

An Investigation on the Fine Structure Levels in the Ground State Configuration for the Antimony Anion

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We have investigated the correlation, relativistic, and isotope shift effects on the fine structure levels in the ground state configuration for the antimony anion (Sb^-). Energies and radiative transition probabilities (for magnetic dipole, M1, and electric quadrupole, E2) have been obtained using the multiconfiguration Hartree–Fock method within the framework of the Breit–Pauli Hamiltonian. Therefore, the most important configuration interaction and relativistic effects have been included. Comparisons with other available works are presented. For some M1 and E2 lines the considered transition probabilities are reported for the first time.

Key words: MCHF Method; Energy Levels; Relativistic Effects; Isotope Effects; Transition Probabilities; Electron Affinity.

1. Introduction

Investigations of the dynamics of negative ions (anions) provide valuable insight into the fundamental problem of many-body motion, which is critical for a detailed understanding of the electronic structure of atoms and molecules. Structural differences between a negative ion and an atom or positive ion originate from the nature of the force binding the extra electron due to the polarization and exchange [1]. The binding energy of the outermost electron is considerably smaller than in the isoelectronic atom due to the absence of the long range Coulomb attraction in negative ions. Therefore electron correlation will be much more important, and negative ions are suitable test objects for various atomic theories [2]. The influences of correlation effects are greatly important in negative ions relative to neutral and positive ions. Relativistic contributions are also important, in particular heavy atomic systems, in addition to correlation contributions. Moreover, the electronic structure calculations of atomic systems need sometimes isotope sensitive calculations. The properties of the nucleus affect the energy level structure of an atomic system and need to be included for an accurate determination of transition energies and other atomic properties [3, 4]. Although the effects of the nucleus are smaller than the uncertainty in the calculation of correlation contributions, the ex-

tended charge correction is important, in particular for heavy atoms [5]. The comparison of theory and experiment through the isotope shift in the electron affinity is of particular interest for probing correlation effects. Experiments considering this effect to be measured are difficult to realize while accurate calculations remain a challenge for atomic theory [6]. Also, the electron affinity has been regarded as one of the hardest atomic or molecular property to produce an ab initio quantum mechanical calculation. In addition, the electron affinity of an atom is a measure of the stability of the corresponding negative ion [1].

Natural antimony (Sb I) consist of two stable isotopes ^{121}Sb ($I = 5/2$) and ^{123}Sb ($I = 7/2$) with natural abundance of 57% and 43%, respectively [7], and has the ground state configuration $[\text{Kr}] 4d^{10}5s^25p^3$. The nuclear moments are $\mu = 3.9796\mu_N$, $Q = -0.36$ barn and $\mu = 2.8812\mu_N$, $Q = -0.49$ barn [7–9] for isotopes 121 and 123, respectively. Single- and multi-photon infrared spectroscopy of Sb^- was studied by Scheer and Haugen [10]. A systematic energy level diagram of the negative ion of antimony was shown by Feldman et al. [11] and obtained a^3P_2 binding energy and $a^3P_2 - a^3P_{1,0}$ fine structure splitting. The $J = 2 - 1$ and $J = 2 - 0$ fine structure and $^3P_2 - ^1D_2$ term splitting had been predicted [12, 13]. In addition, Polak et al. [14] derived an electron affinity by laser photodetached electron spectrum. Negative ions

are atomic systems of growing interest owing to developments in the experimental techniques. The review papers were presented on the structure, dynamics, and collisions in the negative ions [6, 15]. The spectacular experimental developments are leading to the possibility of measuring accurately electron affinities for different isotopes [16, 17]. The comparison of theory and experiment through the isotope shift in the electron affinity is of particular interest for probing correlation effects. Experiments that allow this effect to be measured are difficult to realize while accurate calculations remain a challenge for atomic theory [6]. Some works [18–22] including antimony anion can be also found in the National Institute of Standard and Technology (NIST) [23].

