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RADIAL INTEGRALS, OSCILLATOR STRENGTHS AND POLARIZABILITIES OF THE THALLIUM, LEAD AND BISMUTH ATOMS

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Abstract

The radial integrals for transitions of $6p$-electron to the excited states in the Tl, Pb and Bi atoms have been found by numerical integration of the Dirac equation with an effective potential. The radial integrals for excitation of $6s$- and $5d$-electrons from the closed subshells have been obtained from analysis of the available experimental data on the oscillator strengths in Tl, Hg, Au and polarizability of Hg. Using the obtained radial integrals we determine the polarizabilities of the Tl, Pb, Bi atoms by a simple method similar in essence to the Sternheimer method.

1. Introduction

Calculation of the oscillator strengths for different transitions in the atoms of thallium and lead was the subject of numerous theoretical works (see, e.g., [1-3]). Our interest to this matter is due to calculation of the effects of the parity violation and enhancement of an electrical dipole moment of an electron in the atoms of Tl, Pb and Bi which depend on the values of the radial integrals [4-9]. Although there are extensive experimental and theoretical data on transitions of a valent $6p$-electron in Tl, the data on similar transitions in Pb are incomplete and contradictory; as to Bi, the lifetimes of some levels are known only.

The main purpose of this work is not pure theoretical cal-

culation of the radial integrals but obtaining of the most reliable values of these quantities in the atoms of Tl, Pb and Bi. Therefore, we correct our calculations at each stage *using* the known experimental data on oscillator strengths. Although the calculations were made by us in connection with the parity violation problem in atoms, the obtained results are, in our opinion, of independent interest.

The radial integrals were calculated with the wave functions obtained by numerical integration of the Dirac equation with an effective potential. Comparison with the available experimental data on the oscillator strengths in Tl showed that found by us integrals ζ_{6p-7s} and ζ_{6p-6d} exceed the experimental values by $4-15\%$.

In lead and bismuth the calculated radial integrals were corrected in accordance with the available experimental data on thallium. Using these radial integrals, we calculated several oscillator strengths in Pb and Bi. Agreement with experimental data from the works [10-13] is, in our opinion, quite satisfactory.

The radial integrals connected with the excitations

of $6S$-electrons from the closed subshells are of a special interest, since, in our opinion, the discrepancy in estimate of the effects of the space and time parity violation between the works [4-6] and [7-9] is due mainly to the difference in the magnitudes of the used radial integrals ζ_{6S-6P}. These integrals were obtained by us for Au, Hg and Tl from the analysis of available experimental data and extrapolated to Pb and Bi.

In the present paper we calculated also the polarizabilities of the Tl, Pb and Bi atoms by using a simple method sim-

ilar in essence to the Sternheimer method [14].

2. Calculation of the single-electron wave functions. The technique of calculation of polarizability in many-electron atoms

The Dirac spinor of an electron with the total angular momentum j and orbital angular momentum l in the central potential looks as follows

$$\Psi_{jl\rangle_z} = \frac{1}{z}\left(\begin{array}{c} g_{jl}(z)\,\Omega_{jl\rangle_z} \\ i\,f_{jl}(z)\,\Omega_{\tilde{j}\tilde{l}\rangle_z} \end{array} \right) \tag{1}$$

Here $\Omega_{jl\rangle_z}$ is a spherical spinor, $\tilde{l} = 2j - l$. In these notations the radial integral determining an amplitude of EI-transition may be written in the following way

$$\zeta_{njl,\,n'j'l'} = \int\limits_0^\infty \left[g_{njl}(z)\,g_{n'j'l'}(z) + f_{njl}(z)f_{n'j'l'}(z) \right] z\,dz \tag{2}$$

In this paper all the values of the radial integrals are given in the units of Bohr radius.

We find the radial wave functions f and g [1] by numerical integration of the Dirac equation with the two-parametric effective potential proposed in [15]:

$$U(z) = -\frac{e^2}{z}\left[\frac{Z-1}{H(\exp(z/d)-1)+1} + 1 \right] \tag{3}$$

Z is the charge of a nucleus. We have chosen the following values of parameters:

$$\begin{array}{llll} H_{Hg} = 16.037 & H_{Tl} = 15.041 & H_{Pb} = 14.045 & H_{Bi} = 12.049 \\ d_{Hg} = 1.632a_B & d_{Tl} = 1.580a_B & d_{Pb} = 1.538a_B & d_{Bi} = 1.401a_B \end{array} \tag{4}$$

a_B is the Bohr radius. Obtained in this potential values of the mean energies and the fine splitting constants of $6p$-el-

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1) The sign of the radial functions was chosen so that $g > 0$ at $z \to 0$.

ectrons as well as the energies of ns $(n \geq 7)$-electrons agree with experiment with an accuracy not worse than 5%. Fitting the energies of valent electrons we obtain a true behavior of the wave functions at long distances, whereas the fine splitting serves as the criterion of their correct behavior at short distances. Good agreement between the experimental and calculated in [16] constants of the hyperfine structure of the levels of ground configurations in Tl, Pb and Bi is an additional test for the found wave functions.

In further calculations of the oscillator strengths and polarizabilities of many-electron atoms it is convenient to use the secondary quantization representation. Let us introduce the necessary notations: b_μ is the destruction operator for $6p_{1/2}$ electron with the projection of the total angular momentum on the axis z $j_z = \mu$, c_μ is the destruction operator for $6p_{3/2}$-electron, $a_{n,\mu}$ for ns -electron, $f_{n,\mu}$ for $nd_{3/2}$-electron, $h_{n,\mu}$ for $nd_{5/2}$-electron. The operators of the electrical dipole moment in this representation have the following form

$$\mathcal{D}_z(6p_{1/2} \to ns) = \frac{1}{3} z_{n,1}\left(-a^+_{n,\frac{1}{2}} b_{\frac{1}{2}} + a^+_{n,-\frac{1}{2}} b_{-\frac{1}{2}}\right) + h.c.$$

$$\mathcal{D}_z(6p_{3/2} \to ns) = \frac{\sqrt{2}}{3} z_{n,3}\left(a^+_{n,\frac{1}{2}} c_{\frac{1}{2}} + a^+_{n,-\frac{1}{2}} c_{-\frac{1}{2}}\right) + h.c.$$

$$\mathcal{D}_z(6p_{1/2} \to nd_{3/2}) = \frac{\sqrt{2}}{3} z_{n,13}\left(b^+_{\frac{1}{2}} f_{n,\frac{1}{2}} + b^+_{-\frac{1}{2}} f_{n,-\frac{1}{2}}\right) + h.c.$$

$$\mathcal{D}_z(6p_{3/2} \to nd_{3/2}) = \frac{1}{5} z_{n,33}\left(-c^+_{\frac{3}{2}} f_{n,\frac{3}{2}} - \frac{1}{3}c^+_{\frac{1}{2}} f_{n,\frac{1}{2}} + \frac{1}{3} c^+_{-\frac{1}{2}} f_{n,-\frac{1}{2}} + c^+_{-\frac{3}{2}} f_{n,-\frac{3}{2}}\right) + h.c. \tag{5}$$

$$\mathcal{D}_z(6p_{3/2} \to nd_{5/2}) = \frac{1}{5} z_{n,35}\left(2c^+_{\frac{3}{2}} h_{n,\frac{3}{2}} + \sqrt{6}c^+_{\frac{1}{2}} h_{n,\frac{1}{2}} + \sqrt{6}c^+_{-\frac{1}{2}} h_{n,-\frac{1}{2}} + 2c^+_{-\frac{3}{2}} h_{n,-\frac{3}{2}}\right) + h.c.$$

where the values z_i are the corresponding radial integrals. We use the jj scheme since the radial integrals for $6p_{3/2}$ - and $6p_{1/2}$-electrons differ considerably.

