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Analysis of the 4d105s7p, 4d105s8p, and 4d105p7s Configurations of Triply Ionized Antimony (Sb Iv)

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ABSTRACT

The 3-m normal incidence vacuum spectrograph was used to record the Antimony spectrum in the 300-2080A0 region. Previous Sb IV analyses were updated. Two configurations were created that were stimulated by electrons: 4d10 5s7p, 4d105s8p, and 4d105p7s. To properly understand the Spectrum, multi-configuration Hartree-Fock calculations with relativistic corrections (HFR) and least square fitting calculations (LSF) were performed.

Keywords: *Singly Ionized Antimony Atoms, Isoelectronic Sequence, Triggered Spark Source, Ions, Atoms, Energy Level, Spectrograph, Theoretical Study*

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1. INTRODUCTION

The fourth spectrum of Antimony has relatively simpler two electron structure with its electronic distribution as:

$$1s^2, \quad 2s^2\, 2p^6, \quad 3s^2\, 3p^6\, 3d^{10}, \quad 4s^2\, 4p^6\, 4d^{10}, \quad 5s^2$$

Thus $5s^2$ is the ground configuration and the resulting energy level is $^1S_0$. The first work on this spectrum was reported by Green and Lang [1] followed by Gibbs and Vieweg [2]. Badami [3] extended the earlier work and reported levels of the $5s^2$, $5p^2$, 5sns (n=6, 7), 5snp (n=5, 6) and 5s4f configurations classifying 74 lines in the 456 Å – 3922 Å region. He also calculated ionization limit of Sb IV as 356156 cm^{-1}. Chan [4] re observed the spectrum in the 300 Å – 8000 Å region and did major extensions to both even and odd parities systems by establishing the 5s7d, 5sng (n=5, 6), 5pnp (n=6, 7) and 5p4f configurations of the even system, and 5p6s, 5p5d and 5s5f configurations of the odd parity system and reported ionization limit about 800 cm^{-1} higher than that of Badami [3]. **My investigation is here to confirm the analysis and to provide a satisfactory theoretical interpretation of the energy levels of odd parity Configuration 5s7p, 5s8p and 5p7s**. Even these configurations were present in Chan's [4] work but our preliminary Hartree- Fock calculations [11] showed that almost all of Chan's [4] levels were shifted a few thousand wave number from the predicted values from the intrapolation of sequence from La X to Sb IV. **Therefore, present investigation is here the energy levels of 5s7p, 5s8p and 5p7s configuration with very accurate values to confirm the analysis and to provide a satisfactory theoretical interpretation as well.**

2. EXPERIMENTAL PROCEDURES

Almost all of the data in this paper is based on plates obtained on a 3-m normal incidence vacuum spectrograph in Professor Y.N Joshi's laboratory at the Physics Department, St. Francis Xavier University, Antigonish, Nova Scotia, Canada. The author time and worked in the laboratory and helped record numerous Spectra. The Spectrograph features a 3-m osmium-coated holographic concave grating with 2400 lines per millimeter. It is blazed at 1200 Å. The spectrograph has an inverse dispersion of 1.385 Å/mm in the first order. The dispersion is relatively steady throughout the range, ranging by less than 0.5 percent from 250Å to 2100 Å.

The plate holder is 76 cm long and can accommodate two 15-inch plates. A single setting allows for photography in the 1000Å wavelength range. Two Spectrograph settings: i=9.5˚ and 17.5˚, with ranges of 230 Å - 1224 Å and 1100 Å - 2100 Å, are taken setting, the device in almost stigmatic, causing particular discrimination in Photographing the Antimony discharge plasma between the electrodes. The plate holder measures 76 cm in length, allowing it to accommodate two plates, each 15 inches long. In a single configuration, it is possible to capture images in the approximately 1000 Å wavelength range. The slit is oriented vertically, measuring 3 mm in length, with a width adjusted to 20 - 25 µm using aluminum foil strips of known thickness. To achieve varying exposures on the photographic plate, the holder can be adjusted vertically from the outside, allowing for up to six exposures. As the instrument was constructed at the Antigonish laboratory, the photographic plate chamber cannot be isolated from the rest of the tank. Typically, it takes 3 to 4 hours for the tank pressure to decrease to 5×10^{-5} Torr, which is adequate for capturing images down to 220 Å. It is widely recognized that the reflectivity of gratings decreases at shorter wavelengths in normal incidence spectrographs, resulting in the visibility of only the most prominent lines in the region below 350 Å. The data collected from the 3-meter spectrograph were enhanced by a line list derived from exposures taken with a hollow cathode source at the 6.65-meter normal incidence spectrograph located at the Zeeman Laboratory, University of Amsterdam. This data was also available at the Antigonish laboratory, along with NIST Plates, which were recorded using a sliding spark source**.**

