² 5p5d	R ¹ (5p,5p; 5s,5d)	20549	339	30746	0.668
5s5p ³ -5s ² 5p6d	R ¹ (5p,5p; 5s,6d)	10273	170	15371	0.668
5s5p ³ -5s ² 5p7d	R ¹ (5p,5p; 5s,7d)	6739	111	10084	0.668
5s5p ³ -5s ² 5p6s	R ¹ (5p,5p; 5s,6s)	-1544	-25	-2309	0.668
5s5p ³ -5s ² 5p7s	R ¹ (5p,5p; 5s,7s)	-926	-15	-1385	0.668
5s5p ³ -5s ² 5p8s	R ¹ (5p,5p; 5s,8s)	-647	-11	-968	0.668

Table :2 continued

5s ² 5p5d-5s ² 5p6d	R ⁰ (5p,5d; 5p,6d)	0	0	0	
	R ² (5p,5d; 5p,6d)	5381	89	8052	0.668
	R ¹ (5p,5d; 6d,5p)	6609	109	9888	0.668
	R ³ (5p,5d; 6d,5p)	4185	69	6262	0.668
5s ² 5p5d-5s ² 5p7d	R ⁰ (5p,5d; 5p,7d)	0	0	0	
	R ² (5p,5d; 5p,7d)	3245	54	4855	0.668
	R ¹ (5p,5d; 7d,5p)	4259	70	6372	0.668
	R ³ (5p,5d; 7d,5p)	2713	45	4059	0.668
5s ² 5p5d-5s ² 5p6s	R ² (5p,5d; 5p,6s)	-7308	-121	-1093	0.668
	R ¹ (5p,5d; 6s,5p)	-2985	-49	-4466	0.668
5s ² 5p5d-5s ² 5p7s	R ² (5p,5d; 5p,7s)	-3026	-50	-4528	0.668
	R ¹ (5p,5d; 7s,5p)	-1601	-26	-2395	0.668
5s ² 5p5d-5s ² 5p8s	R ² (5p,5d; 5p,8s)	-1899	-31	-2841	0.668
	R ¹ (5p,5d; 8s,5p)	-1071	-18	-1602	0.668
5s25p6d-5s25p7d	R0(5p,6d;5 p,7d)	0	0	0	
	R2(5p,6d;5 p,7d)	2319	38	3469	0.668
	R1(5p,6d;7 d,5p)	2176	36	3256	0.668
	R3(5p,6d;7 d,5p)	1428	24	2136	0.668
5s25p6d-5s25p6s	R2(5p,6d;5 p,6s)	-1057	-17	-1581	0.668
	R1(5p,6d;6 s,5p)	-909	-15	-1360	0.668
5s25p6d-5s25p7s	R2(5p,6d;5 p,7s)	-2040	-34	-3052	0.668
	R1(5p,6d;7 s,5p)	-579	-10	-866	0.668
5s25p6d-5s25p8s	R2(5p,6d;5 p,8s)	-1385	(fixed)	-1732	0.800
	R1(5p,6d;8 s,5p)	-454	(fixed)	-605	0.750
5s25p7d-5s25p6s	R2(5p,7d;5 p,6s)	-271	(fixed)	-362	0.750
	R1(5p,7d;6 s,5p)	-537	(fixed)	-716	0.750
5s25p7d-5s25p7s	R2(5p,7d;5 p,7s)	-969	(fixed)	-1292	0.750
	R1(5p,7d;7 s,5p)	-367	(fixed)	-489	0.750
5s25p7d-5s25p8s	R2(5p,7d;5 p,8s)	-972	(fixed)	-1295	0.750
	R1(5p,7d;8 s,5p)	-261	(fixed)	-349	0.750
5s25p6s-5s25p7s	R0(5p,6s;5 p,7s)	0	(fixed)	0	
	R1(5p,6s;7 s,5p)	1541	(fixed)	2054	0.750
5s25p6s-5s25p8s	R0(5p,6s;5 p,8s)	0	(fixed)	0	
	R1(5p,6s;8 s,5p)	997	(fixed)	1329	0.750
5s25p7s-5s25p8s	R0(5p,7s;5 p,8s)	0	(fixed)	0	
	R1(5p,7s;8 s,5p)	545	(fixed)	727	0.750
σ (mean error)		=		268	