Come now to calculation of the polarizability. Let us consider the contribution of the excitations of a valent $6p_{1/2}$-electron from the configuration $6p^k$ to the configuration $6p^{k-1}ns$ (for example, in lead this is transition from $6p^2$ to $6p\,ns$). Let $|i\rangle$ be the wave function of the ground state. Then the contribution to the polarizability from the indicated excitations can be written as follows (all energies are expressed in Rydbergs):

$$\alpha_n(\varepsilon) = \frac{4a_B^3}{2j_i+1} \sum_{j_{iz}} \sum_{\gamma} \frac{(E_{n\gamma} - E_i)\langle i, j_{iz}|\mathcal{D}_z(6p_{1/2} \to ns)|n,\gamma\rangle\langle n,\gamma|\mathcal{D}_z(6p_{1/2} \to ns)|i, j_{iz}\rangle}{(E_{n\gamma} - E_i)^2 - \varepsilon^2} \tag{6}$$

where j_i is the angular momentum of the ground state, and the index γ numerates the levels of the configuration $6p^{k-1}ns$. If now we neglect the splitting of the levels inside the configuration $6p^{k-1}ns$ and take into account the completeness of the set $|n,\gamma\rangle$ for the operator $\mathcal{D}_z(6p_{1/2} \to ns)$, then (6) is transformed in such a way:

$$\alpha_n(\varepsilon) = \frac{4a_B^3}{2j_i+1} \sum_{j_{iz}} \frac{(\tilde{E}_n - E_i)\langle i, j_{iz}|\mathcal{D}_z^2(6p_{1/2} \to ns)|i, j_{iz}\rangle}{(\tilde{E}_n - E_i)^2 - \varepsilon^2}$$

$$= \frac{4}{3}a_B^3 \frac{(\tilde{E}_n - E_i)\langle i, j_{iz}|\mathcal{D}^2(6p_{1/2} \to ns)|i, j_{iz}\rangle}{(\tilde{E}_n - E_i)^2 - \varepsilon^2} \tag{7}$$

where $\mathcal{D}^2 = \mathcal{D}_x^2 + \mathcal{D}_y^2 + \mathcal{D}_z^2$, $\tilde{E}_n$ is some effective energy for the given configuration [2]. Since $\mathcal{D}^2$ is the scalar, the projection j_{iz}

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2) In each particular case, it is easy to understand to what is equal the quantity $\tilde{E}_n$, taking into account that for the excited states in Tl, Pb and Bi jj -coupling is realized with a good accuracy. For example, for the excitation under consideration in lead $\tilde{E}_n = E(6p_{1/2}\,ns)$. Note also that the error arizing when passing from formula (6) to (7) at small ε does not exceed several percents.

in the last formula may be chosen arbitrarily.

The calculation of the contributions of the excitations of valent electrons $6p_{3/2} \to ns$, $6p_{1/2,3/2} \to nd$, as well as the excitations of electrons from the closed subshells $6S \to np_{1/2,3/2}$ and $5d \to np_{1/2,3/2}$ is reduced just analogously to the calculation of the mean values of the corresponding operators $\mathcal{D}^2$ over the ground state. It is easy to obtain expressions for the values $\mathcal{D}^2$ from (5). Excluding the creation and destruction operators of all electrons except the valent ones we get

$$\mathcal{D}^2(6p_{1/2} \to ns) = \frac{1}{3} \tau_{n,1}^2 \, b_\mu^+ b_\mu$$

$$\mathcal{D}^2(6p_{3/2} \to ns) = \frac{1}{3} \tau_{n,3}^2 \, c_\mu^+ c_\mu$$

$$\mathcal{D}^2(6p_{1/2} \to nd_{3/2}) = \frac{2}{3} \tau_{n,13}^2 \, b_\mu^+ b_\mu$$

$$\mathcal{D}^2(6p_{3/2} \to nd) = \frac{2}{3} \tau_{n,35}^2 \, c_\mu^+ c_\mu \qquad\qquad (8)$$

$$\mathcal{D}^2(6s \to 6p) = \frac{1}{3} \tau_{6s}^2 \, (b_\mu b_\mu^+ + c_\mu c_\mu^+)$$

$$\mathcal{D}^2(5d \to 6p) = \frac{2}{3} \tau_{5d}^2 \, (b_\mu b_\mu^+ + c_\mu c_\mu^+)$$

The summation should be carried out over the repeating index μ . In these formulae we neglected the fine splitting of d -electrons, i.e. we put $\tau_{n,33} \approx \tau_{n,35}$. For transitions from the closed subshells the difference between the radial integrals for $6p_{1/2}$ - and $6p_{3/2}$ -electrons is neglected also. The equality of these integrals follows from the analysis of experimental data on the oscillator strengths and ~~finite~~ numerical calculations (see below). We do not consider transitions from the closed subshells to the higher states than $6p$ -states, since, as the estimates show, their contribution to the polarizability is very small.

The further calculation of polarizabilities depend on a concrete form of the wave functions of the ground state and may

be carried out fairly simply by the formulae (7) and (8).

Deriving the formula (7) we neglected the configuration mixing. Validity of this approximation is discussed in Appendix in detail.

In conclusion of this section we want to note that if to assume that all the electrons move in the same effective potential then one-electron sums of the type $\sum_n \frac{\tau_{in}^2}{E_n - E_i \pm \mathcal{E}}$ which enter the polarizability can be reduced, as it was done in [14]. However, there are no physical grounds to think that by means of the same effective potential it is possible to describe correctly not only external electrons but also electrons from the closed $6S^2$ and, all the more, $5d^{10}$ subshells. In particular, the potential (3), (4) overestimates considerably the energies and especially the radial integrals for $6S$ - and $5d$ -electrons. For this reason, we shall calculate manifestly the sums entering the polarizability , using, if possible, the available experimental data.

3. Radial integrals and polarizabilities for mercury and thallium

The excitations of $6S$ - and $5d$ -electrons give a significant contribution to the polarizability of Tl. As has been noted at the end of the preceding section the numerical calculation overestimates considerably the corresponding radial integrals. At the same time, if there are quite reliable experimental data on the transition $6S \to 6p$, then for the transition $5d \to 6p$ such data are absent. For this reason, we shall find the radial integral $5d \to 6p$, based on the known value of the polarizability for Hg with the subsequent extrapolation of the obtained value to Tl.

