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TRANSITIONS FROM AUTOIONIZED SINGLE-IONIZED TIN STATES: A THEORETICAL STUDY OF THE $5s5p$ ($^3P^o$) nl ($nl = 5d$, $6s$) LEVELS OF Sn II

A. ALONSO-MEDINA AND C. COLÓN
Departamento de Física Aplicada, EUIT Industrial, Universidad Politécnica de Madrid, Calle Ronda de Valencia 3, E-28012 Madrid, Spain

AND

C. HERRÁN MARTÍNEZ
Departamento de Astronomía y Astrofísica II, Facultad de Ciencias Físicas, Universidad Complutense de Madrid, Avenida Complutense s/n, E-28040 Madrid, Spain
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ABSTRACT

Lines corresponding to several transitions from autoionized states of single-ionized tin were identified in a laser-produced plasma generated by 10640 Å irradiation of an Sn target at a flux of 2×10^{10} W cm^{-2}. Spectra were recorded and analyzed between 2000 and 7000 Å. Theoretical analysis of Sn II was extended using relativistic Hartree-Fock calculations and configuration interactions in an intermediate-coupling scheme with the support of the Cowan code. Our calculations support the experimental value obtained by Schectman et al. in 2000 of the lifetime of $5s^25d\ ^2D_{3/2}$ and the absorption oscillator strength of the resonance transition to this level at 1400.45 Å. The parametric description of $5s5p$ ($^3P^o$) nl ($nl = 5d$, $6s$) of Sn II levels is improved by taking into account the far $5p^3$ configuration mixing effects. The results obtained in this study will allow a substantial improvement in the interpretation of the data of the ultraviolet spectrum of Sn II observed by the Goddard High Resolution Spectrograph aboard the *Hubble Space Telescope*.
Subject headings: atomic data — methods: laboratory

1. INTRODUCTION

The data obtained by the Goddard High Resolution Spectrograph (GHRS) aboard the *Hubble Space Telescope* are fundamental for the knowledge of interstellar space. Interstellar single-ionized tin was first detected (in several stars: 15 Mon, 23 Ori, Φ Sco, 1 Sco, and ζ Oph) through absorption at the 1400.45 Å line by Hobbs et al. (1993). Sofía, Meyer, & Cardelli (1999) determined the gas-phase interstellar abundance of Sn II in diffuse clouds toward 14 stars. Their measures demonstrated that tin is exchanged between the gas and dust phases of the diffuse interstellar medium. They found a tin abundance that appears to be greater than solar, a situation not known to exist for any other element. Hobbs indicates that future GHRS observations of several weaker lines of Sn II such as the 1757.905 Å line can be used to corroborate the identification of the 1400.45 Å line. Thus, reliable Sn II data in the UV range are needed to derive different astrophysical parameters.

The levels of single-ionized tin have been the subject of both experimental and theoretical studies (McCormick & Sawyer 1938; Wujec & Musielok 1976; Wujec & Weniger 1977; Miller, Roig, & Bengtson 1979; Kunisz & Migdalek 1974; Migdalek 1976; Miller & Bengtson 1980; Marcinek & Migdalek 1994). Both types of studies are relevant. Several recent works have been devoted to the analysis of the transition probabilities (Alonso-Medina & Colón 2000), Stark broadening (Martínez & Blanco 1999), and lifetimes of Sn II (Schectman et al. 2000).

The application of laser ablation for chemical element analysis of a solid sample is one of the most attractive and important applications of laser-produced plasmas (LPPs) in science and technology. In the above-mentioned work (Alonso-Medina & Colón 2000), a source of LPP was used in order to analyze the spectrum of single-ionized tin.

Unfortunately, Sn II analysis remains incomplete. There are several energy levels that have not been identified, and a precise study of the mixed configurations in both parities does not exist. In the works mentioned above, certain remarkable discrepancies between the experimental values of some parameters and the corresponding theoretical calculations have been justified with this argument.