In this work, the energies and magnetic dipole (M1) and electric quadrupole (E2) transition probabilities between the fine-structure levels in the ground configuration state have been carried out by the multiconfiguration Hartree–Fock method within the frame work of the Breit–Pauli Hamiltonian. Calculations include correlation, relativistic, and isotope contributions. The negative ion of antimony (Sb^-) has the ground state configuration of $[\text{Kr}] 4d^{10}5s^25p^4$. The $5s^25p^4$ ground configuration of antimony anion gives rise to five levels $^3P_{2,1,0}$, 1D_2 , 1S_0 . All levels of this ground configuration are metastable. Therefore, weak M1 and E2 transitions are allowed in this configuration since electric dipole (E1) transitions are forbidden between states of the same parity. Both of M1 and E2 transition types of radiation are permitted in second-order theory [5, 7]. Due to the computer and method constraints, we have fixed the core $[\text{Kr}] 4d^{10}$ and only considered the valence correlation including excitation from $5s^25p^4$. Therefore we have taken the configurations of $5s^25p^4$, $5s5p^45d$, $5s5p^46s$, $5s^25p^34f$, $5s^25p^35f$, $5s^25p^36p$, $5s5p^34f5d$, $5s5p^35d5f$, $5s5p^35d6p$, $5s5p^36s6p$, $5p^44f5f$, $5p^56p$, $5p^44f^2$, $5p^6$, $5p^45d^2$, $5p^44f^2$, $5p^45f^2$, $5p^46s^2$, $5p^46p^2$, $5s^25p^24f5f$, $5s^25p^24f6p$, $5s^25p^25d6s$, $5s^25p^25f6p$, $5s^25p^24f^2$, $5s^25p^25d^2$, $5s^25p^25f^2$, $5s^25p^26s^2$, $5s^25p^26p^2$ for the antimony anion (Sb^-). And, we have taken the configuration set $5s^25p^3$, $5s^25p^26p$, $5s^25p^24f$, $5s^25p^25f$, $5s^25p^26f$, $5s^25p5d^2$, $5s^25p4f^2$, $5s5p^35d$, $5s5p^36d$, $5s5p^36s$, $5p^5$, $5p^35d^2$, $5s5p^25d4f$, $5s5p^25d5f$, $5p^34f^2$ for the neutral antimony (Sb I) since the electron affinity of antimony has been obtained. We studied the fine structure levels of the ground state for some anions

including the antimony anion by different configuration sets [24]. In the present study we have obtained better results for fine structure levels using different configuration sets. We also investigated isotope effects on energy levels and electron affinity, and M1 and E2 lines for this anion.

2. Calculation Method

In the multiconfiguration Hartree–Fock (MCHF) approximation [5], the Hamiltonian is used for obtaining the best radial functions for the set of non-relativistic energies of the interacting terms. The basic concept and features of this method have already been presented in various publications [5, 25]. In this method, the wavefunction $\Psi(\gamma LS)$ is expanded as a linear combination of configuration state functions (CSFs) $\Phi(\gamma_i LS)$,

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

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

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

The variational MCHF method and the configuration interaction (CI) correlation models are based on the concept of orbital and configuration spaces. The exact solution can be approximated with arbitrary accuracy if enough CSFs in (2) are taken into account. However, this case is often constrained by computing capacities, and limitations for the expansion must be used. This method also includes the relativistic effects. These effects are included in the Breit–Pauli operators used by the CI method [5, 25]. When the non-relativistic MCHF method is used to obtain radial functions, a subsequent configuration interaction calculation in terms of the Breit–Pauli Hamiltonian is performed in order to include relativistic effects in the LSJ coupling. The total energies are eigenvalues of an interaction matrix and the associated eigenvector defines the wave function expansion. This Hamiltonian can be written as

$$H_{\text{BP}} = H_{\text{NR}} + H_{\text{RS}} + H_{\text{FS}}, \quad (3)$$

Table 1. Non-relativistic energy E_{MCHF} , relativistic energy $E_{\text{MCHF+BP}}$, and isotope shift contributions (ΔE_{nms} , ΔE_{sms} , ΔE_{fs}) (in a.u.) for $5s^25p^3$ and $5s^25p^4$ ground state of neutral and antimony anion, respectively.