According to [17] the refraction index of Hg-vapour under normal conditions and the 5893 Å wavelength (i.e. $\mathcal{E} = 0.1546$ Ry) is equal to 1.000933. Whence $\alpha(0.1546) = 37.3\, a_B^3$. The oscillator strengths corresponding to two transitions $6S \to 6p$ are known from experiment: $f(^1S_0 \to {}^3P_1) = 0.0247 \pm 0.0002$, $E_{{}^3P_1} - E_{1S_0} = 0.3591$; $f(^1S_0 \to {}^1P_1) = 1.174 \pm 0.07$, $E_{1P_1} - E_{1S_0} = 0.4927$ [18, 19]. The contribution to polarizability from $5d \to 6p$ transitions is calculated by means of formulae (7) and (8). As a result, we get

$$\alpha(\mathcal{E}) = 4 a_B^3 \left\{ \frac{f(^1S_0 \to {}^3P_1)}{(E_{{}^3P_1} - E_{1S_0})^2 - \mathcal{E}^2} + \frac{f(^1S_0 \to {}^1P_1)}{(E_{1P_1} - E_{1S_0})^2 - \mathcal{E}^2} + \frac{\frac{4}{3} \tau_{5d}^2 (\widetilde{E}_{5d^9 6p} - E_{5d^{10}})}{(E_{5d^9 6p} - E_{5d^{10}})^2 - \mathcal{E}^2} \right\} \quad (9)$$

As has been already noted, the contribution of excitations of $6S$ - and $5d$-electrons to the states higher than $6p$ is very small, therefore, it is neglected. From formula (9), taking into account that $\widetilde{E}_{5d^9 6p} - E_{5d^{10}} \approx 0.794$ [20] we find $\tau_{5d} = 1.44$ (the sign is determined from the numerical calculation).

Computing the configuration $6S6p$ in a standard way and using the known oscillator strengths we find the radial integrals: $\tau_{6,1} = -1.80 \pm 0.04$; $\tau_{6,3} = -1.98 \pm 0.07$. In the following we shall not take account of a relatively small difference between these integrals, i.e. we take $\tau_{6,1} \approx \tau_{6,3} \equiv \tau_{6S} \approx -1.9$. Note that the computation with the potential (3), (4) gives the following values for these quantities: $\tau_{6,1} \approx \tau_{6,3} = \tau_{6S} \equiv -3.2$, i.e. overestimates them about 1.7 times.

Now we pass to the determination of the radial integral τ_{6S} in Tl which is connected with excitations $6S^2 6p \to 6S 6p^2$. Numerical calculation gives $\tau_{6,1} \approx \tau_{6,3} = \tau_{6S} = -3.0$. We assume that the overestimating of this value in comparison to the real one is the same as in Hg: then $\tau_{6S} = -3.0/1.7 = -1.75$. Now we verify whether this value of the radial integral is in a good

agreement with available experimental data. The wave functions of the states of the configurations $6S6p^2$ in the intermediate coupling approximation are presented in the work [4]. The transitions from the ground state to six levels of this configuration are allowed. By means of the functions from [4] at $\tau_{6S} = -1.75$ we get the following oscillator strengths for five of them lying in a continuous spectrum:

$f_{1233} = 0.0422\, \tau_{6S}^2 = 0.129$ $f_{1302} = 0.079\, \tau_{6S}^2 = 0.242$

$f_{1489} = 0.0840\, \tau_{6S}^2 = 0.257$ $f_{1610} = 0.135\, \tau_{6S}^2 = 0.413$

$f_{2007} = 0.00031\, \tau_{6S}^2 = 0.00095$

The wavelengths in vacuum given as the indices for oscillator strengths are presented in Å. Calculated values are in a good agreement with experimental data from [21]:

$$f_{1610} = 0.39 \qquad f_{2007} = 0.0011$$

Note that the results obtained by us differ considerably from experimental data of the work [22].

A very reliable test of the correctness of the values $\tau_{6,1} = \tau_{6,3} = \tau_{6S} = -1.75$ is calculation of the oscillator strengths of the transitions to the state $|{}^4P'_{1/2}\rangle$ of the configuration $6S6p^2$ lying in the discrete spectrum. As was noted in the papers [23,24], because of the nearness of energies ($\Delta E = 77$ cm^{-1}) this state mixes strongly by the Coulomb interaction with the level $|6S^2 10S\rangle$, i.e.

$$|\widetilde{{}^4P_{1/2}}\rangle = \sqrt{1 - \beta^2}\, |{}^4P'_{1/2}\rangle + \beta\, |10S\rangle$$
$$|\widetilde{10S}\rangle = \sqrt{1 - \beta^2}\, |10S\rangle - \beta\, |{}^4P_{1/2}\rangle \qquad (10)$$

We determine an absolute value of the mixing coefficient β by using the known hyperfine structure of the levels $|10S\rangle$ and $|{}^4P_{1/2}\rangle$. Since the probability density of $6S$-electron on the nucleus is by two order of magnitude higher than that of $10S$-electron, the hyperfine structure of both the levels is determined by

a contribution of the state $|6S6p^2, {}^4P_{1/2}\rangle$ with a non-paired $6S$-electron. Taking advantage of the experimental values of the hyperfine splitting constants from [24] we get

$$\frac{\beta^2}{1-\beta^2} = \frac{A_{1\widetilde{0S}}}{A_{\widetilde{4P}_{1/2}}} = 0.285 \tag{11}$$

from here $\beta = \pm 0.47^{3)}$. We put $\beta = +0.47$, since at a negative β all the calculated oscillator strengths disagree drastically with experiment. To calculate the oscillator strengths for the transitions from states $6S^2 6P_{1/2}$ and $6S^2 6P_{3/2}$ to $\widetilde{10S}$ and $\widetilde{4P}_{1/2}$ besides ζ_{6S} it is necessary to know the radial integrals $6p-10S$. As we shall see below they are : $\zeta_{10,1} = 0.255$; $\zeta_{10,3} = 0.245$. Taking advantage of an explicit form of the wave function $^4P_{1/2}'$ from [4] we calculate the oscillator strengths of interest by us. Their values are given in Table 1. As seen from this Table the calculation is in a good agreement with experiment [25,26]. (Since in [25,26] only the relative oscillator strengths are measured, we got their absolute values, based on the data from [27]).

A value of the radial integral ζ_{5d} (transition $5d \to 6p$) we shall get by the extrapolation from Hg assuming that it decreases the same times as ζ_{6S}, i.e. $\zeta_{5d} = 1.44 \frac{1.75}{1.9} = 1.33$. The validity of such an extrapolation is based on the smallness of the variation of the principal quantum numbers from Hg to Tl and the numerical calculations.

