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Abstract
We report on extensive relativistic multiconfiguration Dirac–Hartree–Fock (MCDHF) spectrum calculations for Sb IV. Energies, LS-compositions and Landé g_J-factors for 60 odd- and even-parity states are computed along with lifetimes and rates for transitions between these states. Results for the $5s^2\ ^1S_0$–$5s5p\ ^3P_0^o$ hyperfine-induced transition are also presented. Valence and core-valence electron correlation effects are accounted for by explicit configuration interaction. The calculated energies agree very well with experiment, but the labelling of some of the odd states is ambiguous due to close degeneracies between the 5p5d, 5s7p and 5p6s configurations. Computed lifetimes of the excited states are compared with values from cascade-corrected beam-foil measurements.

1. Introduction

Three-times ionized antimony (Sb IV) belongs to the Cd isoelectronic sequence and the ground state is $5s^2\ ^1S_0$. A revised and extended analysis by Rana *et al* [1] established 48 low lying levels. Based on multiconfiguration Hartree–Fock calculations with relativistic corrections (HFR) and least-squares-fitting (LSF) calculations, the same authors predicted some additional eight level positions. Pinnington *et al* [2] performed decay-curve analysis, incorporating the arbitrarily normalized decay curve (ANDC) method to correct for cascade effects, on beam-foil spectra to derive lifetimes for nine upper states involved in the resonance transitions.

On the theoretical side, work has been devoted to the allowed and spin-forbidden $5s^2\ ^1S$–$5s5p\ ^{1,3}P_1^o$ transitions, but comparatively little is known for more excited states. Migdalek and Baylis [3] used a limited relativistic configuration mixing and a polarization model to obtain rates of $5s^2\ ^1S$–$5s5p\ ^{1,3}P_1^o$ in the Cd isoelectronic sequence. Chou and Huang [4] applied the multiconfiguration relativistic random-phase approximation on the same transitions. Other theoretical results are due to Lavin *et al* [5] who used the relativistic quantum defect orbital method with and without an explicit account for core-valence correlation with the singlet–singlet transition and to Biémont *et al* [6] who used the relativistic Hartree–Fock approach, including a core-polarization potential, and the multiconfiguration Dirac–Fock method, taking the valence and core-valence correlation effects into account.

The purpose of this work is to improve and complement the dataset for Sb IV, especially for the more excited states, and to explore the capacity of the GRASP2K multiconfiguration Dirac–Hartree–Fock (MCDHF) package [7, 8] to predict transition rates in 'spectrum calculations' including states high up in the Rydberg series. Sb IV remains a challenge due to close degeneracies between the 5p5d, 5s7p and 5p6s odd-parity configurations. To facilitate a comparison with experimental data in this case, a transformation between the jj- and LSJ-coupling schemes becomes crucial [9, 10].

2. Computational procedure

The relativistic MCDHF method is described in great detail in a recent book by Grant [11]. Here we just give a brief outline of the method. Starting from the Dirac–Coulomb Hamiltonian for an N-electron system

$$H_{DC} = \sum_{i=1}^{N} \left(c\,\boldsymbol{\alpha}_i \cdot \boldsymbol{p}_i + (\beta_i - 1)c^2 + V_i^N \right) + \sum_{i>j}^{N} \frac{1}{r_{ij}}, \quad (1)$$

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where V^N is the monopole part of the electron–nucleus Coulomb interaction, the atomic state functions (ASFs) describing the studied fine-structure states are obtained as linear combinations of symmetry adapted configuration state functions (CSFs),

$$|\gamma PJM_J\rangle = \sum_{j=1}^{\text{NCSFs}} c_j |\gamma_j PJM_J\rangle. \tag{2}$$

In the expression above, P, J and M_J are the parity and the angular quantum numbers. γ denotes other appropriate labelling of the CSF, for example, orbital occupancy, and coupling scheme. The CSFs are built from products of one-electron Dirac orbitals. In the relativistic self-consistent field (RSCF) procedure, both the radial parts of the Dirac orbitals and the expansion coefficients are optimized to self-consistency. The Breit interaction

$$H_{\text{Breit}} = -\sum_{i<j}^{N} \left[\boldsymbol{\alpha}_i \cdot \boldsymbol{\alpha}_j \frac{\cos(\omega_{ij} r_{ij}/c)}{r_{ij}} \right.$$
$$\left. + (\boldsymbol{\alpha}_i \cdot \boldsymbol{\nabla}_i)(\boldsymbol{\alpha}_j \cdot \boldsymbol{\nabla}_j) \frac{\cos(\omega_{ij} r_{ij}/c) - 1}{\omega_{ij}^2 r_{ij}/c^2} \right] \tag{3}$$

as well as leading quantum electrodynamic (QED) corrections can be included in subsequent relativistic configuration interaction (RCI) calculations [12]. Calculations can be performed for single levels, but also for portions of a spectrum in the extended optimal level (EOL) scheme, where optimization is on a weighted sum of energies [13]. Using the latter scheme, a balanced description of a number of fine-structure states belonging to one or more configurations can be obtained in a single calculation. All calculations were performed with a new release [7] of the GRASP2K code [8].

3. Computation of atomic properties

Once the ASFs have been obtained, measurable properties such as hyperfine structures, Landé g_J-factors and transition rates can be expressed in terms of reduced matrix elements of tensor operators of different rank,

$$\langle \gamma PJ \| \mathbf{T}^{(k)} \| \gamma' P'J' \rangle. \tag{4}$$

Inserting the CSF expansions, the expression above reduces to a sum over matrix elements between CSFs. Using Racah algebra techniques, these matrix elements, in turn, can be obtained as sums over radial integrals [14].

3.1. Hyperfine structure

In atoms with non-zero nuclear spin, I, the fine-structure levels are split into closely spaced hyperfine levels. The splittings of the fine-structure levels are to first order given by the magnetic dipole, A_J, and electric quadrupole, B_J, hyperfine interaction constants,

$$A_J = \frac{\mu_I}{I} \frac{1}{\sqrt{J(J+1)}} \langle \gamma PJ \| \sum_{j=1}^{N}$$
$$- i\sqrt{2}\alpha \, r_j^{-2} (\boldsymbol{\alpha}_j \mathbf{C}^{(1)}(j))^{(1)} \| \gamma PJ\rangle, \tag{5}$$

$$B_J = 2Q\sqrt{\frac{J(2J-1)}{(J+1)(2J+3)}} \langle \gamma PJ \| \sum_{j=1}^{N} -r_j^{-3} \mathbf{C}^{(2)}(j) \| \gamma PJ\rangle, \tag{6}$$

where the reduced matrix elements are defined in the Brink and Satchler sense [15, 16]. The hyperfine levels of closely spaced fine-structure levels are also affected by the off-diagonal hyperfine interaction that mixes states with different J values and opens forbidden decay channels such as $5s^2 \, ^1S_0$–$5s5p \, ^3P_0^o$, see for example [17–19]. The nuclear magnetic dipole moments, μ_I, and the nuclear quadrupole moments, Q, for the different isotopes were taken from a compilation by Stone [20].

3.2. Landé g_J-factors

The Landé g_J-factors are given by

$$g_J = \frac{2}{\sqrt{J(J+1)}} \langle \gamma PJ \| \sum_{j=1}^{N}$$
$$\times \left[-i\frac{\sqrt{2}}{2\alpha^2} r_j (\boldsymbol{\alpha}_j \mathbf{C}^{(1)}(j))^{(1)} + \frac{g_s - 2}{2} \beta_j \boldsymbol{\Sigma}_j \right] \| \gamma PJ\rangle, \tag{7}$$

and determine the splitting of magnetic sub-levels in external magnetic fields. In addition, they give valuable information about the coupling conditions in the system [21]. The Landé g_J-factors were calculated using the Zeeman module of GRASP2K [22].

3.3. Isotope shift

Corrections to the calculated energy structure due to isotope-dependent recoil motion of the nucleus and finite nuclear volume effects were included in first-order perturbation theory with the ASFs as zero-order functions. The corrections, within the lowest-order relativistic approximation (v^2/c^2) and to first order in m_e/M, can be written [23, 24] as

$$E_M = (S_{\text{nms}} + S_{\text{sms}}) \frac{1}{M} + \frac{2}{3}\pi Z\rho(0)\langle r_M^2\rangle, \tag{8}$$

where

$$S_{\text{nms}} = \langle \gamma PJM_J | \frac{1}{2} \sum_{j=1}^{N} \left(\mathbf{p}_j^2 - \frac{\alpha Z}{r_j} \boldsymbol{\alpha}_j \cdot \mathbf{p}_j \right.$$
$$\left. - \frac{\alpha Z}{r_j} (\boldsymbol{\alpha}_j \cdot \mathbf{C}_j^1) \mathbf{C}_j^1 \cdot \mathbf{p}_j \right) | \gamma PJM_J\rangle \tag{9}$$

and

$$S_{\text{sms}} = \langle \gamma PJM_J | \frac{1}{2} \sum_{i \neq j}^{N} \left(\mathbf{p}_i \cdot \mathbf{p}_j - \frac{\alpha Z}{r_i} \boldsymbol{\alpha}_i \cdot \mathbf{p}_j \right.$$
$$\left. - \frac{\alpha Z}{r_i} (\boldsymbol{\alpha}_i \cdot \mathbf{C}_i^1) \mathbf{C}_i^1 \cdot \mathbf{p}_j \right) | \gamma PJM_J\rangle \tag{10}$$

are, respectively, the normal and specific mass shift parameters. The expectation value

$$\rho(0) = \langle \gamma PJM_J | \sum_{j=1}^{N} \delta(\mathbf{r}_j) | \gamma PJM_J\rangle \tag{11}$$

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gives the electron density at the site of the nucleus. M is the mass of the nucleus and $\langle r_M^2 \rangle$ is the root-mean-square radius, both in atomic units. From these quantities, the transition isotope shift $\Delta E_{M',M}$ between two isotopes M' and M was obtained as

$$\Delta E_{M',M} = (\Delta S_{\mathrm{nms}} + \Delta S_{\mathrm{sms}}) \left(\frac{1}{M'} - \frac{1}{M} \right)$$
$$+ \frac{2\pi}{3} Z \Delta \rho(0) \left(\langle r_{M'}^2 \rangle - \langle r_M^2 \rangle \right), \tag{12}$$

where the differences in the electronic quantities are between the values of upper and lower levels in the transition. The isotope shift parameters were calculated using a new isotope shift module RIS [25] of the GRASP2K package.