(i) Light Source:

The excitation of the antimony ions plasma was primarily achieved using a triggered spark. Spectroscopically pure Antimony powder, with a purity of approximately 99.99%, was placed into the cavity of an aluminum electrode, which served as the lower electrode within the spark chamber and was grounded. The upper electrode consisted of a pure aluminum electrode. Aluminum was selected as the electrode material due to its machinability and the simplicity of its well-documented spectral characteristics. To ensure proper alignment of the spark's center with the center of the slit and the grating, a laser beam was employed, with its alignment having been established in advance with respect to the slit and grating.

(ii) Photographic Plates and Recording:

The spectra were captured using two varieties of photographic plates, specifically Kodak SWR and Kodak 101 - 105 plates. The latter exhibits significantly greater sensitivity in the wavelength range below 400Å, there by requiring fewer exposures for satisfactory spectral development. Both plate types were processed using a 50% diluted D-19 developer and fixed with F-5 fixer. However, the development procedures differ between the two. For the SWR plates, both the developer and fixer were maintained at approximately 20 ºC, with a development duration of 2 to 3 minutes. In contrast, the 101 - 105 plates were first immersed in chilled water (5-10ºC) for 10 to 15 minutes before being developed in a chilled developer for around 3 minutes.

(iii) Measurements:

In the process of measuring the plates, the semi-automatic mode is typically favored. This mode requires the operator to adjust the stage (plate holder) by turning a wheel. Two identical densitometric traces of the spectral line are displayed on either side of the center of the oscilloscope. When the desired line to be measured is precisely positioned at the center of the slit, these two traces coincide, appearing as a single trace. This alignment indicates the exact location of the spectral line. At this point, pressing the space bar on the computer keyboard automatically records the position of the line. The operator must then input the intensity and characteristics of the line, along with any necessary comments. The process is then repeated for the subsequent line. Ultimately, the data is saved and transferred to another computer for wavelength calibration.

3. RESULTS AND DISCUSSION

Ab initio calculations were performed using interpolations of the Slater energy parameters obtained from Te V - La X [6 - 10]. The even parity configuration set included $5s^2$, 5s(5d + 6d), $5p^2$, 5sns (where n = 6 - 8). Conversely, the odd parity configuration set consisted of 5snp (where n = 5 - 8), 5p5d, 5p6s and 5p7s. The analysis began with a comprehensive verification of each reported level [12, 4]. Recent measurements have resulted in a notable improvement in the multiplet intervals and their associated level values. **I have investigated twelve new energy levels in odd parity system**. The experimental and fitted energy level values (cm^{-1}) and other LS- Percentage compositions of even parity and odd parity configurations of Sb IV are presented in Table 1 and Table 2.

The Fitted and HFR parametric values (cm^{-1}) and Scaling factors with the even parity Configurations of Sb IV are shown in Table 3 and Table 4.

Table 1. The experimental and fitted energy level values (cm-1) and other LS- Percentage compositions of even parity configurations of Sb IV

E(obs)	E(LSF)	diff.	LS-composition.
J=0			
0.00	0.0	-0.4	98% 5s2
152063.2	152063.0	0.2	94% 5p2 <2>3P+ 5% 5p2 <0>1S
184429.5	184429.0	0.5	92% 5p2 <0>1S+ 6% 5p2 <2>3P
193948.4	193948.0	0.4	100% 5s 6s 1S
259327.3	259327.0	0.3	100% 5s 7s 1S
291405.8	291406.0	-0.2	100% 5s 8s 1S
J=1			
156381.7	156562	-	100% 5p2 <2>3P
178913.3	178911	2.3	100% 5s 5d 3D
188632.3	188632	0.3	100% 5s 6s 3S
254678.4	254680	-1.6	100% 5s 6d 3D
257771.9	257772	-0.1	100% 5s 7s 3S
290488.5	290489	-0.5	100% 5s 8s 3S
J=2			
155947.6	155948	-0.4	56% 5p2 <2>1D+ 23% 5p2 <2>3P+ 21% 5s 5d 1D
163521.4	163521	0.4	77% 5p2 <2>3P+ 14% 5p2 <2>1D+ 9% 5s 5d 1D
179264.7	179269	-4.3	100% 5s 5d 3D
193445.6	193449	-3.4	70% 5s 5d 1D+ 28% 5p2 <2>1D
254829.0	254827	2.0	99% 5s 6d 3D
256513.6	256813	-300	98% 5s 6d 1D
J=3			
179820.9	179819.0	1.9	100% 5s 5d 3D
255081.6	255082.0	-0.4	100% 5s 6d 3D