Table 3 : The experimental and fitted energy level values (cm⁻¹) and their LS- percentage compositions of Odd parity configurations of Sb II

E(obs)	E(LSF)	Diff.	LS-composition
J=0			
69137.0	69142.0	-5.0	98% 5s ² 5p6s ³ P
76862.0	77039.0	-177.0	63% 5s5p ³ (² P) ³ P+34% 5s ² 5p5d ³ P
91125.0	91100.0	25.0	65% 5s ² 5p5d ³ P + 34% 5s5p ³ (² P) ³ P
101321.0	101317.0	4.0	100% 5s ² 5p7s ³ P
	112617.0		97% 5s ² 5p6d ³ P
113796.0	113901.0	-105.0	99% 5s ² 5p8s ³ P
122933.0n	122999.0	-66.0	99% 5s²5p7d³P
J=1			
66291.0	66369.0	-78.0	65% 5s5p ³ (² D) ³ D+ 27% 5s ² 5p5d ³ D 74% 5s ² 5p6s ³ P + 25% 5s ² 5p6s ³ P
69536.0	69530.0	6.0	
75898.0	75887.0	11.0	56% 5s ² 5p6s ³ P + 16% 5s ² 5p6s ³ P + 11% 5s5p ³ (² P) ³ P + 9% 5s ² 5p5d ³ P
85094.0	85207.0	-113.0	48% 5s ² 5p5d ³ D+ 20% 5s5p ³ (² D) ³ D +12% 5s ² 5p5d ³ P + 9% 5s ² 5p5d ³ P
90323.0	90004.0	319.0	59% 5s ² 5p5d ³ P + 16% 5s ² 5p5d ³ D +15%5s5p ³ (² P) ¹ P
91360.0	91223.0	137.0	51% 5s ² 5p5d ³ P + 27% 5s5p ³ (² P) ³ P+7% 5s ² 5p5d ³ D + 4%5s 5p ³ (² D) ³ D
97636.0	97558.0	78.0	85% 5s5p ³ (² S) ³ S + 5% 5s ² 5p5d ³ P
101531.0	101537.0	-6.0	70% 5s ² 5p7s ³ P+29% 5s ² 5p7s ³ P
	104942.0		34% 5s ² 5p6d ³ P + 24% 5s5p ³ (² P) ¹ P + 22% 5s ² 5p6d ³ D + 8% 5s ² 5p6d ³ P
107461.0	107642.0	-181.0	45% 5s ² 5p6d ³ D + 35% 5s5p ³ (² P) ¹ P+8% 5s ² 5p 6d ³ P + 5% 5s ² 5p5d ³ P
108309.0	108311.0	-2.0	68% 5s ² 5p7s ³ P +28% 5s ² 5p7s ³ P
112647.0	112525.0	122.0	78% 5s ² 5p6d ³ P+19% 5s ² 5p6d ³ D
114050.0	113905.0	145.0	61% 5s ² 5p8s ³ P+30% 5s ² 5p8s ³ P+4% 5s ² 5p6d ³ P
	114713.0		38% 5s²5p6d³P+20% 5s²5p7d³P+11% 5s²5p7d³D + 7% 5s²5p6d³D
116776.0n	116796.0	-20.0	46% 5s²5p7d³D+18% 5s²5p6d³P+14% 5s²5p7d³P + 8% 5s5p³(²P)¹P
120013.0n	120032.0	-19.0	67% 5s²5p8s³P + 30% 5s²5p8s³P
123138.0n	122965.0	173.0	75% 5s²5p7d³P+24% 5s²5p7d³D
124130.0n	124193.0	-63.0	69% 5s²5p7d³P+ 16% 5s²5p7d³D+6% 5s²5p7d³P
J=2			
51723.0	51806.0	-83.0	98% 5s5p ³ (⁴ S) ³ S
66502.0	66459.0	43.0	63% 5s5p ³ (² D) ³ D+ 25% 5s ² 5p5d ³ D +6% 5s5p ³ (² P) ³ P
72390.0	72386.0	4.0	54% 5s ² 5p5d ³ D + 19% 5s ² 5p5d ³ F +10% 5s5p ³ (² D) ¹ D + 7% 5s ² 5p5d ³ P
75275.0	75259.0	16.0	81% 5s ² 5p6s ³ P + 5% 5s ² 5p5d ³ F +5% 5s5p ³ (² P) ³ P + 5% 5s ² 5p5d ³ P
76692.0	76737.0	-45.0	61% 5s ² 5p5d ³ F +11% 5s ² 5p6s ³ P +9% 5s ² 5p5d ³ P + 6% 5s5p ³ (² P) ³ P

