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# Fine, hyperfine and Zeeman structures of levels of $^{123}$Sb I

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**Abstract.** The hyperfine and Zeeman structures of 14 lines of isotope $^{123}$Sb covering the UV-NIR spectral range have been measured. The experimental data have been used in order to reanalyse and revise Sb I energy levels. We named majority of them for the first time since they were previously labelled only by their energy values, without any term designations. In both cases of odd- and even-parity levels we took into consideration up to 7 interacting configurations; the set of fine structure parameters and the leading eigenvector percentages of levels as well as their calculated Landé-factors are given. Semi-empirical hfs parameter values extracted from experimental data were compared with ab initio results computed by the use of Cowan code.

## 1 Introduction

Natural antimony consists of two stable isotopes $^{121}$Sb ($I = 5/2$) and $^{123}$Sb ($I = 7/2$), with natural abundance of 57% and 43%, respectively. The large nuclear spins in combination with large nuclear moments ($\mu_I = 3.9796\mu_N$, $Q = -0.36$ barn [1] and $\mu_I = 2.8912\mu_N$, $Q = -0.49$ barn [1,2] for isotopes 121 and 123, respectively) lead to a complex hyperfine structure (hfs) of both isotopes.

Hyperfine structure splitting A and B constants for levels of the ground configuration of Sb I have been obtained in a number of experiments [3–11]. Numerous authors had, at the beginning of Sb I electronic structure studies, looked into the emission spectrum. Later, photoabsorption investigations were preferably used with the flash-pyrolyosis technique [12] since the spectrum of atomic antimony is difficult to obtain experimentally because of the tendency for antimony atoms to form dimers and trimers.

The first observation of forbidden lines in antimony was described in reference [3] and the first hfs analysis of the multipole lines of Sb I was performed in reference [4]. In paper [5] the hfs of forbidden lines between levels belonging to the ground configuration of Sb I was studied.

Most of the experimental studies were focused on the hfs of isotope 121, but only a few were dedicated to isotope 123 [6,7]. In addition, the experimental values for $^{123}$Sb are inconsistent (see Ref. [13]).

In this paper we report results of observation of hfs and Zeeman structure of 14 emission lines of $^{123}$Sb I covering the UV-NIR spectral range (363.8÷1074.2) nm.

The new experimental data have been used in order to reanalyse and revise Sb I energy levels. We found designations and leading eigenvector percentages for levels belonging to 7 lowest configurations of odd- and even-parities.

## 2 Experiment

This work is a continuation of our earlier studies of the hfs and Zeeman structures of heavy atoms [13–24]. Measurments were performed to investigate fourteen strongest emission lines in the near visible and infrared region of isotope $^{123}$Sb (see Fig. 1).

In the experiment the metallic isotope $^{123}$Sb was used. A standard experimental arrangement for observation of hfs and Zeeman structures described in details in a series of our previous papers [13–22] was used. An electrodeless discharge tube powered by a RF generator (55 MHz) was the source of radiation. Helium was used as a buffer gas.

The high-resolution spectral apparatus consisted of a silver-coated Fabry-Pérot étalon (2, 4, 5, 7, 8 and 10 mm spacers were used) and Carl Zeiss Jena PGS-2 grating spectrograph (651.5 grooves/mm, resolution 0.8 nm/mm in the first order) combined with a charge-coupled device (CCD) detector (Hamamatsu model S7032-0906 with head device model C7042).

The Zeeman structure study has been proceded by hyperfine structure observations by the use of various Fabry-Perot spacers. The Zeeman effect studies were performed for transverse direction of observation and separated $\pi(\Delta M = 0)$ and $\sigma(\Delta M = \pm 1)$ components of lines. The light source was placed in a gap of a magnet producing fields up to 2,5 kG. Measurements have been performed for six values of the magnetic field: 1.25, 1.50, 1.75, 2.00, 2.25 and 2.50 kG. The field was measured with an accuracy of 2% by the use of a gaussmeter (Applied Magnetics

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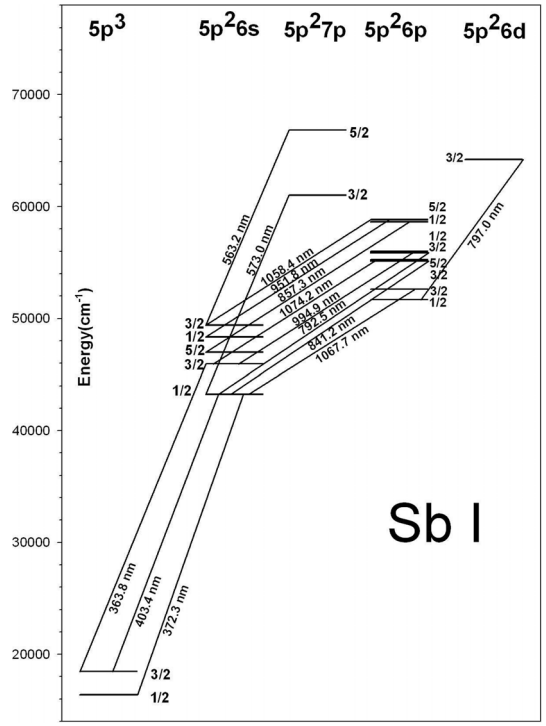


**Fig. 1.** Energy-level diagram of Sb I with level designation introduced in this work.

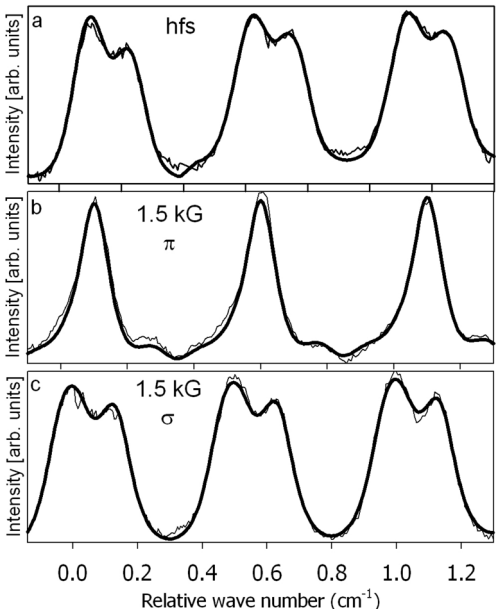


**Fig. 2.** The recorded hyperfine structure (a) of the 792.5 nm line of $^{123}$Sb I obtained with a 10 mm spacer and Zeeman patterns $\pi$-view (b) and $\sigma$-view (c) at 1.50 kG magnetic field. The thin line represents the experimental trace and the thick line shows the computer-generated contour. The line shape parameters $\alpha_1^{-1}$ and $\alpha_2^{-1}$ are 0.10 and 0.15 cm$^{-1}$, respectively.

Laboratory, model GM1A). Using the strong 605.9 nm $\left(6p8p^3\mathrm{P}_0 \rightarrow 6p7s^3\mathrm{P}_1\right)$ line of Pb I, we have calibrated the gaussmeter output to an absolute precision of 1%.

A direct observation of separate hfs Zeeman components is practically unachievable for conditions under which the hfs is barely resolved. What can be observed is an envelope of partially overlapping lines. We assumed that the observed contour is a convolution of Cauchy, Gauss and approximate Airy functions described by the following intensity distribution function [25,26]:

$$I(\nu) = I_0 + C\sum_{i=1}^{N} \frac{I_0^i}{1+\alpha_1^2\left(\widetilde{\nu}_{RL}-\delta\widetilde{\nu}_i\right)^2+\alpha_2^4\left(\widetilde{\nu}_{RL}-\delta\widetilde{\nu}_i\right)^4}, \quad (1)$$

where $I_0$ describes the background noise, $C$ is the scaling factor, $N$ is the number of hfs or hfs Zeeman components, $I_0^i$ is the maximum intensity of the $i$th component (proportional to the theoretical transition probability), $\widetilde{\nu}_{RL}$ is the adjustable parameter in the wave number scale and

$$\delta\widetilde{\nu}_i = \delta\widetilde{\nu}_i^{up} - \delta\widetilde{\nu}_i^{down}, \quad (2)$$

where $\delta\widetilde{\nu}_i^{up}$ and $\delta\widetilde{\nu}_i^{down}$ are shifts of the energy levels in respect to the position of the centre-gravity for the upper and lower hyperfine structure multiplets, respectively. In the case of hfs studies $\delta\widetilde{\nu}_i$ depends on the unknown constants $A(J)$ and $B(J)$. In the analysis of the hf Zeeman structure $\delta\widetilde{\nu}_i$ are functions of the unknown parameters $A_{down}$, $A_{up}$, $B_{down}$, $B_{up}$, $g_J^{down}$ $g_J^{up}$.

Details of the computer program for analysis of the hfs-Zeeman structure have been presented in papers [22,23].

## 3 Experimental results

Figure 2 presents recorded typical hyperfine and Zeeman structures of the observed lines. Thin lines represent the experimental traces and the thick solid lines are best fits described by formula (1).

Computer simulations yielded values of the hyperfine structure constants $A$ and Landé-$g_J$ factors presented in Table 1. From the spectrum analysis we were unable to determine $B(J)$ values with satisfactory precision, so we decided not to present these data.

The $A$ and $g_J$ constants for all levels listed in this table have been obtained in a similar way to yield agreement between calculated and observed line contours. Each value represents the average of several measurements performed in different experimental conditions. The number of analyzed measurements varied between 14 in the case of 363.8 nm line up to 46 in the case of 1058.5 nm line. Figure 3 shows a histogram of 32 individual measurements of $A$ hfs value for the 43 249.3 cm$^{-1}$ level. Similarly in $g_J$ determinations we used 13 recorded Zeeman spectra in the case of 563.2 nm line and for the line 1058.5 nm the number of spectra was 46. Figure 4 shows a histogram of 44 measurements of Landé- $g_J$ factor for the 52 612.4 cm$^{-1}$ level together with the fitted Gaussian curve.

In Table 1 the atomic structure data are presented together with statistical errors. Numbers in brackets give errors corrected by the Student's t-distribution coefficients. In the case of levels 18 464.2, 43 249.3, 45 945.3, 49 391.1 and 58 835.5 cm$^{-1}$ the $A$ and $g_J$-constants were obtained with higher reliability as a weighed mean values from observation of more than only one line.

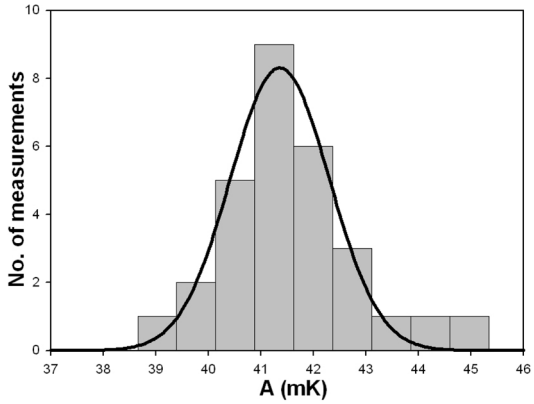


**Fig. 3.** Histogram for distribution of the experimental data for 43 249.3 $cm^{-1}$ level for a total of 32 individual measurements of $A$ value ($A = (41.42 \pm 0.09)$ mK) of 792.5 nm line.

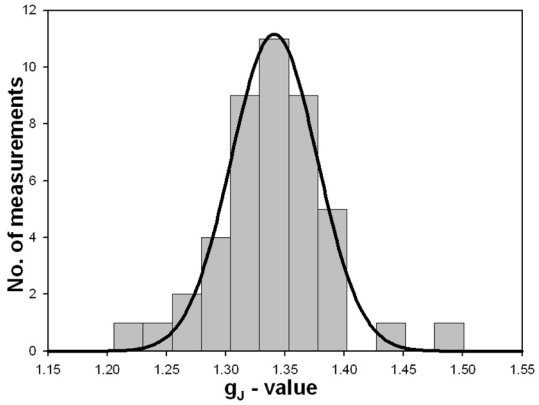


**Fig. 4.** Histogram for distribution of the experimental data for 52 612.4 $cm^{-1}$ level for a total of 44 individual measurements of $g_J$ of 1067.7 nm line ($g_J = (1.339 \pm 0.009)$).

The determined values of hyperfine splitting constant $A$ were found to be consistent with data obtained experimentally for isotope 121 [8]. For a comparison the conversion factor $A_{121}/A_{123} = 1.84661$ [27] should be used.