Table 2. The experimental and fitted energy level values (cm-1) and other LS- Table Percentage compositions of odd parity configurations of Sb IV

E(obs)	E(LSF)	diff.	LS-composition.
J=0			
64437.3	64465.0	-27.7	100% 5s 5p 3P
215387.3	215367.0	20.3	99% 5s 6p 3P
264970*	**264850.0**	**120**	**91% 5s 7p 3P + 7% 5p 5d 3P**
268108.0	268186.0	-78	75% 5p 5d 3P + 22% 5p 6s 3P
272690.0	272808.0	-118	76% 5p 6s 3P + 18% 5p 5d 3P + 6% 5s 7p 3P
291726.0*	**291762.0**	**-36.0**	**100% 5s 8p 3P**
332992.0*	**333011.0**	**-19.0**	**98% 5p 7s 3P**
	338832.0		98% 5p 6d 3P
J=1			
66698.1	66662.0	36.1	98% 5s 5p 3P
95956.7	95957.0	-0.3	96% 5s 5p 1P
215734.1	215756.0	-21.9	86% 5s 6p 3P + 13% 5s 6p 1P
219029.0	219026.0	3.0	84% 5s 6p 1P + 13% 5s 6p 3P
262962.2	262286.0	-	79% 5p 5d 3D + 15% 5p 5d 3P
265094.0*	**264948.0**	**146.0**	**46% 5s 7p 1P + 44% 5s 7p 3P + 6% 5p 6s 1P**
-	265584.0	-	44% 5s 7p 3P + 38% 5s 7p 1P + 7% 5p 6s 1P + 5% 5p 5d 3D
268471.2	268321	150.2	73% 5p 5d 3P + 12% 5p 5d 3D + 9% 5p 6s 3P + 6% 5s 7p 3P
273535.3	273627.0	-91.7	68% 5p 6s 3P + 11% 5p 6s 1P + 7% 5s 7p 1P + 5% 5p 5d 3P
278272.5	278110.0	162.5	44% 5p 5d 1P + 27% 5p 6s 1P + 16% 5p 6s 3P + 4% 5s 7p 1P
286257.7	286365.0	-107.5	43% 5p 6s 1P + 36% 5p 5d 1P + 12% 5s 8p 1P
292030.0*	**291991.0**	**39.0**	**97% 5s 8p 3P**
294010.6*	**293975.0**	**35.6**	**84% 5s 8p 1P + 11% 5p 6s 1P**
	330482.0		75% 5p 6d 3D + 13% 5p 6d 3P + 12% 5p 6d 1P
333432.6*	**333414.0**	**18.6**	**72% 5p 7s 3P + 26% 5p 7s 1P**
	338281.0	-	75% 5p 6d 3P + 19% 5p 6d 3D
341406.6*	**341419.0**	**-12.4**	**41% 5p 7s 1P + 28% 5p 6d 1P + 20% 5p 7s 3P + 8% 5p 6d 3P**
	342709.0	-	55% 5p 6d 1P + 29% 5p 7s 1P + 7% 5p 7s 3P + 4% 5p 6d 3D