There are extensive experimental data concerning the tran-

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3)   Using the wave functions (10) it is possible to calculate not only the ratio of constants $A_{\widetilde{10S}}$ and $A_{\widetilde{4P}_{1/1}}$ but also their absolute values which agree well with experiment. One can obtain a correct value *of the ratio* of isotope shifts of $\widetilde{10S}$ and $\widetilde{4P}_{1/2}$ levels as well.

sitions of a valent electron in Tl [25-27]. The radial integrals calculated by us with the help of the potential (3,4) as well as their values obtained from the data on the oscillator strengths are presented in Table 2. As seen from this Table our calculation overestimates the values of the radial integrals, however, for the main integrals the overestimating is not higher than 15%. The overestimating regularity allows one to refine the calculated values of the radial integrals for Pb and Bi. Extrapolating the overestimating we can find also correct values of the integrals for $6p \to 10s$ transition:

$$\zeta_{10,1} = \frac{0.288}{1.13} = 0.255 \qquad \zeta_{10,3} = \frac{0.314}{1.28} = 0.245$$

Now we calculate the polarizability of Tl. It is made very simply using formulae (7) and (8). The wave function of the ground state has a form $|i\rangle = b_{1/2}^+ |\Psi_0\rangle$ where $|\Psi_0\rangle$ is the wave function of the closed subshells. Let us find, for example, the contribution of excitations $5d^{10}6p_{1/2} \to 5d^9 6p^2$.

$$\alpha \sim \langle i | \mathcal{D}^2 (5d \to 6p) | i \rangle = \frac{2}{3} \zeta_{5d}^2 \langle \Psi_0 | b_{1/2} (b_M b_M^+ + c_N c_N^+) b_{1/2}^+ | \Psi_0 \rangle = \frac{10}{3} \zeta_{5d}^2 \tag{12}$$

In just the same manner we calculate all the remaining contributions and find the following expression for $\alpha(\varepsilon)$

$$\alpha_{Tl}(\varepsilon) = 4a_B^3 \left\{ \sum_{6p \to ns} A_{ns} \frac{1}{9} \frac{\zeta_{n,1}^2}{\varepsilon_{ns}} + \sum_{6p \to nd} A_{nd} \frac{2}{9} \frac{\zeta_{n,13}^2}{\varepsilon_{nd}} + A_{6s} \frac{5}{9} \frac{\zeta_{6s}^2}{\varepsilon_{6s}} + A_{5d} \frac{10}{9} \frac{\zeta_{5d}^2}{\varepsilon_{5d}} \right\} \tag{13}$$

where $\varepsilon_n = \widetilde{E}_n - E_i$, $A_n = \left(1 - \frac{\xi^2}{\varepsilon_n^2}\right)^{-1}$. Note that in each term the factor A is multiplied by the quantity which is in fact the sum of the oscillator strengths of transitions to a given configuration divided by the mean frequency squared $\left(\frac{1}{\varepsilon_n^2} \sum_\lambda f_{n\lambda}\right)$. The numerical values of these quantities and the frequencies ε_n in Rydbergs are given in Table 3. By means of these values

it is not difficult to compute the polarizability at any frequency. For example,

$$\alpha_{Tl}(0) = 48\, a_B^3 \tag{14}$$

4. Radial integrals and polarizabilities of lead and bismuth

Experimental data from which it is possible to determine the radial integrals corresponding to the transitions from the closed subshells in Pb and Bi are unknown. Therefore, we determine these integrals with the help of the extrapolation from Tl and Hg based on the numerical calculation. In this case, in Pb $\zeta_{6S} = -1.6$; $\zeta_{5d} = 1.2$; in Bi $\zeta_{6S} = -1.5$; $\zeta_{5d} = 1.1$. In the preceding section it has been shown that the accuracy of such an extrapolation *for 6S* is not worse than 5% when passing from Hg to Tl. Note that in the opposite case, i.e. when passing from Tl and Hg to Au, we get $\zeta_{6S} = -2.1$, that agrees with experiment[28] very well: $\zeta_{6,1} = -2.24 \pm 0.12$; $\zeta_{6,3} = -2.22 \pm 0.08$.

The radial integrals for the excitations $6p \to 7S$, $8S$ in Pb have been chosen in such a way to get correct values of the oscillator strengths. These integrals are presented in Table 4. All the remaining radial integrals given in this Table have been found by numerical calculation in the potential (3), (4) and we introduced, in each transition, the corresponding correction on overestimating which was taken from Tl (see Table 2). For transitions $6p \to 7S$, $8S$ the values found in this way constitute $\zeta_{6p_{1/2}7S} = 1.85$; $\zeta_{6p_{1/2}8S} = 0.57$; $\zeta_{6p_{3/2}7S} = 2.39$; $\zeta_{6p_{3/2}8S} = 0.57$. Some distinction of these values from the true ones (see Table 4) is probably due to the mixing of $6p\,7S$ and $6p\,8S$ configurations.

Using the radial integrals we can calculate the oscilla-

tor strengths for different transitions and compare them with experiment. Since the number of oscillator strengths is larger than the number of independent radial integrals, such a comparison is reasonable even for the transitions $6p \to 7S$, $8S$, where the radial integrals were chosen in accordance with the experimental values of oscillator strengths. The calculation of the oscillator strengths in Pb is complicated due to the strong mixing between the excited configurations. Therefore, we consider only those transitions which are influenced by this mixing slightly. Moreover, we shall verify two approximate sum rules.

We confine ourselves to the consideration of the transitions to the configurations $6p\,7S$ and $6p_{1/2}6d$ (for transitions to $6p_{1/2}6d$ the oscillator strengths have not been measured). Comparison of the experimental and calculated values of the energies and g-factors shows that the levels $(6p_{1/2}7S)_1$ and $(6p_{1/2}6d_{5/2})_3$ are the pure jj states in practice, and the correct wave function $(6p_{1/2}7S)_1$ has the form $(6p_{1/2}7S)_1 - 0.047\,(6p_{3/2}7S)_1$. The wave functions of the configuration $6p^2$ can be found, for example, in[16]. The oscillator strengths calculated by these functions are presented in Table 5. These values are in full accordance with the experimental ones [10] given in the mentioned Table.

The remaining states of the configurations under study form two groups of the levels which mix strongly ($\sim 20 \div 40\%$) because of the nearness of energies: $6p_{3/2}7S\,(^1P_1')$, $6p_{1/2}8S\,(^3P_1')$ and $6p_{1/2}6d_{3/2}\,(^3D_1')$ with the angular momentum $J = 1$, as well as $6p_{3/2}7S\,(^3P_2)$, $6p_{1/2}6d_{3/2}\,(^3F_2')$ and $6p_{1/2}6d_{5/2}\,(^3D_2')$ with $J = 2$. The conventional LS notations in parentheses correspond to those accepted in[20]. In this case it is comparatively easy to verify only the sum rules for the oscillator strengths which are based on that these levels possess nearly equal energies. There are experimental data necessary for such a verification only

for the transitions $6p^2(^3P_1) \rightarrow |J=1\rangle$ and $6p^2(^3P_2) \rightarrow |J=2\rangle$[10]. They are presented in Table 6. Comparison with the calculated values of the oscillator strengths given in the same Table shows that although, as was to be expected, the calculation for each transition does not agree with experiment, the agreement of the sums of experimental and computed values is quite satisfactory.

The radial integrals for exciting the $6p$-electron in Bi have been found by numerical calculation in the potential (3), (4). For each transition we have introduced the correction on overestimating which equals that for lead. The resulting values of the radial integrals are given in Table 4. To verify these quantities we calculate the lifetimes of those levels for which there are the corresponding experimental data.

