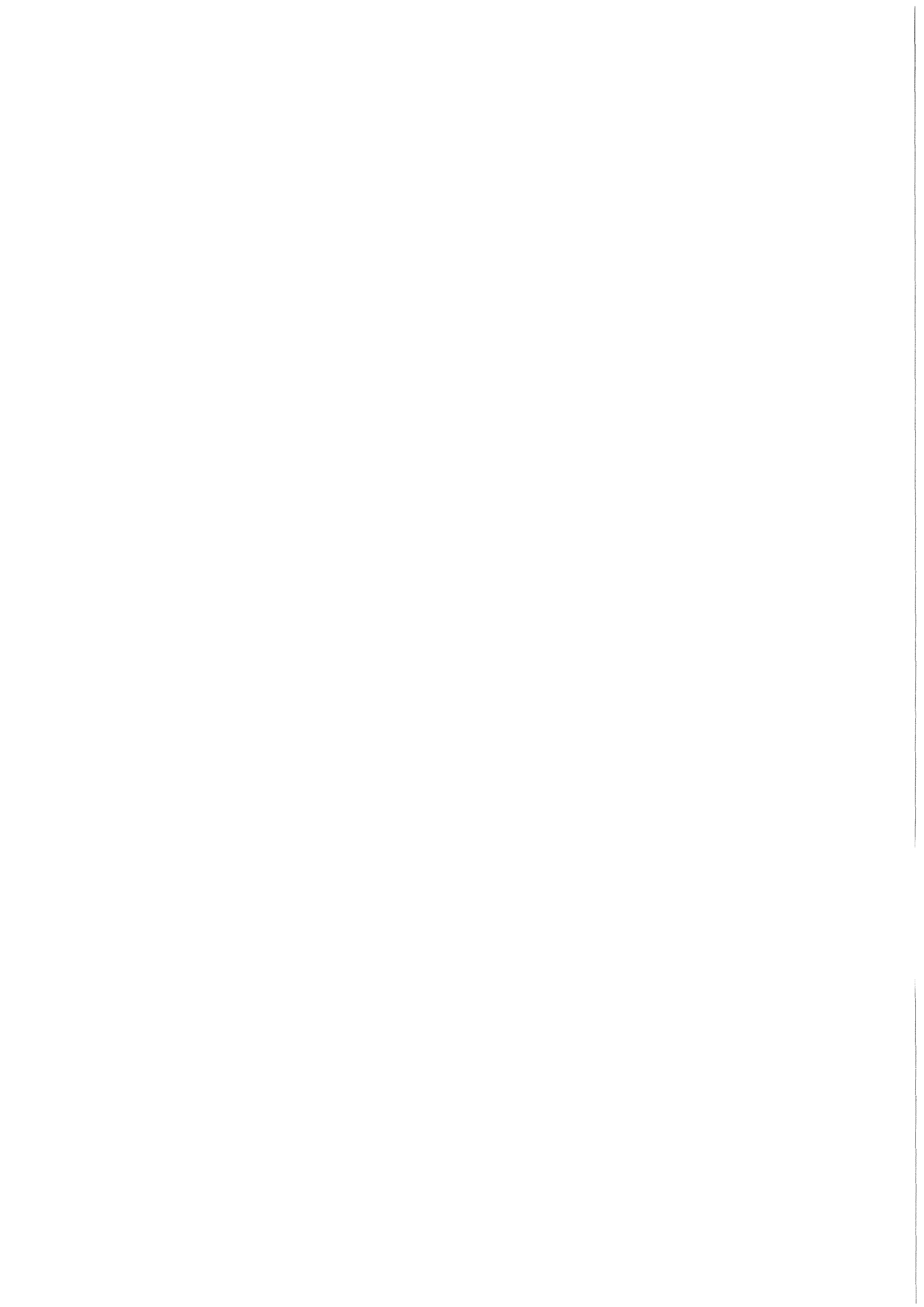


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Rydberg Configurations  $5s^25pn's$   
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 $5s^25pn''$ 'd by the Configuration  $5s5p^3$  in the Spectrum Sn I

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## ABSTRACT

A fine structure analysis for the system  $5s^2 5p n' s$  ( $n' = 6$  to  $11$ ) +  $5s^2 5p n'' d$  ( $n'' = 5$  to  $12$ ) +  $5s 5p^3$  is performed on the basis of available experimental data. The Slater integrals and spin-orbit parameters are determined. For the Slater integrals associated with the Rydberg configurations we find a relation of the type

$$R^t(a,b)/R^t(c,d) = [n^*(a)n^*(b)/(n^*(c) n^*(d))]^{3/2},$$

where  $a, b, c, d$  denote a two-electron configuration  $nln'l'$ , and the  $n^*(nln'l')$  are effective quantum numbers introduced by us for the Rydberg configuration. The configuration  $5s 5p^3$  is shown to influence strongly the odd spectrum Sn I. On the basis of the theoretical results new spectroscopic assignments of the atomic levels involved are given in some cases.

## STÖRUNG DER RYDBERG KONFIGURATIONEN $5s^2 5p n' s$ und $5s^2 5p n'' d$ DURCH DIE KONFIGURATION $5s 5p^3$ IM SPEKTRUM Sn I

Die Feinstruktur des Systems  $5s^2 5p n' s$  ( $n' = 6$  to  $11$ ) +  $5s^2 5p n'' d$  ( $n'' = 5$  to  $12$ ) +  $5s 5p^3$  wurde auf der Basis der verfügbaren experimentellen Daten analysiert. Die Slater-Integrale und Spin-Bahn-Parameter werden bestimmt. Für die Slater-Integrale, die mit Rydberg-Konfigurationen verbunden sind, finden wir eine Relation in der Art

$$R^t(a,b)/R^t(c,d) = [n^*(a)n^*(b)/(n^*(c) n^*(d))]^{3/2},$$

wobei  $a, b, c, d$  die Zwei-Elektron-Konfigurationen  $nln'l'$  und  $n^*(nln'l')$  effektive Quantenzahlen für die Rydberg Konfiguration bezeichnen. Die Konfiguration  $5s 5p^3$  beeinflusst stark das ungerade Spektrum Sn I. Neue spektroskopische Zuordnungen atomarer Zustände werden in einigen Fällen auf der Basis der theoretischen Resultate angegeben.

## 1. INTRODUCTION

In recent years hyperfine structure and isotope shifts of atomic transitions have been experimentally investigated with new experimental tools and methods [1], not only for transitions involving the ground and high-lying metastable levels, but also for Rydberg series [2]. The interpretation of the experimental data requires highly accurate wave functions in an intermediate coupling scheme which can be provided by an semiphenomenological analysis of a sufficiently large body of experimental data for a specific case considered.

In atoms like Sn and Pb with a ground state configuration of the type  $ns^2 np^2$ , states of odd-Rydberg configurations  $ns^2 np n'l'$  are known to be strongly perturbed by the electrostatic interaction with the configuration  $ns np^3$ . Only few percent of admixture from the  $ns np^3$  configuration to levels with  $ns np n''d$  configurations may produce anomalies in the observed hyperfine structure splittings and optical isotope shifts. This appears to be due to the considerably increased density of the  $ns$  electron (e.g.  $5s$  for Sn I) at the nuclear site as compared to other open shell electrons.