Relativistic Hartree-Fock (HFR) calculations using the Cowan (1981) code were presented by Marcinek & Migdalek (1994). A basis set consisting of 12 configurations of odd parity and 20 of even parity was used in these calculations. Appreciable mixing between the experimental $5s^25d$, $5s^26d$, and $5s5p^2$ configurations was indicated in these ab initio calculations. Also detected in this work was mixing between the configuration $5s5p5d$ (with four of its 17 levels experimentally identified) and the configuration $5p^3$ (not experimentally found). Attempts to carry out a least-squares fitting including the complete set proved difficult because of the increase in the number of parameters above the number of experimentally observed energy levels.

In the previously mentioned works, an intermediate solution was to take into account mixing of the configurations $5s^25d$, $6s^26d$, and $5s5p^2$.

In this way, the necessity was suggested (Martínez & Blanco 1999) of including the configuration $5s5p5d$ in the analysis of the $4f$ and $5f$ configurations to explain the discrepancies observed in the Stark broadening corresponding to the transitions $6d$–$6p$ and $7d$–$6p$.

Following this suggestion, in this work we have included this configuration as a test. However, this inclusion alone is unable to explain the relevant discrepancies. In this work we have also included the nonexperimental configuration $5p^3$, which produces a substantial improvement in the identification of the well-known levels (Moore 1958).

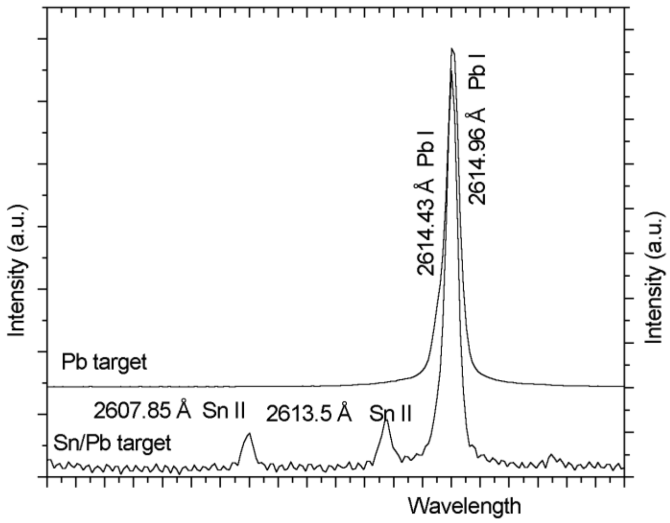

FIG. 1.—Sn II and Pb II experimental spectrum in the Sn/Pb and Pb samples at 6 torr atmosphere of Ar (2.5 μs delay time).

In this work several lines corresponding to transitions of certain levels of Sn II not indexed in the literature have been identified. We report lines corresponding to transitions from $5s5p$ (^3P) $5d$ and $5s5p$ (^3P) $6s$ ^4P to $5s5p^2$ $^2P_{1/2,3/2}$. In Figure 1 the spectrum corresponding to the lines from $5s5p$ (^3P) $5d$ to $5s5p^2$ $^2P_{3/2}$ (with experimental wavelengths 2607.85 and 2613.50 Å) is presented. By means of the theoretical calculations carried out in this work, these lines have been clearly identified.

Improved values for the astrophysically relevant transition probabilities of the 1400.45 and 1489.22 Å lines and the lifetime of the $5s^25d$ $^2D_{3/2}$ level are presented. These values are in good agreement with the experimental ones obtained by Schectman et al. (2000). Other parameters relevant to astrophysical UV transitions will be presented in a future work.

2. PROCEDURE

2.1. *Experimental Setup*

The experimental system is similar to that described in previous works (Alonso-Medina 1997; Colón et al. 1999; Alonso-Medina & Colón 2000; Alonso-Medina, Colón, & Herrán-Martínez 2001). The experiment was carried out by emission of a plasma generated by focusing a laser beam on samples of Pb, Sn, and an Sn-Pb alloy. A lens with a focal distance of 12 cm was used to focus, on a lead/tin target, the laser beam of an Nd:YAG laser, which generated 290 mJ pulses of 7 ns duration at a frequency of 20 Hz and a wavelength of 10640 Å. The laser irradiance on the blank was 2×10^{10} W cm^{-2}, and the diameter of the standard crater was 0.5 mm. The light emitted by the LPP was transmitted through a sapphire window to the input slit of a 1 m Czerny-Turner spectrometer provided with a 2400 groove mm^{-1} holographic grating. The resolution of the spectroscopic system was 0.3 Å to first order.