Calculation of the configuration $6p^2 7s$ in the intermediate coupling scheme does not constitute any difficulty (see, for example,[29] and preprint of the paper[4]). The necessary wave functions in the jj scheme have the form

$$|^4P'_{1/2}7s\rangle = 0.980\left(s\tfrac{1}{2}\tfrac{1}{2}\right)_{1/2} + 0.064\left(s\tfrac{1}{2}\tfrac{3}{2}\right)_{1/2} - 0.186\left(s\tfrac{3}{2}\tfrac{3}{2}\right)_{1/2}$$
$$|^4P'_{3/2}7s\rangle = -0.994\left(s\tfrac{1}{2}\tfrac{3}{2}(1)\right)_{3/2} + 0.108\left(s\tfrac{1}{2}\tfrac{1}{2}(2)\right)_{3/2} - 0.045\left(s\tfrac{1}{2}\tfrac{3}{2}\right)_{3/2} \qquad (15)$$
$$|^2P'_{3/2}7s\rangle = 0.114\left(s\tfrac{1}{2}\tfrac{3}{2}(1)\right)_{3/2} + 0.979\left(s\tfrac{1}{2}\tfrac{1}{2}(2)\right)_{3/2} - 0.159\left(s\tfrac{3}{2}\tfrac{3}{2}\right)_{3/2}$$
$$|^4P'_{5/2}7s\rangle = -0.977\left(s\tfrac{3}{2}\tfrac{3}{2}\right)_{5/2} + 0.217\left(s\tfrac{1}{2}\tfrac{3}{2}\right)_{5/2}$$

The expression $\left(sj_1 j_2(j')\right)_J$ denotes the normalized wave function of one s and two p (with angular momenta j_1 and j_2) electrons, the angular momentum of a pair of p-electrons is equal to j', and the total angular momentum – J. The necessary states of the configurations $6p^2_{1/2}6d$ and $6p^2_{1/2}7d$ are close to the pure jj ones, i.e. $^2D'_{3/2}=\left(d_{3/2}\tfrac{1}{2}\tfrac{1}{2}\right)_{1/2}$, $^2D'_{5/2}=\left(d_{5/2}\tfrac{1}{2}\tfrac{1}{2}\right)_{5/2}$. As to the mixing between the configurations, the state $|^4P'_{1/2}\rangle$ is practically pure, and the remaining states $6p^2 7s$ and $6p^2 6d/7d$ mix sig-

nificantly. Analysis of the known from experiment g-factors of the levels of the configuration $6p^2 7s$[30] [4] as well as the estimates of the Coulomb integrals based on numerical calculation lead to the following wave functions

$$|^4\widetilde{P}_{1/2}\rangle_{7s} = |^4P'_{1/2}\rangle$$
$$|^2\widetilde{D}_{3/2}\rangle_{6d} = 0.946|^2D'_{3/2}\rangle_{6d} + 0.125|^4P'_{3/2}\rangle_{7s} - 0.300|^2P'_{3/2}\rangle_{7s}$$
$$|^4\widetilde{P}_{3/2}\rangle_{7s} = 0.992|^4P'_{3/2}\rangle_{7s} - 0.125|^2D'_{3/2}\rangle_{6d}$$
$$|^2\widetilde{P}_{3/2}\rangle_{7s} = 0.803|^2P'_{3/2}\rangle_{7s} + 0.300|^2D'_{3/2}\rangle_{6d} - 0.515|^2D'_{3/2}\rangle_{7d} \qquad (16)$$
$$|^2\widetilde{D}_{5/2}\rangle_{6d} = 0.991|^2D'_{5/2}\rangle_{6d} + 0.133|^4P'_{5/2}\rangle_{7s}$$
$$|^4\widetilde{P}_{5/2}\rangle_{7s} = 0.940|^4P'_{5/2}\rangle_{7s} - 0.133|^2D'_{5/2}\rangle_{6d} + 0.313|^2D'_{5/2}\rangle_{7d}$$

It should be noted, that not all the coefficients in the wave functions (16) are reliable. Errors can arise due to inexact measurements of g-factors, inaccuracy in determining the wave functions (15) as well as the bad accuracy of the calculation of the Coulomb integrals. However, the lifetimes calculated by using formulae (16) are in a good agreement with experiment. This circumstance allows one to think that the errors in these wave functions are not too large.

Taking advantage of the wave functions for the configuration $6p^3$ (see, e.g.,[16]) it is possible to calculate the oscillator strengths for the transitions from the states (16) to the levels $6p^3$. Their values are given in Table 7. In the latter the oscillator strengths are also presented for the transitions to $6p^2_{1/2}7p_{1/2}$ and $6p^2_{1/2}7p_{3/2}$ which are practically the pure jj states. The corresponding radial integrals are: $\zeta_{7p \cdot 7s} = -6.4$; $\zeta_{7p \cdot 6d} =$

4) We cannot take adtantage of the known g-factors of the levels $|^2\widetilde{D}_{3/2}\rangle_{6d}$ and $|^2\widetilde{D}_{5/2}\rangle_{6d}$ since even a small mixing between different jj states of the configuration $6p^2 6d$ which we do not take into account may influence these g-factors essentially.

= 7.2; $\zeta_{7p\to7d}$ = -3.7. Calculated lifetimes for the states (16) are given in Table 7 too. These values are in a good agreement with the experimental $[11-13]$. It should be noted that although the oscillator strengths for the transitions to the states $6p^2 7p$ are relatively large, a contribution of these transitions to the lifetimes does not exceed 3% because of the smallness of the frequencies.

Using the found radial integrals we determine now the polarizabilities of the atoms of Pb and Bi. It is quite simply, just the same as in Tl, to calculate the contributions of all the types of excitations to the polarizabilities by means of the formulae (7) and (8) and the wave functions of the ground states of these atoms in the secondary quantization representation (see $[16]$). The sums of the oscillator strengths for transitions to a given configuration divided by the mean frequency squared (i.e. $\frac{1}{\varepsilon_n^2}\sum_\alpha f_{n\alpha}$) are given in Table 8 for Pb and in Table 9 for Bi. The polarizabilities are expressed through these values as follows (cf. (13)):

$$\alpha(\varepsilon) = 4a_B^3 \sum_n A_n(\varepsilon)\cdot\left(\frac{1}{\varepsilon_n^2}\sum_\alpha f_{n\alpha}\right) \qquad (17)$$

In the same Tables the corresponding values of ε_n are presented. Energies ε_{6s} and ε_{5d} were obtained by the extrapolation from Hg and Tl since the experimental data for their direct determination are insufficient. From Tables 8 and 9 it is easy to calculate the polarizabilities at any frequency. For example, at $\varepsilon=0$ we get

$$\alpha_{Pb}(0) = 47a_B^3 \qquad \alpha_{Bi}(0) = 53a_B^3 \qquad (18)$$

Thus, the polarizabilities of thallium, lead and bismuth are nearly the same and they are higher considerably than the pola-

rizability of Hg ($\alpha_{Hg}(0) = 34a_B^3$). A sharp increase of the polarizability when passing from Hg to Tl is due to the fact that in Tl the additional contribution arises from the $6p$-electron. In the further motion from Tl to Pb and Bi the polarizability remains to be approximately constant, since although the number of external electrons increases, the contribution of a particular electron cuts down. The polarizabilities of Tl, Pb and Bi at $\varepsilon=0$ have been previously calculated in $[31]$. The results of this work: $\alpha_{Tl}(0) = 43,2a_B^3$; $\alpha_{Pb}(0) = 42.4a_B^3$ $\alpha_{Bi}(0) = 39.5a_B^3$, differ from ours slightly enough, however, according to $[31]$, the polarizability decreases when passing from Hg to Tl, Pb and Bi (in $[31]$ $\alpha_{Hg}(0) = 66.1a_B^3$, that is two times greater than the experimental value).