In this paper we study perturbation effects in the Rydberg configurations  $5s^2 5p n's$  and  $5s^2 5p n''d$  in Sn I from the  $5s5p^3$  configuration. For the case of Sn I a fairly large number of experimental data are available. Early investigations of Sn I summarized by Moore [3] were superseded in 1964 by data in the unpublished theses of Brill [4] and Wilson [5]. In 1977 Brown, Tilford and Ginter [6] studied the absorption spectrum of Sn between 1580 and 2080 Å and published a table of observed odd-energy levels of Sn I. We use their experimental data for a theoretical reanalysis of odd-configurations of Sn I. Our initial calculations, restricted to the system  $5s^2 5p n's + 5s^2 5p n''d + 5s5p^3$  (with  $n' = 6$  and  $7$ , and  $n'' = 5$  and  $6$ ), have not been very successful. The mean error of the least-squares fit of the calculated energy levels to the experimental level values associated with this configuration turned out to exceed  $100 \text{ cm}^{-1}$ . Nevertheless, these calculations showed us that some states associated with the

configurations 5p5d and 5p6d are strongly mixed. From our initial fits, we deduced that the mixing of the states of different configurations 5p5d and 5p6d occurs mainly via the configuration  $5s5p^3$ . This suggested to us that strong natural mixing of many configurations is possible above the states  $5s5p^3 \ ^3D_{1,2,3}$  which are situated in the same region as the Rydberg configurations  $5s^25pn's$  and  $5s^25pn''d$ . From this reason we extended our considerations to the system  $5s^25pn's + 5s^25pn''d + 5s5p^3$  with  $n' = 6$  to 11 and  $n'' = 5$  to 12.

## 2. METHOD

### 2.1 Interactions within each configuration

Energy-level calculations of atomic spectra performed to first-order only of the perturbation theory led to rather poor agreement between the calculated and observed levels. In this approximation, energy matrices including the electrostatic and spin-orbit interactions within a single configuration (or group of adjacent configurations) are constructed and diagonalized. Recently various successful attempts have been made to obtain a more adequate description of the energy levels of  $1^N$  and  $1^N 1'$  configurations through the inclusion of the effective interaction in the energy matrices of the configuration investigated [7,8]. These interactions represent, to second-order of perturbation theory, electrostatic interaction with distant configurations.

The first-order approximation, the electrostatic and spin-orbit interactions are usually taken account of by the following radial parameters:

- (i) for each  $npn's$  configuration by  
 $F^0(np, n's), G^1(np, n's)$  and  $\zeta_{np}(n's),$
- (ii) for each  $npn''d$  configuration by  
 $F^0(np, n''d), F^2(np, n''d), G^1(np, n''d),$   
 $G^3(np, n''d), \zeta_{np}(n d)$  and  $\zeta_{n''d}$   
 $F^0(np^3), F^2(np, np), G^1(np, ns)$  and  $\zeta_{np}(np^3).$

The definitions of the electrostatic interactions parameters

$F^k$  and  $G^k$  (Slater integrals), the spin-orbit parameter  $\zeta_{nl}$ , as well as the coefficients of these parameters indispensable for the construction of the energy matrices, is given in many monographs [9 e.g.].

Second-order effects on the term structure of the configuration  $nl^n'l'$  can be taken into account by including the effective Hamiltonian [10]

$$H_{\text{eff}}^{(2)} = \alpha \vec{l} \cdot \vec{l}' + \beta \vec{s} \cdot \vec{s}' ,$$

where  $\alpha$  and  $\beta$  are adjustable parameters. Such effects play a role in  $npn''d$  and  $nsnp^3$  configurations only. The above effect will be included into our considerations by adding to the first order energy matrix terms diagonal in SL as follows:

- (i) for the configuration  $5s^2 5pn d$   
 $L(L+1) \alpha (5pn''d) + S(S+1) \beta (5pn''d),$
- (ii) for the configuration  $5s5p^3$   
 $L(L+1) \alpha (5s5p^3).$

In the configurations  $npn,s$  effects of interactions with distant configurations are absorbed by the parameters  $F^0$  and  $C^1$ .

## 2.2 Interaction between configurations $ns^2 npn's$ or $ns^2 npn''d$ and $nsnp^3$

For calculations of the Coulomb interaction matrix elements between the above mentioned configurations we have derived the following formulae:

$$\begin{aligned} &\langle ns^2 \ ^1S; nl^n'l' \ SL; SL | G | ns, nl^3 \ S_1 L ; SL \rangle = \\ &= \delta(l', \bar{L}_1) (-1)^{L+1+l'+1} \sqrt{\frac{1}{3}} [S_1, \bar{S}_1]^{1/2} \begin{matrix} \bar{S}_1 & 1/2 & 1/2 \\ S & 1/2 & S_1 \end{matrix} \times \\ &\times (l^3 \ vS_1 L \{ |l^2 \ \bar{v}\bar{S}_1 \bar{L}_1 \} \langle nsn'l'; \bar{S}_1 \bar{L}_1 | G | nl^2; \bar{S}_1 \bar{L}_1 \rangle \end{aligned}$$

where, in our case, the matrix element on the right hand side



takes the following values:

$$\begin{aligned} \langle 5s n's; {}^1S | G | 5p^2; {}^1S \rangle &= - (\sqrt{6}/3) R^1 (5s n's, 5p5p) \\ \langle 5s n''d; {}^1D | G | 5p^2; {}^1D \rangle &= - (2\sqrt{15}/15) R^1 (5s n''d, 5p5p). \end{aligned}$$

Therefore, the electrostatic interaction between the configurations  $5s^2 5p n's$  and  $5s 5p^3$  is proportional to the Slater integrals  $R^1(5s n's, 5p5p)$  and that between the configurations  $5s^2 5p n''d$  and  $5s 5p^3$  to the integrals  $R^1(5s n''d, 5p5p)$ . These integrals will be used as adjustable parameters in our procedure.

### 2.3 Interaction between the configurations $ns^2 np n's$ and $ns^2 np n''d$

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When considering the electrostatic interaction between configurations  $np n's$  and  $np n''d$  two additional parameters  $R^t$  are introduced. The matrix elements of the parameters  $R^t$  in the system studied by us are given by

$$\begin{aligned} \langle 5p n's; {}^3P | G | 5p n''d; {}^3P \rangle &= \\ &= - (\sqrt{2}/5) R^2 (5p n's, 5p n''d) + (\sqrt{2}/3) R^1 (5p n's, n''d 5p), \\ \langle 5p n's; {}^1P | G | 5p n''d; {}^1P \rangle &= \\ &= - (\sqrt{2}/5) R^2 (5p n's, 5p n''d) - (\sqrt{2}/3) R^1 (5p n's, n''d 5p) \end{aligned}$$

### 2.4 Interaction between configurations of the type $ns^2 np n1$ .

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As mentioned a very strong interaction is expected between the configuration  $5s 5p^3$  and each Rydberg configuration  $5p n''d$ . Even if the interaction between configurations  $5p 5d$  and  $5p 6d$  is not taken into account explicitly in the energy matrix, significant admixtures appear in the states of the configurations  $5p 6d$  from the configuration  $5p 5d$ . For example the state  $5p 6d {}^3D_1$  proved to be admixed with the state  $5p 5d {}^1P_1$  roughly by about 15 percent. This indicates that there may be a rather complex mixing. Therefore, in order to solve the problem correctly,

the interactions between different configurations of the type  $5pn''d$  must be included into the energy matrix. The same requirement is indispensable for the configurations  $5pn's$ . The matrix elements of the electrostatic interaction between configuration  $5pn'd$  and  $5pn''d$  are functions of the following radial integrals [11]:

$$R^0(5pn'd, 5pn''d), R^2(5pn'd, 5pn''d), R^1(5pn''d, n'd5p) \text{ and } R^3(5pn''d, n'd5p).$$

Similarly, the interaction between configuration  $5pn's$  and  $5pn''s$  is represented by the radial integrals  $R^0(5pn's, 5pn''s)$  and  $R^1(5pn''s, n's5p)$ . The angular coefficients for the above mentioned parameters are identical with those for the electrostatic interaction within each  $5pnd$  or  $5pns$  configuration. The coefficients at the parameters  $R^0$  are independent of the term SL. Therefore, the terms with radial integrals  $R^0$  can be omitted in the energy matrix. Their effects are absorbed in the first-order diagonal parameters.

## 2.5 Relations between Slater integrals of Rydberg configurations

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Including completely all the interactions considered above for a system consisting of 6 configurations of the type  $5s^25pn's$  ( $n' = 6$  to  $11$ ), 8 of the type  $5s^25pn''d$  ( $n''s = 5$  to  $12$ ) and 1 of the type  $5s5p^3$ , description would necessarily involve 297 parameters. This is an intolerable large number as the system comprises not more than 130 electron levels. In order to reduce the number of parameters.