Level	E_{MCHF}	J	$E_{\text{MCHF+BP}}$	ΔE_{nms}	ΔE_{sms}	ΔE_{fs}
Sb $5s^25p^3$						
4S	-6466.69782429	3/2	-6466.699694	-0.000476715	-0.000145803	0.0010412080
2D	-6466.64995442	3/2	-6466.654661	-0.000476775	-0.000145799	0.0010412078
		5/2	-6466.649842	-0.000476710	-0.000145998	0.0010412082
2P	-6466.61711412	1/2	-6466.617794	-0.000476708	-0.000145796	0.0010412049
		3/2	-6466.611228	-0.000476707	-0.000145795	0.0010412048
Sb ⁻ $5s^25p^4$						
3P	-6466.73016446	2	-6466.7360122	-0.000476716	-0.000145805	0.0010411689
		1	-6466.7259525	-0.000476715	-0.000145803	0.0010411701
		0	-6466.7248719	-0.000476715	-0.000145803	0.0010411702
1D	-6466.70265999	2	-6466.7016971	-0.000476714	-0.000145801	0.0010411695
1S	-6466.66596354	0	-6466.6638835	-0.000476711	-0.000145796	0.0010411687

where H_{NR} , H_{RS} , and H_{FS} is the non-relativistic many-electron Hamiltonian, the relativistic shift Hamiltonian, and the fine structure Hamiltonian, respectively. In atomic units,

$$H_{\text{NR}} = \sum_{i=1}^N \left(-\frac{1}{2} \nabla_i^2 - \frac{Z}{r_i} \right) + \sum_{i>j} \frac{1}{r_{ij}}. \quad (4)$$

H_{RS} is the relativistic shift operator and includes mass correction, one- and two-body Darwin terms, spin-spin contact term, and orbit-orbit term in the form

$$H_{\text{RS}} = H_{\text{MC}} + H_{\text{D1}} + H_{\text{D2}} + H_{\text{SSC}} + H_{\text{OO}}. \quad (5)$$

The fine structure Hamiltonian H_{FS} consists of the spin-orbit, spin-other-orbit, and spin-spin terms,

$$H_{\text{FS}} = H_{\text{SO}} + H_{\text{SOO}} + H_{\text{SS}}. \quad (6)$$

The isotope shift of an energy level arises from the addition of mass shift and field shift. These shifts account for the nuclear motion and the nuclear charge distributions. The mass shift is the sum of the normal mass shift and the specific mass shift (or mass polarization term), and can be interpreted as the kinetic energy of the nuclear motion relative to the centre-of-mass [5]. The normal mass shift E_M^{nms} affects all non-relativistic or relativistic energy levels. The specific mass shift E_M^{sms} may be either positive or negative depending on the electronic state. The field shifts E_M^{fs} are the potential deviations from the Coulomb potential of a point charge Z due to the finite size of the nucleus. The major contribution to the electron density at the origin comes from the inner s-electrons. Thus, the shift between the energy levels of two different isotopes can be given as

$$E_M = E_0 + E_M^{\text{nms}} + E_M^{\text{sms}} + E_M^{\text{fs}}, \quad (7)$$

and the level isotope shift between two isotopes M' and M is obtained by

$$E_{M'M} = E_{M'} - E_M. \quad (8)$$

Radiative properties of atoms are described with an electromagnetic transition between two states and is characterized by the angular momentum and the parity of the corresponding photon. They are very useful in the fields of quantum electronic, atomic physics and laser spectroscopy, plasma physics and astrophysics. Hence, the reliability of the values of these parameters is mainly based on the performance of the calculation methods used. A detail of theoretical background can be found in literature [5, 25]. If the emitted or observed photon has angular momentum k and parity $\pi = (-1)^k$, the transition is an electric multipole transition (E^k), while the transition from the absorbed photon with parity $\pi = (-1)^{k+1}$ is a magnetic multipole transition (M^k). The transition probability for the emission from the upper level to the lower level is given by

$$A^{\pi k}(\gamma J', \gamma J) = 2C_k [\alpha (E_{\gamma J'} - E_{\gamma J})]^{2k+1} \cdot \frac{S^{\pi k}(\gamma J', \gamma J)}{g_{J'}}, \quad (9)$$

where $S^{\pi k}$ is the line strength,

$$S^{\pi k}(\gamma J', \gamma J) = |\langle \gamma J || O^{\pi(k)} || \gamma J' \rangle|^2 \quad (10)$$

and $C_k = (2k+1)(k+1)/k((2k+1)!!)^2$. α is the fine-structure constant, and $O^{\pi(k)}$ is the transition operator. The transition rates (or probabilities) for forbidden

transitions depend on the third (M1) or fifth (E2) power of transition energy.