4. Conclusion

As has been noted in Introduction, our interest in the subject of this paper has arisen in connection with the calculation of the parity violation effects in the atoms of Tl, Pb and Bi. Therefore, we summarize the results concerning the calculation of these effects. Their magnitude depend heavily on the radial integrals and the electron wave functions at zero. As has been shown in this paper, the available experimental data for all three elements are correctly reproduced with values of the radial integrals for excitations $6p \to ns$ used in the papers $[4-6]$. As to the radial integral for the excitations $6s \to 6p$, its value in Au, Hg and Tl is found from the experimental data very reliably and this integral is a monotonic function Z. Therefore, we think that the accuracy of our extrapolation to Pb and Bi (see Table 10) is not worse than $5 \div 10\%$.

Besides the fitting of a fine splitting, we have tested

a behavior of the wave functions of $6p$-electrons in zero at parameters (4) by calculation of the hyperfine splitting in Tl, Pb and Bi[16]. At the same time, for the wave function of $6S$-electron at short distances the quasiclassical Fermi-Segre approximation (see, e.g.,[32]) is good. This follows from calculation of the hyperfine splitting constants $A_{\widetilde{10S}}$ and $A_{\widetilde{4p_{1/2}}}$ in Tl (see footnote after formula (11)). Thus, the present paper and the paper[16], in our opinion, confirm the correctness of the results obtained in[4, 5, 6].

As has been already mentioned in Introduction, the discrepancy in estimating the parity violation effects between [4-6] and [7-9] is probably due to the fact that in the latters the contribution of excitations $6S^2 6p^k \rightarrow 6S 6p^{k+1}$ 6) is overestimated. We have seen indeed that the value of γ_{6S} is 1.7 times less than that found with the effective potential (3), (4). The calculation with the Hartri-Fock wave functions[33, 34] gives approximately the same overestimation. Note, that in the potential (3) the parameters can be chosen, in principal, in such a way ($H \sim 1 \div 2$, $\frac{d}{a_B} \sim 0.4 \div 0.5$) that the calculated value of γ_{6S} becomes closer to the experimental one. However, in this case, the wave functions of the electrons at zero are too large. As the result of this, the effect is overestimated as well.

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6) In the works[7-9] the procedure of inexplicit summation (the Steiheimer method) at which this contribution was not separated directly was used. However, it is evident that this does not influence the essence of the matter.

Appendix
The configuration mixing

Let us consider the question of the influence of the mixing between different configurations on the parity violation effects [4-6] and the polarizabilities calculated in the present work. Firstly, the mixing can occur between the excited configurations over which the summation is carried out when the effect is calculated. Secondly, the admixture to the ground configuration is possible. As to the first case, such a mixing may be quite intensive (20 ÷ 40%), nevertheless, it influences the effects of interest very slightly. It is easy to verify indeed that a relative contribution from this mixing to the parity violation effects and polarizability constitutes $\frac{\Delta P}{P} \sim \frac{\Delta \alpha}{\alpha} \sim \beta \frac{\Delta E}{\widetilde{E}_n - E_i}$, where β is the mixing coefficient; ΔE is the difference of energies of the mixing levels; E_i and $\widetilde{E}_n$ are the energies of the ground and excited configurations.

Since only the close levels mix strongly, i.e. $\Delta E \ll \widetilde{E}_n - E_i$, this contribution does not exceed several percents.

The question of an admixture to the ground configuration is somewhat more complicated. This question is urgent since it is known that the mixing of the configurations $2S^2 2p^k$ and $2p^{k+2}$ in the lightest analogues of lead, bismuth and polonium — carbon, nitrogen and oxigen — is strong enough [36] 7). Nevertheless, it is found, that the admixture to the ground configurations in Tl, Bi and Pb is small. One can judge the range of

7) We are indebted to I.I.Sobelman, I.L.Beigman and L.A.Vainstein who turned our attention to this circumstance.

the configuration mixing in not too heavy atoms by comparing the experimental values of the parameters $R_{2,4} \equiv (E(^1S) - E(^1D))/(E(^1D) - E(^3P))$ for configurations p^2 and p^4, and $R_3 \equiv (E(^2P) - E(^2D))/(E(^2D) - E(^4S))$ for p^3 with the theoretical value found in the one-configuration approximation for LS-coupling[36]. For atoms of C, N and O the difference between the experimental and theoretical values R is quite significant indeed (see Table 11). In this case, the reason of a strong mixing is that due to the nearness of the effective principal quantum numbers the exchange Coulomb integral $2S-2p$ is comparatively large. In the more heavy analogues this integral decreases, and hence the configuration mixing becomes slighter. The agreement of the experimental and theoretical values of the parameters R becomes good (see Table 11). (We do not give R for Pb, Bi and Po since it is evident that the experimental values must differ from the theoretical ones obtained in LS-coupling because of a strong spin-orbital interaction). Thus, in heavy atoms an admixture of the configuration p^{k+2} to s^2p^k is comparatively small. There is no difficulty to calculate directly this admixture. We take into account that the exchange Coulomb integral $G_1(nsnp, nsnp) = \frac{1}{3} \int g_s(z_1) g_p(z_1) g_s(z_2) g_p(z_2) \frac{z_1}{z_2^2} dz_1 d$ which determines the mixing of interest, can be found from the splitting of terms of the configuration $ns\,np^{k+1}$[36]. There are necessary experimental data only for the analogues of mercury (s^2), thallium (s^2p) and lead (s^2p^2)[20]. The exchange integrals obtained in this way are presented in Table 12 (for Si and Pb the necessary data are lacking). In the same Table the distances ΔE between the centres of the mixing configurations are given. We have found them by doubling the distances between the configurations $s^2 p^k$ and sp^{k+1}. The mixing coeffici-

ents α which are defined by the equality

$$|\widetilde{^{2S+1}L}\rangle = |s^2 p^k, {}^{2S+1}L\rangle + \alpha\,|p^{k+2}, {}^{2S+1}L\rangle \tag{19}$$

are equal to

$$s^2 \quad {}^1S \quad \alpha = \sqrt{3}\,\frac{G_1}{\Delta E}; \qquad s^2p^2 \cdot \begin{cases} {}^3P & \alpha = \frac{G_1}{\Delta E} \\ {}^1D & \alpha = \frac{G_1}{\Delta E} \\ {}^1S & \alpha = 2\,\frac{G_1}{\Delta E} \end{cases} \tag{20}$$

$$s^2p \quad {}^2P \quad \alpha = \sqrt{2}\,\frac{G_1}{\Delta E};$$

The numerical values of the mixing coefficients α are given in Table 12. It is seen that the configuration mixing becomes 2-2.5 times lower when passing from the light atoms to their heavy analogues.