We take use of the observations and conclusions of Shenstone and Russell [12] and Edden [13] who studied perturbations and regularities in the Rydberg series. Their conclusions, when generalized, lead to the following relation within particular kinds of Slater integrals, differing only by the principal quantum numbers of the electrons:

$$\frac{R^t(a,b)}{R^t(c,d)} = [n^*(a) n^*(b) / (n^*(c) n^*(d))]^{3/2}, \quad (2.1)$$

where  $a, b, c$  and  $d$  stand for the two-electron configuration  $nln'l'$ ,

with  $n^*(a)$  the effective quantum number of the configuration. Here,  $n^*$  is the effective quantum number of the configuration  $ns^2 nln'l'$  rather than of the electron level.

The effective quantum number  $n^*(nln'l')$  can be determined in the following way: as  $n'$  tends to infinity, the position of the centre of gravity of the configuration  $ns^2 nln'l'$  tends, irrespectively of  $l'$ , to

$$E_{\infty}(nln'l') = \frac{E_{\infty}(^2 1_{1-1/2}) + (l+1) E_{\infty}(^2 1_{1+1/2})}{2l + 1} \quad (2.2)$$

where the  $E_{\infty}(^2 1_{1+1/2})$  are the ionization energy values.

Hence

$$n^*(nln'l') = \left[ \frac{R}{E(nln'l') - E'_{av}(nln'l')} \right]^{1/2} \quad (2.3)$$

where  $E'_{av}(nln'l')$  is the mean energy, to second-order perturbation theory, for all the terms of the configuration  $ns^2 nln'l'$ .

For a configuration of the type  $nln's$  we have

$$E'_{av}(nln's) = F^0(nln's) - (1/6)G^1(nln's), \quad (2.4)$$

whereas for  $nln'd$

$$E'_{av}(nln'd) = F^0 - (1/15)G^1 - (3/70)G^3 - 8\alpha + 1.5\beta \quad (2.5)$$

In calculations of  $n^*(5pn'l')$  for the spectrum Sn I according to Ref. [6] we have taken:

$$E_{\infty}(^2 P_{1/2}) = 59232.69 \text{ cm}^{-1}, \quad E_{\infty}(^2 P_{3/2}) = 63484.18 \text{ cm}^{-1}$$

$$R_{Sn} = 109736.809 \text{ cm}^{-1}.$$

Using the relation (2.1) following relations for particular Slater integrals are found:

(i) for the Slater integrals diagonal in the  $5pn'd$  configuration

$$F^2(5pn'd) = [n^*(5pn'd)/n^*(5p5d)]^3 F^2(5p5d) \quad (2.6)$$

and analogous relations for the exchange integrals  $G^1(5pn'd)$ ,  $G^3(5pn'd)$  as well as for the spin-orbit parameters  $\zeta_{n'd}$  for  $n'd$ -electrons.

(ii) for the Slater integrals diagonal in the  $5pn's$  configuration  $G^1(5pn's) = [n^*(5pn's) / n^*(5p6s)]^3 G^1(5p6s)$ , (2.7)

(iii) for the parameters coupling Rydberg configurations  $5s^2 5pn'd$ :  
 $R^2(5pn'd, 5pn''d) =$   
 $= [n^*(5pn'd) n^*(5pn''d) / (n^*(5p5p) n^*(5p6d))]^{3/2} \times$  (2.8)  
 $\times R^2(5p5d, 5p6d)$

and analogous relations for the exchange integrals  $R^1(5pn'd, n''d5p)$  and  $R^3(5pn'd, n''d5p)$ , (2.9)

(iv) for the parameters coupling Rydberg configurations  $5s^2 5pn's$ :  
 $R^1(5pn's, n''sp5) =$   
 $= [n^*(5pn's) n^*(5pn''s) / (n^*(5p6s) n^*(5p7s))]^{3/2} \times$  (2.10)  
 $\times R^1(5p6s, 7s5p)$ ,

(v) for the parameters representing the interaction between configurations  $5s^2 5pn's$  and  $5s^2 5pn''d$ :  
 $R^2(5pn's, 5pn''d) =$   
 $= [n^*(5pn's) n^*(5pn'd) / (n^*(5p6s) n^*(5p5d))]^{3/2} \times$  (2.11)  
 $\times R^2(5p6s, 5p5d)$

and analogous relations for the exchange integrals  $R^1(5pn's, n''d5p)$ ,

(vi) for the parameters representing interaction between configurations  $5s^2 5pn's$  and  $5s5p^3$ :  
 $R^1(5sn's, 5p5p) =$   
 $= [n^*(5pn's) / n^*(5p6s)]^{3/2} R^1(5s6s, 5p5p)$  (2.12)

(vii) for the parameters representing interaction between configurations  $5s^2 5pn''d$  and  $5s^2 5p^3$ :  
 $R^1(5ns''d, 5p5p) = [n^*(5pn''d) / n^*(5p5d)]^{3/2} \times$  (2.13)  
 $\times R^1(5s5d, 5p5p)$

By using the above relations we were able to reduce the number of free parameters from 297 to 62. This number is much smaller than the number of possible energy levels in the system (130).

### 3. Calculations and results

When taking into account only low-lying configurations it proves to be rather difficult to get a reasonable description of the level spectrum. Nevertheless initial calculations with restrictions of that kind enabled us to evaluate roughly the effective quantum numbers for the configurations  $5p5d$ ,  $5p6d$ ,  $5p6s$  and  $5p7s$  by use of the relation (2.3). Proceeding in the analysis we found, that in particular the successive inclusion of higher-lying configurations  $5s^2 5pn''d$  into the energy matrix leads systematically to an improved agreement between the calculated and experimental values of the energy levels. In this way we have been able to assign the experimental levels [6] by appropriate configurations. Simultaneously, we have been able to correct the effective quantum numbers  $n^*(5pn'l)$  obtained; the results have been subsequently used in the relations (2.6) - (2.13). With respect to reasonable limits in computing time interactions between the distant configurations  $5s^2 5pn's$  and  $5s^2 5pn''d$  have been neglected. Interactions between configurations of the type  $5s^2 5pn''d$  have been restricted to the system  $n'' = 5 \leftrightarrow n'' = 9$ , those between configurations  $5s^2 5pn's$  to the nearest neighbours. However, we took into account the interaction of  $5s5p^3$  with all the configurations  $5s^2 5pn's$  ( $n' = 6$  to  $11$ ) and  $5s^2 5pn''d$  ( $n'' = 5$  to  $12$ ) present in the system under consideration. Finally, calculations<sup>+</sup> for 113 experimental energy levels (ascribed to the system  $5s^2 5pn's$  ( $n'' = 6$  to  $11$ ) +  $5s^2 5pn''d$  ( $n'' = 5$  to  $12$ ) +  $5s5p^3$ ) have been carried out. With 166 parameters, 62 of which were used as free, we achieved a very good fit with a mean deviation of  $22 \text{ cm}^{-2}$ . The results are given in Table 1, where the first column gives the configurations as well as its percent participation in the level, whereas the second column contains the assignment defining the state of the first component. The experimental energy level values given in the fourth column were taken from Ref. [6] except of those marked by "a", which were taken from the compilation of Moore [3]. Column 7 gives the percentage of the first component in the level. Column 8 gives the next component, originating in  $5pn's$  or  $5pn''d$ . Admixtures from  $5s5p^3$  larger than

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<sup>+</sup>We thank Dr. S. Büttgenbach for supplying the computer program.

0.1 percent are given in column 9. In several cases, the same state is present as the first component in two distinct energy levels, e.g.  $7d\ ^3D_1$  is the first component of the level at  $53593\text{ cm}^{-1}$  as well as of the level at  $55073\text{ cm}^{-1}$ . In these cases the letters "a" or "b" have been added to the assignment. If certain states occur twice as first components, others fail to occur in this role. For instance, the state  $5s5p^3\ ^3D_1$  does not occur as the first component in any of the electron levels but is mixed to almost all odd levels with  $J = 1$  in the configurations  $5s^25pn''d$ . In addition Table 1 shows that the quantum numbers  $n'$  and  $l'$  for excited electron states fail to be good quantum numbers in many cases. For example, the level at  $57182\text{ cm}^{-1}$  contains only 21 percent of the configuration  $5p6d$ . The missing 79 percent are distributed over other configurations.