3. Results and Discussion

We have here reported the correlation, relativistic, and isotope effects on fine structure levels in the ground state configuration of the antimony anion (Sb^{-1}). The calculations have been performed using the MCHF atomic structure code [25] based on the multiconfiguration Hartree–Fock method within the framework of the Breit–Pauli Hamiltonian for relativistic effects in addition to correlation effects. In our previous work [24], we obtained the electron affinity value of 0.7305 eV for the antimony anion. This value is in agreement with [9]. In the present work we have found the electron affinity of 7970.96 cm^{-1} . This value is also in agreement with the value of $8436(4) \text{ cm}^{-1}$ given by Polak et al. [14]. In addition, the fine structure levels in the ground state both of neutral and negative ion of antimony are in agreement with other works according to previous results. In calculations we have considered the configuration sets including excited levels from outside core $5s^25p^3$ and $5s^25p^4$ for neutral antimony and its negative ion, respectively, according to valence correla-

tion. We have also considered the core correlation for this atom and anion, but we have a lot of configuration state functions and the convergence calculations for wavefunctions haven't been achieved very difficult. Hence, we have here considered the valence correlation and studied it using the configuration sets of $5s^25p^3$, $5s^25p^26p$, $5s^25p^24f$, $5s^25p^25f$, $5s^25p^26f$, $5s^25p^25d^2$, $5s^25p^24f^2$, $5s^25p^35d$, $5s^25p^36d$, $5s^25p^36s$, $5p^5$, $5p^35d^2$, $5s^25p^25d4f$, $5s^25p^25d5f$ and $5p^34f^2$ for neutral antimony, and $5s^25p^4$, $5s^25p^45d$, $5s^25p^46s$, $5s^25p^34f$, $5s^25p^35f$, $5s^25p^36p$, $5s^25p^34f5d$, $5s^25p^35d5f$, $5s^25p^35d6p$, $5s^25p^36s6p$, $5p^44f5f$, $5p^56p$, $5p^44f^2$, $5p^6$, $5p^45d^2$, $5p^44f^2$, $5p^45f^2$, $5p^46s^2$, $5p^46p^2$, $5s^25p^24f5f$, $5s^25p^24f6p$, $5s^25p^25d6s$, $5s^25p^25f6p$, $5s^25p^24f^2$, $5s^25p^25d^2$, $5s^25p^25f^2$, $5s^25p^26s^2$, and $5s^25p^26p^2$ for antimony anion.

Table 1 displays the non-relativistic energy (E_{MCHF}) including correlation effects, the relativistic energy ($E_{\text{MCHF+BP}}$) including the relativistic effects within the framework of the Breit–Pauli Hamiltonian, the normal mass shift (ΔE_{nms}), the specific mass shift (ΔE_{sms}), and the field shift (ΔE_{fs}) contributions in a.u. for Sb and Sb^{-} . We have obtained the energy value of 6313.4705072 a.u. for the ground state 4S and -6313.5153791 a.u. for the ground state 3P for antimony and antimony anion, respectively, when the ef-

Table 2. Transition energies ΔE (cm^{-1}) and transition probabilities A_{ki} (s^{-1}) for forbidden transitions (M1 and E2) of the ground state configuration $5s^25p^3$ for neutral antimony (Sb I). Numbers in the brackets denote the power of ten.

Transitions	Transition type	ΔE		A_{ki}	
		in this work	in [26], [27]	in this work	in [26]
$^4S_{3/2} - ^2D_{3/2}$	E2	–	8478, 8512	–	8.198(–3)
	M1	–	–	–	1.106
$^4S_{3/2} - ^2D_{5/2}$	E2	10941.17	9881, 9854	1.355(–2)	2.485(–2)
	M1	–	–	2.187(–2)	6.002(–2)
$^4S_{3/2} - ^2P_{1/2}$	E2	17974.84	16413, 16396	1.270(–2)	5.680(–2)
	M1	–	–	2.184	3.458
$^4S_{3/2} - ^2P_{3/2}$	E2	–	18446, 18465	–	1.381(–3)
	M1	–	–	–	5.340
$^2D_{3/2} - ^2D_{5/2}$	E2	1057.58	1403, 1342	0.534(–6)	4.233(–6)
	M1	–	–	1.147(–2)	2.538(–2)
$^2D_{3/2} - ^2P_{1/2}$	E2	8091.25	7983, 7884	1.896(–1)	2.110(–1)
	M1	–	–	0.988	1.166
$^2D_{3/2} - ^2P_{3/2}$	E2	–	9968, 9952	–	1.858(–1)
	M1	–	–	–	4.173
$^2D_{5/2} - ^2P_{1/2}$	E2	7033.67	6532, 6542	6.836(–2)	6.205(–2)
	M1	–	–	–	–
$^2D_{5/2} - ^2P_{3/2}$	E2	8474.83	8565, 8610	2.650(–1)	3.478(–1)
	M1	–	–	0.974	1.485
$^2P_{1/2} - ^2P_{3/2}$	E2	1441.16	2033, 2069	0.170(–5)	1.841(–5)
	M1	–	–	2.380(–2)	6.278(–2)

