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Research Article

ISOTOPE SHIFT EFFECTS ON THE GROUND-STATE LEVELS FOR NEUTRAL TIN

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ABSTRACT

Isotope shift effects including mass shift and field shift on the levels for the levels of $^3P_{0,1,2}$, $^1D_2$ and $^1S_0$ for the ground-state configuration of the neutral tin (Sn I, Z= 50) have been investigated. In calculations, the multiconfiguration Hartree-Fock method within the frame work of Breit-Pauli Hamiltonian has been used. The calculation of isotope effects for tin has been here performed firstly although there are some works on the atomic structure of tin. The results including isotope shift effects on the levels have been discussed, and new energy values have been compared other available works in literature.

Keywords: MCHF method, normal mass shift, spesific mass shift, field shift.

1. INTRODUCTION

Neutral tin has ten natural isotopes. There are some works on energy levels, oscillator strengths, transition probabilities, lifetimes in neutral tin (Sn I, Z=50) [1-8]. However no work reporting on, in particular theoretical, isotope shift electronic factors including specific mass, normal mass and field have been published. Isotope shift (IS) effects occur that the finite mass and the extended spatial change distribution of the nucleus have been taken into account in Hamiltonian describing an atomic system [9]. Although the isotope shift of spectral lines is small, it is known that the isotope shift plays important role in extracting the changes in mean-square change radii of the atomic nuclei [10-12].

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The aim of this work, the isotope shift effects on the energy levels in Sn I is to calculate using the multiconfiguration Hartree-Fock (MCHF) method [13]. In the calculations we have taken into the configuration set 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 $5s5p^26s$ for correlation effects between electrons. In addition the calculation results include the relativistic effects in frame work of the Breit-Pauli Hamiltonian.

2. COMPUTATIONAL PROCEDURE

The MCHF method [13], as implemented in the MCHF atomic structure package [14] is one of the configuration interaction methods. It can calculate the correlation between electrons and the relativistic effects in the frame work of the Breit-Pauli Hamiltonian. In addition hyperfine interactions, isotope shift effects and radiative transitions can be calculated using this package. The MCHF method is employed to obtain wave functions (or atomic state functions- ASFs). In the MCHF method the ASF is a lineer combination of the configuration state functions (CSFs), $\Phi(\gamma_i LS)$:

$$\Psi(\gamma LS) = \sum_{i}^{m} c_i \Phi(\gamma_i LS) \qquad (1)$$

Isotope shift in a spectral line can be expressed in as

$$E_M = E_0 + E_M^{NMS} + E_M^{SMS} + E_M^{FS} \qquad (2)$$

In this formula, these terms are non-relativisti energy, normal mass shift, specific mass shift, and field shift, respectively. The mass shift is the sum of the normal mass shift (NMS) and specific mass shift (SMS), and can be interpreted as the kinetic energy of the nuclear motion relative to the centre-of-mass. The NMS is given by

$$E_M^{NMS} = -\frac{m}{M+m} E_0 \qquad (3)$$

where E_0 is non-relativistic the zeroth order Hamiltonian. The specific mass shift (or mass-polarization correction) is expressed as

$$E_M^{SMS} = \left\langle \Psi_0 \middle| -\frac{\mu}{Mm} \sum_{i<j}^{N} \boldsymbol{\nabla}_i . \boldsymbol{\nabla}_j \middle| \Psi_0 \right\rangle \qquad (4)$$

and in fact, independent of the nuclear mass and depends only on the electronic wave function. The SMS is caused by influence of correlations in the motion of electrons on the recoil energy of the nucleus.

The potential deviates from the Coulomb potential of a point charge Z due to the finite size of the nucleus. This potential deviation leads to an energy shift (called as field shift-FS):

$$E_M^{FS} = -\frac{2}{3}\pi Z \rho_e(\mathbf{0}) < r_M^2 > \quad (5)$$

The SMS can be calculated in the gradient form or Slater form. The two forms of the SMS operator produce same results. But, in general, the gradient form gives more reliable values of the shift [13].

3. RESULTS AND DISCUSSION

In this work, the isotope shift effect, including normal mass, specific and field shifts, on the energy levels of the ground-state configuration for neutral tin has been calculated. We have taken into correlation and relativistic effects in the frame work of Breit-Pauli Hamiltonian. For correlation effects, the configuration set 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 $5s5p^26s$ has been considered. And we have also added the isotope effects to the first order energy not the zeroth order. For heavy atoms, the inner s electrons are appreciably influenced by relativistic effects leading to higher densities [13]. For this reason, the non-relativistic density should be multiplied with correction factor, f(Z). The f(Z) and the change in the the nuclear radii, $\delta\langle r^2\rangle$, were taken from [15]. Table 1 displays mass, abundance spin and magnetic moment for natural isotopes for tin.

The normal mass shift (NMS), specific mass shift (SMS) and field shift (FS) contributions(in cm^{-1}) on the ground-state configuration levels of $^3P_{0,1,2}$, $^1D_2$ and $^1S_0$ of neutral tin have been given in Table 2. Table 3 includes the energy levels including isotope shift effects for ground-state configuration. We have compared our results with [15] and [16]. In Table 3, the energies E_0 and $E_{rel.}$ represent the non-relativistic including correlation and relativistic energies, respectively. In addition, we have reported the relativistic effects within the frame work of Breit-Pauli Hamiltonian in this table. As seen in table, the isotope effects are smaller than relativistic effects. Of course, this is the expected case. However, the isotope effects should be considered for describing the transitions and atomic properties in theory, in particular heavy atoms.