3.4. Transition parameters

The transition parameters, such as rates for spontaneous decay, for multipole transitions between two atomic states $\gamma P J M_J$ and $\gamma' P' J' M_J'$ can be expressed in terms of the reduced matrix elements,

$$\langle \gamma P J \| \mathbf{Q}_k^{(\lambda)} \| \gamma' P' J' \rangle, \tag{13}$$

where $\mathbf{Q}_k^{(\lambda)}$ is the electromagnetic multipole operator of order k in length (Babushkin) or velocity (Coulomb) gauge [26]. The superscript designates the type of multipole: $\lambda = 1$ for electric multipoles and $\lambda = 0$ for magnetic multipoles. Standard Racah algebra assumes that the ASFs are built from the same orthogonal radial orbital set [14]. However, this restriction can be relaxed. To compute transition matrix elements between two ASFs described by independently optimized orbital sets, transformations of the ASFs are performed in such a way that the orbital sets become biorthogonal, in which case the calculation can be handled using standard techniques [27, 28].

4. Calculations

4.1. Spectrum

It is, from some perspectives, desirable to perform separate calculations for each of the studied fine-structure states. This approach, however, is impractical and time consuming when considering large portions of a spectrum. In this work, the ASFs were instead determined simultaneously in EOL calculations on the weighted energy average of the fine-structure states [13]. As a starting point, two MCDHF calculations were performed in the EOL scheme: one calculation with CSFs describing the 24 even-parity states from the $5s^2\ ^1S_0$ ground state up to $5s8s\ ^1S_0$, and one calculation with CSFs describing the 36 odd-parity states from $5s5p\ ^3P_0^o$ up to $5p6s\ ^1P_1^o$. To correct for electron correlation effects, these calculations were followed by calculations with expansions including CSFs obtained by single (S) and double (D) excitations from, respectively, the studied even- and odd-state reference configurations to active sets of orbitals. Of the excitations from the even- and odd-state reference configurations, at most one was allowed from the outer 4d core shell. The 1s, 2s, . . . , 4s, 4p core shells are all kept closed. The active sets for the even- and odd-parity states,

consisting of spectroscopic orbitals from the initial MCDHF calculations, were consecutively enlarged by adding four layers of correlation orbitals. Each layer contained orbitals with s, p, d, f, g symmetries (in non-relativistic notation). Two layers also included orbitals with h symmetry. Due to stability problems in the RSCF procedure, only the outermost layers of orbitals could be optimized each time. The largest calculation for the even-parity states included 66 relativistic orbitals and more than 217 000 CSFs distributed over the $J = 0, 1, 2, 3, 4, 5$ symmetries. The largest calculation for the odd-parity states was based on 68 relativistic orbitals and around 373 000 CSFs with symmetries $J = 0, 1, 2, 3, 4$. The MCDHF calculations were complemented by final RCI calculations, where the Breit interaction was added to the electron–electron Coulomb interaction.

4.2. Ground and first excited states

In EOL calculations, the included correlation orbitals correct the wavefunctions for a number of fine-structure states at the same time. Obviously this will give less accurate results compared with the case where the correlation orbitals are obtained in separate calculations for each of the states. To check the accuracy of the spectrum calculations described above, separate calculations were performed for the $5s^2\ ^1S_0$ ground state and the excited $5s5p\ ^3P_{0,1,2}^o$, $^1P_1^o$ states. The expansions for the ground state were obtained by allowing SD excitations from the $5s^2$, $5p^2$ and $5d^2$ complex to an active set. As for the full spectrum calculations, at most one excitation was allowed from the outer 4d core shell. The $5s5p\ ^3P_{0,1,2}^o$, $^1P_1^o$ states were treated together in an EOL scheme. The expansions for these states were obtained by allowing SD excitations from the $5s5p$ and $5p5d$ complex to an active set. The active sets were increased by adding five layers of correlation orbitals. All calculations were followed by RCI calculations including the Breit interaction. To account for spin- and orbital-polarization, additional RCI calculations were performed with the expansions from the previous RCI calculations augmented by CSFs generated by allowing single excitations from all core shells of the initial reference configurations to the active set of orbitals [29]. Although the radial orbitals are optimized on valence- and core-valence effects, and thus do not have the optimal location for accounting for spin-polarization effects, this approach has previously been shown to be quite successful [30].

5. Results and discussion

5.1. Spectrum properties

Energy values from the spectrum calculations are displayed in table 1. The inclusion of the valence and core-valence correlation effects within the CSF basis, on which the four layers of correlation orbitals are optimized, improves the energies dramatically, and the final energies are in very good agreement with experiment with an average difference of only 0.12%. The majority of the levels are a few hundred cm^{-1} too high relative to the $5s^2\ ^1S_0$ ground level. The $5p^2\ ^1S_0$ and $5p6s\ ^1P_1^o$ levels are around 900 cm^{-1} too high, but they

Table 1. Calculated and experimental energy levels in cm^{-1}. Columns 2 and 3 present respectively the *LS*-compositions and Landé g_J-factors. Column 5 displays experimental energies and energies from HFR calculations by Rana *et al* [1]. The latter energies are denoted by ∗. The last column, labelled 'Diff', gives differences in energy between experiment and the largest calculation-based four layers of correlation orbitals. In some cases, the level designations do not agree with the ones given by Rana *et al* [1]. Whenever this is the case, the designation from the latter work is given in parentheses on the line below. Note that we have retained the designation 5p5d $^3P_2^o$ suggested by Rana *et al* for the level at 265 094.3 cm^{-1}.