Table 3. Transition energies ΔE (cm^{-1}) and transition probabilities A_{ki} (s^{-1}) for forbidden transitions (M1 and E2) of the ground state configuration $5s^25p^4$ for antimony anion (Sb^-). Numbers in the brackets denote the power of ten.

Transitions	Transition type	ΔE		A_{ki}	
		in this work	in [10]	in this work	in [10]
$^3P_2 - ^3P_1$	E2	2207.84	2516	0.30(-3)	0.9(-3)
	M1			0.23	0.4
$^3P_2 - ^3P_0$	E2	2445.01	2831	0.74(-3)	2.0(-3)
	M1			-	
$^3P_2 - ^1S_0$	E2	15830.36	16700	0.53	-
	M1			-	
$^3P_0 - ^1D_2$	E2	5086.26	-	0.44(-4)	-
	M1			-	
$^1D_2 - ^3P_1$	E2	5323.43	-	0.61(-3)	-
	M1			0.085	
$^1D_2 - ^1S_0$	E2	8299.09	-	0.98	-
	M1			-	
$^1S_0 - ^3P_1$	E2		-	-	-
	M1	13622.52		3.78	
$^3P_1 - ^3P_0$	E2		-	-	-
	M1	237.17		0.70(-3)	
$^3P_2 - ^1D_2$	E2	7531.31	7628	-	-
	M1			-	

fects mentioned above have not been considered. The isotope effects are very small corresponding to the correlation and relativistic effects.

The electric quadrupole (E2) and magnetic dipole (M1) transitions between the fine structure levels of ground state have been given in Tables 2 and 3 for antimony and antimony anion, respectively. In Table 2, the energy differences (in cm^{-1}) and transition probabilities (in s^{-1}) for M1 and E2 transitions in neutral antimony have been presented and compared with those presented by Biemont [26] and Hassini et al. [27] in [23]. The most of our results are in agreement. It is seen in Table 2 that there is no our values for $^4S_{3/2} - ^2D_{3/2}$, $^4S_{3/2} - ^2P_{3/2}$ and $^2D_{3/2} - ^2P_{3/2}$ transitions. We haven't obtained these transitions in this work due to the forbidden of $J - J' = 0$ transitions in this computer code. For antimony anion, Table 3 includes also the energy differences and transition probabilities. We have compared the transition energies and the transition probabilities for some transitions can be compared with the values from [10] In Tables 2 and 3 we have omitted the core $[\text{Kr}]4d^{10}$ and only given the levels excited of $5s^25p^3$ and $5s^25p^4$ for neutral antimony and antimony anion, respectively.

4. Conclusion

In this work, we have performed the atomic structure calculations including correlation, relativistic, and isotope shift effects on antimony anion using the multiconfiguration Hartree–Fock method developed by Fischer [5, 25]. In calculations the configuration sets have been generated according to the valence correlation by single or double excitation from $5s^25p^3$ and $5s^25p^4$ for neutral antimony and its anion. We studied the transition energies and electron affinities for some atomic systems using this method, further the transition energies, electron affinities, and forbidden transitions for some atomic systems [24, 28–31]. Transition parameters for atoms and ions are fundamental quantities for many scientific applications. Especially, forbidden transitions such as M1 and E2 are of great interest for the plasma diagnostics since the photons from such transitions may carry information from large optical depths within the plasma. Some M1 and E2 transitions have been presented for the first time for Sb^- . Therefore, we hope that our results on M1 and E2 transitions for Sb, and especially for Sb^- , will provide theoretical supports for further other theoretical and experimental researchers.

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