The Zeeman effect studies delivered 11 new $g_J$-constants.

## 4 Fine structure considerations for odd-parity levels

First theoretical studies of the hfs in the antimony atom were performed in references [8,9]. At the same time some fine structure (fs) analyses were achieved [28–30]. The last paper [8], which considers both configurations has added thirty-two new energy levels and revised $J$ values for several energy levels. Nevertheless up to now the odd-parity $5s^25p^2$(np + nf) configuration levels are not yet well defined since designation terms are missing, as well as calculated Landé-factor values, which are very useful for comparison with experimental data in order to check the validity of level assignments. Furthermore the accuracy of the amplitude of the energy level eigenvector is known to have particularly a strong influence on the determination of the effective mono-electronic hyperfine structure parameters deduced from magnetic dipole $A$ and electric quadrupole $B$ constants, experimentally obtained. For these reasons we propose to extend previous fs studies, using a method successfully tested for atoms: Si I [31], Hf I [32], Zr I [33], and ions: Nb II [34] Ta II [35], V II [36]. This method should find particular application for systems composed of many Rydberg configurations mutually interacting. Here, in the case of odd-parity levels we took into consideration the configuration basis set-up consisted of the following seven configurations: $5s^25p^3$, $5s^25p^26p$, $5s^25p^27p$, $5s^25p^28p$, $5s^25p^29p$, $5s^25p^24f$, $5s^25p^25f$. Although the total number of interaction integrals required for this basis is large, the situation was made tractable by recurring to physically realistic ratios of radial integrals as constraints [31]. For this reason we included in our fitting procedure additional assumptions, selected mainly from Hartree-Fock calculations. The totality of the experimental known odd-parity levels, located up to 90 000 $cm^{-1}$ were fitted. Thus, the fs least square fitting procedure has been carried out over 68 energy levels listed in reference [8]. With 263 parameters, 16 of which were treated as free, a very good fit has been achieved (standard deviation: 4.8 $cm^{-1}$).

The coupling scheme used to describe the levels is usually $LS$ coupling, also known as Russell Saunders coupling, $L$ and $S$ designating, respectively, the orbital and spin angular momenta of the state. Entire fs parameter sets of the configurations $5s^25p^3$, and $5s^25p^26p$ were adjusted. With regard to the configurations $5s^25p^27p$, $5s^25p^28p$, $5s^25p^29p$, $5s^25p^24f$, $5s^25p^25f$ only the average energies of configuration centers of gravity $E_{av}$ and the main Slater integrals were fitted. The other parameters are weighed by factor: $0.778 = \frac{28\,170}{36\,199} = \frac{F^2(5p,5p)(fs)}{F^2(5p,5p)(\text{ab initio})}$, i.e. by the ratio between Slater integrals $F^2(5p, 5p)$ of the main configuration $5p^3$, obtained thanks to the fs study and ab initio calculations. In Table 2, the energy levels, calculated eigenvalues, the resulting $LS$-percentages of the first and second components of the wavefunctions, and the new $LS$-term designations are given. In this table, the calculated $g_J$-factors, deduced from the eigenvector compositions, are compared with experimental ones (when the latter are available) and with ab initio Landé-factor values computed by means of Cowan code [37]. For further extensions of this work we give predicted positions of missing experimental levels up to 89 000 $cm^{-1}$ as well as their corresponding designation terms and calculated Landé-factor values. Tables 3 and 4 display fitted fs parameter values. Some of the fs parameters, which are expected to be small, have been fixed to zero and are not listed in these two tables.

## 5 Fine structure considerations for even-parity levels

When we decided to interpret Sb I hfs data of ground configuration levels we, at first, did not insert $5s5p^4$ in

**Table 1.** Experimental hfs constants $A$ and Landé $g_J$-factors of $^{123}$Sb I levels.

| Energy ($cm^{-1}$) | Level† | Line (nm) | $A$ (mK) | Landé factor |
|---|---|---|---|---|
| 16 395.4 | $5p^3\ ^2P_{1/2}$ | 372.3 | **89.16(0.41)** | **0.676(0.010)** |
| 18 464.2 | $5p^3\ ^2P_{3/2}$ | 363.8 | 14.60(0.40) | 1.274(0.009) |
| | | 403.4 | 11.60(0.13) | 1.280(0.005) |
| | | | **11.89(0.13)*** | **1.279(0.005)*** |
| 43 249.3 | $5p^2 6s^4P_{1/2}$ | 372.3 | 41.31(0.25) | 2.328(0.011) |
| | | 403.4 | 42.03(0.50) | 2.332(0.009) |
| | | 563.2 | 41.54(0.14) | 2.352(0.018) |
| | | 792.5 | 41.59(0.24) | 2.345(0.013) |
| | | 1067.7 | 41.24(0.19) | 2.357(0.023) |
| | | 841.2 | 41.31(0.38) | 2.338(0.011) |
| | | | **41.42(0.09)*** | **2.343(0.008)*** |
| 45 945.3 | $5p^2 6s^4P_{3/2}$ | 363.8 | 9.52(0.27) | 1.722(0.008) |
| | | 994.9 | 9.38(0.23) | 1.675(0.006) |
| | | 1074.2 | 9.40(0.18) | 1.675(0.015) |
| | | | **9.42(0.13)*** | **1.690(0.005)*** |
| 48 332.4 | $5p^2 6s^4P_{5/2}$ | 951.8 | **31.59(0.25)** | **1.536(0.008)** |
| 46 991.1 | $5p^2 6s^2P_{1/2}$ | 857.3 | **−18.22(0.26)** | **1.007(0.010)** |
| 49 391.1 | $5p^2 6s^2P_{3/2}$ | 573.0 | 23.78(0.36) | 1.271(0.011) |
| | | 1058.5 | 23.32(0.38) | 1.277(0.010) |
| | | | **23.56(0.27)*** | **1.274(0.008)*** |
| 51 676.4 | $5p^2 6p\ ^4D_{1/2}$ | 797.0 | **8.18(0.27)** | **0.711(0.007)** |
| 52 612.4 | $5p^2 6p\ ^4D_{3/2}$ | 1067.7 | **0.84(0.12)** | **1.339(0.009)** |
| 55 134.3 | $5p^2 6p\ ^4D_{3/2}$ | 841.2 | **1.07(0.21)** | **1.347(0.028)** |
| 55 993.9 | $5p^2 6p\ ^4P_{1/2}$ | 994.9 | **−19.99(0.41)** | **2.240(0.017)** |
| 55 864.8 | $5p^2 6p\ ^2D_{3/2}$ | 792.5 | **5.06(0.14)** | **1.223(0.009)** |
| 55 252.1 | $5p^2 6p\ ^4D_{5/2}$ | 1074.2 | **−2.12(0.16)** | **1.375(0.009)** |
| 58 835.5 | $5p^2 6p\ ^2D_{5/2}$ | 951.8 | 18.62(0.24) | 1.298(0.007) |
| | | 1058.5 | 18.62(0.20) | 1.298(0.007) |
| | | | **18.62(0.16)*** | **1.298(0.005)*** |
| 58 653.0 | $5p^2 6p\ ^2P_{1/2}$ | 857.3 | **69.38(0.39)** | **0.978(0.018)** |
| 61 000.3 | $5p^2 7p\ ^4D_{3/2}$ | 563.2 | **0.26(0.09)** | **1.336(0.010)** |
| 64 220.6 | $5p^2 6d\ ^2P_{3/2}$ | 797.0 | **0.61(0.26)** | **0.827(0.005)** |
| 66 837.6 | $5p^2 7p\ ^2D_{5/2}$ | 573.0 | **18.45(0.11)** | **1.279(0.009)** |

† Level designations introduced in this work (largest eigenvalue component).
* Weighted mean value.

the studied configuration basis set-up, thinking that this latter configuration is enough far. Furthermore the paper of Hassini et al. [8] which is the last one devoted to Sb I fine and hyperfine structures confirmed the farness of $5s5p^4$.

Unfortunately when fitting experimental energy levels to determine fine structure (fs) parameters we have noticed that this fit for highest levels is poor. We then introduced $5s5p^4$ to our studied configuration set and this time a notable improvement has occurred.

Three decades ago one of us (S.B.) performed hyperfine structure measurements of arsenic and was surprised by experimental data obtained in the laboratory: magnetic $A$ factor values of $4s^24p^25s$ levels were smaller than expected [38]; antimony is placed in the same column as

**Table 2.** Comparison between observed and calculated energy levels and $g_J$-factors for odd-parity levels.

| Observed energy [8] ($cm^{-1}$) | Calculated eigenvalue ($cm^{-1}$) | Largest eigenvalue component (%) | Next largest component (%) | Theoretical $g_J$ calc. | Theoretical $g_J$ ab initio* | Observed $g_J$ |
|---|---|---|---|---|---|---|
| $J = 1/2$ | | | | | | |
| 16 395.359 | 16 294.312 | a 99.43 2P | b 0.38 3P; 2P | 0.666 | 0.666 | 0.676† |
| 51 676.438 | 51 679.059 | b 54.89 3P; 4D | b 17.71 3P; 2S | 0.725 | 0.703 | 0.711† |
| 54 196.617 | 54 245.906 | b 50.74 3P; 2S | b 35.91 3P; 4D | 1.320 | 1.369 | |
| 55 993.859 | 55 952.148 | b 73.06 3P; 4P | b 16.5 3P; 2P | 2.244 | 2.214 | 2.240† |
| 58 653.012 | 58 733.266 | b 62.54 3P; 2P | b 14.69 3P; 2S | 0.947 | 0.962 | 0.978† |
| 60 765.293 | 60 786.535 | c 54.13 3P; 4D | c 13.49 3P; 2P | 0.666 | 0.663 | |
| 63 606.332 | 63 636.129 | c 39.4 3P; 2S | c 33.88 3P; 4D | 1.407 | 1.538 | |
| 64 098.355 | 64 094.273 | d 35.69 3P; 4D | c 15.96 3P; 4P | 1.009 | 0.768 | |
| 64 209.430 | 64 249.219 | c 34.67 3P; 4P | c 23.26 3P; 2P | 1.415 | 1.514 | |
| 65 479.617 | 65 479.168 | b 70.59 1D; 2P | c 9.06 3P; 2S | 0.981 | 0.968 | |
| 65 863.297 | 65 888.914 | f 51.09 3P; 4D | f 19.88 3P; 2P | 0.694 | 0.707 | |
| 66 685.102 | 66 801.648 | c 23.33 3P; 2P | c 16.38 3P; 2S | 1.038 | 1.068 | |
| 67 192.000 | 67 109.945 | d 44.46 3P; 4P | d 25.22 3P; 4D | 1.761 | 1.806 | |
| 67 401.602 | 67 521.586 | d 30.82 3P; 2P | d 28.54 3P; 4P | 1.453 | 1.397 | |
| | 68057.656 | f 85.7 3P; 4D | g 14.11 1D; 2P | 0.093 | 0.088 | |
| 68 945.703 | 68 926.609 | f 36.33 3P; 4D | f 31.65 3P; 2S | 1.402 | 1.518 | |
| 69 042.297 | 69 068.617 | f 44.33 3P; 2P | f 44.18 3P; 4P | 1.676 | 1.573 | |
| | 69 869.367 | d 38.88 3P; 2S | d 29.73 3P; 2P | 1.401 | 1.395 | |
| | 70 627.461 | h 85.23 3P; 4D | h 14.69 1D; 2P | 0.096 | 0.089 | |
| | 71 593.969 | f 43.44 3P; 2S | f 26.98 3P; 2P | 1.460 | 1.457 | |
| | 73 964.656 | c 82.58 1D; 2P | c 6.42 3P; 2S | 0.786 | 0.788 | |
| | 74 937.258 | b 61.54 1S; 2P | g 23.78 1D; 2P | 0.643 | 0.628 | |
| | 75 738.742 | g 61.63 1D; 2P | b 25.04 1S; 2P | 0.600 | 0.614 | |
| | 77 018.828 | d 86.33 1D; 2P | d 7.49 3P; 2S | 0.802 | 0.796 | |
| | 78 083.32 | h 84.3 1D; 2P | h 14.34 3P; 4D | 0.570 | 0.578 | |
| | 78 813.078 | f 85.56 1D; 2P | f 8.03 3P; 2S | 0.811 | 0.801 | |
| | 84 013.781 | c 94.27 1S; 2P | c 2.82 3P; 4D | 0.666 | 0.666 | |
| | 87 211.328 | d 94.71 1S; 2P | d 2.8 3P; 4D | 0.666 | 0.666 | |
| | 89 070.938 | f 94.66 1S; 2P | f 2.89 3P; 4D | 0.666 | 0.666 | |
| $J = 3/2$ | | | | | | |
| 0.000 | –41.867 | a 94.88 4S | a 4.5 2P | 1.965 | 1.973 | 1.967†† |
| 8 512.125 | 8 612.421 | a 83.71 2D | a 13.7 2P | 0.900 | 0.888 | 0.889†† |
| 18 464.201 | 18 506.084 | a 81.27 2P | a 15.48 2D | 1.270 | 1.275 | 1.279† |
| 52 612.484 | 52 581.539 | b 43.53 3P; 4D | b 24.68 3P; 4P | 1.342 | 1.341 | |
| 55 134.254 | 55 157.109 | b 48.41 3P; 4D | b 18.27 3P; 4S | 1.373 | 1.356 | 1.347† |
| 55 864.828 | 55 913.828 | b 62.63 3P; 2D | b 20.26 3P; 4S | 1.176 | 1.157 | 1.223† |
| 58 075.535 | 57 972.023 | b 43.16 3P; 4S | b 41.57 3P; 4P | 1.776 | 1.818 | |
| 58 589.512 | 58 636.996 | b 66.27 3P; 2P | b 20.29 1D; 2D | 1.229 | 1.246 | |
| 61 000.297 | 60 972.555 | c 30.68 3P; 4D | c 25.13 3P; 4P | 1.338 | 1.341 | 1.336† |
| 63 798.445 | 63 797.047 | c 31.31 3P; 4S | c 24.65 3P; 4D | 1.491 | 1.441 | |
| 63 900.527 | 63 831.758 | c 42.03 3P; 2D | c 26.03 3P; 4D | 1.063 | 1.097 | |
| 64 273.855 | 64 257.734 | d 23.85 3P; 2D | d 23 3P; 4D | 1.322 | 1.312 | |
| 64 984.586 | 65 058.238 | b 44.84 1D; 2D | c 12.64 3P; 2D | 1.067 | 1.076 | |
| 65 565.234 | 65 575.539 | g 62.99 3P; 4F | g 18.34 3P; 2D | 0.622 | 0.622 | |
| 65 959.000 | 65 916.891 | b 33.23 1D; 2P | c 17.73 3P; 2P | 1.302 | 1.278 | |
| 66 029.789 | 66 021.359 | f 21.74 3P; 4D | f 21.05 3P; 4P | 1.324 | 1.339 | |
| 66 541.555 | 66 483.555 | c 42.92 3P; 4S | c 35.72 3P; 4P | 1.756 | 1.780 | |
| 66 957.805 | 67 011.477 | d 31.31 3P; 4D | c 17.3 3P; 2P | 1.288 | 1.265 | |
| 67 375.227 | 67 331.57 | d 48.92 3P; 2D | d 22.79 3P; 4S | 1.297 | 1.415 | |

