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M1 and E2 Transitions in the Ground-State Levels of Neutral Tin

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Abstract: We have reported the magnetic dipole (M1) and electric quadrupole (E2) transition parameters such as transition energies, logarithmic weighted oscillator strengths and transition probabilities between the fine structure levels in the ground-state configuration of $5s^25p^2$ for neutral tin (Sn I, Z=50) using the multiconfiguration Hartree-Fock approximation within the framework of the Breit-Pauli Hamiltonian (MCHF+BP). The results obtained for Sn I have been compared with other available results. Also, new results on oscillator strengths for Sn I have been presented.
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Introduction

Although the atomic kinetics depend, in particular, on optical allowed transitions, electric dipole (E1), the weak forbidden transitions (in particular, magnetic dipole, M1 and electric quadrupole, E2) have been linked to dominant features in the optical spectra of planetary nebulae and aurora [1-3]. M1 and E2 transition rates (or probabilities) are of several orders of magnitude smaller than those for E1 transitions with a similar energy-level separation.

The forbidden transition lines (especially, magnetic dipole, M1, and electric quadrupole, E2) have great importance in astrophysics which includes the determination of the elemental abundances in different celestial objects and also in laboratory astrophysics and plasma physics studies, since they carry valuable information such as thermal Doppler effects of heavenly bodies. These lines are particularly sensitive to the collisional de-excitation and serve as indicators of electron density and temperature in the emission spectrum. They are used as the best diagnostic tools in both astrophysics and laboratory plasma research [4].

The aim of this work is to investigate the forbidden transitions (M1 and E2) between the fine structure energy levels within the ground state configuration of atomic tin (Sn I, Z=50) using the multiconfiguration Hartree-Fock (MCHF) approach within the framework of the Breit-Pauli Hamitonian [5]. Sn I has the ground state configuration of [Pd] $5s^25p^2$. There are a few works on forbidden transitions (M1 and E2) [6-9], whereas the allowed transitions (electric dipole, E1) (for example, [10-14]) are widely investigated in literature. In calculations, we have selected the configuration set for including valence correlation effect. Other correlation methods (core and core-valence correlations) produce a lot of states, and in this case, the convergence problems in the radial functions occur. For valence correlation, we have only taken into account the configurations including one electron excitation from valence to other high subshells: $5s^25p^2$, $5s5p^25d$, $5s^25d^2$, $5p^25d^2$, $5s^25p5f$, $5p^4$, $5s^25p4f$, $5p^24f^2$, $5p^34f$, $5p^35f$, $5p^25f^2$, $5s^24f^2$ and $5s5p^26s$. Since the parity of upper and lower levels within the ground state configuration is the same, the electric dipole (E1) transitions are forbidden. The lowest-order

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metastable levels radiatively decay corresponding to magnetic dipole (M1) and electric quadrupole (E2) transitions. M1 and E2 transition rates are several orders of magnitude smaller than those for electric dipole (E1) transitions with a similar energy level separation.

Computational Procedure

A detail of theoretical background on radiative transitions can be also found in the literature (for example, [5, 15]). If the emitted or observed photon has angular momentum k and parity $\pi = (-1)^k$, the transition is an electric multipole transition (Ek), while the transition from absorbed photon with parity $\pi = (-1)^{k+1}$ is a magnetic multipole transition (Mk).

The transition probability (or rate) for the emission from the upper level to the lower level is given by:

$$A^{\pi k}\left(\gamma' J', \gamma J\right) = 2C_k \left[\alpha\left(E_{\gamma' J'} - E_{\gamma J}\right)\right]^{2k+1} \frac{S^{\pi k}(\gamma' J', \gamma J)}{g_{J'}}, \qquad (1)$$

where $g_{J'}$ denotes statistical weight of the upper level; namely $g_{J'} = 2J'+1$ and $S^{\pi k}$ is the line strength,

$$S^{\pi k}\left(\gamma' J', \gamma J\right) = \left| < \gamma J \| \mathbf{O}^{\pi(k)} \| \gamma' J' > \right|^2, \qquad (2)$$

$C_k = (2k+1)(k+1)/k((2k+1)!!)^2$ and $\mathbf{O}^{\pi(k)}$ is the transition operator which describes each multipole. The transition probabilities for forbidden transitions depend on the third (in M1 transition) or fifth (in E2 transition) power of transition energy.