J=2			
72555.7	72563.0	-7.3	100% 5s 5p 3P
217804.8	217806.0	-1.2	99% 5s 6p 3P
227059.0	226981.0	78.0	93% 4f 5s 3F + 7% 5p 5d 3F
254143.8	254259.0	-	58% 5p 5d 3F + 34% 5p 5d 1D + 5% 4f 5s 3F
258835.2	258920.0	-84.8	49% 5p 5d 1D + 25% 5p 5d 3F + 12% 5p 5d 3D + 11% 5p 5d 3P
265094.3	265083	11.3	44% 5p 5d 3D + 25% 5p 5d 3P + 15% 5p 5d 1D + 8% 5s 7p 3P
265950.0*	**266118.0**	**-168.0**	**77% 5s 7p 3P + 19% 5p 5d 3D**
	267841.0	-	94% 5s 5f 3F
269195.4	269126.0	69.4	59% 5p 5d 3P + 24% 5p 5d 3D + 13% 5s 7p 3P
279778.0	279790.0	-12.0	97% 5p 6s 3P + 2% 5s7p ^{3}P +1% 5p5d ^{3}P
292512.7*	**292546.0**		**99% 5s 8p 3P**
	328480.0		64% 5p 6d 3F + 32% 5p 6d 1D
	329773.0		43% 5p 6d 3D + 30% 5p 6d 3P + 17% 5p 6d 1D + 9% 5p 6d 3F
-	335934.0	-	43% 5p 6d 1D + 28% 5p 6d 3D + 26% 5p 6d 3F
-	337844.0	-	62% 5p 6d 3P + 27% 5p 6d 3D + 8% 5p 6d 1D
341078.7*	**341071.0**	**7.7**	**96% 5p 7s 3P**
J=3			
227144.0	227145.0	-1.0	93% 4f 5s 3F + 6% 5p 5d 3F
228438.0	228439.0	-1.0	90% 4f 5s 1F + 8% 5p 5d 1F
257840.1	257836.0	4.1	83% 5p 5d 3F + 7% 5p 5d 3D + 5% 4f 5s 3F
	266267.0	-	42% 5s 5f 1F + 38% 5p 5d 3D + 9% 5s 5f 3F + 7% 5p 5d 1F
	267223.0		46% 5s 5f 1F + 41% 5p 5d 3D + 9% 5s 5f 3F
	268380.0		79% 5s 5f 3F + 14% 5p 5d 3D + 7% 5p 5d 3F
285536.4	284618.0	-918.4	70% 5p 5d 1F + 11% 5s 6f 1F + 9% 5s 5f 1F + 6% 4f 5s 1F
	330535.0		60% 5p 6d 3F + 29% 5p 6d 3D + 10% 5p 6d 1F
	336764.0		66% 5p 6d 3D + 34% 5p 6d 3F
-	341847.0	-	85% 5p 6d 1F + 6% 5p 6d 3F + 5% 5p 6d 3D

J=4			
227304.0	227380.0	-76.0	95% 4f 5s 3F + 4% 5p 5d 3F
262631.5	262735.0	-104	86% 5p 5d 3F + 9% 5s 5f 3F + 4% 4f 5s 3F
	268156.0		90% 5s 5f 3F + 9% 5p 5d 3F
	336935.0	-	99% 5p 6d 3F

Table 3: Fitted and HFR parametric values (cm^{-1}) and Scaling factors the even parity Configurations of Sb IV

Conf.	Parameter	LSF	Accuracy	HF	LSF/HF
5s2	E0(5s2)	4351.3	5.0	4355.0	
5p2	E0(5p2)	164174.8	3.0	159611.4	1.029
	F2(5p, 5p)	34203.3	15.0	45618.7	0.750
	alfa(5p)	694.0	2.0		
	zeta(5p)	5351.7	3.0	4710.6	1.136
5s 6s	E0(5s 6s)	189989.9	4.0	185487.4	1.025
	G0(5s, 6s)	2684.3	3.0	3753.9	0.715
5s 7s	E0(5s 7s)	258138.5	4.0	253349.0	1.019
	G0(5s, 7s)	744.6	3.0	1245.8	0.598
5s 8s	E0(5s 8s)	290701.8	4.0	285545.9	1.018
	G0(5s, 8s)	435.5	3.0	587.6	0.741
5s 9s	E0(5s 9s)	303523.9	4.0	303531.9	1.000
	G0(5s, 9s)	242.4	3.0	329.2	0.736
5s 5d	E0(5s 5d)	181097.3	3.0	176214.6	1.02
	zeta(5d)	363.5	2.0	268.1	1.356
	G2(5s, 5d)	16271.8	(fixed)	21695.9	0.75
5s 6d	E0(5s 6d)	255362.0	3.0	250572.6	1.019
	zeta(6d)	161.0	2.0	115.5	1.394
	G2(5s, 6d)	4464.6	(fixed)	5952.9	0.750
5s 7d	E0(5s 7d)	284295.7	2.0	284305.9	1.000
	zeta(7d)	60.5	2.0	60.6	0.998
	G2(5s, 7d)	1925.4	13.0	2660.8	0.724

5s 8d	E0(5s 8d)	302855.7	2.0	302862.5	1.000
	zeta(8d)	34.8	2.0	36.0	0.967
	G2(5s, 8d)	1092.4	(fixed)	1456.6	0.750

Table 4: Fitted and HFR parametric values (cm^{-1}) and Scaling factors the even parity Configurations of Sb IV