**Table 2.** Continued.

| Observed energy [8] ($cm^{-1}$) | Calculated eigenvalue ($cm^{-1}$) | Largest eigenvalue component (%) | Next largest component (%) | Theoretical $g_J$ calc. | Theoretical $g_J$ ab initio* | Observed $g_J$ |
|---|---|---|---|---|---|---|
| 67 465.102 | 67 480.094 | d 25.37 3P; 4D | c 18.79 3P; 2P | 1.235 | 1.128 | |
| 68 024.688 | 68 048.766 | g 42.83 3P; 2D | h 24.31 3P; 4F | 0.719 | 0.693 | |
| 68 070.102 | 68 052.133 | g 51.69 3P; 4D | g 13.04 3P; 2D | 1.008 | 1.084 | |
| | 68 137.992 | h 27.15 3P; 4F | g 18.56 3P; 4F | 0.715 | 0.662 | |
| 68 966.898 | 68 986.156 | f 56.65 3P; 4D | f 20.63 3P; 2P | 1.348 | 1.397 | |
| 69 053.797 | 69 051.445 | f 56.23 3P; 2D | f 21.9 3P; 4P | 1.243 | 1.186 | |
| | 69 754.797 | d 45.92 3P; 4S | d 35.6 3P; 4P | 1.777 | 1.785 | |
| | 69 886.039 | d 58.57 3P; 2P | d 14.81 1D; 2D | 1.220 | 1.224 | |
| | 70 618.562 | h 55.05 3P; 2D | h 28.98 3P; 4D | 0.987 | 1.071 | |
| | 70 649.562 | h 41 3P; 4D | h 29.12 3P; 4F | 0.850 | 0.766 | |
| | 71 560.992 | f 42.83 3P; 4S | f 38.29 3P; 4P | 1.760 | 1.782 | |
| | 71 602.758 | f 59.7 3P; 2P | f 14.04 1D; 2D | 1.230 | 1.223 | |
| | 73 560.992 | c 67.86 1D; 2D | c 12.76 1D; 2P | 0.985 | 1.015 | |
| | 74 263.219 | c 66.67 1D; 2P | c 12.07 1D; 2D | 1.305 | 1.267 | |
| | 75 047.555 | b 52.89 1S; 2P | g 32.81 1D; 2P | 1.312 | 1.300 | |
| | 75 391.531 | g 85.12 1D; 2D | g 5.09 3P; 4F | 0.799 | 0.799 | |
| | 75 802.297 | g 52.59 1D; 2P | b 34.02 1S; 2P | 1.303 | 1.311 | |
| | 76 876.625 | d 69.71 1D; 2D | d 13.94 1D; 2P | 0.977 | 1.019 | |
| | 77 149.758 | d 70.3 1D; 2P | d 12.98 1D; 2D | 1.310 | 1.261 | |
| | 77 973.727 | h 84.84 1D; 2D | h 5.13 3P; 2D | 0.798 | 0.799 | |
| | 78 085.664 | h 84.1 1D; 2P | h 7.3 3P; 4D | 1.287 | 1.291 | |
| | 78 732.953 | f 68.86 1D; 2D | f 15.54 1D; 2P | 0.986 | 1.014 | |
| | 78 898.766 | f 68.8 1D; 2P | f 14.88 1D; 2D | 1.301 | 1.263 | |
| | 84 076.703 | c 94.37 1S; 2P | c 1.58 3P; 4P | 1.334 | 1.334 | |
| | 87 247.719 | d 94.72 1S; 2P | d 1.46 3P; 4P | 1.334 | 1.334 | |
| | 89 097.078 | f 94.67 1S; 2P | f 1.48 3P; 4P | 1.334 | 1.334 | |
| $J = 5/2$ | | | | | | |
| 9 854.018 | 10 100.023 | a 99.8 2D | b 0.13 3P; 2D | 1.200 | 1.200 | 1.205†† |
| 55 252.133 | 55 246.453 | b 72.43 3P; 4D | b 19 3P; 4P | 1.401 | 1.407 | 1.375† |
| 57 410.340 | 57 384.125 | b 36.5 3P; 4P | b 22.85 3P; 2D | 1.358 | 1.385 | |
| 58 835.488 | 58 837.426 | b 53.81 3P; 2D | b 30.93 3P; 4P | 1.291 | 1.276 | 1.298† |
| 62 462.406 | 62 463.227 | g 41.35 3P; 4G | g 18.05 3P; 2D | 0.856 | 0.856 | |
| 63 790.945 | 63 791.48 | c 50.61 3P; 4D | c 18.04 3P; 4P | 1.371 | 1.379 | |
| 64 512.391 | 64 471.82 | b 57.39 1D; 2D | b 16.11 1D; 2F | 1.214 | 1.104 | |
| 64 878.957 | 64 884.242 | b 63.73 1D; 2F | b 12.13 3P; 2D | 1.002 | 1.093 | |
| 64 973.820 | 64 949.758 | h 40.98 3P; 4G | h 17.91 3P; 2D | 0.856 | 0.856 | |
| 65 460.148 | 65 466.785 | g 46.83 3P; 4G | g 38.27 3P; 2D | 0.908 | 0.913 | |
| 65 568.312 | 65 571.734 | g 34.62 3P; 2F | g 29.63 3P; 4D | 1.083 | 1.078 | |
| 66 361.633 | 66 365.695 | c 36.26 3P; 4P | c 28.51 3P; 4D | 1.372 | 1.408 | |
| 66 837.570 | 66828.227 | c 47.47 3P; 2D | c 24.99 3P; 4P | 1.293 | 1.262 | 1.279† |
| 67 307.000 | 67 259.797 | d 54.4 3P; 4D | d 22.62 3P; 4P | 1.389 | 1.393 | |
| 67 994.383 | 68 008.938 | h 45.33 3P; 4G | h 40.12 3P; 2D | 0.901 | 0.914 | |
| 68 023.867 | 68 039.844 | h 20.26 3P; 4D | h 17.96 3P; 4F | 1.127 | 1.151 | |
| 68 148.219 | 68 132.734 | g 26.88 3P; 4F | g 25.47 3P; 2F | 0.968 | 0.995 | |
| 68 157.109 | 68 141.992 | g 26.28 3P; 4D | h 14.68 3P; 2F | 1.149 | 1.086 | |
| 69 037.297 | 68 997.672 | f 58.84 3P; 4D | f 24.52 3P; 4P | 1.400 | 1.401 | |
| | 69 669.414 | d 33.31 3P; 4D | d 30.85 3P; 4P | 1.357 | 1.398 | |
| | 69 892.633 | d 51.29 3P; 2D | d 32.87 3P; 4P | 1.308 | 1.270 | |
| | 70 646.578 | h 30.73 3P; 4D | h 28.94 3P; 2F | 1.139 | 1.208 | |
| | 70 665.969 | h 40 3P; 4F | h 16.96 3P; 4D | 1.029 | 0.964 | |