The oscillator strength is a dimensionless quantity. It expresses the probability of absorption or emission of electromagnetic radiation in transitions between energy levels. For absorption, the oscillator strength is expressed by:

$$f^{\pi k}(\gamma J, \gamma' J') = \frac{1}{\alpha} C_k \left[\alpha (E_{\gamma' J'} - E_{\gamma J})\right]^{2k-1} \frac{S^{\pi k}(\gamma J, \gamma' J')}{g_J}. \qquad (3)$$

A similar expression can be written for the emission oscillator strength, where $\gamma' J'$ and γJ are interchanged, making the emission oscillator strength negative. The weighted oscillator strength, or *gf*-value, is completely symmetrical (except sign) between the two levels. The weighted oscillator strength is given by:

$$gf^{\pi k}(\gamma' J', \gamma J) = g_{J'} f^{\pi k}(\gamma' J', \gamma J). \qquad (4)$$

The weighted oscillator strength or gf-value is an important property. The intensity of the special line is proportional to the line strength and also to the gf-value.

In the MCHF method, the wave function (or atomic state function, ASF) in the equations above is expressed as a linear combination of configuration state functions (CSFs) $\Phi(\gamma_i LS)$,

$$\Psi(\gamma LS) = \sum_{i=1}^{M} c_i \Phi\left(\gamma_i LS\right), \quad \sum_{i=1}^{M} c_i^2 = 1, \qquad (5)$$

where γ represents electronic configuration. The mixing coefficients c_i and the one-electron radial wave functions of Φ are obtained in a self-consistent procedure by optimization of the energy function based on the non-relativistic Hamiltonian of an atom,

$$H_{NR} = \sum_{j=1}^{N} \left(\frac{1}{2} \nabla_j^2 - \frac{Z}{r_j} \right) + \sum_{j<k} \frac{1}{r_{jk}}. \qquad (6)$$

In this method, the relativistic effects were included as a first-order correction to the MCHF approximation by evaluating Breit-Pauli Hamiltonian using CI method [16]. The Breit-Pauli Hamiltonian consists of a non-relativistic many-electron Hamiltonian(H_{NR}), a relativistic shift Hamiltonian (H_{RS}) including a mass correction, one- and two-body Darwin terms, a spin-spin contact term, an orbit-orbit term; and fine structure Hamiltonian (H_{FS}) including spin-orbit, spin-other-orbit and spin-spin terms. A detail for these terms in the Breit-Pauli Hamiltonian can be found in reference [5] (in Chapter 7). Also, this method includes correlation effects between electrons together with relativistic effects. The wave functions are obtained as a linear combination of CSFs in LSJ coupling and the matrix eigenvalue problem becomes:

$$\boldsymbol{Hc} = E\boldsymbol{c}, \quad (7)$$

where $\boldsymbol{H}$ is the Hamiltonian matrix with elements

$$H_{ij} = \left\langle \gamma_i L_i S_i JM \left| H_{BP} \right| \gamma_j L_j S_j JM \right\rangle \quad (8)$$

and $\boldsymbol{c} = (c_1, ..., c_M)^t$ is the column vector of the expansion coefficients. The Breit-Pauli Hamiltonian is a first-order perturbation correction to the non-relativistic Hamiltonian.

Results and Discussion

In this work, the results of transition energies, ΔE (in cm^{-1}), logarithmic weighted oscillator strengths(or logarithmic gf-value, log(gf)) and transition probabilities, A_{ki} (s^{-1}), for magnetic dipole, M1 and electric quadrupole, E2 transitions between the fine structure levels of the ground-state configuration $5s^25p^2$ in Sn I have been reported using the MCHF atomic-structure package [17]. In calculations, the correlation and relativistic effects in the frame work of the Breit-Pauli Hamiltonian mentioned in section Computational Procedure have been considered. M1 and E2 transitions combine the states with the same parity. Therefore, we have taken into account the configurations of $5s^25p^2$, $5s5p^25d$, $5s^25d^2$, $5p^25d^2$, $5s^25p5f$, $5p^4$, $5s^25p4f$, $5p^24f^2$, $5p^34f$, $5p^35f$, $5p^25f^2$, $5s^24f^2$ and $5s5p^26s$ outside the core [Pd] for considering correlation effects. In MCHF calculations, for avoiding computer constraints, we have only selected the states of $^3P_{2,\ 1,\ 0}$, $^1D_2$ and $^1S_0$ for all considered configurations. These are also the states of the ground-state configuration. We have obtained 139 energy levels including only these states for all of configurations. The transition energies obtained from M1 and E2 transitions between the levels of ground configuration have been listed and compared with [6, 8, 10] in Table 1. We have given $\left(\frac{E_{this\ work} - E_{other\ work}}{E_{other\ work}}\right) \times 100$, where the differences are in per cent (%), for the accuracy of energy results obtained from this work, as presented in Table 1. When the differences (%) between our results and other results have been investigated, the differences with [6], [8] and [10] are in the range of 1.23-18.23, 1.11-16.78 and 0.50-5.12, respectively. In Table 2, we have presented the logarithmic weighted oscillator strengths, log(gf), and transition probabilities, A_{ki}, for M1 and E2 transitions between the ground levels. The A_{ki} values have been compared with those in [7]. A_{ki} values obtained from this work are in agreement with those obtained from work [7]. The weighted oscillator strength values for these lines from M1 and E2 transitions have been presented here firstly. Atomic tin has a high-Z atom and the correlation effects are dominant for this atom. The transition energy results obtained from this work are in agreement with the values available in literature in general. We have not obtained J-J'=0 transitions due to the constraint in MCHF code.