Table 3 : Continued

78391.0	78265.0	126.0	31% 5s5p ³ (² P) ³ P+ 22% 5s ² 5p5d ³ P + 21% 5s ² 5p5d ³ D + 12% 5s ² 5p5d ³ F
86025.0	85817.0	208.0	46% 5s ² 5p5d ³ D + 20% 5s ² 5p5d ³ P +15% 5s5p ³ (² P) ³ P +13% 5s5p ³ (² D) ³ D
91243.0	91044.0	199.0	33% 5s ² 5p5d ³ P + 26% 5s ² 5p5d ³ D +25% 5s5p ³ (² P) ³ P +11% 5s5p ³ (² D) ³ D
98856.0	99147.0	-291.0	62% 5s5p ³ (² D) ¹ D +16% 5s ² 5p5d ³ D+14% 5s ² 5p6d ³ D
104723.0	104798.0	-75.0	80% 5s ² 5p6d ³ F +10% 5s ² 5p6d ³ D +4% 5s ² 5p6d ³ D
105536.0	105881.0	-345.0	44% 5s ² 5p6d ³ P +28% 5s ² 5p6d ³ D+18% 5s ² 5p6d ³ D+6% 5s5p ³ (² D) ¹ D
107825.0	107826.0	-1.0	99% 5s25p7s ³ P
	111687.0		42% 5s ² 5p6d ³ D + 35% 5s ² 5p6d ³ D +17% 5s ² 5p6d ³ F + 4% 5s5p ³ (² D) ¹ D
	112461.0		53% 5s ² 5p6d ³ F +16% 5s ² 5p7d ³ D +5% 5s ² 5p7d ³ D
115820.0n	115774.0	46.0	47% 5s ² 5p7d ³ P+33% 5s ² 5p7d ³ D+18% 5s ² 5p7d ³ D
119832.0	119812.0	20.0	100% 5s ² 5p8s ³ P
122499.0n	122488.0	11.0	57% 5s ² 5p7d ³ D + 19% 5s ² 5p7d ³ D
123248.0n	122909.0	339.0	49% 5s ² 5p7d ³ P + 42% 5s ² 5p7d ³ D+7% 5s ² 5p7d ³ D
J=3			
67885.0	67643.0	242.0	72% 5s5p ³ (² D) ³ D+ 26% 5s ² 5p5d ³ D
77727.0	77741.0	-14.0	92% 5s25p5d ³ F
88259.0	88245.0	14.0	60% 5s ² 5p5d ³ D + 20% 5s5p ³ (² D) ³ D+13% 5s ² 5p5d ³ F +5% 5s ² 5p5d ³ F
91226.0	91569.0	-343.0	80% 5s ² 5p5d ³ F+ 12% 5s ² 5p5d ³ D
	105580.0		59% 5s ² 5p6d ³ F+ 21% 5s ² 5p6d ³ D +18% 5s ² 5p6d ³ F
	111606.0		60% 5s ² 5p6d ³ D 34%5s ² 5p6d ³ F
	113137.0		68% 5s ² 5p6d ³ F + 17% 5s ² 5p6d ³ D+5% 5s ² 5p6d ³ F + 5% 5s ² 5p7d ³ F
116410.0n	116008.0	402.0	50% 5s ² 5p7d ³ F + 22% 5s ² 5p7d ³ D+20% 5s ² 5p7d ³ F + 6% 5s ² 5p6d ³ F
122433.0n	122616.0	-183.0	59% 5s ² 5p7d ³ D + 38% 5s ² 5p7d ³ F
123319.0n	123534.0	-215.0	71% 5s ² 5p7d ³ F +18%5s ² 5p7d ³ D +9% 5s ² 5p7d ³ F
J=4			
81083.0	81226.0	-143.0	100% 5s ² 5p5d ³ F
	111110.0		99% 5s ² 5p6d ³ F
	122310.0		100% 5s ² 5p7d ³ F