**Table 2.** Continued.

| Observed energy [8] ($cm^{-1}$) | Calculated eigenvalue ($cm^{-1}$) | Largest eigenvalue component (%) | Next largest component (%) | Theoretical $g_J$ calc. | Theoretical $g_J$ ab initio* | Observed $g_J$ |
|---|---|---|---|---|---|---|
| | 71 508.406 | f 34.14 3P; 4D | f 26.87 3P; 4P | 1.338 | 1.390 | |
| | 71 630.258 | f 47.57 3P; 2D | f 36.63 3P; 4P | 1.325 | 1.279 | |
| | 73 513 | c 74.8 1D; 2D | c 11.12 3P; 4P | 1.216 | 1.065 | |
| | 73 682.188 | c 74.7 1D; 2F | c 10.22 3P; 2D | 0.956 | 1.095 | |
| | 75 272.781 | g 84.28 1D; 2F | g 5.33 3P; 4F | 0.879 | 0.878 | |
| | 75 393.188 | g 85.1 1D; 2D | g 7.6 3P; 4D | 1.200 | 1.199 | |
| | 76 826.75 | d 68.32 1D; 2D | d 16.59 1D; 2F | 1.181 | 1.080 | |
| | 76 870.031 | d 68.06 1D; 2F | d 16.48 1D; 2D | 0.984 | 1.080 | |
| | 77 897.867 | h 84.33 1D; 2F | h 5.3 3P; 4F | 0.879 | 0.878 | |
| | 77 974.531 | h 84.84 1D; 2D | h 7.82 3P; 4D | 1.200 | 1.190 | |
| | 78 716.789 | f 56.06 1D; 2D | f 28.6 1D; 2F | 1.133 | | |
| | 78 729.586 | f 55.91 1D; 2F | f 28.55 1D; 2D | 1.034 | | |
| $J = 7/2$ | | | | | | |
| 57 555.355 | 57 506.301 | b 85.74 3P; 4D | b 13.41 1D; 2F | 1.391 | 1.395 | |
| 62 465.945 | 62 464.562 | g 24.36 3P; 2G | g 22.97 3P; 4D | 1.141 | 1.143 | |
| 64 957.230 | 64 950.938 | h 23.44 3P; 2G | h 22.21 3P; 4F | 1.142 | 1.179 | |
| 64 978.246 | 64 966.285 | b 81.53 1D; 2F | b 11.82 3P; 4D | 1.183 | 1.144 | |
| 65 467.215 | 65 471.711 | g 47.2 3P; 4D | g 29.54 3P; 2G | 1.181 | 1.184 | |
| 65 531.000 | 65 529.789 | g 40.45 3P; 4G | g 26.4 3P; 2F | 1.024 | 1.020 | |
| 66 405.383 | 66 382.117 | c 83.74 3P; 4D | c 14.79 1D; 2F | 1.386 | 1.390 | |
| 67 997.023 | 68 011.773 | h 46.79 3P; 4D | h 31.09 3P; 2G | 1.178 | 1.159 | |
| | 68 032.055 | h 33.08 3P; 4G | h 22.33 3P; 2F | 1.033 | 1.069 | |
| | 68 137.273 | g 27.31 3P; 2F | g 24.3 3P; 4F | 1.198 | 1.227 | |
| 68 164.055 | 68 144.484 | g 27.67 3P; 4F | g 18.65 3P; 2F | 1.087 | 1.043 | |
| | 69 695.461 | d 84.79 3P; 4D | d 14.47 1D; 2F | 1.388 | 1.390 | |
| | 70 658.297 | h 53.08 3P; 2F | h 16.32 3P; 2G | 1.060 | 1.086 | |
| | 70 670.648 | h 52.81 3P; 4F | h 19.93 3P; 4D | 1.228 | 1.206 | |
| | 71 533.18 | f 84.59 3P; 4D | f 15.02 1D; 2F | 1.386 | 1.390 | |
| | 73 706.133 | c 84.75 1D; 2F | c 14.72 3P; 4D | 1.186 | 1.182 | |
| | 75 235.273 | g 84.11 1D; 2G | g 7.64 3P; 2F | 0.920 | 0.920 | |
| | 75 273.195 | g 84.25 1D; 2F | g 7.35 3P; 4F | 1.160 | 1.156 | |
| | 76 890.367 | d 85.08 1D; 2F | d 14.51 3P; 4D | 1.185 | 1.183 | |
| | 77 871.938 | h 84.19 1D; 2G | h 7.65 3P; 2F | 0.919 | 0.921 | |
| | 77 898.383 | h 84.26 1D; 2F | h 7.48 3P; 4F | 1.160 | 1.154 | |
| | 78 745.922 | f 84.76 1D; 2F | f 15.05 3P; 4D | 1.186 | 1.183 | |
| $J = 9/2$ | | | | | | |
| 65 527.793 | 65 534.508 | g 47.8 3P; 4G | g 34.64 3P; 4F | 1.218 | 1.219 | |
| | 68 042.992 | h 37.89 3P; 4G | h 28.78 3P; 4F | 1.217 | 1.151 | |
| | 68 056.703 | g 63.79 3P; 2G | g 15.78 3P; 4G | 1.102 | 1.180 | |
| | 68 144.547 | g 47.36 3P; 4F | g 19.76 3P; 4G | 1.244 | 1.236 | |
| | 70 615.656 | h 64.03 3P; 2G | h 20.82 3P; 4G | 1.094 | 1.109 | |
| | 70 667.602 | h 54.31 3P; 4F | h 23.82 3P; 4G | 1.247 | 1.235 | |
| | 75 234.539 | g 84.1 1D; 2G | g 10.04 3P; 4F | 1.136 | 1.134 | |
| | 75 383.852 | g 85.27 1D; 2H | g 10.7 3P; 2G | 0.941 | 0.939 | |
| | 77 871.938 | h 84.21 1D; 2G | h 9.92 3P; 4F | 1.136 | 1.134 | |
| | 77 958.906 | h 84.94 1D; 2H | h 10.89 3P; 2G | 0.942 | 0.939 | |
| $J = 11/2$ | | | | | | |
| | 68 064.047 | g 85.25 3P; 4G | g 14.74 1D; 2H | 1.246 | 1.248 | |
| | 70 624.445 | h 84.92 3P; 4G | h 15.07 1D; 2H | 1.246 | 1.248 | |
| | 75 385.352 | g 85.24 1D; 2H | g 14.74 3P; 4G | 1.118 | 1.116 | |
| | 77 960.391 | h 84.93 1D; 2H | h 15.06 3P; 4G | 1.119 | 1.116 | |

a: $5p^3$; b: $5p^2 6p$; c: $5p^2 7p$; d: $5p^2 8p$; f: $5p^2 9p$; g: $5p^2 4f$; h: $5p^2 5f$.
† Present work, †† NIST data, * ab initio results obtained by the use of Cowan code.

**Table 3.** Values of fs-parameters of odd-parity levels of Sb I. The uncertainties given in parentheses are the standard deviations.

| Configuration | $E_{av}$ | $F^2(5p,5p)$ | $F^2(5p,np)$ $F^2(5p,nf)$ | $\xi_{5p}$ | $\xi_{np}$ | $G^0(5p,np)$ | $G^2(5p,np)$ | $G^2(5p,nf)$ |
|---|---|---|---|---|---|---|---|---|
| $5p^3$ | 10033 (28) | 26302 (133) | | 3270 (44) | | | | |
| $5p^26p$ | 60683 (16) | 27950 (243) | 4159 (127) | 3630 (28) | 261[a] | 753[a] | 888[a] | |
| $5p^27p$ | 69153 (25) | 28404 (247) | 1543 (47) | 3656 (29) | 80[a] | 233[a] | 212[a] | |
| $5p^28p$ | 72404 (43) | 28440 (247) | 600 (24) | 3652 (47) | 42[a] | 113[a] | 90[a] | |
| $5p^29p$ | 74203 (22) | 28448 (247) | 325 (13) | 3652 (48) | 23[a] | 65[a] | 60[a] | |
| $5p^24f$ | 70750 (21) | 28661 (249) | 631 (26) | 3671 (49) | 0[a] | | | 11[a] |
| $5p^25f$ | 73340 (29) | 28786 (250) | 395 (16) | 3671 (49) | 0[a] | | | 9[a] |

[a] Fixed.

**Table 4.** Values of configuration interaction parameters for odd-parity levels.

| | $R^0$ ($cm^{-1}$) | $R^2$ ($cm^{-1}$) | $D^2$ ($cm^{-1}$) | $E^0$ ($cm^{-1}$) | $E^2$ ($cm^{-1}$) | $E^4$ ($cm^{-1}$) |
|---|---|---|---|---|---|---|
| $5p^3$-$5p^26p$ | 587 (70) | 1614 (85) | | | | |
| $5p^3$-$5p^27p$ | 260 (31) | 1210 (64) | | | | |
| $5p^3$-$5p^28p$ | 245 (30) | 969 (51) | | | | |
| $5p^3$-$5p^29p$ | 179 (22) | 789 (42) | | | | |
| $5p^3$-$5p^24f$ | | –989 (111) | | | | |
| $5p^3$-$5p^25f$ | | –200 (22) | | | | |
| $5p^26p$-$5p^27p$ | | | 1825[a] | 485[a] | 500[a] | |
| $5p^26p$-$5p^28p$ | | | 980[a] | 330[a] | 352[a] | |
| $5p^26p$-$5p^29p$ | | | 700[a] | 238[a] | 250[a] | |
| $5p^26p$-$5p^24f$ | | | 912[a] | –21[a] | | |
| $5p^26p$-$5p^25f$ | | | 680[a] | –21[a] | | |
| $5p^27p$-$5p^28p$ | | | 570[a] | 180[a] | 200[a] | |
| $5p^27p$-$5p^29p$ | | | 455[a] | 130[a] | 147[a] | |
| $5p^27p$-$5p^24f$ | | | 230[a] | –7[a] | | |
| $5p^27p$-$5p^25f$ | | | 100[a] | –7[a] | | |
| $5p^28p$-$5p^29p$ | | | 340[a] | 87[a] | 100[a] | |
| $5p^28p$-$5p^24f$ | | | 84[a] | 0[a] | | |
| $5p^28p$-$5p^25f$ | | | 70[a] | 0[a] | | |
| $5p^29p$-$5p^24f$ | | | 60[a] | 0[a] | | |
| $5p^29p$-$5p^25f$ | | | 56[a] | 0[a] | | |
| $5p^24f$-$5p^25f$ | | | 335[a] | | 33[a] | 21[a] |

[a] Fixed.

arsenic in the periodic table. In the EGAS Conference held in Liege in 1982 Voss and Winkler, Howard and Andrew had been facing the same problem: what is the real impact of close $4s4p^4$ configuration [39], whose levels have very large magnetic structure (because of high influence of Fermi-contact hfs parameter $a^{10}_{4s}$)? Let us point out that $a^{10}_{ns}$ is inversely proportional to the square of principal quantum number $n$.

Some years later the levels of the latter configuration have been revised and corrected [40–42] and it has been proven that levels of these two configurations mix only very weakly (less than 1%) because they are not as close as previously indicated in reference [39].

Similar situation one of us (J.K.) met performing several years ago calculations of the level structure of the ground $6s^26p^2$ configuration of lead [43]. It was found that a large impact on the fit of the energy levels had to consider the interaction with distant configuration $6p^4$.

As for many elements, Sb I was first investigated by Meggers and Humphreys [3]. Later Mazzoni and Joshi [28], Joshi et al. [29], Zaidi, Makdisi and Bhatia [12], Beigang and Wynne [30] extended and revised in turn this first analysis. The last but not the least work was done by Hassini et al. [8] who reported 138 levels derived from 617 spectral lines in the range 2536 to 24 786 $cm^{-1}$.

The method applied here for fine and hyperfine structure studies was successfully used previously as regards neutral and singly ionized atoms: Zr I, Hf I, Nb II, Ta II, V II, Ti II [34–36,44,45], gathering the set of their studied configurations in model space when it was possible. In the fs calculations we took into account the basis set-up consisted of the 7 interacting configurations: $5s^25p^26s$,

$5s^2 5p^2 7s$, $5s^2 5p^2 8s$, $5s5p^4$, $5s^2 5p^2 5d$, $5s^2 5p^2 6d$ and $5s^2 5p^2 7d$. The procedure of fs analysis includes spin-dependent and electrostatic interactions, represented by Slater integrals $F^k$, $G^k$ and $R^k$. The spin-orbit integrals $\xi_{nd}$ and $\xi_{5p}$ effect the interactions with distant configurations. We have taken also into account two-body parameters $\alpha$ and $\beta$ standing for one- and two-electron excitations, respectively. Parametric calculations were performed with the use of the Russel-Saunders ($LS$) coupling scheme where $L$ and $S$ represent the total angular momentum and the resulting spin quantum numbers for a system of electrons, respectively. The fs least square fitting procedure has been carried out first over all even-parity levels available in literature [3,8,12,28–30], but in the second step we discarded three levels of poor accuracy: 65 945.699 $cm^{-1}$ ($J = 1/2$), 66 113.217 $cm^{-1}$ ($J = 3/2$) and 66 535.190 $cm^{-1}$ ($J = 3/2$). With 53 parameters, 15 of which were treated as free, an excellent fit has been achieved. Tables 5 and 6 contain the values of fs radial parameters obtained thanks to the fitting procedure. When some fs parameters are given without uncertainties this means that to these parameters were given simply ab initio values or were deduced by links with other parameters thanks to ab initio ratio of the corresponding parameters. Let us add that values of some parameters, although predicted by theory but expected to be small in this study were fixed to zero and then are not listed in Tables 5 and 6. In Table 7 the experimental energy levels, calculated eigenvalues, resulting $LS$-percentage of first and second components of the wave functions, and the corresponding $LS$-term designations are given. In this table our experimental Landé $g_J$-factors, as well as those found in literature are compared to those deduced from the eigenvector compositions and those computed by ab initio procedure, recurring to Cowan code [37].

## 6 Hyperfine interaction

The hyperfine structure of atomic energy levels is caused by the interaction between electrons and the electromagnetic multipole moments of the nucleus.

The hyperfine interaction Hamiltonian can be represented usually by a multipole expansion as follows [46]:

$$H_{hfs} = \sum_{k=1} T^{(k)} M^{(k)} \tag{3}$$

where $T^{(k)}$ and $M^{(k)}$ are spherical tensor operators of rank $k$ in the electronic and nuclear spaces, respectively. In the nonrelativistic framework, the electronic tensor operators in atomic units can be written as:

$$T^{(1)} = \frac{\alpha^2}{2} \sum_{i=1}^{N} \left\{ 2g_l l^{(1)}(i) r_i^{-3} - g_s \sqrt{10} \left[ C^{(2)}(i) \times s^{(1)}(i) \right]^{(1)} \right] r_i^{-3} + g_s \frac{8}{3} \pi \delta(r_i) s^{(1)}(i) \right\} \tag{4}$$

and

$$T^{(2)} = -\sum_{i=1}^{N} C^{(2)}(i) r_i^{-3}, \tag{5}$$

where $g_l$ and $g_s$ are the orbital and electron spin $g$-factors. The three terms in equation (4) are usually called *orbital*, *spin-dipole*, and *Fermi-contact term*, respectively.