A chamber was used to generate the plasma in a vacuum or in a gas atmosphere. After a vacuum of 10^{-5} torr had been attained inside the chamber by means of a turbomolecular pump, it was filled with argon and maintained at a pressure of 6 torr throughout the measurement, using a small continuous flow of gas to maintain the purity of the atmosphere.

Spectra were recorded and analyzed between 2000 and 7000 Å by a time-resolved optical multichannel analyzer that allowed the recording of spectra at a preset delay from the laser pulse with a selected time length. Spectra were obtained at a 2.5 μs delay from the laser pulse, and light was collected during 0.1 μs in synchronism with the electronic trigger of the laser Q-switch. In each data acquisition period, a correction was made with regard to the dark signal in the absence of the laser plasma. The instrumental profile of the line was determined with a precision of 97%; the instrumental width (FWHM) was 0.11 Å to second order for a wavelength of 3000 Å.

To calibrate the spectral response of the system in the range studied (2000–7000 Å), a deuterium lamp was used for the 2000–4000 Å range, and a tungsten lamp was used for the 3500–7000 Å range. The instrumental profile was predetermined by observation of various narrow lines emitted by hollow cathode lamps.

The same experimental system was used to study the homogeneity of the plasma in order to have spatial resolution and to determine where the different atomic species of tin were located in the plasma. The light was focused by means of a lens on a 1 mm light guide, by which we were able to select the point of the plasma where the light emission was observed. The measurements were taken by scanning the plasma emission in two perpendicular directions: through the axis of the plasma, with a distance from the target in the 0.25–2.75 mm range, to study the evolution of the plasma in space, and parallel to the surface of the target, with a radial distance in the range of 0.0–1.12 mm.

In our experimental conditions, lines corresponding to transitions from autoionized levels of Sn II were observed (corresponding to levels 3^o and 4^o of Moore 1958). Lines corresponding to transitions from $5s5p6s$ $^4P_{1/2,3/2}$ were also observed. Several spectra corresponding to different tin and lead concentrations were obtained, to assure a correct identification of the different lines studied and to be used in later works to obtain transition probabilities. This situation can be observed in Figure 1. In Figure 2 a partial diagram of levels of Sn II is presented. In this figure, 3^o, 4^o, and 5^o are the arbitrary labels used by Moore (1958) for certain energy levels whose configurations were not clearly identified. The transitions corresponding to the lines (3074.3, 3441.1, 3418.9, 3448.2, 2607.9, and 2613.5 Å) observed experimentally in our work with appreciable intensities are shown.

2.2. *Theoretical Calculations*

Single-ionized tin involves a single optical electron whose energy levels are well separated. This structure must allow us to obtain a suitable comparison between experimental and theoretical results with relativistic central field calculations using the *LS* coupling scheme. Nevertheless, this scheme is not enough to describe the $5s5p^2$ configuration (Marcinek & Migdalek 1994), and a more detailed description is necessary to take into account some results. For comparison with and interpretation of experimental results, we have obtained theoretical values of transition probabilities in an intermediate-coupling (IC) scheme and by using ab initio HFR calculations.

For the IC calculations we used the standard method of least-squares fitting of experimental energy levels by means