n = new levels

CONCLUSIONS

Using the scaling from the isoelectronic sequence members from Te III - La VIII [1-6] multi-configuration interaction calculations were performed to predict the 5p²- (5s5p³ + 5p5d + 5p6d + 5p7d + 5p6s + 5p7s + 5p8s) transition array. The analysis is considerably extended to complete the 5p7d, and 5p8s configurations for the first time. Arcimowicz et al had classified 88 lines of Sb II for 5p²- (5s5p³ + 5p5d + 5p6s +

5p7s) array while presently I have identified more lines in Sb II and have added two more configurations namely 5p7d, and 5p8s in the 446–2076 region.

ACKNOWLEDGMENT

By the name of Allah I feel so grateful of His blessings, I finally completed this paper. I am thankful to the Natural sciences and Engineering Research Council of Canada (NSERC) for the financial assistance which made my stay possible in Antigonish laboratory in 2002. I am very much thankful to Deanship of Educational Services for providing me all facilities in Qassim University, KSA. I am thankful to Aligarh Muslim University for their continued support to the research program on Atomic Spectra. I would like to express my humble gratitude to Prof. Rahimullah Khan and Dr. Tauheed Ahmad of Aligarh Muslim University (India) for his constant guidance that helped me to complete this paper.

REFERENCES

- [1] Y.N. Joshi, A. Tauheed and I.G. Davison, *Canad. J. Phys.* 70, 740 (1992)
- [2] A. Tauheed, Y.N Joshi, and V. Kaufman, *J.Phys. B: At. Mol. Opt. Phys.* 24, 3701 (1991).
- [3] E.H Pinnington, R.N.Gosselin, Q. Ji, J.A. Kernahan and B.Guo; *Physica Scripta.* 46, 40 (1992).
- [4] A. Tauheed and Y.N Joshi, *Physica Scripta.* 46, 403 (1992).
- [5] A.Tauheed and Y.N Joshi, *Physica Scripta.* 46, 403 (1992)
- [6] R.R. Churilov, and Y.N Joshi, *Phys. Scr.* 58, 441 (1998)
- [7] R. J Lang and E. H. Vestine, *Phys. Rev.* 42, 233 (1932)
- [8] S. G Krishnamurty, *Indian J. Phys.* 10, 83 (1936)
- [9] K.Murakawan and S. Suwa, *Reports Inst. Sci Tech Tokyo university* 1, 121 (1947)
- [10] C.E Moore, *Atomic energy levels*, 3, N.B.S.Circular 467 (U.S.Government Printing Bureau, Washington, D.C) 1957
- [11] B. Arcimowicz, Y.N Joshi and V. Kaufman, *Canad. J. Phys.* 67, 572 (1989)
- [12] Tazeen Rana, A. Tauheed and Y.N. Joshi, *Physics Scripta.* Vol 63, 108- 112, (2001)
- [13] R.L; Kelly *Atomic and ionic lines below 2000Å*; *J. Phys. Chem. Ref. Data*, 16 [Suppl 1] (1987). R.D. Cowan, "Theory of Atomic Structure and Spectra, Berkeley ,CA,
- [14] University of California Press (1981) and Cowan code programs.