Hyperfine interaction couples electronic angular momentum $\mathbf{J}$ and nuclear angular momentum $\mathbf{I}$ to a total angular momentum $\mathbf{F} = \mathbf{I} + \mathbf{J}$. In this representation the diagonal and off-diagonal hyperfine energy corrections are given by:

$$W_{M1}(J, J) = \frac{1}{2} A_J C, \tag{6}$$

$$W_{M1}(J, J-1) = \frac{1}{2} A_{J,J-1} [(K+1)(K-2F) \times (K-2I)(K-2J+1)]^{1/2}, \tag{7}$$

$$W_{E2}(J, J) = B_J \frac{3/4C(C+1) - I(I+1)J(J+1)}{2I(2I-1)J(2J-1)}, \tag{8}$$

where $C = F(F+1) - J(J+1) - I(I+1)$ and $K = I+J+F$.

The coupling constants are:

$$A_J = \frac{\mu_I}{I} \frac{1}{[J(J+1)(2J+1)]^{1/2}} \langle \gamma J || T^{(1)} || \gamma J \rangle, \tag{9}$$

$$A_{J,J-1} = \frac{\mu_I}{I} \frac{1}{[J(2J-1)(2J+1)]^{1/2}} \langle \gamma J || T^{(1)} || \gamma (J-1) \rangle, \tag{10}$$

$$B_J = 2Q \left[ \frac{2J(2J-1)}{(2J+1)(2J+2)(2J+3)} \right]^{1/2} \times \langle \gamma J || T^{(2)} || \gamma J \rangle. \tag{11}$$

The nuclear magnetic dipole moment $\mu_I$ and nuclear electric quadrupole moment $Q$ are defined through the expectation values of the nuclear tensor operators $M^{(1)}$ and $M^{(2)}$ in the state with the maximum component of the nuclear spin, $M_I = I$:

$$\left\langle \gamma_I II \middle| M_0^{(1)} \middle| \gamma_I II \right\rangle = \mu_I, \tag{12}$$

$$\left\langle \gamma_I II | M_0^{(2)} | \gamma_I II \right\rangle = \frac{Q}{2}. \tag{13}$$

Together with the nuclear magnetic dipole and electric quadrupole moments the $A$ and $B$ hfs coupling constants yield values of the electronic hyperfine parameters $a_l$, $a_{sd}$, $a_c$ and $b_q$:

$$a_l = \left\langle \gamma LSM_L M_S \middle| \sum_{i=1}^{N} l_0^{(1)}(i) r_i^{-3} \middle| \gamma LSM_L M_S \right\rangle, \quad (orbital) \tag{14}$$

**Table 5.** Values of fs parameters for even-parity levels of Sb I. The uncertainties given in parentheses are the standard deviations.

| Config. | $5s^25p^26s$ | $5s^25p^27s$ | $5s^25p^28s$ | $5s5p^4$ | Config. | $5s^25p^25d$ | $5s^25p^26d$ | $5s^25p^27d$ |
|---|---|---|---|---|---|---|---|---|
| | | | | | | Fit | Fit | Fit |
| $E_{av}$ | 51756 (26) | 66274 (32) | 71218 (41) | 78138 (203) | $E_{av}$ | 62552 (25) | 69468 (41) | 72610 (59) |
| $F^2(5p,5p)$ | 28170 (120) | 28170 (120) | 28170 (120) | 28170 (120) | $F^2(5p,5p)$ | 26988 (226) | 26988 (226) | 26988 (226) |
| $G^1(5pns,ns5p)$ | 2390 (65) | 400 (60) | 0.00 | 35052 | $F^2(5p,nd)$ | 6650 (134) | 1786 (372) | 900 (170) |
| $\xi_{5p}$ | 3560 (19) | 3567(19) | 3645 (21) | 3000 | $\xi_{5p}$ | 3579 (19) | 3631(20) | 3642(21) |
| $\alpha$ | 4.5 (2.5) | 4.5 (2.5) | 4.5 (2.5) | 4.5 (2.5) | $\xi_{nd}$ | 18 | 6 | 3 |
| | | | | | $\alpha$ | 4.5 (2.5) | 4.5 (2.5) | 4.5 (2.5) |
| | | | | | $G^1(5p,nd)$ | 3773 (87) | 1519 (182) | 650 (103) |
| | | | | | $G^3(5p,nd)$ | 1652 (147) | 927 (239) | 420 (97) |

**Table 6.** Values of configuration interaction parameters for even-parity levels.

| Interacting configurations | $E^1$ ($cm^{-1}$) | $D^2$ ($cm^{-1}$) | $R^1$ ($cm^{-1}$) | $E^3$ ($cm^{-1}$) |
|---|---|---|---|---|
| $5s^25p^26s$-$5s^25p^27s$ | 890 | | | |
| $5s^25p^26s$-$5s^25p^28s$ | 550 | | | |
| $5s^25p^26s$-$5s^25p^25d$ | –3206 (113) | –4627 (213) | | |
| $5s^25p^26s$-$5s^25p^26d$ | –780 (160) | –2412 (410) | | |
| $5s^25p^26s$-$5s^25p^27d$ | –560 | –1190 | | |
| $5s^25p^26s$-$5s5p^4$ | | | –1978 (150) | |
| $5s^25p^27s$-$5s^25p^28s$ | 261 | | | |
| $5s^25p^27s$-$5s^25p^25d$ | –750 | –1632 | | |
| $5s^25p^27s$-$5s^25p^26d$ | –395 | –1210 | | |
| $5s^25p^27s$-$5s^25p^27d$ | –260 | –820 | | |
| $5s^25p^27s$-$5s5p^4$ | | | –750 | |
| $5s^25p^28s$-$5s^25p^25d$ | –500 | –1000 | | |
| $5s^25p^28s$-$5s^25p^26d$ | –250 | –628 | | |
| $5s^25p^28s$-$5s^25p^27d$ | –178 | –495 | | |
| $5s^25p^28s$-$5s5p^4$ | | | –500 | |
| $5s^25p^25d$-$5s^25p^26d$ | 2394(71) | 3413 (114) | | 1795 (108) |
| $5s^25p^25d$-$5s^25p^27d$ | 1750 | 2160 | | 800 |
| $5s^25p^25d$-$5s5p^4$ | | | 8587 (98) | 611 |
| $5s^25p^26d$-$5s^25p^27d$ | 948 (81) | 1255 (190) | | |
| $5s^25p^26d$-$5s5p^4$ | | | 7305 (165) | |
| $5s^25p^27d$-$5s5p^4$ | | | 6573 (249) | |

$$a_{sd} = \left\langle \gamma LSM_LM_S \left| \sum_{i=1}^{N} 2C_0^{(2)}(i)s_0(i)r_i^{-3} \right| \gamma LSM_LM_S \right\rangle, \quad (spin\text{-}dipole) \quad (15)$$

$$a_c = \left\langle \gamma LSM_LM_S \left| \sum_{i=1}^{N} 8\pi\delta^3(r_i)s_0(i) \right| \gamma LSM_LM_S \right\rangle, \quad (Fermi\ contact) \quad (16)$$

$$b_q = \left\langle \gamma LSM_LM_S \left| \sum_{i=1}^{N} 2C_0^{(2)}(i)r_i^{-3} \right| \gamma LSM_LM_S \right\rangle, \quad (electric\text{-}quadrupole) \quad (17)$$

where $M_L = L$ and $M_S = S$.

## 7 Hyperfine structure considerations for odd-parity levels

Optical hfs investigations started early [6] for this medium heavy element ($Z = 51$). A spectroscopy team from Berlin extended previous investigations using pressure-scanned Fabry-Pérot interferometers [7,9] and some years later, recurring to Fourier-transform spectrometer, the wavelengths of 617 lines have been measured and the hyperfine-structure splitting factors of 77% of these lines were determined by Hassini et al. [8].

Table 8 contains values of fitted hfs parameters with regard to magnetic factor $A$ only. Concerning the hfs analysis, we follow the many-body parameterization method. The radial parameters $a_{nl}^{\kappa k}$, $b_{nl}^{\kappa k}$ have been evaluated by fitting them to experimentally determined hfs constants $A$ and $B$ using the theoretical expressions (Eqs. (4) and (5) of [45] for example). In this aim we used experimental hfs values of Table 1 and some selected ones from paper [8],

**Table 7.** Comparison between observed and calculated even-parity energy levels and $g_J$-factors.

| $J$ | Observed energy [8] ($cm^{-1}$) | Calculated eigenvalue ($cm^{-1}$) | Largest eigenvalue component (%) | Next largest component (%) | Theoretical $g_J$ calc. | Theoretical $g_J$ ab initio* | Experimental $g_J$ this work | Experimental $g_J$ others† |
|---|---|---|---|---|---|---|---|---|
| 0.5 | 43 249.336 | 43 229.395 | a 80.94 3P4P | a 13.64 3P2P | 2.356 | 2.350 | 2.343 | 2.332 |
| 0.5 | 46 991.059 | 47 027.316 | a 79.57 3P2P | a 15.58 3P4P | 0.984 | 0.990 | 1.007 | 1.004 |
| 0.5 | 56 698.609 | 56 642.598 | d 36.68 3P4P | d 32.63 3P4D | 1.526 | 1.396 | | |
| 0.5 | 57 597.203 | 57 678.273 | d 21.65 3P4D | d 21.14 3P2P | 1.471 | 1.479 | | |
| 0.5 | 58 132.656 | 58 150.008 | b 55.60 3P4P | b 21.89 3P2P | 1.914 | 1.823 | | |
| 0.5 | 59 737.625 | 59 735.121 | d 50.66 3P2P | d 32.04 3P4D | 0.609 | 0.851 | | |
| 0.5 | 61 386.508 | 61 290.504 | b 67.32 3P2P | b 24.47 3P4P | 1.166 | 1.132 | | |
| 0.5 | 62 960.316 | 62 985.121 | c 62.03 3P4P | c 30.62 3P2P | 1.994 | 2.043 | | |
| 0.5 | 63 825.758 | 63 757.918 | e 34.15 3P4D | e 20.16 3P4P | 1.411 | 0.846 | | |
| 0.5 | 64 769.176 | 64 731.531 | e 41.41 3P4D | g 14.95 3P4P | 1.257 | 1.904 | | |
| 0.5 | 65 654.406 | 65 624.992 | a 73.74 1S2S | d 9.19 1D2S | 2.002 | 1.852 | | |
| 0.5 | 66 009.711 | 65 986.711 | c 62.13 3P2P | c 31.98 3P4P | 1.325 | 1.264 | | |
| 0.5 | 66 353.859 | 66 299.922 | e 43.20 3P2P | d 22.01 1D2P | 0.699 | 0.739 | | |
| 0.5 | 67 427.023 | 67 382.953 | d 61.27 3P4D | f 15.50 3P2P | 0.625 | 0.454 | | |
| 0.5 | | 68 451.250 | d42.80 1D2P | e 14.54 3P2P | 0.864 | 0.670 | | |
| 0.5 | | 68 670.328 | d 23.02 3P4P | f 22.54 3P4P | 1.941 | 2.106 | | |
| 0.5 | | 69 086.992 | d 62.79 1D2S | a 13.99 1S2S | 1.942 | 2.161 | | |
| 0.5 | | 70 040.359 | f 60.08 3P2P | f 15.79 3P4D | 0.625 | 0.616 | | |
| | | | | | | | | |
| 1.5 | 45 945.340 | 45 942.695 | a 92.52 3P4P | a 6.76 3P2P | 1.705 | 1.705 | 1.690 | 1.713 |
| 1.5 | 49 391.133 | 49 347.133 | a 67.45 3P2P | a 16.64 1D2D | 1.253 | 1.265 | 1.274 | 1.277 |
| 1.5 | 53 527.957 | 53 489.625 | d 58.53 3P4F | d 10.87 3P4D | 0.719 | 0.740 | | |
| 1.5 | 55 232.965 | 55 247.754 | a 46.83 1D2D | d 13.38 3P2P | 1.051 | 1.015 | | 0.991 |
| 1.5 | 56 151.801 | 56 196.727 | d 28.20 3P4P | a 25.65 1D2D | 1.224 | 1.250 | | 1.302 |
| 1.5 | 56 733.160 | 56 655.125 | d 49.60 3P2P | d 12.24 3P4P | 1.285 | 1.256 | | 1.311 |
| 1.5 | 58 746.355 | 58 773.828 | d 70.99 3P4D | g 6.79 3P4P | 1.218 | 1.226 | | |
| 1.5 | 60 580.898 | 60 544.223 | d 27.83 3P2D | e 22.37 3P4F | 0.840 | 0.854 | | |
| 1.5 | 60 964.672 | 60 981.961 | b 84.58 3P4P | b 13.02 3P2P | 1.678 | 1.166 | | |
| 1.5 | 61 808.699 | 61 867.086 | d 32.89 3P2D | e 19.65 3P4F | 0.881 | 0.838 | | |
| 1.5 | 63 193.031 | 63 222.086 | e 22.51 3P4F | e 17.39 3P4P | 1.294 | 1.147 | | |
| 1.5 | 63 649.461 | 63 667.332 | b 61.30 3P2P | b 13.48 1D2D | 1.301 | 1.315 | | |
| 1.5 | 64 220.605 | 64 257.441 | f 29.04 3P4F | e 18.80 3P2P | 0.878 | 0.884 | 0.827 | |
| 1.5 | 64 432.395 | 64 586.117 | d 20.60 1D2D | e 19.61 3P2P | 0.970 | 0.884 | | |
| 1.5 | 64 843.422 | 64 862.508 | d 35.62 1D2D | e 11.04 3P2P | 0.999 | 1.126 | | |
| 1.5 | 65 143.602 | 65 231.434 | e 56.73 3P4D | e 10.34 3P2D | 1.177 | 1.312 | | |
| 1.5 | 66 023.102 | 66 022.602 | c 81.48 3P4P | c 16.76 3P2P | 1.661 | 1.627 | | |
| 1.5 | | 66 952.930 | e 34.07 3P2D | f 9.28 3P2D | 0.960 | 0.949 | | |
| 1.5 | | 67 253.469 | f 32.38 3P4F | f 17.34 3P2P | 1.133 | 1.101 | | |
| 1.5 | | 67 857.016 | f 22.64 3P2P | e 16.74 3P2D | 1.135 | 1.182 | | |
| 1.5 | | 68 411.617 | c 47.77 3P2P | d 16.49 1D2P | 1.301 | 1.247 | | |
| 1.5 | | 68 776.828 | f 36.47 3P4D | e 18.80 3P4P | 1.325 | 1.307 | | |
| 1.5 | | 69 205.336 | d 53.86 1D2P | c 14.44 3P2P | 1.309 | 1.419 | | |
| 1.5 | | 69 943.539 | f 36.96 3P2D | f 20.12 3P2P | 0.947 | 0.948 | | |
| 1.5 | | 70 895.719 | b 69.60 1D2D | b 11.38 3P2P | 0.933 | 0.914 | | |
| 1.5 | | 71 464.836 | f 41.94 3P4P | g 23.27 3P4P | 1.566 | 1.622 | | |
| 1.5 | | 72 628.797 | e 50.38 1D2D | d 10.20 1D2D | 0.910 | 0.882 | | |