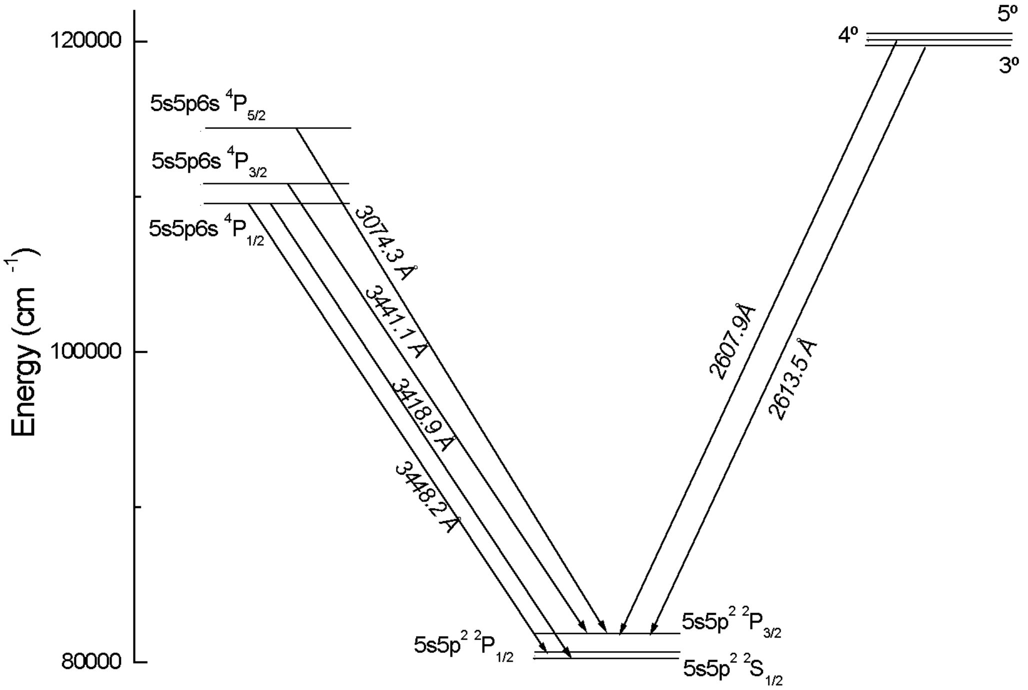

FIG. 2.—Partial energy level diagram of Sn II showing transitions in this study, 3^o, 4^o, and 5^o, including experimental wavelengths

of computer codes from Cowan (1981). In this way we obtained the *LS* composition of each level and the degree of configuration mixing, when considering their interaction. For the HFR calculations, the Cowan computer code provided us with the radial parts for the determination of transition probabilities and initial estimates of the parameters for the IC fittings. The radial integrals for calculations of transition probabilities were obtained from the HFR wave functions.

The basis set used in the present work consists of three configurations of even parity, namely, $5s5p^2$-$5s^25d$-$5s^26d$, and six configurations of odd parity, namely, $5s^25p$-$5p^3$-$5s5p5d$-$5s5p6s$-$5s^24f$-$5s^25f$.

3. RESULTS AND DISCUSSION

3.1. $5s5p^2$-$5s^25d$-$5s^26d$ *Configuration Interaction*

The calculations carried out in this work refine those presented in a previous paper (Alonso-Medina & Colón 2000). Those calculations pursued a comparison with our own experimental values obtained in the range from 2000 to 7000 Å. The current calculations that use a mixture of three single configurations give a relative improvement when discarding the adjustment of the levels $5s5p^2\ ^2S_{1/2}$ and $5s5p^2\ ^2P_{1/2}$, and they overcome the inconveniences that we indicated in the earlier work. However, the resulting parameters and energy levels from the least-squares fitting are very similar to those given in that work.

3.2. $5s^25p$-$5p^3$-$5s5p5d$-$5s5p6s$-$5s^24f$-$5s^25f$ *Configuration Interaction*

Ab initio HFR calculations (without fitting) show small energy splitting between the $5s^2\ nf\ ^2F_{5/2}$ and $5s^2\ nf\ ^2F_{7/2}$ doublet. Experimental data also present small energy splitting, but the doublets are inverted. Although the discrepancies are small in energy terms ($\sim$4 cm^{-1}), the parameters that depend on the wave functions of these levels present a wide disagreement between the calculations and the experimental values (Martínez & Blanco 1999). The inclusion of $5s5p5d$-$5s5p6s$ in the configuration allows us to solve these discrepancies. Although four of the 17 levels of the configuration $5s5p5d$ were clearly assigned by Moore (1958), there were several levels (some autoionized levels) without clear assignment. We were able to assign these levels in this study. Our first attempt was fruitless because of the impossibility of explaining the assigned experimental energy levels. Following Marcinek & Migdalek (1994), we introduced into our calculations the configuration $5p^3$. These calculations allowed us to achieve a complete assignment of the Sn II energy levels.

Additional details of the above calculations are given in Tables 1A, 1B, and 2. Tables 1A and 1B include the values found for the different parameters involved in the IC calculations, while Table 2 displays energy levels and mixing effects.