Table 2 gives the values of the effective quantum numbers and values of the diagonal radial parameters for the configurations studied. The parameters with their standard deviation (given in parentheses) have been used as adjustable parameters in the fit procedure.

Table 3 gives only those values of the off-diagonal Slater integrals which have been used as free parameters. The values of the other off-diagonal Slater integrals, which have been used as dependent parameters, can be easily obtained by means of the relations 2.8 - 2.13 and Table 2. The upper limits of the off-diagonal integrals determined on the basis of the Racah criterion [14] are also given in Table 3.

In Table 4 calculated  $g$ -factor values are compared to experimental values available in the literature, demonstrating the good agreement. It is worthwhile to note that the agreement could be significantly improved when taking into account, in some cases, the interaction between configurations of the type  $5s^25pn''d$  (relations 2.8 and 2.9) in the energy matrix. For the level  $6p6d\ ^3D_1$ , the direct coupling between  $5s^25p5d$  and  $5s^25p6d$  decreases the difference  $g_J(\text{exp}) - g_J(\text{calc})$  from about 0.09 to 0.006. This corroborates the importance of the direct coupling between Rydberg configuration, particularly in cases when they additionally mix via another strongly interacting configurations (in the above case by  $5s5p^3$ ) configurations.

#### 4. Discussion

##### 4.1 Energy level scheme

In Table 1 (column 2) the levels with an assignment changed as compared to Moore's compilation [3] are marked with the letter "c", whereas those supplied by us with an n'l' SL-assignment are marked "N". In the light of the present calculations, the changes in the classification of levels as proposed in Ref. [6] are by no means justified. Thus, the level at  $49487 \text{ cm}^{-1}$  is  $5d^3 P_0$  (92.5 %) in agreement with Moore's compilation, and not  $5s5p^3^3 P_0$  (only 4.5 %). Similarly, the proposed assignment of the levels at  $50125 \text{ cm}^{-1}$ ,  $51010 \text{ cm}^{-1}$  and  $57283 \text{ cm}^{-1}$  to the configuration  $5s5p^3$  proved to be not justified. Our calculations clearly show that they belong to the Rydberg configurations  $5pn'l'$ , whereas the terms  $5s5p^3^3 P$  and  $^3 S$  are found much higher (see Table 1). The term  $5s5p^3^2 D$  turns out to be localized in the region about  $53600 \text{ cm}^{-1}$ . However, the levels at  $53592 \text{ cm}^{-1}$ ,  $53621 \text{ cm}^{-1}$  and  $53826 \text{ cm}^{-1}$  contain only 21, 21.5 and 23.4 percent, respectively, of the  $5s5p^3^3 D_{1,2,3}$  states.

The Slater integrals  $R^1(5sn''d, 5p5p)$ , which determine the strength of interaction between the configurations  $5s5p^3$  and  $5s^2 5pn''d$  are significantly greater (see Table 3) than the other off-diagonal Slater integrals. This is the reason for a coupling of the configuration  $5s5p^3$  with many Rydberg configurations  $5s^2 5pn''d$ . As a result of the fact that the terms  $5s5p^3^3 D$  and  $^3 P$  are found in the same region as the configuration  $5s^2 5pn''d$ , the states  $5s5p^3^3 D_J$  and  $^3 P_J$  undergo a decomposition among many states of configurations  $5s^2 5pn''d$ . For example, the respective admixtures of  $5s5p^3^3 D_1$  are: 11.06% to  $5d^3 D_1$ , 7.12 % to  $5d^3 P_1$ , 5.41 % to  $5d^1 P$ , 6.08 % to  $7d^3 D_1$ , 5.86 % to  $6d^1 P_1$ , 6.17 % to  $9d^3 D_1$ , and range from 5 to 0.1 percent in all the other states with  $J = 1$  within the system under consideration.

The interaction of the configuration  $5s5p^3$  with the Rydberg configurations  $5s^2 5pn's$  is much weaker than previously expected. The theoretical limit for the Slater integrals  $R^1(5sn's, 5p5p)$  deduced on the basis of the Racah criterion [14] is considerably higher (see Table 3) than the values obtained by the fit procedure.

The admixture of the configuration  $5s5p^3$  to states in the configurations  $5pn'$ s does not exceed 4 percent and occurs in the level  $9s^3P_1$ .

In order to confirm the values of the parameters  $R^1$  ( $5sn'$ s,  $5p5p$ ), we changed the values of these parameters by a factor of 1.5 - 2.0 and studied their effect on the fit result. The fits obtained in this way lead to a significantly worse description with a considerable admixture of  $5s5p^3^5S_2$  to the state  $6s^3P_2$ . This admixture increases the g-factor value calculated for the level  $6s^3P_2$ . The values obtained for  $g_J(6s^3P_2)$  were about 10 % larger than the experimental value 1.501 [3]. This is due to the fact that the interaction of the configuration  $5s5p^3$  with  $5s^25pn'$ s is much weaker than with  $5s^25pn'$ 'd configurations.

#### 4.2 Test of relations between Slater integrals

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In order to check the relation (2.2) we carried out series of fits varying the relations (2.2) - (2.13) between Slater integrals within  $\pm 20$  percent. When the relations were varied within limits of  $\pm 5$  percent the residuum and mean error in our fits remained practically unchanged. A variation within  $\pm 10$  percent led to an increase of about 20 percent whereas variations within  $\pm 20$  percent caused an increase in the residuum of a factor of about 2. It should be also noted that the values of the effective quantum numbers  $n^*(5pn'1')$  obtained along these lines varied quite slightly. For low - lying configurations ( $n' = 5, 6$  and  $7$ ) the changes in  $n^*(5pn'1')$  did not exceed  $\pm 0.01$ , whereas for higher-lying configurations they were of the order of 0.04 in the maximum. We note, however, that in the case of larger  $n'$ -values ( $n' > 10$ ) a shift of several  $\text{cm}^{-1}$  in the position of centre of gravity  $E'_a(5pn'1')$  of the configuration, the position of which is determined on the basis of semi-empirical values of the parameters (relation 2.5), leads to essential modifications in value of the effective quantum number  $n^*(5pn'1')$  of the configuration. This results immediately from the relation

$$\Delta n^* = [n^*/2 (E_\infty - E'_{av})] \Delta E'_{av}$$

where  $\Delta E'_{av}$  represents the accuracy with which the positions of the



centra of gravity of the Rydberg configuration are determined, and with  $E_{\infty}$  the centre of gravity of the two ionization limits of  $5s^2 5p$  ( $^2P_{1/2}$ ) and  $5s^2 5p$  ( $^2P_{3/2}$ ).

Hence, it is not reasonable to ascribe any physical meaning to fluctuations [3,6] in  $(n'-n^*)$  along Rydberg configurations (Table 2).

We carried out another test of the relation (2.1) by removing the relation (2.13) between Slater integrals  $R^1(5sn''d, 5p5p)$ . In this procedure the value of  $R^1(5s5d, 5p5p)$  was not varied, whereas the other parameters  $R^1(5sn''d, 5p5p)$  were assumed to be adjustable. Despite of the fact that the number of free parameters is increased by 6, no significant decrease of the residuum was obtained and the values calculated for the parameters remained almost unchanged. For comparison, Table 5 gives the values of the integrals  $R^1$  obtained with and without using relation (2.13).

The small differences in parameter values obtained with these two procedures, as well as the insensitivity on the magnitude of the residuum when dropping the relation (2.13) allows the statement that the general relation (2.1) between the Slater integrals of Rydberg configurations is well justified and confirmed. Further studies of regularities along Rydberg configurations require additional experimental work checking the energies of certain electron levels (Table 1) and completing the experimental information about the system under configuration.