Level	*LS*-composition	g_J	E	Exp/HFR	Diff
5s^2 $^1S_0$	0.95 5s^2 ^{1}S + 0.02 5p^2 ^{1}S				
5s5p $^3P_0^o$	0.98 5s5p ^{3}P^o		64 735	64 437.3	−298
5s5p $^3P_1^o$	0.96 5s5p ^{3}P^o	1.493	66 952	66 698.1	−255
5s5p $^3P_2^o$	0.98 5s5p ^{3}P^o	1.501	72 727	72 555.7	−172
5s5p $^1P_1^o$	0.93 5s5p ^{1}P^o	1.008	95 551	95 956.7	405
5p^2 $^3P_0$	0.93 5p^2 ^{3}P + 0.04 5p^2 ^{1}S		152 137	152 063.2	−74
5p^2 $^1D_2$	0.56 5p^2 ^{1}D + 0.27 5p^2 ^{3}P + 0.12 5s5d ^{1}D	1.140	156 322	155 947.6	−375
5p^2 $^3P_1$	0.97 5p^2 ^{3}P	1.501	156 339	156 381.7	42
5p^2 $^3P_2$	0.70 5p^2 ^{3}P + 0.19 5p^2 ^{1}D + 0.07 5s5d ^{1}D	1.359	163 548	163 521.4	−27
5s5d $^3D_1$	0.82 5s5d ^{3}D + 0.15 5s6d ^{3}D	0.499	178 895	178 913.3	18
5s5d $^3D_2$	0.82 5s5d ^{3}D + 0.15 5s6d ^{3}D	1.167	179 244	179 264.7	20
5s5d $^3D_3$	0.83 5s5d ^{3}D + 0.14 5s6d ^{3}D	1.334	179 877	179 820.9	−57
5p^2 $^1S_0$	0.87 5p^2 ^{1}S + 0.04 5p^2 ^{3}P		185 345	184 429.5	−916
5s6s $^3S_1$	0.84 5s6s ^{3}S + 0.08 5s7s ^{3}S + 0.05 5s8s ^{3}S	2.002	188 837	188 623.0	−214
5s5d $^1D_2$	0.67 5s5d ^{1}D + 0.21 5p^2 ^{1}D + 0.06 5s6d ^{1}D	1.002	193 679	193 445.6	−234
5s6s $^1S_0$	0.85 5s6s ^{1}S + 0.06 5s7s ^{1}S		194 313	193 948.4	−365
5s6p $^3P_0^o$	0.87 5s6p ^{3}P^o + 0.10 5s7p ^{3}P^o		215 581	215 387.3	−194
5s6p $^3P_1^o$	0.76 5s6p ^{3}P^o + 0.12 5s6p ^{1}P^o + 0.08 5s7p ^{3}P^o	1.433	215 922	215 734.1	−189
5s6p $^3P_2^o$	0.87 5s6p ^{3}P^o + 0.10 5s7p ^{3}P^o	1.501	217 960	217 804.8	−156
5s6p $^1P_1^o$	0.75 5s6p ^{1}P^o + 0.12 5s6p ^{3}P^o + 0.07 5s7p ^{1}P^o	1.068	219 187	219 029.0	−158
5s4f $^3F_2^o$	0.58 5s4f ^{3}F^o + 0.35 5s5f ^{3}F^o + 0.05 5p5d ^{3}F^o	0.666	227 203	227 059.0	−144
5s4f $^3F_3^o$	0.58 5s4f ^{3}F^o + 0.33 5s5f ^{3}F^o + 0.04 5p5d ^{3}F^o	1.081	227 264	227 144.0	−120
5s4f $^3F_4^o$	0.62 5s4f ^{3}F^o + 0.33 5s5f ^{3}F^o + 0.03 5p5d ^{3}F^o	1.250	227 420	227 304.0	−116
5s4f $^1F_3^o$	0.58 5s4f ^{1}F^o + 0.30 5s5f ^{1}F^o + 0.07 5p5d ^{1}F^o	1.002	228 499	228 438.0	−61
5p5d $^3F_2^o$	0.66 5p5d ^{3}F^o + 0.26 5p5d ^{1}D^o + 0.03 5s4f ^{3}F^o	0.764	254 321	254 143.8	−178
5s6d $^3D_1$	0.82 5s6d ^{3}D + 0.15 5s5d ^{3}D	0.499	254 958	254 678.4	−280
5s6d $^3D_2$	0.82 5s6d ^{3}D + 0.15 5s5d ^{3}D	1.166	255 094	254 829.0	−265
5s6d $^3D_3$	0.83 5s6d ^{3}D + 0.14 5s5d ^{3}D	1.334	255 373	255 081.6	−292
5s6d $^1D_2$	0.84 5s6d ^{1}D + 0.14 5s5d ^{1}D	1.001	256 934	256 513.6	−421
5s7s $^3S_1$	0.66 5s7s ^{3}S + 0.19 5s8s ^{3}S + 0.13 5s6s ^{3}S	2.002	258 061	257 771.9	−290
5p5d $^3F_3^o$	0.85 5p5d ^{3}F^o + 0.06 5p5d ^{3}D^o + 0.04 4f5s ^{3}F^o	1.098	258 051	257 840.1	−212
5p5d $^1D_2^o$	0.51 5p5d ^{1}D^o + 0.18 5p5d ^{3}F^o + 0.15 5p5d ^{3}P^o	1.035	258 962	258 835.2	−127
5s7s $^1S_0$	0.70 5s7s ^{1}S + 0.17 5s8s ^{1}S + 0.11 5s6s ^{1}S		259 666	259 327.3	−339
5p5d $^3F_4^o$	0.93 5p5d ^{3}F^o + 0.04 5s4f ^{3}F^o	1.250	262 878	262 631.5	−247
5p5d $^3D_1^o$	0.72 5p5d ^{3}D^o + 0.18 5p5d ^{3}P^o + 0.05 5p5d ^{1}P^o	0.729	262 971	262 962.2	−10
5p5d $^3P_2^o$	0.28 5p5d ^{3}P^o + 0.40 5p5d ^{3}D^o + 0.20 5p5d ^{1}D^o	1.198	265 146	265 094.3	−52
5p5d $^3P_0^o$	0.45 5p5d ^{3}P^o + 0.44 5s7p ^{3}P^o + 0.08 5s6p ^{3}P^o		268 390	268 108.0	−282
5p5d $^3P_1^o$ (5s7p $^1P_1^o$)	0.36 5p5d ^{3}P^o + 0.31 5s7p ^{3}P^o + 0.13 5p5d ^{3}D^o (0.28 5s7p ^{1}P^o + 0.26 5p5d ^{3}P^o + 0.19 5p6s ^{3}P^o)	1.306	268 675	268 471.2	−204
5p5d $^3D_3^o$	0.85 5p5d ^{3}D^o + 0.07 5p5d ^{3}F^o	1.299	268 407	268 547.5	140
5p6s $^3P_0^o$ (5s7p $^3P_0^o$)	0.60 5p6s ^{3}P^o + 0.26 5p5d ^{3}P^o + 0.11 5s7p ^{3}P^o (0.58 5s7p ^{3}P^o + 0.41 5p6s ^{3}P^o)		270 527	269 052∗	−1475
5s7p $^1P_1^o$ (5s7p $^3P_1^o$)	0.40 5s7p ^{1}P^o + 0.21 5p6s ^{1}P^o + 0.16 5p6s ^{3}P^o (0.28 5s7p ^{3}P^o + 0.25 5p5d ^{3}P^o + 0.16 5s7p ^{1}P^o)	1.111	269 160	269 078∗	−82
5p5d $^3D_2^o$	0.39 5p5d ^{3}D^o + 0.34 5p5d ^{3}P^o + 0.19 5s7p ^{3}P^o	1.356	269 232	269 195.4	−37
5s7p $^3P_1^o$	0.33 5s7p ^{3}P^o + 0.32 5p5d ^{3}P^o + 0.16 5p6s ^{3}P^o	1.407	271 320	270 319∗	−1002
5s5f $^1F_3^o$	0.46 5s5f ^{1}F^o + 0.36 5s4f ^{1}F^o + 0.11 5p5d ^{1}F^o	1.015	271 941	270 947∗	−994
5s7p $^3P_2^o$	0.65 5s7p ^{3}P^o + 0.18 5p5d ^{3}P^o + 0.06 5s6p ^{3}P^o	1.481	271 995	271 375∗	−620
5s5f $^3F_2^o$	0.60 5s5f ^{3}F^o + 0.36 5s4f ^{3}F^o	0.667	272 673	272 126∗	−547
5s5f $^3F_3^o$	0.61 5s5f ^{3}F^o + 0.34 5s4f ^{3}F^o	1.084	272 664	272 175∗	−490
5s5f $^3F_4^o$	0.63 5s5f ^{3}F^o + 0.33 5s4f ^{3}F^o	1.251	272 695	272 262∗	−434
5s7p $^3P_0^o$ (5p6s $^3P_0^o$)	0.34 5s7p ^{3}P^o + 0.36 5p6s ^{3}P^o + 0.26 5p5d ^{3}P^o (0.38 5p6s ^{3}P^o + 0.33 5s7p ^{3}P^o + 0.28 5p5d ^{3}P^o)		272 917	272 690.0	−227
5p6s $^3P_1^o$	0.41 5p6s ^{3}P^o + 0.22 5s7p ^{1}P^o + 0.18 5s7p ^{3}P^o	1.327	273 778	273 535.3	−244
5p5d $^1P_1^o$	0.45 5p5d ^{1}P^o + 0.22 5p6s ^{1}P^o + 0.19 5p6s ^{3}P^o	1.102	278 635	278 272.5	−363
5p6s $^3P_2^o$	0.95 5p6s ^{3}P^o + 0.02 5s7p ^{3}P^o	1.501	279 949	279 778.0	−172
5s5g $^1G_4$	0.50 5s5g ^{1}G + 0.48 5s5g ^{3}G	1.025	281 639		
5s5g $^3G_3$	0.98 5s5g ^{3}G	0.749	281 640		

Table 1. (Continued.)

Level	*LS*-composition	g_J	E	Exp/HFR	Diff
$5s5g\ ^3G_4$	$0.50\ 5s5g\ ^3G + 0.48\ 5s5g\ ^1G$	1.025	281 688		
$5s5g\ ^3G_5$	$0.98\ 5s5g\ ^3G$	1.200	281 690		
$5p5d\ ^1F_3^o$	$0.73\ 5p5d\ ^1F^o + 0.19\ 5s5f\ ^1F^o$	1.005	285 989	285 536.4	−453
$5p6s\ ^1P_1^o$	$0.44\ 5p6s\ ^1P^o + 0.39\ 5p5d\ ^1P^o + 0.05\ 5s7p\ ^1P^o$	1.020	287 180	286 257.7	−922
$5s8s\ ^3S_1$	$0.74\ 5s8s\ ^3S + 0.24\ 5s7s\ ^3S$	2.002	290 771	290 488.5	−283
$5s8s\ ^1S_0$	$0.77\ 5s8s\ ^1S + 0.21\ 5s7s\ ^1S$		291 447	291 405.8	−41

seem to be moving in the right direction as the orbital set is increased. Included in the comparison in table 1, there are eight predicted energy levels, denoted by asterisks, from the semi-empirical multiconfiguration Hartree–Fock calculation with relativistic corrections (HFR) by Rana *et al* [1]. The agreement with the HFR values is not as good as with experiment, reaching 1500 cm^{-1} for the $5p6s\ ^3P_0^o$ state (this state is labelled $5s7p\ ^3P_0^o$ in the HFR calculations). These differences reflect the combined uncertainty of the two calculations. The labels for some of the levels are not consistent with the ones given by Rana, and in these cases, the corresponding label from the latter work is given in parentheses on the line below.

In relativistic calculations, the states are normally given in jj-coupling. To obtain more appropriate labels, we have performed a transformation to the LSJ coupling scheme. The transformation procedure was developed by Gaigalas and co-workers [9, 10] and adapted for large-scale calculations in the new release of the GRASP2K code [7]. In table 1, we give LS-compositions of the even and odd states. We also give the Landé g_J-factors, which provide information about the splittings of magnetic sub-levels in external magnetic fields. The 5p5d, 5p7p and 5p6s odd configurations overlap, with average energies of 266 210, 271 183 and 276 773 cm^{-1}, respectively, and there is considerable configuration mixing for several states, making it difficult to assign a proper label. In the analysis by Rana *et al,* the positions of the levels of the 5s7p configuration could not be experimentally established and they had to guess the average energy in the HFR calculation. As commented by Rana *et al,* a slight shift in the average position of 5s7p has a dramatic effect on the LS-composition. Traces of this problem can be seen for the $5p5d\ ^3P_1^o$, $5p6s\ ^3P_0^o$, $5s7p\ ^1P_1^o$, $5s7p\ ^3P_0^o$ states. Here the current LS-composition does not match the one from the HFR calculation. The composition from the latter calculation is given in parentheses on the line below. In addition, although not as severe, there is also an inconsistency in the labelling of the $5p5d\ ^3D_2^o$ state. One should keep in mind that the labelling is not anything absolute, but in some cases with close degeneracies dependent on the calculation and the correlation effects included.

Table 2 gives the calculated lifetimes for all the states, where the length gauge has been used for the electric dipole transitions. The longest lifetimes are the ones of the $5s5p\ ^3P^o$ term. In table 2, averaged calculated lifetimes of states belonging to nine terms (value in parentheses) are compared with values from cascade-corrected beam-foil measurements by Pinnington *et al* [2] and from other theory. The agreement between the current averaged lifetimes and experimental lifetimes is very good. The only exceptions are the $5s4f\ ^{1,3}F^o$

terms, where theory gives shorter lifetimes. We note that the Coulomb approximation gives unreliable values of the lifetimes [2].

Weighted oscillator strengths and transition rates for spontaneous emission are presented in table 3. Rates are based on computed transition energies. Length gauge has been used for the transitions. To assess the accuracy of the computed values, also the ratios, R, between the rates in the length and velocity gauges are given. In most cases, the ratio is close to 1, but for some of the weaker transitions, values in the two gauges differ substantially, giving ratios far from 1. The weakness of a transition frequently comes out as a result of cancellation between a number of large contributions or between different parts of the radial transition integrals [31]. A small imbalance due to correlation effects may thus change the calculated transition probabilities dramatically in one of the gauges. It is difficult to infer the accuracy of the computed transition parameters, but weak transitions with values of R far from 1 are associated with rather large uncertainties.