**Table 7.** Continued.

| $J$ | Observed energy [8] ($cm^{-1}$) | Calculated eigenvalue ($cm^{-1}$) | Largest eigenvalue component (%) | Next largest component (%) | Theoretical $g_J$ calc. | Theoretical $g_J$ ab initio* | Experimental $g_J$ this work | Experimental $g_J$ others† |
|---|---|---|---|---|---|---|---|---|
| 1.5 | | 74 514.812 | e 75.74 1D2P | e 11.05 3P4P | 1.364 | 1.354 | | |
| 1.5 | | 75 728.305 | c 82.77 1D2D | c 12.70 3P2P | 0.899 | 0.901 | | |
| 2.5 | 48 332.426 | 48 328.031 | a 86.49 3P4P | a 12.84 1D2D | 1.549 | 1.553 | 1.536 | 1.547 |
| 2.5 | 53 442.969 | 53 342.336 | d 38.77 3P4P | g 16.25 3P4P | 1.417 | 1.432 | | |
| 2.5 | 55 120.941 | 55 181.488 | d 42.71 3P4F | a 21.50 1D2D | 1.205 | 1.196 | | |
| 2.5 | 55 728.266 | 55 759.969 | a 57.57 1D2D | d 10.85 3P4F | 1.262 | 1.257 | | 1.277 |
| 2.5 | 57 287.051 | 57 342.688 | d 58.15 3P2F | d 19.11 3P4F | 0.935 | 0.946 | | |
| 2.5 | 58 862.891 | 58 885.988 | d 56.82 3P4D | d 12.14 3P2F | 1.287 | 1.263 | | |
| 2.5 | 60 404.477 | 60 502.965 | d 24.08 3P2D | d 13.06 1D2F | 1.218 | 1.168 | | |
| 2.5 | 61 631.066 | 61 642.484 | d 31.54 3P2D | d 12.50 1D2D | 1.284 | 1.282 | | |
| 2.5 | 62 501.727 | 62 436.797 | e 24.87 3P4F | g 16.08 3P4P | 1.274 | 1.330 | | |
| 2.5 | 63 516.281 | 63 541.152 | b 81.89 3P4P | b 14.09 1D2D | 1.537 | 1.494 | | |
| 2.5 | 64 213.707 | 64 220.074 | e 18.10 3P4F | f 13.23 3P4F | 1.187 | 1.136 | | |
| 2.5 | 64 513.703 | 64 624.145 | e 28.60 3P2F | d 21.96 1D2D | 1.124 | 1.185 | | |
| 2.5 | 65 243.250 | 65 160.602 | e 28.18 3P2F | d 18.64 1D2D | 1.133 | 1.095 | | |
| 2.5 | | 65 543.594 | e 24.02 3P4F | e 20.79 3P4D | 1.206 | 1.271 | | |
| 2.5 | | 66 472.805 | e 26.81 3P2D | d 25.66 1D2F | 1.087 | 1.100 | | |
| 2.5 | | 66 997.102 | e 21.28 3P4D | f 19.78 3P4F | 1.300 | 1.267 | | |
| 2.5 | | 67 884.172 | f 31.84 3P2F | f 23.30 3P4F | 1.028 | 1.028 | | |
| 2.5 | | 68 385.461 | e 25.03 3P2D | d 11.22 1D2F | 1.168 | 1.430 | | |
| 2.5 | | 68 586.609 | c 74.88 3P4P | c 13.06 1D2D | 1.499 | 1.201 | | |
| 2.5 | | 68 841.891 | f 24.37 3P4D | f 12.99 3P4F | 1.273 | 1.332 | | |
| 2.5 | | 70 232.789 | f 29.35 3P2D | f 16.57 3P4D | 1.179 | 1.183 | | |
| 2.5 | | 70 575.656 | f 29.06 3P4P | f 17.58 3P2D | 1.361 | 1.407 | | |
| 2.5 | | 70 749.977 | b 73.11 1D2D | b 12.22 3P4P | 1.257 | 1.259 | | |
| 2.5 | | 72 783.438 | e 45.18 1D2D | g 8.16 1D2D | 1.250 | 1.224 | | |
| 3.5 | 56 528.133 | 56 573.910 | d 72.34 3P4F | d 19.73 3P4D | 1.270 | 1.278 | | |
| 3.5 | 58 944.148 | 58 919.750 | d 40.56 3P4D | d 17.84 3P4F | 1.266 | 1.289 | | |
| 3.5 | 61 125.742 | 61 035.402 | d 59.99 3P2F | d 25.52 3P4D | 1.188 | 1.174 | | |
| 3.5 | 64 120.879 | 64 112.078 | e 46.30 3P4F | e 30.28 3P4D | 1.284 | 1.276 | | |
| 3.5 | 65 403.797 | 65 383.625 | d 55.01 1D2F | d 14.11 1D2G | 1.152 | 1.135 | | |
| 3.5 | | 66 622.445 | d 48.26 1D2G | e 17.58 3P2F | 1.013 | 1.039 | | |
| 3.5 | 66 743.125 | 66 787.117 | e 47.80 3P4D | e 23.56 3P4F | 1.281 | 1.261 | | |
| 3.5 | 67 358.203 | 67 363.070 | f 35.59 3P4F | f 22.61 3P4D | 1.238 | 1.266 | | |
| 3.5 | 68 079.695 | 68 003.930 | e 31.68 3P2F | f 14.63 3P4F | 1.175 | 1.164 | | |
| 3.5 | | 69 963.523 | f 38.62 3P4F | f 38.59 3P4D | 1.280 | 1.287 | | |
| 3.5 | | 70 400.375 | f 64.14 3P2F | f 13.94 3P4D | 1.152 | 1.153 | | |
| 4.5 | | 58 572.621 | d 86.09 3P4F | d 11.07 1D2G | 1.309 | 1.312 | | |
| 4.5 | 66 428.102 | 66 346.453 | d 52.47 1D2G | e 40.22 3P4F | 1.208 | 1.163 | | |
| 4.5 | | 66 820.094 | e 41.45 3P4F | d 35.78 1D2G | 1.229 | 1.276 | | |
| 4.5 | | 69 965.961 | f 82.58 3P4F | f 15.68 1D2G | 1.299 | 1.304 | | |

a: $5p^2 6s$; b: $5p^2 7s$; c: $5p^2 8s$; d: $5p^2 5d$; e: $5p^2 6d$; f: $5p^2 7d$; g: $5s5p^4$.
† Data from NIST, * ab initio results obtained by the use of Cowan code.

**Table 8.** The fitted hfs parameters for the magnetic dipole interaction for odd-parity levels; in parentheses are the standard deviations.

| Config. | $a^{01}_{5p}$ (mK) | $a^{12}_{5p}$ (mK) | $a^{10}_{5p}$ (mK) | $a^{01}_{np}$ (mK) | $a^{12}_{np}$ (mK) |
|---|---|---|---|---|---|
| $5s^25p^3$ | 27.51 (0.07) | 37.41 (0.09) | –6.88 (0.02) | | |
| $5s^25p^26p$ | 32.78 (0.14) | 44.58 (0.19) | –6.01 (0.45) | 2.42(0.08) | 3.28 (0.11) |
| $5s^25p^27p$ | 33.43 (0.14) | 45.47 (0.19) | –6.01 (0.45) | 0.80 (0.03) | 1.08 (0.04) |
| $5s^25p^28p$ | 33.76 (0.14) | 45.91 (0.19) | –6.01 (0.45) | 0.37 (0.01) | 0.41 (0.02) |
| $5s^25p^29p$ | 34.09 (0.14) | 46.36 (0.19) | –6.01 (0.45) | 0.08 (0.07) | 0.09(0.09) |
| $5s^25p^24f$ | 34.09 (0.14) | 46.36 (0.19) | –0.98 (0.46) | 0.00 | 0.00 |
| $5s^25p^25f$ | 34.09 (0.14) | 46.36 (0.19) | –1.27 (0.66) | 0.00 | 0.00 |

**Table 9.** The calculated parameters for the magnetic dipole interaction for odd-parity levels.

| Config. | $\langle r^{-3}\rangle_{5p}$ (a.u.) | $a^{01}_{5p}$ (mK) | $a^{12}_{5p}$ (mK) | $\langle r^{-3}\rangle_{np}$ (a.u.)<br>$\langle r^{-3}\rangle_{nf}$ (a.u.) | $a^{01}_{np}$ (mK)<br>$a^{01}_{nf}$ (mK) | $a^{12}_{np}$ (mK)<br>$a^{12}_{nf}$ (mK) |
|---|---|---|---|---|---|---|
| $5s^25p^3$ | 10.52 | 27.63 | 37.58 | | | |
| $5s^25p^26p$ | 12.55 | 32.96 | 44.83 | 0.78 | 2.05 | 2.79 |
| $5s^25p^27p$ | 12.59 | 33.07 | 44.98 | 0.26 | 0.68 | 0.92 |
| $5s^25p^28p$ | 12.62 | 33.12 | 45.04 | 0.12 | 0.32 | 0.44 |
| $5s^25p^29p$ | 12.61 | 33.12 | 45.04 | 0.07 | 0.18 | 0.24 |
| $5s^25p^24f$ | 12.62 | 33.15 | 45.08 | 4.60e-4 | 0.00 | 0.00 |
| $5s^25p^25f$ | 12.62 | 33.15 | 45.08 | 2.40e-4 | 0.00 | 0.00 |

which seem be not affected by false fs designation and not questionable about their accuracy. Since these latter values were measured for $^{121}$Sb isotope we converted them, introducing the ratio: $A_{121}/A_{123} = g_{I\ 121}/g_{I\ 123} = 1.84661$ [27] confirmed in a precision atomic beam magnetic resonance experiment [11]. It should be noted that the converted data neglect possible effects of hfs-anomalies different for different levels [47]; such an effect was observed for the ground level of antimony [11,27].