Table 1. Natural isotopes for tin (Sn)

Isotope	Mass	Abundance (%)	Spin	Magnetic Moment
^{112}Sn	111.904826	0.97	0	-
^{114}Sn	113.902784	0.65	0	-
^{115}Sn	114.903348	0.36	1/2	-0.918
^{116}Sn	115.901747	14.53	0	-
^{117}Sn	116.902956	7.68	1/2	-1.000
^{118}Sn	117.901609	24.22	0	-
^{119}Sn	118.903310	8.,58	1/2	-1.046
^{120}Sn	119.902220	32.59	0	-
^{122}Sn	121.903440	4.63	0	-
^{124}Sn	123.905724	5.79	0	-

Table 2.The isotope shift effects for the ground-state configuration levels of neutral tin: Normal mass shift (NMS), specific mass shift (SMS) and field shift (FS) contributions (in cm^{-1}). NMS and SMS values are considered as negative

	$^3P_0$	$^3P_1$	$^3P_2$	$^1D_2$	$^1S_0$
NMS					
112-120	441.72881565	441.72835578	441.72784476	441.72603461	441.72298043
114-120	325.48441844	325.48407960	325.48370305	325.48236926	325.48011881
115-120	268.87844388	268.87816396	268.87785290	268.87675108	268.87489201
116-120	213.24842978	213.24820777	213.24796107	213.24708721	213.24561277
117-120	158.56935163	158.56918655	158.56900310	158.56835331	158.56725693
118-120	104.81703321	104.81692409	104.81680283	104.81637330	104.81564858
119-120	51.968110933	51.968056833	51.967996712	51.967783755	51.967424431
120-122	101.38042462	101.38031908	101.38020179	101.37978635	101.37908539
120-124	199.49052743	199.49031975	199.49008897	199.48927148	199.48789217
SMS					
112-120	134.30148214	134.29985513	134.29844993	134.29557246	134.2926840
114-120	98.95898680	98.95778795	98.95675253	98.95463232	98.95250403
115-120	81.74872823	81.74773787	81.74688253	81.74513105	81.74337289
116-120	64.83519825	64.83441279	64.83373442	64.83234531	64.83095092

117-120	48.21078844	48.21020438	48.20969995	48.20866703	48.20763017
118-120	31.86814829	31.86776222	31.86742878	31.86674600	31.86606062
119-120	15.80017436	15.79998295	15.79981763	15.79947911	15.79913930
120-122	30.82329097	30.82291756	30.82259505	30.82193466	30.82127175
120-124	60.65228223	60.65154745	60.65091284	60.64961336	60.64830892
FS					
112-120	6293.42835317	6293.43064396	6293.43163538	6293.43210765	6293.42367831
114-120	4647.44841441	4647.45010606	4647.45083819	4647.45118694	4647.44496220
115-120	4127.25078676	4127.25228907	4127.25293925	4127.25324897	4127.24772097
116-120	2974.84483187	2974.84591471	2974.84638334	2974.84660658	2974.84262211
117-120	2416.59482363	2416.59570327	2416.59608396	2416.59626531	2416.59302855
118-120	556.801162952	556.801365624	556.801453334	556.801495122	556.800749347
119-120	909.796775641	909.797106802	909.797250125	909.797318405	909.796099836
120-122	1228.88017717	1228.88062447	1228.88081806	1228.88091028	1228.87926433
120-124	2315.40006750	2315.40091029	2315.40127505	2315.40144880	2315.39834758
E_{IS}(NMS+SMS+FS)					
112-120	5766.81265759	5766.80646761	5766.80129987	5766.79712225	5766.87654241
114-120	4259.41576865	4259.41121131	4259.40740509	4259.40653816	4259.46253408
115-120	3806.89969580	3806.69886191	3806.69534152	3791.66299082	3791.68509519
116-120	2720.61652902	2720.61351769	2720.61101293	2720.61043968	2720.64741704
117-120	2227.55325873	2227.55110394	2227.54926367	2227.54885275	2227.57607477
118-120	457.628346396	457.627397091	457.626642724	457.626361560	457.639870482
119-120	844.841972953	847.841306387	847.840715080	847.840603763	847.849363063
120-122	1102.34698972	1108.01603770	1107.90491158	1108.01451227	1108.03233997
120-124	2055.25731184	2055.25904309	2055.26027324	2055.26256396	2055.26214649

Table 3. Comparison between energy levels ($E_{rel.}$+E_{IS}) (in cm^{-1}) including isotope effects and other works([16] and [5]) for neutral tin

	$^3P_0$	**$^3P_1$**	**$^3P_2$**	**$^1D_2$**	**$^1S_0$**
E_0	0.0	0.0	0.0	5831.129	15153.572
E_{rel}	0.0	1408.322	2973.328	8516.881	17870.282
112-120	0.0	1408.316	2973.317	8516.865	17870.346
114-120	0.0	1408.318	2973.320	8516.871	17870.328
115-120	0.0	1408.121	2973.141	8501.651	17855.067
116-120	0.0	1408.319	2973.323	8516.874	17870.312

117-120	0.0	1408.320	2973.332	8516.876	17870.304
118-120	0.0	1408.321	2974.076	8516.878	17870.293
119-120	0.0	1411.322	2976.321	8519.879	17873.289
120-122	0.0	1413.991	2978.886	8522.548	17875.967
120-124	0.0	1408.324	2973.331	8516.886	17870.286
[16]	0.0	1685	3428	8606	17164
[5]	0.0	1605	3411	8275	17365

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