One may note that there are several strong transitions between states belonging to configurations differing by more than one electron. One example is the $5s7p\ ^1P_1^o$–$5p^2\ ^1D_2$ transition with the rate 1.19×10^9 s^{-1}. These transition rates are identically zero in the independent particle model, and become allowed only due to configuration interaction effects [29].

5.2. The resonance transition

In table 4, energies and rates in length and velocity gauges for the $5s^2\ ^1S_0$–$5s5p\ ^3P_1^o$ and $5s^2\ ^1S_0$–$5s5p\ ^1P_1^o$ electric dipole (E1) transitions are shown. In addition, values are given for the weak $5s^2\ ^1S_0$–$5s5p\ ^3P_2^o$ magnetic quadrupole (M2) transition. The values were obtained from increasingly large RCI calculations including the Breit interaction and leading QED effects. The transition parameters converge rapidly with the active sets, and basically only two layers of correlation orbitals are needed. Comparing the transition energies and rates with the ones from the spectrum calculation, we see that there is a very good consistency. The good overall agreement strengthens our confidence in the spectrum calculations, indicating that these include the same correlation effects as do the calculations targeted for the individual states. In table 4, values from the HFR and MCDHF calculations of Biémont *et al* [6] are also presented. The MCDHF calculations include the same correlation effects as the present calculations, but the $^1P_1^o$ state is separately optimized in one calculation and the three $^3P^o$ states in another. One notes the large effect of the optimization scheme on the rate of the allowed transition in

Table 2. Lifetimes in ns. τ_{RCI}: this work; τ_{exp}: beam foil; τ_C: Coulomb approximation; τ_{HFR}: Hartree–Fock calculation including configuration interaction. The calculated lifetimes in the Coulomb approximation and using the HFR approximation are quoted from the paper by Pinnington *et al* [2]. When the level designation does not agree with the one given by Rana *et al* [1], the designation from the latter work is given in parentheses.

State	τ_{RCI}	τ_{exp}^a	τ_C^a	τ_{HFR}^a
$5s5p\ ^3P_1^o$	66.73			
$5s5p\ ^1P_1^o$	0.32	0.38 ± 0.04	0.23	0.20
$5p^2\ ^3P_0$	0.41			
$5p^2\ ^1D_2$	1.15	1.40 ± 0.25	0.52	1.23
$5p^2\ ^3P_1$	0.38			
$5p^2\ ^3P_2$	0.46			
$5s5d\ ^3D_1$	$0.21(0.22)^a$	0.25 ± 0.05	0.21	0.18
$5s5d\ ^3D_2$	$0.21(0.22)^a$	0.25 ± 0.05	0.21	0.18
$5s5d\ ^3D_3$	$0.23(0.22)^a$	0.25 ± 0.05	0.21	0.18
$5p^2\ ^1S_0$	0.46			
$5s6s\ ^3S_1$	0.21			
$5s5d\ ^1D_2$	0.16	0.19 ± 0.04	0.35	0.12
$5s6s\ ^1S_0$	0.22			
$5s6p\ ^3P_0^o$	$1.81(1.55)^a$	1.30 ± 0.20	3.04	1.54
$5s6p\ ^3P_1^o$	$1.47(1.55)^a$	1.30 ± 0.20	3.04	1.54
$5s6p\ ^3P_2^o$	$1.56(1.55)^a$	1.30 ± 0.20	3.04	1.54
$5s6p\ ^1P_1^o$	1.00			
$5s4f\ ^3F_2^o$	$1.60(1.56)^a$	2.0 ± 0.4	1.13	1.48
$5s4f\ ^3F_3^o$	$1.56(1.56)^a$	2.0 ± 0.4	1.13	1.48
$5s4f\ ^3F_4^o$	$1.55(1.56)^a$	2.0 ± 0.4	1.13	1.48
$5s4f\ ^1F_3^o$	0.91	1.37 ± 0.20	2.76	1.47
$5p5d\ ^3F_2^o$	0.48			
$5s6d\ ^3D_1$	$0.84(0.88)^a$	0.90 ± 0.20	0.72	0.53
$5s6d\ ^3D_2$	$0.86(0.88)^a$	0.90 ± 0.20	0.72	0.53
$5s6d\ ^3D_3$	$0.92(0.88)^a$	0.90 ± 0.20	0.72	0.53
$5s6d\ ^1D_2$	0.73	0.60 ± 0.20	1.03	0.49
$5p5d\ ^3F_3^o$	0.48			
$5s7s\ ^3S_1$	0.35			
$5p5d\ ^1D_2^o$	0.26			
$5s7s\ ^1S_0$	0.41			
$5p5d\ ^3F_4^o$	0.52			
$5p5d\ ^3D_1^o$	0.14			
$5p5d\ ^3P_2^o$	0.17			
$5p5d\ ^3P_0^o$	0.56			
$5p5d\ ^3D_3^o$	0.13			
$5p5d\ ^3P_1^o(5s7p\ ^1P_1^o)$	0.29			
$5s7p\ ^1P_1^o(5s7p\ ^3P_1^o)$	0.36			
$5p5d\ ^3D_2^o$	0.20			
$5p6s\ ^3P_0^o(5s7p\ ^3P_0^o)$	0.14			
$5s7p\ ^3P_1^o$	0.19			
$5s5f\ ^1F_3^o$	0.45			
$5s7p\ ^3P_2^o$	0.37			
$5s5f\ ^3F_3^o$	3.20			
$5s5f\ ^3F_2^o$	3.11			
$5s5f\ ^3F_4^o$	3.73			
$5s7p\ ^3P_0^o(5p6s\ ^3P_0^o)$	0.66			
$5p6s\ ^3P_1^o$	0.57			
$5p5d\ ^1P_1^o$	0.31			
$5p6s\ ^3P_2^o$	0.24			
$5s5g\ ^1G_4$	0.87			
$5s5g\ ^3G_3$	0.86			
$5s5g\ ^3G_4$	0.86			
$5s5g\ ^3G_5$	0.86			
$5p5d\ ^1F_3^o$	0.13			

Table 2. (Continued.)

State	τ_{RCI}	τ_{exp}^a	τ_C^a	τ_{HFR}^a
$5p6s\ ^1P_1^o$	0.12			
$5s8s\ ^3S_1$	0.57			
$5s8s\ ^1S_0$	0.68			

^{a} The experimental and other theoretical lifetimes are term averaged. The reported values in parentheses are the term-averaged lifetimes from our RCI calculation.

velocity gauge. Overall, the different calculations agree very well. For $5s^2\ ^1S_0$–$5s5p\ ^1P_1^o$, the theoretical transition rates seem to be somewhat larger than the rate derived from the beam-foil lifetime measurement by Pinnington *et al* [2].

Hyperfine-structure constants obtained from the RCI wavefunctions including spin polarization are displayed in table 5. Both diagonal and off-diagonal parameters are shown. The diagonal and off-diagonal constants show a similar convergence pattern, and are fairly stable after three layers of correlation orbitals.

In table 6, the differences ΔS_{nms}, ΔS_{sms} and $\Delta \rho(0)$ between the upper and lower state isotope shift parameters in the $5s^2\ ^1S_0$–$5s5p\ ^3P_1^o$ transition are shown as functions of the increasing active set of orbitals. The computed quantities converge after three layers of correlation orbitals. Combining the computed differences in electronic quantities with differences in nuclear masses and charge radii according to equation (12), we obtain the isotope shift

$$\Delta \nu = \nu_{123} - \nu_{121} = \underbrace{(0.1208)}_{\Delta\nu_{nms}}$$
$$+ \underbrace{(0.3159)}_{\Delta\nu_{sms}} + \underbrace{-1.0278}_{\Delta\nu_{vol}} = -0.5911 \text{ GHz.} \quad (14)$$

For the nuclear charge radii, we use the values proposed by Angeli [32] $\langle r_{121}^2 \rangle = 21.904\,272\,04$ fm^2 and $\langle r_{123}^2 \rangle = 21.976\,406\,41$ fm^2. The nuclear masses were taken from the tables by Audi *et al* [33]. As expected for such a heavy system, the shift is dominated by the volume effect. To estimate the accuracy of the calculated isotope shift, we may look at the isotope shift for the $5s^2\ ^1S_0$–$5s5p\ ^3P_1^o$ transition in In II. Calculations similar to the ones presented here predicted the ^{115,113}In isotope shift to be -0.515 GHz [30]. This should be compared with the most recent values of the shift that gives $-0.695\,76(0.168)$ GHz [34], i.e. indicating an error of around 30% in the calculations. Provided that the difference in charge radii for Sb is known with the same accuracy as the difference in charge radii for In, we can expect that the calculated ^{123,121}Sb isotope shift is associated with an error of the same magnitude.

5.3. The $5s^2\ ^1S_0$–$5s5p\ ^3P_0^o$ hyperfine-induced transition

The hyperfine interaction, although weak, not only shifts and splits individual J levels, but also mixes wavefunctions with different J quantum numbers. The wavefunction for the $5s5p\ ^3P_0^o$ state can, when the hyperfine interaction is included, be written as

$$|\text{'}5s5p\ ^3P_0^o\ IF\text{'}\rangle = c_0|5s5p\ ^3P_0^o\ IF\rangle + \sum_i c_i|\gamma_i PJ_i IF\rangle, \quad (15)$$

Table 3. Weighted oscillator strengths and transition rates for spontaneous emission in units of s^{-1}. Rates are based on computed transition energies. Length gauge has been used for E1 transitions. R is the ratio between transition rates in length and velocity gauge. When the level designation does not agree with the one given by Rana *et al* [1], the designation from the latter work is given in parentheses.