The number of experimental hfs $A$-values is larger than the number of many-body parameters required by theory and then no additional assumptions had to be included in our hfs fitting procedure. To check the validity of the hfs many-body parameter values for *p-electrons* one can use, for instance, the well-established relations (in mK): $a^{\kappa k}_{nl} = 2\mu_0\mu_B\mu_I\langle r^{-3}\rangle^{\kappa k}_{nl}/4\pi I = 3.180 g_I\langle r^{-3}\rangle^{\kappa k}_{nl}$ where the computed expectation values $\langle r^{-3}\rangle^{\kappa k}_{nl}$ are given in Table 9 thanks to Cowan code. Here we have $g_I = \mu_I/I = 2.8912/3.5$.

Regarding *f-electrons* there is no hfs splitting since Sb I spin-orbit constants of $4f$ and $5f$ are equal to zero.

We can compare the calculated hfs many-body parameter values of Table 9 with those from Table 6 deduced by fitting them to experimentally determined hfs constants $A$ of Table 10. One can notice that the agreement is very satisfactory. Regarding the B-factor, the dispersion of published experimental values and particularly their signs, due to different precisions of the applied methods, is so big that we have decided not to look into this problem now. Moreover, in paper [8] the B-factor contribution for many levels is out right neglected.

## 8 Hyperfine structure considerations for even-parity levels

For hfs analysis we follow the many-body parameterization method described in reference [48] which allows us to take advantage of similarities between configuration interaction effects observed independently in spin-orbit and hyperfine splitting.

Table 11 contains values of fiited hfs parameters with regard to magnetic factor $A$ only. The fitted values were compared with our experimental data and data from paper [8] obtained for isotope $^{121}$Sb and converted for isotope 123. The converted data neglects the $A$-hfs anomalies which can vary between diffrent levels [11,27,47].

The radial parameters $a^{\kappa k}_{nl}$ and $b^{\kappa k}_{nl}$ have been evaluated by fitting them to experimentally determined hfs constants $A$ and $B$ using the theoretical expressions (Eqs. (4) and (5) of [45] for example). A good fit, with a root mean square deviation of 0.55 mK was obtained for selected accurate hfs values given in reference [8] gathered with our data given in Table 1. Table 12 contains the values of fitted hfs parameters quoted with their uncertainties with regard to magnetic dipole interaction only: the hfs parameters relative to electric factor $B$ present more uncertainties because some experimental values given in literature seem doubtful, particularly their sign. In order to check validity of these fitted parameters we have compared some of them to ab initio values obtained by means of Cowan code [37]. For instance one can use the well-established relation

$$a^{\kappa k}_{nl}\,(mK) = \frac{2\mu_0\mu_B\mu_I\langle r^{-3}\rangle^{\kappa k}_{nl}}{4\pi I} = 3.18 g_I\langle r^{-3}\rangle^{\kappa k}_{nl}.$$

**Table 10.** Comparison between experimental and calculated $A$ hfs magnetic factors for odd-parity levels of $^{123}$Sb.

| Energy | $A^{Exp.}$(mK) | | $A$(mK) | Energy | $A^{Exp.}$(mK) | | $A$ (mK) | Energy | $A^{Exp.}$(mK) | | $A$ (mK) |
|---|---|---|---|---|---|---|---|---|---|---|---|
| level cm$^{-1}$ | this work | other* | calc | level cm$^{-1}$ | this work | other* | calc | level cm$^{-1}$ | this work | other* | calc |
| $J = 1/2$ | | | | 67 465.10 | | | 10.03 | 71 508.41 | | | 23.08 |
| 16 395.35 | 89.16 | 88.65 | 89.05 | 68 024.68 | | | –21.49 | 71 630.26 | | | 18.17 |
| 51 676.43 | 8.18 | 8.06 | 8.10 | 68 070.10 | | | 1.44 | 73 513.00 | | | 15.42 |
| 54 196.61 | | –15.65 | –14.94 | 68 137.99 | | | 3.60 | 73 682.19 | | | 19.62 |
| 55 993.85 | –19.99 | –19.66 | –20.07 | 68 966.89 | | | –3.57 | 75 272.78 | | | 6.70 |
| 58 653.01 | 69.38 | 69.05 | 69.34 | 69 053.79 | | | –1.97 | 75 393.19 | | | 0.35 |
| 60 765.29 | | 7.31 | 7.20 | 69 754.80 | | | 27.52 | 76 826.75 | | | 16.44 |
| 63 606.33 | | –12.89 | –12.45 | 69 886.04 | | | 27.39 | 76 870.03 | | | 18.84 |
| 64 098.35 | | | 1.41 | 70 618.56 | | | –22.46 | 77 897.87 | | | 6.51 |
| 64 209.43 | | | –3.91 | 70 649.56 | | | 3.40 | 77 974.53 | | | 0.57 |
| 65 479.61 | | | 47.98 | 71 560.99 | | | 25.31 | 78 716.79 | | | 17.88 |
| 65 863.29 | | | 1.40 | 71 602.76 | | | 31.42 | 78 729.59 | | | 17.42 |
| 66 685.10 | | | 51.26 | 73 560.99 | | | 26.04 | $J = 7/2$ | | | |
| 67 192.00 | | | –7.01 | 74 263.22 | | | 19.96 | 57 555.35 | | 15.98 | 16.23 |
| 67401.60 | | | 10.79 | 75 047.56 | | | –6.64 | 62 465.94 | | –0.38 | 0.14 |
| 68 057.66 | | | –39.92 | 75 391.53 | | | 0.02 | 64 957.23 | | 11.70 | 7.31 |
| 68 945.70 | | | –8.09 | 75 802.30 | | | –7.22 | 64 978.24 | | 1.52 | 6.99 |
| 69 042.29 | | | 0.87 | 76 876.63 | | | 27.28 | 65 467.21 | | –0.27 | –0.25 |
| 69 869.37 | | | 60.38 | 77 149.76 | | | 20.97 | 65 531.00 | | –1.95 | –1.22 |
| 70 627.46 | | | –40.23 | 77 973.73 | | | –1.23 | 66 405.38 | | 11.81 | 16.17 |
| 71 593.97 | | | 60.38 | 78 085.66 | | | –15.38 | 67 997.02 | | –0.70 | 1.82 |
| 73 964.66 | | | 51.11 | 78 732.95 | | | 27.84 | 68 032.06 | | | 2.72 |
| 74 937.26 | | | –6.39 | 78 898.77 | | | 21.27 | 68 137.27 | | | 2.60 |
| 75 738.74 | | | –18.83 | 84 076.70 | | | 0.12 | 68 164.05 | | | 8.79 |
| 77 018.83 | | | 50.35 | 87 247.72 | | | 0.15 | 69 695.46 | | | 16.39 |
| 78 083.32 | | | –33.06 | 89 097.08 | | | –0.05 | 70 658.30 | | | 9.02 |
| 78 813.08 | | | 50.41 | $J = 5/2$ | | | | 70 670.65 | | | 8.92 |
| 84 013.78 | | | 2.80 | 9 854.01 | | 26.54 | 26.69 | 71 533.18 | | | 16.56 |
| 87 211.33 | | | 0.61 | 55 252.13 | –2.12 | –2.27 | –2.20 | 73 706.13 | | | 13.92 |
| 89 070.94 | | | 0.06 | 57 410.34 | | 22.53 | 22.32 | 75 235.27 | | | 9.32 |
| $J = 3/2$ | | | | 58 835.48 | 18.62 | 18.79 | 18.55 | 75 273.20 | | | 5.67 |
| 0.00 | | –5.52 | –4.92 | 62 462.40 | | | 0.04 | 76 890.37 | | | 14.12 |
| 8 512.12 | | 10.21 | 10.79 | 63 790.94 | | –0.43 | 0.50 | 77 971.94 | | | 9.26 |
| 18 464.20 | 11.89 | 12.30 | 11.85 | 64 512.39 | | 14.08 | 13.54 | 77 898.38 | | | 5.74 |
| 52 612.48 | 0.84 | 0.81 | 1.38 | 64 878.95 | | 17.11 | 17.12 | 78 745.92 | | | 14.09 |
| 55 134.25 | 1.07 | 1.19 | 1.41 | 64 973.82 | | –0.11 | 0.03 | $J = 9/2$ | | | |
| 55 864.82 | 5.06 | 5.20 | 5.36 | 65 460.14 | | –0.70 | –0.12 | 65 527.79 | | –1.03 | –0.89 |
| 58 075.53 | | 27.51 | 27.57 | 65 568.31 | | 1.19 | 0.80 | 68 042.99 | | | 12.63 |
| 58 589.51 | | 19.12 | 19.15 | 66 361.63 | | 11.00 | 22.72 | 68 056.70 | | | 1.07 |
| 61 000.29 | 0.26 | 0.38 | 0.36 | 66 837.57 | 18.45 | 17.98 | 17.42 | 68 144.55 | | | 7.36 |
| 63 798.44 | | –3.25 | –4.02 | 67 307.00 | | | –1.84 | 70 615.66 | | | 12.59 |
| 63 900.52 | | 5.09 | 5.10 | 67 994.38 | | –0.97 | 0.25 | 70 667.60 | | | 9.67 |
| 64 273.85 | | | 1.45 | 68 023.86 | | | –0.99 | 75 234.54 | | | 7.63 |
| 64 984.58 | | 16.03 | 15.78 | 68 148.21 | | | 5.98 | 75 383.85 | | | 11.07 |
| 65 565.23 | | 1.90 | 1.38 | 68157.10 | | | 5.22 | 77 871.94 | | | 7.54 |
| 65 959.00 | | | 19.66 | 69 037.29 | | | –2.96 | $J = 11/2$ | | | |
| 66 029.78 | | | 3.01 | 69 669.41 | | | 22.95 | 68 064.05 | | | 11.01 |
| 66 541.55 | | | 28.36 | 69 892.63 | | | 17.85 | 70 624.45 | | | 11.05 |
| 66 957.80 | | | 8.58 | 70 646.58 | | | 1.15 | 75 385.35 | | | 9.11 |
| 67 375.22 | | | –0.64 | 70 665.97 | | | 8.08 | 77 960.39 | | | 9.07 |

* Data converted from experimental results for isotope $^{121}$Sb [8] using the ratio $\frac{A_{121}}{A_{123}} = \frac{g_I(121)}{g_I(123)} = 1.84661$ [27].