Finally, we calculate the parameters R for the configuration $s^2 p^2$, taking account of the mixing under consideration. Using (20) we get

$$R = \frac{E(^1S) - E(^1D)}{E(^1D) - E(^3P)} = 1.5 - \frac{3G_1^2}{\Delta E(E(^1D) - E(^3P))} \tag{21}$$

Whence $R_{calc}(C) = 1.07$; $R_{calc}(Sn) = 1.43$, that agrees well with experimental values $R(C) = 1.13$; $R(Sn) = 1.41$.

The parameters R for the configurations $2s^2 2p^k$ have been previously found[37] with the configuration mixing taken into account. Unfortunately, in the mentioned paper the found coefficients of the configuration mixing were not presented.

The calculations presented here and the calculation of a hyperfine structure[16] allowing to determine an admixture of the configuration $6s6p^k ns$ to $6s^2 6p^k$ show that admixtures to the ground configurations of Tl, Pb and Bi do not exceed probably 10%. Besides the above-mentioned arguments a smallness of mixing with the ground configuration in Tl, Pb and Bi is confirmed by the agreement of experimental and calculated values of g -

-factors (in the case of jj -coupling the Coulomb mixing influences g -factor), the agreement of experimetal and calculated values of the oscillator strengths in Tl, Pb and Bi, and nearness of the values ζ_{6s-6p} in Tl, Hg and Au (if in Tl and Hg the state $6s^2$ may be mixed with $6p^2$, in Au such a mixing is impossible).

transition	$6p_{1/2}→\widetilde{10s}$	$6p_{1/2}→\sideset{}{^4}{\widetilde{p}}_{1/2}$	$6p_{3/2}→\widetilde{10s}$	$6p_{3/2}→\sideset{}{^4}{\widetilde{p}}_{1/2}$
$\lambda(\mathring{A})$	2208	2211	2666	2672
calculation	0.0100	0.0057	0.0035	~ 0.0001
experiment	0.0103 ±0.0007	0.0057 ±0.0006	0.0031 ±0.0003	—

Table 1

Oscillator strengths for transitions $6p_{1/2}, 6p_{3/2}→\widetilde{10s}, \sideset{}{^4}{\widetilde{p}}_{1/2} (6s6p^2)$ in Tl.

		$7s$	$8s$	$9s$	$10s$	$6d_{3/2}$	$6d_{5/2}$	$7d$	$8d$	$9d$
$6p_{1/2}$	calculation	2.31	0.74	0.42	0.29	-2.13	—	-1.08	-0.70	-0.51
	exper.	2.23	0.67	0.38	—	-1.99	—	-0.93	-0.56	-0.39
	calc./exper.	1.04	1.10	1.12	—	1.07	—	1.16	1.25	1.31
$6p_{3/2}$	calculation	3.22	0.85	0.47	0.31	-2.91	-2.85	-1.34	-0.84	-0.61
	exper.	2.83	0.66	0.37	—	-2.64	-2.58	-1.14	-0.65	-0.46
	calc./exper.	1.14	1.29	1.27	—	1.10	1.11	1.18	1.30	1.31

Table 2

Calculated and experimental (from oscillator strengths [27]) radial integrals in Tl and their ratios.

	7S	8S	ns-lev-els,n>8	cont. spect.	$6d_{3/2}$	$7d_{3/2}$	nd-lev-els,n>7	cont. spect.	$6S6p^2$	$5d^9 6S^2 6p^2$
$\frac{1}{\varepsilon_n^2}\sum_\delta \beta_{n\delta}$	2.28	0.14	0.08	0.13	2.67	0.51	0.26	1.09	2.93	1.72
ε_n	0.241	0.353	0.40	0.61	0.329	0.383	0.41	0.56	0.58	1.14

Table 3

Contributions of different excitations to polarizability of Tl.
$\alpha(\varepsilon) = 4a_\delta^3 \sum_n A_n \left(\frac{1}{\varepsilon_n^2} \sum_\delta \beta_{n\delta} \right)$, $A_n = \frac{1}{1 - \varepsilon^3/\varepsilon_n^2}$. A quantity ε_{sd} is taken from [35].

		7S	8S	9S	10S	$6d_{3/2}$	$6d_{5/2}$	7d	8d	9d
Pb	$6p_{1/2}$	1.75	0.89	0.32	0.22	-1.82		-0.84	-0.50	-0.36
	$6p_{3/2}$	2.55	0.90	0.33	0.20	-2.41	-2.32	-1.02	-0.58	-0.42
Bi	$6p_{1/2}$	1.45	0.78	0.29	0.19	-1.66		-0.77	-0.46	-0.32
	$6p_{3/2}$	2.19	0.79	0.30	0.19	-2.20	-2.11	-0.94	-0.53	-0.38

Table 4

Radial integrals for excitations of $6p$-electron in Pb and Bi.

transition	$6p^2(^3P_0)' \to$ $\to (6p_{1/2} 7S)_1$	$6p^2(^3P_1) \to$ $\to (6p_{1/2} 7S)_0$	$6p^2(^3P_1) \to$ $\to (6p_{1/2} 7S)_1'$	$6p^2(^3P_2)' \to$ $\to (6p_{1/2} 7S)_1'$	$6p^2(^3P_2)' \to$ $\to (6p_{1/2} 6d_{5/2})_3$
$\lambda(\overset{\circ}{A})$	2834	3685	3641	4059	2803
calculation	0.214	0.119	0.063	0.148	0.305
experiment	0.212 ±0.003	0.116 ±0.003	0.063 ±0.002	0.153 ±0.004	0.30 ±0.02

Table 5

Calculated and experimental [10] oscillator strengths in Pb.

	$J=1$	$(6p_{3/2} 7S)_1'$	$(6p_{1/2} 6d_{3/2})_1$	$(6p_{1/2} 8S)_1$	sum f_i
$6p^2(^3P_1)$	calcul-ation	0.0174	0.0378	0.0109	0.066
	exper-iment	0.024 ±0.002	0.019 ±0.007	0.0134 ±0.0008	0.0564 ±0.007
	$J=2$	$(6p_{1/2} 7S)_2$	$(6p_{1/2} 6d_{3/2})_2$	$(6p_{1/2} 6d_{5/2})_2$	sum f_i
$6p^2(^3P_2)'$	calcul-ation	0.131	0.0347	0.0217	0.187
	exper-iment	0.107 ±0.006	0.051 ±0.003	0.036 ±0.003	0.194 ±0.007

Table 6

The sum rules for oscillator strengths in Pb.
Experimental data are taken from [10]