Upper	Lower	ΔE_{calc} (cm^{-1})	λ (nm)	gf	A	R
$5s5p\ ^1P^o_1$	$5s^2\ ^1S_0$	95 551	104.66	1.55E+00	3.15E+09	0.93
$5p^2\ ^3P_1$	$5s5p\ ^3P^o_0$	91 604	109.17	5.52E−01	1.03E+09	0.94
$5s5d\ ^3D_1$	$5s5p\ ^3P^o_0$	114 160	87.60	9.39E−01	2.72E+09	0.96
$5s6s\ ^3S_1$	$5s5p\ ^3P^o_0$	124 101	80.58	1.53E−01	5.24E+08	1.04
$5p^2\ ^3P_0$	$5s5p\ ^3P^o_1$	85 184	117.39	4.96E−01	2.40E+08	0.94
$5p^2\ ^1D_2$	$5s5p\ ^3P^o_1$	89 370	111.89	2.70E−01	2.88E+08	0.94
$5p^2\ ^3P_1$	$5s5p\ ^3P^o_1$	89 386	111.87	3.92E−01	6.97E+08	0.94
$5p^2\ ^3P_2$	$5s5p\ ^3P^o_1$	96 595	103.53	4.66E−01	5.80E+08	0.94
$5s5d\ ^3D_1$	$5s5p\ ^3P^o_1$	111 942	89.33	7.06E−01	1.97E+09	0.96
$5s5d\ ^3D_2$	$5s5p\ ^3P^o_1$	112 291	89.05	2.09E+00	3.52E+09	0.96
$5s6s\ ^3S_1$	$5s5p\ ^3P^o_1$	121 884	82.05	4.77E−01	1.58E+09	1.03
$5p^2\ ^1D_2$	$5s5p\ ^3P^o_2$	83 595	119.62	5.07E−01	4.73E+08	0.93
$5p^2\ ^3P_1$	$5s5p\ ^3P^o_2$	83 611	119.60	5.89E−01	9.16E+08	0.93
$5p^2\ ^3P_2$	$5s5p\ ^3P^o_2$	90 820	110.11	1.41E+00	1.55E+09	0.94
$5s5d\ ^3D_2$	$5s5p\ ^3P^o_2$	106 516	93.88	7.46E−01	1.13E+09	0.96
$5s5d\ ^3D_3$	$5s5p\ ^3P^o_2$	107 149	93.33	4.01E+00	4.39E+09	0.95
$5s6s\ ^3S_1$	$5s5p\ ^3P^o_2$	116 109	86.13	9.11E−01	2.73E+09	1.03
$5s7s\ ^3S_1$	$5s5p\ ^3P^o_2$	185 334	53.96	1.43E−01	1.09E+09	1.05
$5p^2\ ^1D_2$	$5s5p\ ^1P^o_1$	60 771	164.55	2.23E−01	1.10E+08	0.92
$5p^2\ ^1S_0$	$5s5p\ ^1P^o_1$	89 793	111.37	3.89E−01	2.09E+09	0.95
$5s5d\ ^1D_2$	$5s5p\ ^1P^o_1$	98 128	101.91	4.91E+00	6.31E+09	0.95
$5s6s\ ^1S_0$	$5s5p\ ^1P^o_1$	98 761	101.25	6.96E−01	4.53E+09	1.02
$5s6d\ ^1D_2$	$5s5p\ ^1P^o_1$	161 383	61.96	1.59E−01	5.54E+08	0.87
$5p5d\ ^3D^o_1$	$5p^2\ ^3P_0$	110 834	90.23	1.87E+00	5.12E+09	0.96
$5s7p\ ^1P^o_1(5s7p\ ^3P^o_1)$	$5p^2\ ^3P_0$	117 023	85.45	1.13E−01	3.43E+08	1.01
$5s7p\ ^3P^o_1$	$5p^2\ ^3P_0$	119 183	83.90	1.38E−01	4.35E+08	1.03
$5s6p\ ^1P^o_1$	$5p^2\ ^1D_2$	62 864	159.07	2.97E−01	2.62E+08	1.04
$5s4f\ ^1F^o_3$	$5p^2\ ^1D_2$	72 176	138.55	1.43E+00	7.09E+08	0.95
$5p5d\ ^3F^o_2$	$5p^2\ ^1D_2$	97 998	102.04	6.43E−01	8.24E+08	0.95
$5p5d\ ^3F^o_3$	$5p^2\ ^1D_2$	101 728	98.30	2.29E−01	2.26E+08	0.96
$5p5d\ ^1D^o_2$	$5p^2\ ^1D_2$	102 639	97.43	1.16E+00	1.63E+09	0.95
$5p5d\ ^3P^o_2$	$5p^2\ ^1D_2$	108 823	91.89	3.27E−01	5.17E+08	0.93
$5p5d\ ^3D^o_3$	$5p^2\ ^1D_2$	112 084	89.22	1.94E+00	2.32E+09	0.96
$5p5d\ ^3P^o_1(5s7p\ ^1P^o_1)$	$5p^2\ ^1D_2$	112 352	89.01	2.62E−01	7.36E+08	1.03
$5s7p\ ^1P^o_1(5s7p\ ^3P^o_1)$	$5p^2\ ^1D_2$	112 837	88.62	4.19E−01	1.19E+09	1.13
$5p5d\ ^3D^o_2$	$5p^2\ ^1D_2$	112 909	88.57	3.96E−01	6.74E+08	0.96
$5s7p\ ^3P^o_1$	$5p^2\ ^1D_2$	114 997	86.96	1.57E−01	4.62E+08	0.93
$5s7p\ ^3P^o_2$	$5p^2\ ^1D_2$	115 672	86.45	1.73E−01	3.10E+08	0.99
$5p5d\ ^1P^o_1$	$5p^2\ ^1D_2$	122 312	81.76	1.28E−01	4.26E+08	0.91
$5p6s\ ^3P^o_2$	$5p^2\ ^1D_2$	123 626	80.89	2.58E−01	5.26E+08	1.04
$5p5d\ ^1F^o_3$	$5p^2\ ^1D_2$	129 666	77.12	1.10E+00	1.76E+09	0.95
$5p6s\ ^1P^o_1$	$5p^2\ ^1D_2$	130 857	76.42	1.65E−01	6.27E+08	1.02
$5p5d\ ^1D^o_2$	$5p^2\ ^3P_1$	102 622	97.44	9.18E−01	1.29E+09	0.97
$5p5d\ ^3D^o_1$	$5p^2\ ^3P_1$	106 632	93.78	3.88E−01	9.80E+08	0.96
$5p5d\ ^3P^o_2$	$5p^2\ ^3P_1$	108 806	91.91	2.52E+00	3.98E+09	0.96
$5p5d\ ^3P^o_0$	$5p^2\ ^3P_1$	112 050	89.25	1.57E−01	1.31E+09	0.95
$5p5d\ ^3P^o_1(5s7p\ ^1P^o_1)$	$5p^2\ ^3P_1$	112 335	89.02	5.90E−01	1.66E+09	0.96
$5p5d\ ^3D^o_2$	$5p^2\ ^3P_1$	112 892	88.58	4.71E−01	8.00E+08	0.96
$5p6s\ ^3P^o_0(5s7p\ ^3P^o_0)$	$5p^2\ ^3P_1$	114 187	87.58	6.74E−01	5.86E+09	1.01
$5s7p\ ^3P^o_1$	$5p^2\ ^3P_1$	114 981	86.97	6.04E−01	1.78E+09	0.98
$5p6s\ ^3P^o_2$	$5p^2\ ^3P_1$	123 610	80.90	3.24E−01	6.60E+08	1.04
$5s6p\ ^1P^o_1$	$5p^2\ ^3P_2$	55 638	179.73	1.52E−01	1.05E+08	1.03
$5s4f\ ^1F^o_3$	$5p^2\ ^3P_2$	64 950	153.96	5.96E−01	2.40E+08	0.96
$5p5d\ ^3F^o_3$	$5p^2\ ^3P_2$	94 503	105.82	1.93E−01	1.65E+08	0.95
$5p5d\ ^1D^o_2$	$5p^2\ ^3P_2$	95 413	104.81	2.14E−01	2.60E+08	0.92
$5p5d\ ^3P^o_2$	$5p^2\ ^3P_2$	101 598	98.43	2.23E−01	3.07E+08	0.96
$5p5d\ ^3D^o_3$	$5p^2\ ^3P_2$	104 858	95.37	3.53E+00	3.70E+09	0.95
$5p5d\ ^3P^o_1(5s7p\ ^1P^o_1)$	$5p^2\ ^3P_2$	105 126	95.12	1.54E−01	3.79E+08	0.91
$5p5d\ ^3D^o_2$	$5p^2\ ^3P_2$	105 684	94.62	1.68E+00	2.50E+09	0.96

Table 3. (Continued.)