TABLE 1. Energy differences, ΔE (in cm^{-1}), between the fine structure levels of $5s^25p^2$ in atomic tin (Sn I). A:The differences (%) by comparing with [6], B: The differences (%) by comparing with [8] and C: The differences (%) by comparing with [10].

Transitions	$\Delta E(cm^{-1})$				
	This work	Other works	A	B	C
$^1D_2 - {}^3P_1$	7109	6901[a], 6921[b], 7034[c]	3.01	2.71	1.06
$^1D_2 - {}^3P_0$	8517	8623[a], 8613[b], 8475[c]	1.23	1.11	0.50
$^1D_2 - {}^1S_0$	9353	8547[a], 8550[b], 8897[c]	9.43	9.39	5.12
$^3P_2 - {}^3P_1$	1565	1695[a], 1736[b], 1628[c]	7.66	9.85	3.86
$^3P_2 - {}^3P_0$	2973	3417[a], 3428[b], 3069[c]	12.99	13.27	3.12
$^3P_2 - {}^1S_0$	14897	13753[a], 13735[b], 14303[c]	8.31	8.46	4.15
$^3P_1 - {}^3P_0$	1408	1722[a], 1692[b], 1441[c]	18.23	16.78	2.19
$^3P_1 - {}^1S_0$	16461	15448[a], 15471[b], 15931[c]	6.56	6.40	3.33

[a][6], [b][8], [c][10]

TABLE 2. Logarithmic weighted oscillator strengths, log(*gf*), and transition probabilities, A_{ki} (s^{-1}), for the magnetic dipole (M1) and electric quadrupole (E2) transitions between the fine structure levels of $5s^25p^2$ in atomic tin (Sn I). The numbers in brackets represent the power of 10.

Transitions		log(*gf*)	A_{ki}	
		This work	This work	Other works
$^3P_1 - {}^1D_2$	E2	-9.3	1.548 (-3)	4.710 (-3)[a], 4.3(-3)[b]
	M1	-7.44	2.435(-1)	4.518 (-1)[a], 4.6(-1)[b]
$^3P_0 - {}^1D_2$	E2	-10.3	5.231 (-5)	1.654 (-4)[a], 8.1(-5)[b]
	M1	-	-	-
$^1D_2 - {}^1S_0$	E2	-7.9	0.79	1.155[a], 0.95[b]
	M1	-	-	-
$^3P_1 - {}^3P_2$	E2	-10.08	1.305 (-5)	3.742(-5)[a], 3.6(-5)[b]
	M1	-6.9	4.185(-2)	5.926(-2)[a], 6.2(-2)[b]
$^3P_0 - {}^3P_2$	E2	-9.6	1.628(-4)	6.842(-4)[a], 5.9(-4)[b]
	M1	-	-	–
$^3P_2 - {}^1S_0$	E2	-8.8	2.406 (-1)	6.831(-1)[a], 5.7(-1)[b]
	M1	-	-	–
$^3P_0 - {}^3P_1$	E2	-	-	-
	M1	-7.0	4.267(-2)	8.903 (-2)[a], 8.3(-2)[b]
$^3P_1 - {}^1S_0$	E2	-		
	M1	-7.7	4.288	7.076[a], 7.0[b]

[a][6], [b][7]

Conclusion

Through a systematic MCHF study within the framework of the Breit-Pauli Hamiltonian of transition energies, logarithmic weighted oscillator strengths and transition probabilities for the magnetic dipole, M1 and electric quadrupole, E2 transitions between the fine structure levels of $[Pd]5s^25p^2$ ground state configuration of neutral tin (Sn I, Z=50) have been reported. There is a requirement of atomic data of neutral tin, even its charged ions, to understand the erosion of vessel wall tiles in fusion power plants [1], in special, and for plasma diagnostics and modeling. These ground state levels perform weak spectral lines and they decay *via* magnetic dipole (M1) and electric quadrupole (E2) transitions. It is seen that there is an agreement when comparing our results with those presented in other available works. Some differences among other works [6-8, 10] also appear. The studies on M1 and E2 transition parameters, such as oscillator strengths and transition probabilities for Sn I, are limited in number in the literature. Hence, we hope that the results obtained from this work will be useful for other works in the future for Sn I spectrum and provide support to further research on this atom.

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