**Table 11.** Comparison of experimental and calculated $A$ hfs for even-parity levels of $^{123}$Sb.

| $J$ | Energy levels ($cm^{-1}$) | $A^{Exp.}$ (mK) this work | other* | $A^{Calc}$ (mK) | $J$ | Energy levels ($cm^{-1}$) | $A^{Exp.}$ this work | other* | $A^{Calc}$ (mK) |
|---|---|---|---|---|---|---|---|---|---|
| 0.5 | 43 249.33 | 41.42 | 41.05 | 41.40 | 1.5 | 71 464.83 | | – | 31.12 |
| 0.5 | 46 991.05 | –18.22 | –18.41 | –18.77 | 1.5 | 72 628.79 | | – | 7.64 |
| 0.5 | 56 698.60 | | 9.53 | 10.21 | 1.5 | 74 514.81 | | – | 8.64 |
| 0.5 | 57 597.20 | | 81.61 | 81.32 | 1.5 | 75 728.30 | | – | 25.19 |
| 0.5 | 58 132.65 | | 49.12 | 20.98 | 2.5 | 48 332.42 | 31.59 | 31.52 | 30.79 |
| 0.5 | 59 737.62 | | –15.00 | –10.97 | 2.5 | 53 442.96 | | 20.63 | 16.91 |
| 0.5 | 61 386.50 | | –11.21 | –8.37 | 2.5 | 55 120.94 | | 16.84 | 15.19 |
| 0.5 | 62 960.31 | | 4.98 | 6.17 | 2.5 | 55 728.26 | | 27.02 | 23.47 |
| 0.5 | 63 825.75 | | 20.36 | 14.24 | 2.5 | 57 287.05 | | 15.60 | 15.76 |
| 0.5 | 64 769.17 | | 83.02 | 98.19 | 2.5 | 58 862.89 | | 22.53 | 21.69 |
| 0.5 | 65 654.40 | | – | 48.86 | 2.5 | 60 404.47 | | 6.23 | 7.03 |
| 0.5 | 66 009.71 | | –13.21 | –10.08 | 2.5 | 61 631.06 | | 4.55 | 6.66 |
| 0.5 | 66 353.85 | | – | -24.36 | 2.5 | 62 501.72 | | 17.87 | 18.13 |
| 0.5 | 67 427.02 | | – | 1.92 | 2.5 | 63 516.28 | | 24.64 | 23.04 |
| 0.5 | 68 451.25 | | – | 13.94 | 2.5 | 64 213.70 | | – | 0.83 |
| 0.5 | 68 670.32 | | – | 53.24 | 2.5 | 64 513.70 | | 13.65 | 10.58 |
| 0.5 | 69 086.99 | | – | 33.27 | 2.5 | 65 243.25 | | 19.71 | 16.80 |
| 0.5 | 70 040.35 | | – | –21.10 | 2.5 | 65 543.59 | | – | 18.24 |
| 0.5 | 72 125.93 | | – | 105.09 | 2.5 | 66 472.80 | | – | 3.85 |
| 1.5 | 45 945.34 | 9.42 | 9.37 | 9.45 | 2.5 | 66 997.10 | | – | 7.62 |
| 1.5 | 49 391.13 | 23.56 | 23.50 | 22.59 | 2.5 | 67 884.17 | | – | 2.26 |
| 1.5 | 53 527.95 | | 5.31 | 4.40 | 2.5 | 68 385.46 | | – | 13.01 |
| 1.5 | 55 232.96 | | 5.69 | 9.23 | 2.5 | 68 586.60 | | – | 22.00 |
| 1.5 | 56 151.80 | | 16.52 | 14.89 | 2.5 | 68 841.89 | | – | 21.11 |
| 1.5 | 56 733.16 | | 8.83 | 3.68 | 2.5 | 70 232.78 | | – | 18.36 |
| 1.5 | 58 746.35 | | 26.21 | 25.04 | 2.5 | 70 575.65 | | – | 15.76 |
| 1.5 | 60 580.89 | | 8.29 | 7.10 | 2.5 | 70 749.97 | | – | 18.41 |
| 1.5 | 60 964.67 | | –1.62 | –2.67 | 2.5 | 72 783.43 | | – | 19.19 |
| 1.5 | 61 808.69 | | 14.95 | 14.67 | 3.5 | 56 528.13 | | – | -0.48 |
| 1.5 | 63 193.03 | | 11.86 | 12.80 | 3.5 | 58 944.14 | | 11.86 | 12.32 |
| 1.5 | 63 649.46 | | 26.70 | 29.64 | 3.5 | 61 125.74 | | 12.35 | 12.58 |
| 1.5 | 64 220.60 | 0.61 | 2.27 | 1.56 | 3.5 | 64 120.87 | | –1.25 | -1.74 |
| 1.5 | 64 432.39 | | –3.25 | –0.45 | 3.5 | 65 403.79 | | – | 10.07 |
| 1.5 | 64 843.42 | | – | 6.17 | 3.5 | 66 622.44 | | – | 13.71 |
| 1.5 | 65 143.60 | | – | 24.83 | 3.5 | 66 743.12 | | 11.43 | 12.58 |
| 1.5 | 66 023.10 | | – | -1.77 | 3.5 | 67 358.20 | | – | 3.12 |
| 1.5 | 66 113.21 | | – | 13.87 | 3.5 | 68 079.69 | | – | 8.53 |
| 1.5 | 67 253.46 | | – | -0.57 | 3.5 | 69 963.52 | | – | 14.62 |
| 1.5 | 67 857.01 | | – | 4.08 | 3.5 | 70 400.37 | | – | 14.21 |
| 1.5 | 68 411.61 | | – | 23.19 | 4.5 | 58 572.62 | | – | 11.51 |
| 1.5 | 68 776.82 | | – | 32.39 | 4.5 | 66 428.10 | | 10.83 | 11.78 |
| 1.5 | 69 205.33 | | – | 14.87 | 4.5 | 66 820.09 | | – | 11.32 |
| 1.5 | 69 943.53 | | – | 15.35 | 4.5 | 69 965.96 | | – | 12.71 |

* Data converted from experimental results for isotope $^{121}$Sb [8] using the ratio $\frac{A_{121}}{A_{123}} = \frac{g_I(121)}{g_I(123)} = 1.84661$ [27].

**Table 12.** The fitted hfs parameters for the magnetic dipole interaction for even-parity levels. The uncertainties given in parentheses are the standard deviations.

| Configuration | $a^{01}_{5p}$ (mK) | $a^{12}_{5p}$ (mK) | $a^{10}_{5p}$ (mK) | $a^{10}_{ns}$ (mK) | $a^{01}_{nd}$ (mK) | $a^{12}_{nd}$ (mK) |
|---|---|---|---|---|---|---|
| $5s^25p^26s$ | 30.16 (0.32) | 40.73 (0.44) | –1.02 (0.55) | 49.09 (0.59) | | |
| $5s^25p^27s$ | 30.76 (0.32) | 41.54 (0.45) | –1.02 (0.55) | 14.30 (0.15) | | |
| $5s^25p^28s$ | 30.76 (0.32) | 41.54 (0.45) | –1.02 (0.55) | 7.45 (0.09) | | |
| $5s5p^4$ | 26.15 (0.28) | 35.31 (0.38) | –0.83 (0.45) | 472.69 (4.95) | | |
| $5s^25p^25d$ | 30.34 (0.32) | 40.97 (0.44) | –1.02 (0.55) | | 0.21 (0.03) | 0.20 (0.03) |
| $5s^25p^26d$ | 31.97 (0.34) | 43.17 (0.47) | –1.02 (0.55) | | 0.00 | 0.00 |
| $5s^25p^27d$ | 31.97 (0.34) | 43.17 (0.47) | –1.02 (0.55) | | 0.00 | 0.00 |

**Table 13.** The calculated parameters for the magnetic dipole interaction for even-parity levels.

| Configuration | $\langle r^{-3}\rangle_{np}$ (a.u.) | $\langle r^{-3}\rangle_{nd}$ (a.u.) | $\xi_{np}$ | $\xi_{nd}$ | $a^{01}_{5p}$ (mK) | $a^{12}_{5p}$ (mK) | $a^{01}_{nd}$ (mK) | $a^{12}_{nd}$ (mK) |
|---|---|---|---|---|---|---|---|---|
| $5p^26s$ | 12.29 | | 3421 | | 29.63 | 40.01 | | |
| $5p^27s$ | 12.54 | | 3491 | | 30.12 | 40.68 | | |
| $5p^28s$ | 12.59 | | 3504 | | 30.22 | 40.81 | | |
| $5s5p^4$ | 10.66 | | 2967 | | 25.69 | 34.64 | | |
| $5p^25d$ | 12.36 | 0.09 | 3439 | 18.9 | 29.80 | 40.24 | 0.20 | 0.20 |
| $5p^26d$ | 12.54 | 0.03 | 3489 | 7.0 | 30.24 | 40.84 | 0.07 | 0.07 |
| $5p^27d$ | 12.58 | 0.02 | 3502 | 3.5 | 30.35 | 40.99 | 0.04 | 0.04 |

**Table 14.** Pseudo-relativistic Hartree-Fock estimates of $4\pi|\Psi(0)|^2$ (in a.u.) for studied in the present paper even-parity configurations, using the PSUHFR code [51].

| Configuration | $5s5p^4$ | $5p^26s$ | $5p^27s$ | $5p^28s$ |
|---|---|---|---|---|
| $1s$ | 944 880.00 | 94 4886.00 | 944 883.00 | 944 880.00 |
| $2s$ | 104 264.00 | 104 267.00 | 104 268.00 | 104 268.00 |
| $3s$ | 20 225.00 | 20 230.00 | 20 229.00 | 20 229.00 |
| $4s$ | 3 906.00 | 3 917.00 | 3 917.00 | 3 917.00 |
| $5s$ | 414.38 | 429.00 | 429.00 | 429.00 |
| $6s$ | | 27.14 | | |
| $7s$ | | | 8.05 | |
| $8s$ | | | | 3.52 |
| Total *s-electron* density[a] | 2 146 963.00 | 2 147 485.00 | 2 147 462.00 | 2 147 449.00 |

[a] Totals are contributions from all *s-orbitals* weighted by their occupation number.

To give it experimental significance we have to weight it by the ratio of spin-orbit constants obtained thanks to fs study and ab initio calculations, i.e. to multiply it by $\xi_{nl}(fs)/\xi_{nl}$ (ab initio) as we did for instance in previous work [35]. Using the expectation values of Table 13, knowing that the magnetic dipole moment of $^{123}$Sb is equal to 2.8912 $\mu_n$ one gets the $a^{01}_{nl}$ and $a^{12}_{nl}$ values of Table 13 which are very close to experimental ones (Tab. 12). We used $a^{12}_{nl} = 1.35a^{01}_{nl}$ for *p-electron* and $a^{12}_{nl} = 0.97a^{01}_{nl}$ for *d-electron* keeping the ratio obtained experimentally.

To test exactness of the most influential hfs parameters $a^{10}_{ns}$ of $5p^2ns$ and $5s5p^4$ configurations it is interesting to compare the corresponding ratio $a^{10}_{ns}/\mu_I$ for Sb I, to those of its neighbours Sn I and Te I and usually $a^{10}_{ns}/\mu_I$ (Sn I) $< a^{10}_{ns}/\mu_I$ (Sb I) $< a^{10}_{ns}/\mu_I$ (Te I). Unfortunately some of these parameter values are not available in literature. There is one solution left: to use $a^{10}_{ns}(\text{mK}) = 3.18g_I\langle r^{-3}\rangle ns = 2.12g_I 4\pi|\psi(0)|^2$. We give in Table 14 a summary of the Pennsylvania state University Hartree-Fock relativistic code (PSUHFR) values of the charge density at the nucleus, $4\pi|\psi(0)|^2$, for each of Sb I configurations of interest here. In absence of Sb I isotope shift calculations (like those done by Aufmuth for other elements [49,50]) and particularly the scaling-factor value we are not able to use this equation directly except to compare the Sb I ratios of $a^{10}_{8s}\ (4p^28s)/a^{10}_{6s}(4p^26s) = 3.52/27.14 = 0.130$, $a^{10}_{7s}\ (4p^27s)/a^{10}_{6s}(4p^26s) = 8.05/27.14 = 0.297$, and $a^{10}_{5s}(5s5p^4)/a^{10}_{6s}(4p^26s) = 414.38/27.14 = 15.26$. The agreement with corresponding ratios of the experimental values of Table 12 is very satisfactory for two first calculated ratios but rather worse for the last one, maybe because we did not exploit directly some experimental $A$ hfs constants of the $5s5p^4$ levels (not available up to now)

but only some bits existing in levels of other configurations (see index g in Tab. 7) when determining hfs single-electron parameters given in Table 12.

## 9 Conclusion

New Landé factors and hfs constants of 12 odd-parity and 6 even-parity levels of $^{123}$Sb were determined experimentally. Using a linked-parameter technique of level-fitting calculations in a multiconfiguration basis a parametric analysis of fs structure involving in both cases of even and odd-parity levels up to seven configurations have been performed. The calculated $g_J$-factors deduced from the eigenvector compositions were compared with available experimental data and with ab initio Landé factor values computed by means of Cowan code. The agreements of the observed and calculated energy levels and $g_J$ factors are very satisfactory.

Thanks to deduced eigenvectors, the expansions of hfs constants in intermediate coupling and extraction of mono-electronic parameter values semi-empirically were possible. Finally a complete list of the predicted hfs constants $A$ of all levels of the studied system was generated.

The ab initio data computed by means of Cowan code for lowest configurations are highly similar to the experimental data. However it is known, that for high excited levels and Rydberg states the results of Cowan code are rather questionable and calculations should take into account second order perturbations, spin polarization and so on.

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