Upper	Lower	ΔE_{calc} (cm^{-1})	λ (nm)	*gf*	*A*	*R*
5s7p ^{3}P$_1^o$	5p^2 ^{3}P$_2$	107 772	92.79	4.73E−01	1.22E+09	1.02
5s5f ^{1}F$_3^o$	5p^2 ^{3}P$_2$	108 392	92.26	3.63E−01	4.06E+08	0.98
5s7p ^{3}P$_2^o$	5p^2 ^{3}P$_2$	108 446	92.21	8.31E−01	1.31E+09	0.98
5p5d ^{1}P$_1^o$	5p^2 ^{3}P$_2$	115 086	86.89	2.46E−01	7.24E+08	0.98
5p6s ^{3}P$_2^o$	5p^2 ^{3}P$_2$	116 401	85.91	7.30E−01	1.32E+09	1.04
5p5d ^{1}F$_3^o$	5p^2 ^{3}P$_2$	122 441	81.67	6.65E−01	9.50E+08	0.95
5p6s ^{1}P$_1^o$	5p^2 ^{3}P$_2$	123 631	80.89	1.55E−01	5.27E+08	1.02
5s6p ^{3}P$_0^o$	5s5d ^{3}D$_1$	36 685	272.59	3.97E−01	3.57E+08	1.03
5s6p ^{3}P$_1^o$	5s5d ^{3}D$_1$	37 026	270.08	2.58E−01	7.87E+07	1.03
5s4f ^{3}F$_2^o$	5s5d ^{3}D$_1$	48 307	207.01	1.69E+00	5.27E+08	1.00
5p5d ^{3}F$_2^o$	5s5d ^{3}D$_1$	75 426	132.58	1.19E+00	9.05E+08	0.94
5p5d ^{1}D$_2^o$	5s5d ^{3}D$_1$	80 066	124.90	2.41E−01	2.06E+08	0.96
5p5d ^{3}D$_1^o$	5s5d ^{3}D$_1$	84 076	118.94	2.04E−01	3.21E+08	0.93
5p5d ^{3}P$_2^o$	5s5d ^{3}D$_1$	86 250	115.94	3.39E−01	3.36E+08	0.94
5p5d ^{3}P$_0^o$(5s7p ^{1}P$_1^o$)	5s5d ^{3}D$_1$	89 779	111.38	2.34E−01	4.19E+08	0.90
5p5d ^{3}D$_2^o$	5s5d ^{3}D$_1$	90 336	110.70	1.91E−01	2.08E+08	0.92
5s7p ^{3}P$_1^o$	5s5d ^{3}D$_1$	92 424	108.20	2.73E−01	5.19E+08	0.99
5s7p ^{3}P$_0^o$(5p6s ^{3}P$_0^o$)	5s5d ^{3}D$_1$	94 021	106.36	1.59E−01	9.39E+08	1.05
5s6p ^{3}P$_1^o$	5s5d ^{3}D$_2$	36 678	272.64	7.83E−01	2.34E+08	1.03
5s6p ^{3}P$_2^o$	5s5d ^{3}D$_2$	38 716	258.29	2.98E−01	5.97E+07	1.02
5s6p ^{1}P$_1^o$	5s5d ^{3}D$_2$	39 942	250.36	1.07E−01	3.81E+07	1.03
5s4f ^{3}F$_2^o$	5s5d ^{3}D$_2$	47 958	208.52	3.03E−01	9.28E+07	1.00
5s4f ^{3}F$_3^o$	5s5d ^{3}D$_2$	48 019	208.25	2.50E+00	5.49E+08	1.00
5p5d ^{3}F$_2^o$	5s5d ^{3}D$_2$	75 077	133.20	3.61E−01	2.72E+08	0.94
5p5d ^{3}F$_3^o$	5s5d ^{3}D$_2$	78 807	126.89	2.05E+00	1.21E+09	0.94
5p5d ^{1}D$_2^o$	5s5d ^{3}D$_2$	79 717	125.44	1.55E−01	1.31E+08	0.92
5p5d ^{3}D$_1^o$	5s5d ^{3}D$_2$	83 727	119.44	4.65E−01	7.25E+08	0.94
5p5d ^{3}D$_3^o$	5s5d ^{3}D$_2$	89 162	112.16	7.55E−01	5.72E+08	0.94
5p5d ^{3}D$_2^o$	5s5d ^{3}D$_2$	89 987	111.13	6.07E−01	6.56E+08	0.92
5s7p ^{3}P$_1^o$	5s5d ^{3}D$_2$	92 076	108.61	2.46E−01	4.63E+08	1.05
5s7p ^{3}P$_2^o$	5s5d ^{3}D$_2$	92 750	107.82	2.93E−01	3.36E+08	1.01
5s5f ^{3}F$_3^o$	5s5d ^{3}D$_2$	93 420	107.04	1.19E−01	9.87E+07	0.94
5s6p ^{3}P$_2^o$	5s5d ^{3}D$_3$	38 083	262.58	1.67E+00	3.23E+08	1.05
5s4f ^{3}F$_3^o$	5s5d ^{3}D$_3$	47 386	211.03	2.96E−01	6.35E+07	1.00
5s4f ^{3}F$_4^o$	5s5d ^{3}D$_3$	47 542	210.34	3.85E+00	6.45E+08	1.00
5p5d ^{3}F$_3^o$	5s5d ^{3}D$_3$	78 174	127.92	7.09E−01	4.13E+08	0.98
5p5d ^{1}D$_2^o$	5s5d ^{3}D$_3$	79 084	126.45	3.41E−01	2.85E+08	0.94
5p5d ^{3}F$_4^o$	5s5d ^{3}D$_3$	83 001	120.48	3.79E+00	1.94E+09	0.96
5p5d ^{3}P$_2^o$	5s5d ^{3}D$_3$	85 269	117.28	6.04E−01	5.85E+08	0.92
5p5d ^{3}D$_3^o$	5s5d ^{3}D$_3$	88 529	112.96	1.03E+00	7.68E+08	0.93
5s7p ^{3}P$_2^o$	5s5d ^{3}D$_3$	92 117	108.56	4.59E−01	5.20E+08	1.09
5s5f ^{3}F$_4^o$	5s5d ^{3}D$_3$	92 818	107.74	1.68E−01	1.07E+08	0.92
5p5d ^{1}P$_1^o$	5p^2 ^{1}S$_0$	93 290	107.19	5.30E−01	1.03E+09	0.95
5p6s ^{1}P$_1^o$	5p^2 ^{1}S$_0$	101 835	98.20	1.39E+00	3.21E+09	0.99
5s6p ^{3}P$_0^o$	5s6s ^{3}S$_1$	26 744	373.92	4.12E−01	1.97E+08	1.01
5s6p ^{3}P$_1^o$	5s6s ^{3}S$_1$	27 085	369.21	1.08E+00	1.77E+08	1.01
5s6p ^{3}P$_2^o$	5s6s ^{3}S$_1$	29 123	343.37	2.23E+00	2.52E+08	1.01
5s6p ^{1}P$_1^o$	5s6s ^{3}S$_1$	30 350	329.49	1.85E−01	3.79E+07	1.02
5s7p ^{1}P$_1^o$(5s7p ^{3}P$_1^o$)	5s6s ^{3}S$_1$	80 323	124.50	1.36E−01	1.95E+08	0.93
5p6s ^{3}P$_0^o$(5s7p ^{3}P$_0^o$)	5s6s ^{3}S$_1$	81 690	122.41	1.61E−01	7.17E+08	0.92
5s7p ^{3}P$_1^o$	5s6s ^{3}S$_1$	82 483	121.24	1.34E−01	2.02E+08	0.90
5s7p ^{3}P$_0^o$(5p6s ^{3}P$_0^o$)	5s6s ^{3}S$_1$	84 080	118.93	1.01E−01	4.74E+08	0.96
5p6s ^{3}P$_1^o$	5s6s ^{3}S$_1$	84 941	117.73	3.61E−01	5.78E+08	0.96
5p5d ^{1}P$_1^o$	5s6s ^{3}S$_1$	89 798	111.36	1.72E−01	3.08E+08	0.95
5p6s ^{3}P$_2^o$	5s6s ^{3}S$_1$	91 112	109.76	1.42E+00	1.58E+09	0.95
5s6p ^{1}P$_1^o$	5s5d ^{1}D$_2$	25 507	392.05	6.62E−01	9.57E+07	0.97
5s4f ^{1}F$_3^o$	5s5d ^{1}D$_2$	34 819	287.20	1.08E+00	1.25E+08	1.08
5p5d ^{3}F$_3^o$	5s5d ^{1}D$_2$	64 371	155.35	1.81E−01	7.13E+07	0.96
5p5d ^{3}D$_3^o$	5s5d ^{1}D$_2$	74 727	133.82	1.49E−01	7.95E+07	0.98
5s5f ^{1}F$_3^o$	5s5d ^{1}D$_2$	78 261	127.78	2.78E+00	1.62E+09	0.98
5p5d ^{1}F$_3^o$	5s5d ^{1}D$_2$	92 310	108.33	6.00E+00	4.88E+09	0.95
5p6s ^{1}P$_1^o$	5s5d ^{1}D$_2$	93 500	106.95	1.16E+00	2.26E+09	0.99
5s6p ^{3}P$_1^o$	5s6s ^{1}S$_0$	21 609	462.77	1.26E−01	1.31E+07	1.00

Table 3. (Continued.)