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Table 1. Observed and calculated odd-parity energy levels of Sn I.

Configuration First component %	Designation	J	Energy in cm <sup>-1</sup>			Leading component %		
			Observed	Calculated	O - C	First	Next	Admixture from the conf. 5s5p <sup>3</sup>
1	2	3	4	5	6	7	8	9
99.8 5s <sup>2</sup> 5p6s	6s 3P	0	34640.76	34652	-11	99.8		0.1 3P
99.6 5s <sup>2</sup> 5p6s	6s 3P	1	34914.28	34903	11	74.9	24.7 6s 1P	0.1 3P
96.6 5s <sup>2</sup> 5p6s	6s 3P	2	38628.88	38642	-13	96.6		2.6 5s
98.3 5s <sup>2</sup> 5p6s	6s 1P	1	39257.05	39244	13	73.5	24.8 6s 3P	
96.5 5s5p <sup>3</sup>	5p <sup>3</sup> 5S	2	39625.51	39625	0	93.8	3.1 6s 3P	
97.0 5s <sup>2</sup> 5p5d	5d 3F	2	43682.74	43685	-3	54.8	39.0 5d 1D	0.7 1D
89.1 5s <sup>2</sup> 5p5d	5d 3D	2	44144.37	44157	-13	45.8	20.0 5d 3P	7.4 3D
86.1 5s <sup>2</sup> 5p5d	5d 3D	1	44508.68	44517	-8	68.7	9.1 5d 3P	11.1 3D+0.9 3P
94.2 5s <sup>2</sup> 5p5d	5d 3F C	3	44576.00	44558	18	50.5	32.6 5d 3D	4.5 3D
88.3 5s <sup>2</sup> 5p5d	5d 1D	2	47145.68	47137	8	36.8	32.8 5d 3F	6.7 3D
83.5 5s <sup>2</sup> 5p5d	5d 3D C	3	47487.70	47461	26	44.9	37.6 5d 3F	14.0 3D
98.5 5s <sup>2</sup> 5p5d	5d 3F N	4	48107.27	48120	-13	98.5	1.1 6d 3F	
96.8 5s <sup>2</sup> 5p7s	7s 3P	0	48216.36	48198	18	96.8	2.4 5d 3P	0.6 3P
95.5 5s <sup>2</sup> 5p7s	7s 3P	1	48222.16	48241	-19	64.7	30.8 7s 1P	0.4 3P+0.3 3D
89.0 5s <sup>2</sup> 5p5d	5d 3P	2	48669.41	48682	-12	71.7	12.7 5d 3D	4.7 3D+1.3 3P

Table 1.

1	2	3	4	5	6	7	8	9	
84.5	5s <sup>2</sup> 5p5d	5d <sup>3</sup> P	1	48981.93	48945	37	59.4	16.0 5d <sup>1</sup> P	7.1 <sup>3</sup> D+1.2 <sup>3</sup> P
92.5	5s <sup>2</sup> 5p5d	5d <sup>3</sup> P	0	49487.13	49515	-28	92.5	2.8 7s <sup>3</sup> P	4.5 <sup>3</sup> P
76.7	5s <sup>2</sup> 5p5d	5d <sup>1</sup> F	3	49893.80 <sup>a</sup>	49909	-15	68.5	8.3 6d <sup>1</sup> F	1.9 <sup>3</sup> D
68.5	5s <sup>2</sup> 5p5d	5d <sup>1</sup> P	1	50125.97	50097	29	42.2	25.0 5d <sup>3</sup> P	5.4 <sup>3</sup> D+3.5 <sup>3</sup> P
76.1	5s <sup>2</sup> 5p6d	6d <sup>3</sup> D	2	51010.94	51009	2	35.6	23.4 6d <sup>3</sup> P	7.2 <sup>3</sup> D+3.1 <sup>3</sup> P
95.4	5s <sup>2</sup> 5p6d	6d <sup>3</sup> F	2	51160.52	51134	27	54.7	32.6 6d <sup>1</sup> D	0.3 <sup>3</sup> P
54.9	5s <sup>2</sup> 5p6d	6d <sup>3</sup> D	1	51474.74	51532	-57	35.5	18.3 5d <sup>1</sup> P	2.9 <sup>3</sup> D+0.7 <sup>3</sup> P
74.7	5s <sup>2</sup> 5p6d	6d <sup>3</sup> F C	3	51754.67	51747	8	37.9	23.6 6d <sup>3</sup> D	1.7 <sup>3</sup> D
97.7	5s <sup>2</sup> 5p7s	7s <sup>3</sup> P	2	52415.83	52417	-1	97.7	0.5 6d <sup>3</sup> D	0.1 <sup>3</sup> P
65.7	5s <sup>2</sup> 5p7s	7s <sup>1</sup> P	1	52706.80	52697	10	47.8	17.9 7s <sup>3</sup> P	0.1 <sup>3</sup> D+0.1 <sup>3</sup> P
99.4	5s <sup>2</sup> 5p8s	8s <sup>3</sup> P N	0	52919.77	52929	-9	99.4	0.2 7s <sup>3</sup> P	0.2 <sup>3</sup> P
76.6	5s <sup>2</sup> 5p8s	8s <sup>3</sup> P	1	53020.97	53011	10	52.0	24.6 8s <sup>1</sup> P	0.8 <sup>3</sup> D+0.2 <sup>3</sup> P
38.2	5s <sup>2</sup> 5p7d	7d a <sup>3</sup> D	1	53592.77	53650	-58	24.7	19.0 6d <sup>1</sup> P	21.0 <sup>3</sup> D+1.9 <sup>3</sup> P
24.6	5s5p <sup>3</sup>	5p <sup>3</sup> <sup>3</sup> D C	2	53631.83	53606	26	21.5	19.3 7d <sup>3</sup> D	2.9 <sup>3</sup> P
23.4	5s5p <sup>3</sup>	5p <sup>3</sup> <sup>3</sup> D C	3	53826.55	53844	-17	23.4	15.0 7d <sup>3</sup> D	
96.1	5s <sup>2</sup> 5p7d	7d <sup>3</sup> F	2	54211.76	54221	-9	60.2	28.7 7d <sup>1</sup> D	0.1 <sup>1</sup> D
56.7	5s <sup>2</sup> 5p7d	7d <sup>3</sup> F C	3	54653.86	54631	22	33.0	18.2 7d <sup>1</sup> F	7.2 <sup>3</sup> D
42.9	5s <sup>2</sup> 5p6d	6d <sup>1</sup> D C	2	54713.32	54690	22	22.0	16.5 7d <sup>3</sup> P	4.6 <sup>3</sup> D+0.4 <sup>1</sup> D
38.5	5s <sup>2</sup> 5p7d	7d b <sup>3</sup> D C	1	55073.21	55064	9	20.0	19.8 9s <sup>3</sup> P	6.1 <sup>3</sup> D

Table 1.