Table 7

init. state \ final state		6p³					6p²7p		lifetime (nsec)	
		$^2P_{1/2}'$	$^4S_{3/2}'$	$^2D_{3/2}'$	$^2P_{3/2}'$	$^2D_{5/2}$	$(4\frac{1}{2})7p_{1/2}$	$(4\frac{1}{2})7p_{3/2}$	calculation	experiment
$7S, {}^4\tilde{P}_{1/2}$	λ	9152	3069	4724					5.05	4.7±1.[a] 4.75±0.18[b] 5.9±0.2[c]
	$-f\cdot10^2$	0.03	27.6	1.24						
$6d, {}^2\tilde{D}_{3/2}$	λ	4494	2277	3078		3512	35868	102881	27.2	27±3.[a] 28±2.[b]
	$-f\cdot10^2$	0.70	1.54	0.04		2.58	13.1	0.91		
$7S, {}^4\tilde{P}_{3/2}$	λ	4310	2229	2990	8547	3398			4.75	4.3±0.4[a] 7±2.[b]
	$-f\cdot10^2$	0.15	10.4	7.34	0.05	3.02				
$7S, {}^2\tilde{P}_{1/2}$	λ	3598	2012	2629	6138	2940	12002	15347	4.5	4.8±0.4[a]
	$-f\cdot10^2$	5.54	0.64	4.32	0.26	16.6	28.1	4.38		
$6d, {}^2\tilde{D}_{5/2}$	λ		2231	2994	8582	3404		53305	2.95	3.8±1.[a] 1.÷2.5[b]
	$-f\cdot10^2$		24.5	1.62	0.13	0.18		11.7		
$7S, {}^2\tilde{P}_{3/2}$	λ		2062	2698		3026		18021	4.80	5.5±0.5[a] 4.9±0.25[b]
	$-f\cdot10^2$		8.31	0.47		10.1		6.70		

Table 7

Oscillator strengths and lifetimes of the levels in Bi.
Oscillator strengths are given for a transition from the
upper level to the lower one.

[a] Ref. 11
[b] Ref. 12
[c] Ref. 13

Table 8

	$6p_{1/2}7S$	$6p_{3/2}7S$	$6p\,8S$	$\sum ns\, n\geqslant9$	cont. spect. S	$6S\,6p^3$
$\frac{1}{\varepsilon_n^2}\sum_8 f_{ns}$	2.01	0.17	0.40	0.09	0.22	1.53
ε_n	0.322	0.451	0.444	0.49	0.71	0.744

	$6p_{1/2}6d$	$6p_{3/2}6d$	$6p\,7d$	$\sum nd\, n\geqslant8$	cont. spect. d	$5d^9 6p^3$
$\frac{1}{\varepsilon_n^2}\sum_8 f_{ns}$	3.23	0.23	0.66	0.44	1.77	0.87
ε_n	0.420	0.542	0.478	0.51	0.67	1.51

Table 8

Contributions of different excitations to polarizability
of Pb.

Table 9

	$\frac{1}{2}\frac{1}{2}7S$	$\frac{1}{2}\frac{3}{2}7S$	$\frac{3}{2}\frac{3}{2}7S$	$\frac{1}{2}\frac{1}{2}8S$	$\frac{1}{2}\frac{3}{2}8S$	$\frac{3}{2}\frac{3}{2}8S$	$\sum ns\, n\geqslant9$	cont. spect. S	$6S\,6p^4$
$\frac{1}{\varepsilon_n^2}\sum_8 f_{ns}$	1.57	1.20	0.11	0.14	0.24	0.02	0.11	0.26	0.79
ε_n	0.299	0.425	0.62	0.43	0.56	0.75	0.56	0.75	0.96

	$\frac{1}{2}\frac{1}{2}6d$	$\frac{1}{2}\frac{3}{2}6d$	$\frac{3}{2}\frac{3}{2}6d$	$\frac{1}{2}\frac{1}{2}7d$	$\frac{1}{2}\frac{3}{2}7d$	$\frac{3}{2}\frac{3}{2}7d$	$\sum nd\, n\geqslant8$	cont. spect. d	$5d^9 6p^4$
$\frac{1}{\varepsilon_n^2}\sum_8 f_{ns}$	2.15	2.30	0.20	0.37	0.44	0.05	0.68	2.10	0.48
ε_n	0.406	0.547	0.74	0.47	0.60	0.79	0.58	0.70	1.80

Table 9

Contributions of different excitations to polarizability
of Bi. $j_1 j_2 ns(nd) \equiv 6p_{j_1} 6p_{j_2} ns(nd).$

element	Au	Hg	Tl	Pb	Bi
Z	79	80	81	82	83
ζ_{6s}	-2.2	-1.9	-1.75	-1.6	-1.5
ζ_{5d}		1.4	1.3	1.2	1.1

Table 10

Radial integrals for $6s \to 6p$ and $5d \to 6p$ excitations

atom	config- uration	R_2	atom	config- uration	R_3	atom	config- uration	R_4
C	$2s^2 2p^2$	1.13	N	$2s^2 2p^3$	0.500	O	$2s^2 2p^4$	1.14
Si	$3s^2 3p^2$	1.48	P	$3s^2 3p^3$	0.646	S	$3s^2 3p^4$	1.43
Ge	$4s^2 4p^2$	1.50	As	$4s^2 4p^3$	0.666	Se	$4s^2 4p^4$	1.50
Sn	$5s^2 5p^2$	1.41	Sb	$5s^2 5p^3$	0.664	Te	$5s^2 5p^4$	1.54
theory	p^2	1.50		p^3	0.667		p^4	1.50

Table 11

Experimental and theoretical values of the relations $R_2 = R_4 \equiv$
$\equiv (E(^1S) - E(^1D))/(E(^1D) - E(^3P))$, $R_3 \equiv (E(^2P) - E(^2D))/(E(^2D) - E(^4S))$.
In order to exclude the fine splitting in linear approximation,
in the configurations p^2 and p^4 it should be taken $E(^3P) =$
$= \frac{1}{2}(E(^3P_1) + E(^3P_2))$. For calculation of R_3 we used the ener-
gies of the levels $^2P_{1/2}$ and $^2D_{\frac{5}{2}}$ since the spin-orbital inter-
action do not influence the latters.

Z	atom	configu- ration	$G_1 \cdot 10^{-3} \text{cm}^{-1}$	$\Delta E \cdot 10^{-3} \text{cm}^{-1}$	mixing coeffi- cients		
4	Be	$2s^2$	10.3	72	0.25		
5	B	$2s^2 2p$	14.6	122	0.17		
6	C	$2s^2 2p^2$	18.0	220	0.08	0.08	0.16
12	Mg	$3s^2$	6.6	72	0.16		
13	Al	$3s^2 3p$	9.2	104	0.13		
14	Si	$3s^2 3p^2$	—		—		
30	Zn	$4s^2$	7.1	81	0.15		
31	Ga	$4s^2 4p$	9.2	123	0.11		
32	Ge	$4s^2 4p^2$	$\leqslant 1.$		$\leqslant 0.01$		
48	Cd	$5s^2$	6.5	80	0.14		
49	In	$5s^2 5p$	7.9	112	0.10		
50	Sn	$5s^2 5p^2$	4.0	112	0.035	0.035	0.07
80	Hg	$6s^2$	5.6	95	0.10		
81	Tl	$6s^2 6p$	8.8	136	0.09		
82	Pb	$6s^2 6p^2$	—		—		

Table 12

Exchange Coulomb integrals, distances between the configu-
rations $s^2 p^\kappa$ and $p^{\kappa+2}$, and coefficients of their mixing
in the analogs of Hg, Tl and Pb. The mixing coefficients
for the configuration $s^2 p^2$ are given in the order ^3P, ^1D, ^1S.

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