Upper	Lower	ΔE_{calc} (cm^{-1})	λ (nm)	gf	A	R
5s6p $^1P^o_1$	5s6s $^1S_0$	24 873	402.04	9.06E−01	1.25E+08	1.01
5s7p $^1P^o_1$(5s7p $^3P^o_1$)	5s6s $^1S_0$	74 847	133.61	2.86E−01	3.56E+08	0.97
5p5d $^1P^o_1$	5s6s $^1S_0$	84 321	118.59	1.43E−01	2.27E+08	0.93
5p6s $^1P^o_1$	5s6s $^1S_0$	92 866	107.68	8.36E−01	1.60E+09	0.98
5s6d $^3D_1$	5s6p $^3P^o_0$	39 376	253.96	1.26E+00	4.34E+08	1.01
5s7s $^3S_1$	5s6p $^3P^o_0$	42 480	235.40	2.58E−01	1.04E+08	1.01
5s6d $^3D_1$	5s6p $^3P^o_1$	39 035	256.18	8.14E−01	2.76E+08	1.01
5s6d $^3D_2$	5s6p $^3P^o_1$	39 171	255.29	2.64E+00	5.40E+08	1.01
5s6d $^1D_2$	5s6p $^3P^o_1$	41 011	243.84	3.05E−01	6.84E+07	1.00
5s7s $^3S_1$	5s6p $^3P^o_1$	42 139	237.31	6.81E−01	2.69E+08	1.01
5s8s $^3S_1$	5s6p $^3P^o_1$	74 849	133.60	1.10E−01	1.37E+08	1.18
5s6d $^3D_2$	5s6p $^3P^o_2$	37 133	269.30	9.54E−01	1.76E+08	1.01
5s6d $^3D_3$	5s6p $^3P^o_2$	37 412	267.29	5.41E+00	7.21E+08	1.01
5s7s $^3S_1$	5s6p $^3P^o_2$	40 101	249.37	1.43E+00	5.12E+08	1.01
5s8s $^3S_1$	5s6p $^3P^o_2$	72 810	137.34	2.11E−01	2.48E+08	1.19
5s6d $^3D_1$	5s6p $^1P^o_1$	35 771	279.56	1.34E−01	3.81E+07	1.01
5s6d $^3D_2$	5s6p $^1P^o_1$	35 907	278.50	2.14E−01	3.67E+07	1.01
5s6d $^1D_2$	5s6p $^1P^o_1$	37 747	264.92	3.36E+00	6.38E+08	1.00
5s7s $^3S_1$	5s6p $^1P^o_1$	38 874	257.24	1.22E−01	4.08E+07	1.02
5s7s $^1S_0$	5s6p $^1P^o_1$	40 479	247.04	7.04E−01	7.69E+08	1.00
5s8s $^1S_0$	5s6p $^1P^o_1$	72 259	138.39	1.10E−01	3.82E+08	1.09
5s6d $^3D_1$	5s4f $^3F^o_2$	27 755	360.30	5.10E−01	8.73E+07	1.01
5s5g $^3G_3$	5s4f $^3F^o_2$	54 437	183.70	3.67E+00	1.04E+09	1.01
5s6d $^3D_2$	5s4f $^3F^o_3$	27 829	359.34	7.04E−01	7.27E+07	1.00
5s5g $^1G_4$	5s4f $^3F^o_3$	54 375	183.91	3.15E+00	6.90E+08	1.01
5s5g $^3G_3$	5s4f $^3F^o_3$	54 376	183.90	3.08E−01	8.68E+07	1.01
5s5g $^3G_4$	5s4f $^3F^o_3$	54 424	183.74	1.70E+00	3.72E+08	1.01
5s6d $^3D_3$	5s4f $^3F^o_4$	27 953	357.74	1.08E+00	8.02E+07	1.00
5s5g $^1G_4$	5s4f $^3F^o_4$	54 219	184.44	1.50E−01	3.28E+07	1.00
5s5g $^3G_4$	5s4f $^3F^o_4$	54 268	184.27	1.65E−01	3.60E+07	1.01
5s5g $^3G_5$	5s4f $^3F^o_4$	54 270	184.26	6.36E+00	1.14E+09	1.01
5s6d $^1D_2$	5s4f $^1F^o_3$	28 435	351.68	8.81E−01	9.50E+07	1.03
5s5g $^1G_4$	5s4f $^1F^o_3$	53 140	188.18	1.90E+00	3.98E+08	1.02
5s5g $^3G_4$	5s4f $^1F^o_3$	53 189	188.01	3.44E+00	7.22E+08	1.02
5p5d $^3P^o_0$	5s6d $^3D_1$	13 431	744.55	3.95E−01	4.76E+07	1.15
5p5d $^3P^o_1$(5s7p $^1P^o_1$)	5s6d $^3D_1$	13 716	729.08	2.16E−01	9.03E+06	1.13
5s7p $^3P^o_1$	5s6d $^3D_1$	16 362	611.17	2.07E−01	1.23E+07	1.18
5s5f $^3F^o_2$	5s6d $^3D_1$	17 715	564.49	3.43E+00	1.44E+08	1.08
5s7p $^3P^o_0$(5p6s $^3P^o_0$)	5s6d $^3D_1$	17 958	556.85	2.95E−01	6.35E+07	1.09
5p6s $^3P^o_1$	5s6d $^3D_1$	18 820	531.35	1.20E−01	9.43E+06	1.06
5p5d $^3P^o_1$(5s7p $^1P^o_1$)	5s6d $^3D_2$	13 580	736.38	6.93E−01	2.84E+07	1.13
5p5d $^3D^o_2$	5s6d $^3D_2$	14 138	707.31	1.21E−01	3.24E+06	1.10
5s7p $^3P^o_1$	5s6d $^3D_2$	16 226	616.29	6.91E−01	4.05E+07	1.15
5s7p $^3P^o_2$	5s6d $^3D_2$	16 900	591.72	4.52E−01	1.72E+07	1.15
5s5f $^3F^o_3$	5s6d $^3D_2$	17 570	569.15	4.94E+00	1.45E+08	1.08
5s5f $^3F^o_2$	5s6d $^3D_2$	17 579	568.86	6.04E−01	2.49E+07	1.07
5p6s $^3P^o_1$	5s6d $^3D_2$	18 684	535.22	2.80E−01	2.17E+07	1.09
5p5d $^3D^o_2$	5s6d $^3D_3$	13 859	721.55	7.36E−01	1.89E+07	1.23
5s7p $^3P^o_2$	5s6d $^3D_3$	16 621	601.65	2.40E+00	8.86E+07	1.13
5s5f $^3F^o_3$	5s6d $^3D_3$	17 291	578.34	6.23E−01	1.78E+07	1.08
5s5f $^3F^o_4$	5s6d $^3D_3$	17 322	577.30	7.23E+00	1.61E+08	1.08
5p5d $^3P^o_1$(5s7p $^1P^o_1$)	5s6d $^1D_2$	11 740	851.79	1.31E−01	4.02E+06	1.01
5s7p $^1P^o_1$(5s7p $^3P^o_1$)	5s6d $^1D_2$	12 225	818.00	9.78E−01	3.25E+07	1.07
5s7p $^3P^o_1$	5s6d $^1D_2$	14 386	695.12	1.38E−01	6.36E+06	0.93
5s5f $^1F^o_3$	5s6d $^1D_2$	15 006	666.40	4.00E+00	8.58E+07	1.06
5p6s $^3P^o_1$	5s6d $^1D_2$	16 844	593.68	6.66E−01	4.20E+07	0.96
5p5d $^1P^o_1$	5s6d $^1D_2$	21 700	460.83	1.43E−01	1.50E+07	0.87
5p5d $^1F^o_3$	5s6d $^1D_2$	29 055	344.17	1.31E+00	1.06E+08	0.96
5p6s $^1P^o_1$	5s6d $^1D_2$	30 245	330.63	1.34E−01	2.73E+07	0.87
5s5g $^1G_4$	5p5d $^3F^o_3$	23 587	423.96	1.55E−01	6.39E+06	1.33
5p5d $^3P^o_0$	5s7s $^3S_1$	10 328	968.24	2.77E−01	1.97E+07	1.05
5p5d $^3P^o_1$(5s7p $^1P^o_1$)	5s7s $^3S_1$	10 613	942.24	5.93E−01	1.49E+07	1.05

Table 3. (Continued.)

Upper	Lower	ΔE_{calc} (cm^{-1})	λ (nm)	gf	A	R
5s7p ^{1}P$^o_1$(5s7p ^{3}P$^o_1$)	5s7s ^{3}S$_1$	11 098	901.06	1.08E−01	2.95E+06	1.04
5p5d ^{3}D$^o_2$	5s7s ^{3}S$_1$	11 170	895.26	6.40E−01	1.07E+07	1.06
5s7p ^{3}P$^o_1$	5s7s ^{3}S$_1$	13 258	754.26	6.91E−01	2.70E+07	1.04
5s7p ^{3}P$^o_2$	5s7s ^{3}S$_1$	13 933	717.72	2.37E+00	6.13E+07	1.03
5s7p ^{3}P$^o_0$(5p6s ^{3}P$^o_0$)	5s7s ^{3}S$_1$	14 855	673.17	2.31E−01	3.40E+07	1.04
5p6s ^{3}P$^o_1$	5s7s ^{3}S$_1$	15 716	636.29	3.79E−01	2.08E+07	1.04
5p5d ^{3}P$^o_1$(5s7p ^{1}P$^o_1$)	5s7s ^{1}S$_0$	9008	1110.12	1.36E−01	2.46E+06	1.00
5s7p ^{1}P$^o_1$(5s7p ^{3}P$^o_1$)	5s7s ^{1}S$_0$	9494	1053.30	7.18E−01	1.44E+07	1.00
5s7p ^{3}P$^o_1$	5s7s ^{1}S$_0$	11 654	858.07	1.49E−01	4.49E+06	1.02
5p6s ^{3}P$^o_1$	5s7s ^{1}S$_0$	14 112	708.62	4.65E−01	2.06E+07	1.01
5p5d ^{1}P$^o_1$	5s7s ^{1}S$_0$	18 968	527.20	1.17E−01	9.35E+06	1.03
5p6s ^{1}P$^o_1$	5s7s ^{1}S$_0$	27 513	363.46	1.19E−01	2.01E+07	1.00
5s5g ^{3}G$_5$	5p5d ^{3}F$^o_4$	18 811	531.60	2.32E−01	4.98E+06	1.47
5s8s ^{3}S$_1$	5p5d ^{3}P$^o_0$	22 381	446.81	1.98E−01	2.20E+07	1.35
5s5g ^{3}G$_4$	5p5d ^{3}D$^o_3$	13 281	752.96	1.71E−01	2.24E+06	1.24
5s8s ^{3}S$_1$	5p5d ^{3}P$^o_1$(5s7p ^{1}P$^o_1$)	22 096	452.57	4.22E−01	4.58E+07	1.33
5s8s ^{1}S$_0$	5p5d ^{3}P$^o_1$(5s7p ^{1}P$^o_1$)	22 771	439.16	1.03E−01	3.55E+07	1.26
5s8s ^{1}S$_0$	5s7p ^{1}P$^o_1$(5s7p ^{3}P$^o_1$)	22 286	448.71	5.58E−01	1.85E+08	1.33
5s8s ^{3}S$_1$	5p5d ^{3}D$^o_2$	21 539	464.27	4.66E−01	4.81E+07	1.38
5s8s ^{3}S$_1$	5s7p ^{3}P$^o_1$	19 451	514.11	4.49E−01	3.77E+07	1.06
5s8s ^{1}S$_0$	5s7p ^{3}P$^o_1$	20 126	496.87	1.01E−01	2.72E+07	1.01
5s5g ^{1}G$_4$	5s5f ^{1}F$^o_3$	9698	1031.14	1.80E+00	1.26E+07	1.14
5s5g ^{3}G$_4$	5s5f ^{1}F$^o_3$	9747	1025.96	1.96E+00	1.38E+07	1.16
5s8s ^{3}S$_1$	5s7p ^{3}P$^o_2$	18 776	532.59	1.60E+00	1.26E+08	1.09
5s5g ^{1}G$_4$	5s5f ^{3}F$^o_3$	8974	1114.33	1.94E+00	1.16E+07	1.13
5s5g ^{3}G$_3$	5s5f ^{3}F$^o_3$	8976	1114.08	2.45E−01	1.88E+06	1.13
5s5g ^{3}G$_4$	5s5f ^{3}F$^o_3$	9024	1108.16	1.75E+00	1.06E+07	1.13
5s5g ^{3}G$_3$	5s5f ^{3}F$^o_2$	8967	1115.20	2.82E+00	2.16E+07	1.13
5s5g ^{1}G$_4$	5s5f ^{3}F$^o_4$	8943	1118.19	1.20E−01	7.12E+05	1.13
5s5g ^{3}G$_4$	5s5f ^{3}F$^o_4$	8992	1112.10	1.25E−01	7.51E+05	1.14
5s5g ^{3}G$_5$	5s5f ^{3}F$^o_4$	8994	1111.85	4.82E+00	2.37E+07	1.14
5s8s ^{3}S$_1$	5s7p ^{3}P$^o_0$(5p6s ^{3}P$^o_0$)	17 854	560.10	1.44E−01	1.02E+07	0.91
5s8s ^{3}S$_1$	5p6s ^{3}P$^o_1$	16 992	588.51	2.51E−01	1.61E+07	0.93
5s8s ^{1}S$_0$	5p6s ^{3}P$^o_1$	17 668	566.00	3.03E−01	6.30E+07	0.92

Table 4. Energies (in cm^{-1}) and rates in length and velocity gauges for the 5s^2 ^{1}S$_0$–5s5p ^{1}P$^o_1$ and 5s^2 ^{1}S$_0$–5s5p ^{3}P$^o_{1,2}$ transitions from RCI calculations with increasingly large configuration expansions. The first active set consists of the 5s, 5p−, 5p, 5d−, 5d orbitals in the complex. The active set is enlarged by up to five layers of correlation orbitals.