1	2	3	4	5	6	7	8	9			
96.2	5s <sup>2</sup> 5p9s	9s <sup>3</sup> P N	0	55131.53	55121	11	96.2	2.9	6d <sup>3</sup> P	0.7	<sup>3</sup> P
61.7	5s <sup>2</sup> 5p9s	9s <sup>3</sup> P	1	55156.74	55178	-22	42.5	19.2	9s <sup>1</sup> P	3.6	<sup>3</sup> D+0.3 <sup>3</sup> P
74.6	5s <sup>2</sup> 5p6d	6d <sup>3</sup> P C	2	55296.28	55275	21	43.9	24.1	6d <sup>1</sup> D	3.4	<sup>3</sup> D+1.3 <sup>3</sup> P
97.7	5s <sup>2</sup> 5p6d	6d <sup>3</sup> F N	4	55444.61	55464	-19	97.7	1.2	5d <sup>3</sup> F		
86.9	5s <sup>2</sup> 5p6d	6d <sup>3</sup> P N	0	55621.89	55651	-29	86.9	3.7	9s <sup>3</sup> P	7.4	<sup>3</sup> P
73.8	5s <sup>2</sup> 5p6d	6d <sup>3</sup> P C	1	55688.37	55660	28	57.1	14.7	6d <sup>3</sup> D	7.1	<sup>3</sup> P+0.3 <sup>3</sup> D
58.3	5s <sup>2</sup> 5p8d	8d a <sup>3</sup> F C	3	55741.17	55737	5	25.3	20.6	8d <sup>1</sup> F	0.4	<sup>3</sup> D
58.2	5s <sup>2</sup> 5p8d	8d <sup>3</sup> P C	2	55805.35	55803	3	28.4	22.4	6d <sup>3</sup> D	3.6	<sup>3</sup> P+0.9 <sup>3</sup> D
93.6	5s <sup>2</sup> 5p8d	8d <sup>3</sup> F N	2	55854.62	55872	-17	69.7	19.9	8d <sup>1</sup> D	0.2	<sup>3</sup> D
62.4	5s <sup>2</sup> 5p8d	8d <sup>3</sup> D C	1	56242.35	56213	29	31.2	20.7	8d <sup>1</sup> P	1.1	<sup>3</sup> D+0.4 <sup>1</sup> S
50.6	5s <sup>2</sup> 5p6d	6d <sup>1</sup> F	3	56297.98	56331	-33	37.8	17.0	8d <sup>3</sup> F	0.1	<sup>3</sup> D
99.3	5s <sup>2</sup> 5p10s	10s <sup>3</sup> P N	0	56358.87	56368	-9	99.3	0.6	6d <sup>3</sup> P		
98.9	5s <sup>2</sup> 5p10s	10s <sup>3</sup> P	1	56390.11	56381	9	66.3	32.6	10s <sup>1</sup> P		
32.8	5s <sup>2</sup> 5p9d	9d a <sup>3</sup> P C	2	56546.14	56538	8	14.5	13.4	9d <sup>3</sup> D	7.6	<sup>3</sup> D+2.4 <sup>3</sup> P
42.5	5s <sup>2</sup> 5p6d	6d <sup>1</sup> P C	1	56659.18	56666	-7	25.2	16.8	9d <sup>3</sup> D	5.9	<sup>3</sup> D+0.9 <sup>3</sup> P
97.9	5s <sup>2</sup> 5p9d	9d <sup>3</sup> F N	2	56779.98	56797	-17	64.2	27.0	9d <sup>1</sup> D	0.2	<sup>3</sup> D
59.8	5s <sup>2</sup> 5p9d	9d a <sup>3</sup> F	3	56838.68	56808	31	25.9	18.1	9d <sup>1</sup> F	5.0	<sup>3</sup> D
40.7	5s <sup>2</sup> 5p9d	9d <sup>3</sup> D C	1	57094.33	57090	4	17.3	16.4	9d <sup>1</sup> P	6.2	<sup>3</sup> D+0.4 <sup>3</sup> P
99.7	5s <sup>2</sup> 5p11s	11s <sup>3</sup> P N	0	57103.95	57100	4	99.7	0.2	6d <sup>3</sup> P		

Table 1.

1	2	3	4	5	6	7	8	9
54.6	5s <sup>2</sup> 5p9d	9d b <sup>3</sup> P C	2	57104.73	57108	-3	22.2	19.4 9d <sup>3</sup> D
69.1	5s <sup>2</sup> 5p11s	11s <sup>3</sup> P N	1	57106.96	57112	-5	59.9	29.3 11s <sup>1</sup> P 0.4 <sup>3</sup> D+0.1 <sup>3</sup> P
88.8	5s <sup>2</sup> 5p8s	8s <sup>3</sup> P	2	57150.16	57146	4	88.8	1.6 10d <sup>3</sup> D 1.1 <sup>3</sup> D
20.8	5s <sup>2</sup> 5p6d	6d <sup>3</sup> D C	3	57181.71	57180	1	17.0	12.9 9d <sup>3</sup> F 12.8 <sup>3</sup> D
78.5	5s <sup>2</sup> 5p8s	8s <sup>1</sup> P	1	57283.66	57289	-5	54.2	24.2 8s <sup>3</sup> P 0.3 <sup>3</sup> D+0.2 <sup>3</sup> P
99.7	5s <sup>2</sup> 5p10d	10d <sup>3</sup> F N	2	57374.56	57369	5	62.9	27.7 10d <sup>1</sup> D
74.0	5s <sup>2</sup> 5p10d	10d a <sup>3</sup> F N	3	57517.71	57528	-11	35.1	24.5 10d <sup>1</sup> F 4.9 <sup>3</sup> D
70.2	5s <sup>2</sup> 5p10d	10d a <sup>3</sup> P C	2	57533.30	57532	2	29.2	25.4 10d <sup>3</sup> D 3.9 <sup>3</sup> D+0.3 <sup>3</sup> P
70.5	5s <sup>2</sup> 5p10d	10d <sup>3</sup> D C	1	57562.44	57562	0	33.9	24.6 10d <sup>1</sup> P 4.1 <sup>3</sup> D+0.3 <sup>3</sup> P
99.7	5s <sup>2</sup> 5p11d	11d <sup>3</sup> F N	2	57775.44	57770	6	61.3	28.2 11d <sup>1</sup> D
90.9	5s <sup>2</sup> 5p11d	11d <sup>3</sup> F C	3	57847.17	57853	-6	41.8	29.8 11d <sup>1</sup> F 1.4 <sup>3</sup> D
80.8	5s <sup>2</sup> 5p11d	11d a <sup>3</sup> P C	2	57856.75	57865	-8	32.5	30.1 11d <sup>3</sup> D 2.2 <sup>3</sup> D
81.1	5s <sup>2</sup> 5p11d	11d <sup>3</sup> D C	1	57898.20	57890	8	39.6	27.7 11d <sup>1</sup> P 2.5 <sup>3</sup> D
99.7	5s <sup>2</sup> 5p12d	12d <sup>3</sup> F N	2	58057.94	58054	4	60.9	28.2 12d <sup>1</sup> D
86.9	5s <sup>2</sup> 5p12d	12d a <sup>3</sup> P C	2	58100.69	58107	-6	34.5	32.8 12d <sup>3</sup> D 1.3 <sup>3</sup> D
95.7	5s <sup>2</sup> 5p12d	12d a <sup>3</sup> F N	3	58100.89	58107	-6	43.6	31.2 12d <sup>1</sup> F 0.5 <sup>3</sup> D
87.3	5s <sup>2</sup> 5p12d	12d <sup>3</sup> D C	1	58143.31	58136	7	42.9	29.4 12d <sup>1</sup> P 2.0 <sup>3</sup> D+0.2 <sup>1</sup> P
89.3	5s <sup>2</sup> 5p7d	7d <sup>1</sup> D N	2	58390.58	58389	1	41.7	39.3 7d <sup>3</sup> P 2.5 <sup>3</sup> P+1.2 <sup>3</sup> D
82.7	5s <sup>2</sup> 5p7d	7d <sup>3</sup> P N	0	58465.59	58476	-10	82.7	3.1 6d <sup>3</sup> P 10.6 <sup>3</sup> P
98.0	5s <sup>2</sup> 5p7d	7d <sup>3</sup> F N	4	58521.91	58528	-6	98.0	1.0 6d <sup>3</sup> F