3.3. *Lifetimes*

Because the $5s^25p\ ^2P_{1/2}$–$5s^25d\ ^2D_{3/2}$ transition at 1400.45 Å is relevant, our primary intention was to calculate the lifetime of the $5s^25d\ ^2D_{3/2}$ level. We obtained a value of 0.41 ns versus an experimental value of 0.44 ± 0.02 ns (Schectman et al. 2000). The value obtained for the lifetime of the $5s^25d\ ^2D_{5/2}$ level is 0.50 ns versus an experimental value of 0.46 ± 0.04 ns (Schectman et al. 2000).

In Table 3 we present the $5s^25p\ ^2P_{1/2,3/2}$–$5s^25d\ ^2D_{3/2,5/2}$ oscillator strength.

The central result of this work has been to determine the importance of including the configurations $5s5p5d$, $5s5p6s$,

TABLE 1A

PARAMETERS RESULTING FROM THE LEAST-SQUARES FITTING OF THE INTERMEDIATE-COUPLING CALCULATIONS: CONFIGURATIONS

Configuration	E_{av} (cm^{-1})	F^k and G^k (cm^{-1})	ζ_{nl} (cm^{-1})
$5s^25p$	$E_{av} = 10642$ (8538)	. . .	$\zeta_{5p} = 3392$ (2666)
$5s^24f$................	$E_{av} = 90607$ (95955)	. . .	$\zeta_{4f} = 4$ (4)
$5s^25f$................	$E_{av} = 100221$ (106433)	. . .	$\zeta_{5f} = 2$ (2)
$5s5p5d$.............	$E_{av} = 125712$ (125908)	$F^1(5p, 5d) = 2175$ (0)	$\zeta_{5d} = 2929$ (3019)
		$F^2(5p, 5d) = 8987$ (20388)	$\zeta_{5p} = 745$ (772)
		$G^1(5s, 5d) = 22405$ (50829)	
		$G^2(5s, 5p) = 4303$ (9762)	
		$G^1(5p, 5d) = 8900$ (20189)	
		$G^2(5p, 5d) = -2550$ (0)	
		$G^3(5p, 5d) = 5504$ (12487)	
$5s5p6s$	$E_{av} = 121603$ (118536)	$G^1(5s, 6s) = 43811$ (51164)	$\zeta_{5p} = 3536$ (3087)
		$G^0(5s, 5d) = 2160$ (2523)	
		$G^1(5d, 6s) = 3621$ (4228)	
$5p^3$	$E_{av} = 139363$ (135771)	$F^2(5p, 5p) = 40578$ (37046)	$\zeta_{5d} = 29667$ (2708)
		$\alpha = 151$	

NOTES.—E_{av} is the multiplet energy, ζ_{nl} is the fine-structure splitting, and F^k and G^k are the Slater integrals. The values in parentheses are ab initio HFR results.

TABLE 1B

PARAMETERS RESULTING FROM THE LEAST-SQUARES FITTING OF THE INTERMEDIATE-COUPLING CALCULATIONS: CONFIGURATION INTERACTIONS

Configuration Interaction	R_d and R_e (cm^{-1})
$5s^25p$-$5p^3$	$R_d^1(5s5s, 5p5p) = 54169$ (49160)
$5s^25p$-$5s5p5d$	$R_d^1(5s5p, 5p5d) = 32902$ (29859)
	$R_e^1(5s5p, 5p5d) = 21685$ (19679)
$5s^25p$-$5s5p6s$..	$R_d^0(5s5s, 5s6s) = 2927$ (2656)
	$R_d^1(5s5p, 5p6s) = -2684$ (-2437)
	$R_e^0(5s5p, 5p6s) = -308$ (-279)
$5p^3$-$5s5p5d$..	$R_d^1(5p5p, 5s5d) = 31727$ (28793)
$5p^3$-$5s5p6s$	$R_d^1(5p5p, 5s6s) = -1953$ (-1773)
$5s5p5d$-$5s5p6s$	$R_d^2(5p5d, 5p6s) = -11562$ (-10493)
	$R_e^1(5p5d, 5p6s) = -4758$ (-4318)
$5s5p5d$-$5s^24f$..	$R_d^1(5p5d, 5s4f) = -15958$ (-14117)
	$R_e^2(5p5d, 5s4f) = -5128$ (-4693)
$5s5p5d$-$5s^25f$..	$R_d^1(5p5d, 5s5f) = -10299$ (-9420)
	$R_e^2(5p5d, 5s5f) = -4074$ (-3753)

NOTES.—R_e and R_d are the configuration interaction Slater integrals. The values in parentheses are ab initio HFR results.