Active set	5s^2 ^{1}S$_0$–5s5p ^{1}P$^o_1$ E1			5s^2 ^{1}S$_0$–5s5p ^{3}P$^o_1$ E1		
	ΔE	A_L	A_V	ΔE	A_L	A_V
Complex	98 037	5.893E+9	3.644E+9	55 536	6.501E+7	2.478E+6
Layer 1	95 316	3.342E+9	3.141E+9	65 598	1.352E+7	1.438E+7
Layer 2	95 673	3.201E+9	3.372E+9	66 881	1.495E+7	1.645E+7
Layer 3	95 613	3.178E+9	3.386E+9	66 996	1.509E+7	1.668E+7
Layer 4	95 597	3.167E+9	3.416E+9	67 004	1.506E+7	1.696E+7
Layer 5	95 575	3.163E+9	3.427E+9	67 005	1.506E+7	1.705E+7
MCDHF[a]	95 566	3.18E+9	3.19E+9	67 283	1.42E+7	1.54E+7
HFR[a]		3.12E+9			1.37E+7	
Exp[b]	95 956.7	2.6 ± 0.3E+9		66 698.1		

	5s^2 ^{1}S$_0$–5s5p ^{3}P$^o_2$ M2	
Active set	ΔE	A
Complex	61 015	2.352E−2
Layer 1	71 338	5.850E−2
Layer 2	72 646	6.533E−2
Layer 3	72 764	6.600E−2
Layer 4	72 772	6.599E−2
Layer 5	72 773	6.600E−2
Exp	72 560	

[a] Biémont *et al* [6].

[b] Pinnington *et al* [2].

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Table 5. Magnetic dipole, A, and electric quadrupole, B, hyperfine interaction constants (in MHz) for 5s5p ^{3}P^o in ^{121}Sb from RCI calculations with increasingly large configuration expansions. The first active set consists of the 5s, 5p−, 5p, 5d−, 5d orbitals in the complex. The active set is enlarged by up to five layers of correlation orbitals. The expansions include CSFs obtained by single excitations from all the core shells. We take the $I = 5/2$, $\mu_I = 3.363(3)$ nm and $Q = -0.45(3)$ barn from the compilation by Stone [20].

Active set	$A(^3P_1^o)$	$B(^3P_1^o)$	$A(^3P_2^o)$	$B(^3P_2^o)$	$A(^3P_1^o, ^3P_2^o)$	$A(^1P_1^o, ^3P_0^o)$	$A(^3P_1^o, ^3P_0^o)$
Complex	12 521	387	8866	−696	10 568	6870	10 568
Layer 1	13 656	413	9137	−757	10 997	6992	10 997
Layer 2	13 678	410	9110	−754	10 986	6882	10 986
Layer 3	13 779	416	9168	−765	11 019	6912	11 018
Layer 4	13 739	414	9138	−762	10 994	6891	10 994
Layer 5	13 756	415	9150	−764	11 006	6898	11 006

where I is the nuclear spin and $F (= I)$ is the total angular momentum quantum number. The use of quotation marks in the left-hand wavefunction emphasizes the fact that the notation is just a label indicating the dominant character of the eigenvector. Clearly, the one-photon 5s5p ^{3}P$_0^o$ → 5s^2 ^{1}S$_0$ transition now becomes allowed via the mixing of functions with J different from zero. $|5s5p\ ^3P_1^o\ IF\rangle$ and $|5s5p\ ^1P_1^o\ IF\rangle$ are the only important contributors to wavefunction expansion and in this work we model the 5s5p ^{3}P$_0^o$ state as

$$|'5s5p\ ^3P_0^o\ IF'\rangle = c_0|5s5p\ ^3P_0^o\ IF\rangle$$
$$+ c_1|5s5p\ ^3P_1^o\ IF\rangle + c_2|5s5p\ ^1P_1^o\ IF\rangle. \qquad (16)$$

The mixing coefficients are obtained by constructing and diagonalizing the Hamiltonian matrix in the presence of the hyperfine interaction. Once the mixing coefficients have been determined, the transition rate can be computed as

$$A(5s5p\ ^3P_0^o \rightarrow 5s^2\ ^1S_0)$$
$$= \frac{2.026\,13 \times 10^{18}}{3\lambda^3}\big|c_1\langle 5s^2\ ^1S_0\|\mathbf{Q}_1^{(1)}\|5s5p\ ^3P_1^o\rangle$$
$$+ c_2\langle 5s^2\ ^1S_0\|\mathbf{Q}_1^{(1)}\|5s5p\ ^1P_1^o\rangle\big|^2, \qquad (17)$$

where the decay rate is in s^{-1} and λ is the wavelength in Å for the transition. $\langle 5s^2\ ^1S_0\|\mathbf{Q}_1^{(1)}\|5s5p\ ^3P_1^o\rangle$ and $\langle 5s^2\ ^1S_0\|\mathbf{Q}_1^{(1)}\|5s5p\ ^1P_1^o\rangle$ are the reduced matrix elements for the electric dipole operator [19]. The reduced transition matrix elements can be obtained as square roots of the corresponding line strengths. The phase is such that we have constructive interference. To obtain a good value for the rate, both the hyperfine interaction and the transition matrix elements must be calculated with high accuracy. The off-diagonal magnetic hyperfine interaction constants needed to construct the Hamiltonian matrix elements are given in table 5. The reader may consult [29] for explicit formulas relating the interaction constants and the matrix elements. For ^{121}Sb, the off-diagonal magnetic hyperfine interaction constants give the mixing coefficients $c_1 = -4.908 \times 10^{-4}$ and $c_2 = -2.212 \times 10^{-5}$. Using the transition matrix elements $\langle 5s^2\ ^1S_0\|\mathbf{Q}_1^{(1)}\|5s5p\ ^3P_1^o\rangle = 2.722 \times 10^{-1}$ and $\langle 5s^2\ ^1S_0\|\mathbf{Q}_1^{(1)}\|5s5p\ ^1P_1^o\rangle = 2.316$ from the calculations reported in table 5, we obtain a transition rate $A = 6.278$ s^{-1} corresponding to a lifetime $\tau = 0.159$ s of the ^{3}P$_0^o$ state. For ^{123}Sb with $I = 7/2$, $\mu = 2.5498(2)$ nm and $Q = 0.49(5)$ barn, similar calculations give the rate $A = 3.314$ s^{-1} and lifetime $\tau = 0.302$ s. To estimate the accuracy of the hyperfine-induced lifetime, we again rely on In II. Calculations similar to the ones

Table 6. Differences ΔS_{sms}, ΔS_{nms} and $\Delta\rho(0)$ between the upper and lower state isotope shift parameters in the 5s^2 ^{1}S$_0$–5s5p ^{3}P$_1^o$ transition from RCI calculations with increasingly large configuration expansions. The first active set consists of the 5s, 5p−, 5p, 5d−, 5d orbitals in the complex. The active set is enlarged by up to five layers of correlation orbitals.

	5s^2 ^{1}S$_0$–5s5p ^{3}P$_1^o$		
Active set	ΔS_{sms}	$\Delta\rho(0)$	ΔS_{nms}
Complex	−0.359 709	−55.9264	−0.244 080
Layer 1	−0.766 530	−57.6157	−0.180 390
Layer 2	−0.657 939	−56.5270	−0.238 064
Layer 3	−0.687 112	−56.9699	−0.202 606
Layer 4	−0.645 979	−56.6869	−0.248 387
Layer 5	−0.650 250	−56.7749	−0.248 675

presented here predicted a lifetime of $\tau = 0.217$ s of the ^{3}P$_0^o$ state in ^{115}In$^+$. This is in excellent agreement with the most recent experimental value $\tau = 0.195(8)$ s [35]. Based on the reasoning that the present calculation predicts hyperfine structure and transition rates with the same accuracy as in In II, we may expect the lifetimes of the ^{3}P$_0^o$ state in ^{121}Sb^{3+} and ^{123}Sb^{3+} to be quite accurate.

6. Conclusion

This work reports on extensive calculations for the level energies, lifetimes, Landé g_J-factors and transitions rates of the triply ionized antimony (Sb IV). Using the new release of GRASP2K [7], we describe 24 even-parity states, from 5s^2 ^{1}S$_0$ to 5s8s ^{1}S$_0$, and 36 odd-parity states, from 5s5p ^{3}P$_0^o$ to 5p6s ^{1}P$_1^o$. The obtained theoretical data are in good agreement with available experimental data. There is also a good consistency with the theoretical calculations by Rana *et al* [1], although some problems of labelling remain due to the close degeneracy between odd-parity configurations. For testing the accuracy of our spectrum calculation, we perform separate calculations, for describing as best as possible the ground and first excited states. There is very good agreement for the predicted properties using either the spectrum or separated calculations. We use the highly correlated wavefunction from the calculations of the ground and first excited states for evaluating the isotope shift in the 5s^2 ^{1}S$_0$–5s5p ^{3}P$_1^o$ transition and the rate of the hyperfine-induced 5s^2 ^{1}S$_0$–5s5p ^{3}P$_0^o$ transition.

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Acknowledgments

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