Config.	Parameter	LSF	Accuracy	HF	LSF/HF
5s2 -5p2	R1(5s, 5s; 5p, 5p)	47675.1	(fixed)	59593.8	0.800
5s2 -5s 6s	R0(5s, 5s; 5s, 6s)	2553.1	(fixed)	3191.4	0.800
5s2 -5s 7s	R0(5s, 5s; 5s, 7s)	1289.8	(fixed)	1612.2	0.800
5s2 -5s 8s	R0(5s, 5s; 5s, 8s)	832.9	(fixed)	1041.1	0.800
5s2 -5s 9s	R0(5s, 5s; 5s, 9s)	602.6	(fixed)	753.3	0.800
5p2 -5s 6s	R1(5p, 5p; 5s, 6s)	1111.2	(fixed)	1388.9	0.800
5p2 -5s 7s	R1(5p, 5p; 5s, 7s)	1267.1	(fixed)	1583.9	0.800
5p2 -5s 8s	R1(5p, 5p; 5s, 8s)	1056.3	(fixed)	1320.4	0.800
5p2 -5s 9s	R1(5p, 5p; 5s, 9s)	862.0	(fixed)	1077.5	0.800
5p2 -5s 5d	R1(5p, 5p; 5s, 5d)	35557.5	(fixed)	44446.9	0.800
5p2 -5s 6d	R1(5p, 5p; 5s, 6d)	16151.8	(fixed)	20189.8	0.800
5p2 -5s 7d	R1(5p, 5p; 5s, 7d)	10121.9	(fixed)	12652.4	0.800
5p2 -5s 8d	R1(5p, 5p; 5s, 8d)	7227.6	(fixed)	9034.5	0.800
5s 6s -5s 7s	R0(5s, 6s; 5s, 7s)	0.0	(fixed)	0.0	
	R0(5s, 6s; 7s, 5s)	1706.7	(fixed)	2133.3	0.800
5s 6s -5s 8s	R0(5s, 6s; 5s, 8s)	0.0	(fixed)	0.0	
	R0(5s, 6s; 8s, 5s)	1155.1	(fixed)	1443.9	0.800
5s 6s -5s 9s	R0(5s, 6s; 5s, 9s)	0.0	(fixed)	0.0	
	R0(5s, 6s; 9s, 5s)	856.0	(fixed)	1070.0	0.800
5s 7s -5s 8s	R0(5s, 7s; 5s, 8s)	0.0	(fixed)	0.0	
	R0(5s, 7s; 8s, 5s)	682.7	(fixed)	853.3	0.800
5s 7s -5s 9s	R0(5s, 7s; 5s, 9s)	0.0	(fixed)	0.0	
	R0(5s, 7s; 9s, 5s)	509.1	(fixed)	636.4	0.800
Table 4 continued……………………………………………………………………………..					
5s 8s -5s 9s	R0(5s, 8s; 5s, 9s)	0.0	(fixed)	0.0	
	R0(5s, 8s; 9s, 5s)	351.6	(fixed)	439.5	0.800

5s 5d -5s 6d	R0(5s, 5d; 5s, 6d)	0.0	(fixed)	0.0	
	R2(5s, 5d; 6d, 5s)	8696.7	(fixed)	10870.9	0.800
5s 5d -5s 7d	R0(5s, 5d; 5s, 7d)	0.0	(fixed)	0.0	
	R2(5s, 5d; 7d, 5s)	5603.4	(fixed)	7004.2	0.800
5s 5d -5s 8d	R0(5s, 5d; 5s, 8d)	0.0	(fixed)	0.0	
	R2(5s, 5d; 8d, 5s)	4050.0	(fixed)	5062.5	0.800
5s 6d -5s 7d	R0(5s, 6d; 5s, 7d)	0.0	(fixed)	0.0	
	R2(5s, 6d; 7d, 5s)	3165.6	(fixed)	3957.0	0.800
5s 6d -5s 8d	R0(5s, 6d; 5s, 8d)	0.0	(fixed)	0.0	
	R2(5s, 6d; 8d, 5s)	2324.8	(fixed)	2906.0	0.800
5s 7d -5s 8d	R0(5s, 7d; 5s, 8d)	0.0	(fixed)	0.0	
	R2(5s, 7d; 8d, 5s)	1572.5	(fixed)	1965.7	0.800

4. CONCLUSION

Recent measurements have resulted in a notable improvement in the multiplet intervals and their associated level values. Total twelve new energy levels have been established in odd parity set. My investigation is here to confirm the analysis and to provide a satisfactory theoretical interpretation of the energy levels of odd parity Configuration 5s7p, 5s8p and 5p7s. Ab initio calculations were performed using interpolations of the Slater energy parameters obtained from Te V - La X [6 - 10]. The even parity configuration set included $5s^2$, 5s(5d + 6d), $5p^2$, 5sns (where n = 6 - 8). Conversely, the odd parity configuration set consisted of 5snp (where n = 5 - 8), 5p5d, 5p6s and 5p7s.

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