Table 1

1		2		3	4	5	6	7	8		9	
52.6	5s <sup>2</sup> 5p7d	7d	<sup>3</sup> P	C	1	58523.55	58512	11	64.9	16.3	7d <sup>3</sup> D	9.2 <sup>3</sup> P
76.3	5s <sup>2</sup> 5p7d	7d	<sup>3</sup> D		2		58820		49.2	11.8	7d <sup>3</sup> F	5.7 <sup>3</sup> D+5.0 <sup>3</sup> P
93.5	5s <sup>2</sup> 5p7d	7d	<sup>1</sup> F		3		58855		50.3	40.0	7d <sup>3</sup> F	1.6 <sup>3</sup> D
74.6	5s <sup>2</sup> 5p7d	7d	<sup>1</sup> P	N	1	59157.01	59156	1	47.9	22.1	7d <sup>3</sup> D	4.0 <sup>3</sup> D+0.5 <sup>3</sup> P
73.4	5s <sup>2</sup> 5p7d	7d	<sup>3</sup> D		3	59230.	59195	35	56.4	14.8	7d <sup>1</sup> F	9.6 <sup>3</sup> D
97.7	5s <sup>2</sup> 5p9s	9s	<sup>3</sup> P	N	2	59375.4	59367	9	97.7	0.8	7d <sup>3</sup> D	0.2 <sup>3</sup> D
88.1	5s <sup>2</sup> 5p9s	9s	<sup>1</sup> P	N	1	59427.	59437	-10	59.8	28.4	9s <sup>3</sup> P	0.2 <sup>3</sup> D
89.5	5s <sup>2</sup> 5p8d	8d	<sup>1</sup> D		2		59975		48.4	32.7	8d <sup>3</sup> P	1.6 <sup>3</sup> P+0.6 <sup>3</sup> D
73.6	5s <sup>2</sup> 5p8d	8d	<sup>3</sup> P	N	0	60013.	60013	0	73.6	8.6	7d <sup>3</sup> P	10.4 <sup>3</sup> P
78.7	5s <sup>2</sup> 5p8d	8d	<sup>3</sup> P		1	60051.4 <sup>a</sup>	60048	4	62.2	16.0	8d <sup>3</sup> D	7.9 <sup>3</sup> P+0.4 <sup>3</sup> D
98.3	5s <sup>2</sup> 5p8d	8d	<sup>3</sup> F		4		60193			0.8	7d <sup>3</sup> F	
91.1	5s <sup>2</sup> 5p8d	8d	<sup>3</sup> D		2		60194		56.3	14.6	8d <sup>3</sup> F	4.3 <sup>3</sup> P+0.4 <sup>3</sup> D
97.3	5s <sup>2</sup> 5p8d	8d	<sup>3</sup> F	N	3	60290.	60267	23	47.6	46	8d <sup>1</sup> F	0.2 <sup>3</sup> D
85.9	5s <sup>2</sup> 5p8d	8d	<sup>1</sup> P		1	60395	60418	-23	55.1	26.7	8d <sup>3</sup> D	1.8 <sup>3</sup> D+0.2 <sup>3</sup> P
83.0	5s <sup>2</sup> 5p8d	8d	<sup>3</sup> D	N	3	60454	60463	-9	63.8	15.2	8d <sup>1</sup> F	3.9 <sup>3</sup> D
97.4	5s <sup>2</sup> 5p10s	10s	<sup>3</sup> P	N	2	60603	60605	-2	97.4	0.9	8d <sup>3</sup> D	0.1 <sup>3</sup> D
98.3	5s <sup>2</sup> 5p10s	10s	<sup>1</sup> P	N	1	60630	60628	2	66.0	32.3	10s <sup>3</sup> P	
90.7	5s <sup>2</sup> 5p9d	9d	<sup>1</sup> D		2		60913		52.9	28.5	9d <sup>3</sup> P	0.9 <sup>3</sup> P+0.5 <sup>3</sup> D
68.7	5s <sup>2</sup> 5p9d	9d	<sup>3</sup> P	N	0	60946	60945	1	68.7	14.7	8d <sup>3</sup> P	7.3 <sup>3</sup> P
74.9	5s <sup>2</sup> 5p9d	9d	<sup>3</sup> P		1	60968	60970	-2	59.7	14.5	9d <sup>3</sup> D	5.5 <sup>3</sup> P+0.4 <sup>3</sup> D

Table 1

1	2	3	4	5	6	7	8	9	
89.7	5s <sup>2</sup> 5p9d	9d <sup>3</sup> D							
			2	61049		55.3	13.5 9d <sup>3</sup> F	3.2 <sup>3</sup> P	
99.0	5s <sup>2</sup> 5p9d	9d <sup>3</sup> F	4	61077		99.0	0.7 8d <sup>3</sup> F		
98.1	5s <sup>2</sup> 5p9d	9d b <sup>3</sup> F	3	61094		50.4	42.6 9d <sup>1</sup> F		
86.3	5s <sup>2</sup> 5p9d	9d <sup>1</sup> P	1	61214.	61212	2	55.0	28.6 9d <sup>3</sup> D	1.6 <sup>3</sup> D+0.1 <sup>3</sup> P
85.6	5s <sup>2</sup> 5p9d	9d <sup>3</sup> D C	3	61245.	61244	1	63.8	18.9 9d <sup>1</sup> F	2.2 <sup>3</sup> D
97.4	5s <sup>2</sup> 5p11s	11s <sup>3</sup> P N	2	61351	61346	5	97.4	1.0 9d <sup>3</sup> D	
95.3	5s <sup>2</sup> 5p11s	11s <sup>1</sup> P N	1	61365	61370	-5	64.0	31.3 11s <sup>3</sup> P	
85.8	5s <sup>2</sup> 5p10d	10d b <sup>3</sup> P C	2	61534.2 a	61543	-9	41.2	29.1 10d <sup>1</sup> D	1.6 <sup>3</sup> P+0.3 <sup>3</sup> D
73.4	5s <sup>2</sup> 5p10d	10d <sup>3</sup> P N	0	61550.	61552	-2	73.4	15.8 9d <sup>3</sup> P	3.4 <sup>3</sup> P
78.3	5s <sup>2</sup> 5p10d	10d <sup>3</sup> P	1	61562.	61558	6	59.4	18.8 10d <sup>3</sup> D	2.9 <sup>3</sup> P+0.1 <sup>3</sup> D
97.8	5s <sup>2</sup> 5p10d	10d <sup>3</sup> D N	2	61600.	61617	-17	41.9	33.6 10d <sup>1</sup> D	0.9 <sup>3</sup> P+0.1 <sup>3</sup> D
100	5s <sup>2</sup> 5p10d	10d <sup>3</sup> F	4		61623		100.		
95.7	5s <sup>2</sup> 5p10d	10d b <sup>3</sup> F N	3	61696.	61687	9	51.3	22.7 10d <sup>3</sup> D	
98.2	5s <sup>2</sup> 5p10d	10d <sup>1</sup> P	1	61747.4	61741	6	65.4	25.8 10d <sup>3</sup> D	0.5 <sup>3</sup> D+0.1 <sup>3</sup> P
92.0	5s <sup>2</sup> 5p10d	10d <sup>3</sup> D C	3	61766	61760	6	46.0	45.1 10d <sup>1</sup> F	1.1 <sup>3</sup> D
87.4	5s <sup>2</sup> 5p11d	11d b <sup>3</sup> P C	2	61963 a	61971	-8	42.7	26.8 11d <sup>1</sup> D	1.4 <sup>3</sup> P+0.3 <sup>3</sup> D
74.4	5s <sup>2</sup> 5p11d	11d <sup>3</sup> P N	0	61964.6	61963	2	74.4	12.1 10d <sup>3</sup> P	3.6 <sup>3</sup> P
80.5	5s <sup>2</sup> 5p11d	11d <sup>3</sup> P	1	61975.	61970	5	60.1	20.4 11d <sup>3</sup> D	2.7 <sup>3</sup> P+0.2 <sup>3</sup> D
98.8	5s <sup>2</sup> 5p11d	11d <sup>3</sup> D N	2	62008.6	62020	-11	39.6	36.8 11d <sup>1</sup> D	0.6 <sup>3</sup> P
100	5s <sup>2</sup> 5p11d	11d <sup>3</sup> F	4		62026		100.		