TABLE 2

ENERGY LEVELS AND MIXING EFFECTS IN Sn II

	ENERGY (cm^{-1})			COMPOSITION					
				First		Second		Third	
LEVELS (MOORE)	Exp.	Cal.	J	Percentage	Level	Percentage	Level	Percentage	Level
1^o	109223.4	109225	3/2	62.4	$5s5p\,(^3P)\,5d\ ^2D$	26.0	$5p^3\ ^2D$	. . .	. . .
2^o	113819.0	113802	1/2	81.0	$5s5p\,(^3P)\,6s\ ^2P$	12.2	$5s5p\,(^3P)\,5d\ ^2P$	. . .	. . .
3^o	119980.9	120297	3/2	65.6	$5s5p\,(^3P)\,5d\ ^4D$	26.0	$5s5p\,(^3P)\,5d\ ^4P$	. . .	. . .
4^o	120063.0	120364	1/2	90.2	$5s5p\,(^3P)\,5d\ ^4D$	6.8	$5s5p\,(^3P)\,5d\ ^4P$	. . .	. . .
5^o	120253.6	120054	5/2	53.3	$5s5p\,(^3P)\,5d\ ^4P$	36.0	$5s5p\,(^3P)\,5d\ ^4D$	4.8	$5s5p\,(^3P)\,5d\ ^4F$
6^o	122491.6	122392	7/2	88.4	$5s5p\,(^3P)\,5d\ ^4D$	10.2	$5s5p\,(^3P)\,5d\ ^4F$	. . .	. . .
7^o	123156.9	123133	3/2	68.9	$5s5p\,(^3P)\,5d\ ^4P$	27.0	$5s5p\,(^3P)\,5d\ ^4D$	. . .	. . .
8^o	124246.4	123827	5/2	90.2	$5s5p\,(^3P)\,5d\ ^2F$	6.2	$5s5p\,(^1P)\,5d\ ^2F$	. . .	. . .
9^o	124627.7	124603	3/2	65.6	$5p^3\ ^4S$	18.5	$5s5p\,(^3P)\,5d\ ^2P$	7.3	$5s5p\,(^3P)\,6s\ ^2P$
10^o	132168.0	132591	3/2	70.6	$5s5p\,(^1P)\,5d\ ^2D$	13.7	$5s5p\,(^3P)\,5d\ ^2D$	11.6	$5p^3\ ^2D$
11^o	132708.3	132437	5/2	72.2	$5s5p\,(^1P)\,5d\ ^2D$	12.2	$5s5p\,(^3P)\,5d\ ^2D$	12.2	$5p^3\ ^2D$

TABLE 3

$5s^25p\ ^2P_{1/2,3/2}$—$5s^25d\ ^2D_{3/2,5/2}$ Oscillator Strength

Transition	Wavelength (Å)	*f* Oscillator Strength	
		This Work	Others
$5s^25p\ ^2P_{1/2}$–$5s^25d\ ^2D_{3/2}$	1400.52	1.25	1.04(5),[a] 0.80,[b] 1.38[c]
$5s^25p\ ^2P_{3/2}$–$5s^25d\ ^2D_{3/2}$	1489.22	0.104	0.170(14),[a] 0.086,[b] 0. 130[c]
$5s^25p\ ^2P_{3/2}$–$5s^25d\ ^2D_{5/2}$	1475.00	0.97	1.06(9),[a] 0.74,[b] 1.18[c]

Note.—Parentheses denote uncertainties.
[a] Schectman et al. 2000.
[b] Migdalek 1976.
[c] Marcinek & Migdalek 1994.

and $5p^3$ in the study of the parameters of Sn II. Thanks to this inclusion, we have been able to carry out a correct identification of several spectral lines not indexed in the literature and a precise calculation of the lifetime of the level $5s^25d\ ^2D_{3/2}$ in excellent agreement with the measurements of Schectman et al., thus reaffirming the conclusions of their work.

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