Table 1

1	2	3	4	5	6	7	8	9
96.6	5s <sup>2</sup> 5p11d	11d 3 <sub>F</sub> N	3	62080	62071	9	52.5	25.3 11d 1 <sub>F</sub> 0.4 3 <sub>D</sub>
98.7	5s <sup>2</sup> 5p11d	11d 1 <sub>P</sub>	1	62112.7	62110	3	65.9	24.8 11d 3 <sub>D</sub> 0.3 3 <sub>D</sub>
91.2	5s <sup>2</sup> 5p11d	11d 3 <sub>D</sub> C	3	62125.3	62124	1	48.8	41.1 11d 1 <sub>F</sub> 0.9 3 <sub>D</sub>
81.8	5s <sup>2</sup> 5p12d	12d 3 <sub>P</sub> N	0	62260.5	62261	0	81.8	11.7 11d 3 <sub>P</sub> 2.3 3 <sub>P</sub>
91.4	5s <sup>2</sup> 5p12d	12d b 3 <sub>P</sub> C	2	62263.9 <sup>a</sup>	62269	-5	46.7	29.1 12d 3 <sub>D</sub> 1.0 3 <sub>P</sub> +0.2 3 <sub>D</sub>
86.8	5s <sup>2</sup> 5p12d	12d 3 <sub>P</sub>	1	62269.	62266	3	46.2	22.6 12d 3 <sub>D</sub> 1.6 3 <sub>P</sub> +0.1 3 <sub>D</sub>
99.6	5s <sup>2</sup> 5p12d	12d 1 <sub>D</sub> N	2	62297.7	62302	-4	48.2	29.2 12d 3 <sub>D</sub> 0.2 3 <sub>P</sub> +0.1 3 <sub>D</sub>
100	5s <sup>2</sup> 5p12d	12d 3 <sub>F</sub>	4		62299			
97.0	5s <sup>2</sup> 5p12d	12d b 3 <sub>F</sub> N	3	62350.	62340	10	52.8	25.4 12d 1 <sub>F</sub> 0.5 3 <sub>D</sub>
99.3	5s <sup>2</sup> 5p12d	12d 1 <sub>P</sub>	1	62374.4	62373	1	66.4	23.7 12d 3 <sub>D</sub> 0.2 3 <sub>D</sub>
94.0	5s <sup>2</sup> 5p12d	12d 3 <sub>D</sub> C	3	62382.98	62388	-5	52.4	41.5 12d 1 <sub>F</sub> 1.2 3 <sub>D</sub>
48.9	5s5p <sup>3</sup>	5p <sup>3</sup> 3 <sub>P</sub>	0		63085		48.9	12.4 12d 3 <sub>P</sub>
57.2	5s5p <sup>3</sup>	5p <sup>3</sup> 3 <sub>P</sub>	1		63388		48.8	4.9 9d 3 <sub>P</sub> 7.5 3 <sub>D</sub> +0.8 3 <sub>S</sub>
67.3	5s5p <sup>3</sup>	5p <sup>3</sup> 3 <sub>P</sub>	2		63844		52.1	2.7 9d 3 <sub>P</sub> 12.4 3 <sub>D</sub> +1.8 1 <sub>D</sub>
96.3	5s5p <sup>3</sup>	5p <sup>3</sup> 1 <sub>D</sub>	2		74692		93.0	1.2 5d 1 <sub>D</sub> 3.1 3 <sub>P</sub>
99.2	5s5p <sup>3</sup>	5p <sup>3</sup> 3 <sub>S</sub> N	1	75952.	75952	0	69.9	27.8 1 <sub>P</sub>
98.8	5s5p <sup>3</sup>	5p <sup>3</sup> 1 <sub>P</sub>	1		81874		68.7	28.7 3 <sub>S</sub>

Table 2 Effective quantum numbers and other fine structure parameters for the odd configuration of Sn I.

Conf. 5pn'l'	n*(5pn'l')	E' <sub>av</sub> (5pn'l')	Values of the parameters obtained from the fit in cm <sup>-1</sup>								
			F <sup>0</sup> (5pn'l')	F <sup>2</sup> (np,n'l')	G <sup>1</sup> (5pn'l')	G <sup>3</sup> (5pn'l')	ζ <sub>5p</sub> (5pn'l')	ζ(n'l'd) n'd	α(5pn'l')	β(5pn'l')	
5p6s	2.1188	37623.95	37871(29)		1480(61)			2687(20)			
5p7s	3.166	51117.24	51191(25)		444			2782(23)			
5p8s	4.175	55771.85	55804(17)		192			2802(20)			
5p9s	5.181	57978.81	57996(16)		101			2814(21)			
5p10s	6.193	59206.22	59216(13)		59			2826(16)			
5p11s	7.182	59939.32	59946(13)		33			2830(16)			
5p5d	2.7717	47783.11	48127(51)	6098(119)	3908(49)	2132(158)	2707(14)	19(8)	-20(4)	110(29)	
5p6d	3.763	54318.07	54251(47)	2420	1551	846	2787(16)	7.5	-4(3)	161(27)	
5p7d	4.773	57249.74	57293(40)	1195	766	418	2831(19)	3.7	-9(4)	67(32)	
5p8d	5.789	58792.18	58663(35)	675	433	236	2832(17)	2.1	-2(3)	124(36)	
5p9d	6.762	59666.64	59555(55)	420	266	146	2812(22)	1.3	-4(5)	109(32)	
5p10d	7.753	60241.34	60241(39)	279	179	98	2824(13)	0.87	3(3)	-5(27)	
5p11d	8.750	60633.78	60636(38)	194	124	68	2829(12)	0.60	2(3)	-2(24)	
5p12d	9.723	60906.14	60922(36)	141	90	49	2828(11)	0.43	1(3)	-11(20)	
5snp <sup>3</sup>			26826(273)	19587(970)	27946(110)		3334(183)		-301(56)		

Table 3

Experimental values, and their theoretical limits deduced from the Racah criterion for the off-diagonal Slater integrals of Sn I

	Experimental cm <sup>-1</sup>	Limit cm <sup>-1</sup>
$R^1(5s6s, 5p5p)$	1925(583)	6431
$R^1(5s5d, 5p5p)$	-7565(77)	-10450
$R^2(5p6s, 5p5d)$	-2527(171)	
$R^1(5p6s, 5d5p)$	-1106(98)	-2405
$R^2(5p5d, 5p6d)$	2797(254)	3842
$R^1(5p5d, 6d5p)$	2200(122)	2462
$R^3(5p5d, 6d5p)$	598(200)	1343
$R^1(5p6s, 7s5p)$	518(104)	810

Table 4

Experimental and calculated values of the g-factors

Designation according to Table 1.	Experimental [3]	Calculated	Exp.- Calc.
5p6s $^3P_1$	1.380	1.37596	0.004
5p6s $^1P_1$	1.121	1.12454	-0.003
5p5d $^3D_1$	0.635	0.64431	-0.009
5p7s $^3P_1$	1.316	1.32736	-0.011
5p5d $^3P_1$	1.229	1.20518	0.024
5p5d $^1P_1$	1.066	1.09259	-0.027
5p6d $^3D_1$	0.863	0.85705	0.006
6p6s $^3P_2$	1.501	1.51394	-0.013
5p5d $^3F_2$	0.865	0.82915	0.036
5p5d $^3D_2$	1.131	1.16726	-0.036
5p5d $^1D_2$	0.941	0.94293	-0.002
5p5d $^3D_2$	1.406	1.40480	0.001
5p5d $^3F_3$	1.167	1.16855	-0.002
5p5d $^3D_3$	1.246	1.23573	0.010
5p5d $^1F_3$	1.043	1.03468	0.008

Table 5

Comparison of the values of some Slater integrals obtained with the relation 2.1 and without it.

Configuration	$R^1(5s^n d, 5p5p)$ with use of relation 2.1	$R^1(5s^n d, 5p5p)$ applied as free parameters
$5s^2 5p5d$	-7565 (77)	-7565 -
$5s^2 5p6d$	-4766	-4815 (92)
$5s^2 5p7d$	-3349	-3525 (72)
$5s^2 5p8d$	-2517	-2512 (112)
$5s^2 5p9d$	-1981	-1980 (118)
$5s^2 5p10d$	-1618	-1637 (127)
$5s^2 5p11d$	-1349	-1374 (145)
$5s^2 5p12d$	-1147	-1191 (146)