УДК 539.182; 539.184.52

NATURAL LIFETIMES OF EXCITED STATES IN THE GROUP II IONS

I. L. Glukhov, E. A. Nikitina and V. D. Ovsiannikov

Voronezh State University

Поступила в редакцию 18.07.2013 г.

Аннотация: демонстрируется хорошая точность метода модельного потенциала Фьюса для расчета скоростей спонтанных радиационных распадов A_{nl}, определяющих времена жизни $\tau_{nl} = 1/A_{nl}$ возбужденных nS, nP, nD и nF состояний однократно ионизованных атомов второй группы периодической системы. Численные результаты расчетов времен жизни и квантовых дефектов возбужденных состояний ионов основной подгруппы второй группы IIa (щелочно-земельные металлы): Be^+, Mg^+, Ca^+, Sr^+, Ba^+ — и побочной подгруппы IIb: Zn^+, Cd^+, Hg^+ — приведены в сравнении с литературными данными. Представленные в статье таблицы демонстрируют значительные расхождения между результатами в различных статьях и таким образом проясняют надежность наиболее цитируемых ранее опубликованных работ. Согласие рассчитанных времен жизни с наиболее надежными данными, опубликованными к настоящему моменту, демонстрирует применимость метода модельного потенциала и возможность получения на его основе времен жизни произвольно высоких состояний ионов подгрупп IIa и IIb.

Ключевые слова: ридберговские состояния, щелочно-земельные ионы, времена жизни, модельный потенциал.

Abstract: a good precision of the Fues' model potential is demonstrated in calculating rates A_{nl} of spontaneous radiation decays determining lifetimes $\tau_{nl} = 1/A_{nl}$ of excited nS, nP, nD and nF states in singly ionized atoms of the group II elements. Numerical results for lifetimes and quantum defects of excited states in the group IIa (alkaline-earth-metal) ions Be^+, Mg^+, Ca^+, Sr^+, Ba^+ and in the group IIb ions Zn^+, Cd^+, Hg^+ are presented in comparison with data available from the literature. The tables of this article demonstrate significant discrepancies between the data of different papers available in the literature and so clarify reliability of the most cited previously published works. Agreement of calculated lifetimes with the most reliable data of current literature demonstrates applicability of the model potential method and availability of the data for lifetimes of arbitrary excited states in ions of groups IIa and IIb elements.

Keywords: Rydberg states, alkaline-earth ions, lifetimes, model potential.

INTRODUCTION

Intense researches on the possibilities of the use of alkaline-earth-metal atoms and ions in designing new time-frequency standards [1] – [3] and quantum information processors [4] – [9] stimulate detailed studies of optical properties of these particles in their ground and excited states [10], [11]. Together with position on the energy scale, the lifetime of an excited state is one of the most important optical characteristics. Despite a great number of works on experimental measurements and theoretical calculations, the data of the literature on the lifetimes of excited

---

states in positive ions still remain either unknown or contradictory (see e.g. [12] – [15]). However, the most reliable recommended data is already tabulated in widely renowned and internationally approved data bases, such as [16], [17]. But these data are confined to a small number of lowest energy levels and cannot give information on the natural widths of highly excited Rydberg states, now considered as rather promising objects both for quantum computations and for optical time-frequency standards [18] – [20].

The high-precision methods taking into account all many-body and relativistic effects on the level widths in the alkaline-earth ions were used in the last years for determining lifetimes of only a limited number of the lowest excited states in some ions of the group II elements [10], [21] – [23]. The results of these calculations may serve as control data for other computative methods extending significantly the possibilities of numerical evaluations. However, the number of ions and their excited states considered so far were quite limited, so a bulk of new calculations is required to derive quantitative information for every additional state. A few model-potential approaches were proposed for estimating the lifetimes of excited states, but they were also used for only a small number of states with rather low principal quantum numbers [13], [15]. The need of the data for the lifetimes of arbitrary states in singly ionized atoms of the group II elements stimulated generation of approximations, such as in refs. [12], [14], which could be used for simple estimates. But the use of these approximations in the regions of their applicability gives significant discrepancies with the most reliable data of the literature, up to a factor of 100. These contradictions and discrepancies make indispensable further calculations and derivation of rather accurate asymptotic approximations on the basis of a method already approved in calculations for atoms with well-pronounced single-electron spectra, e.g. alkali-metal atoms.

In this article, we propose to use the Fues model potential (FMP) approximation [24], [25] for estimating rates of radiation transitions in the ions of alkaline-earth-like elements. The FMP was widely used in previous decades for calculating electromagnetic susceptibilities of alkali-metal and inert-gas atoms [26], [27], [28]. Quite similar structure of the single-electron spectra in alkali atoms and in alkaline-earth ions ensures satisfactory accuracy of the FMP in estimating radiation-transition matrix elements in the ions.

There exist a number of differently grounded and differently entitled methods, where the non-integer part of the effective principal quantum number is transferred to corresponding orbital momentum (see for example [12], [15], [25], [26], [29]). All these methods are intimately related with the semiempirical quantum defect method [30], [31] and use the data on the spectrum of energies for single-electron excitations in atoms. However, the existing data on atomic energy levels is confined to small numbers of levels in every particular series of states. Therefore, asymptotic equations are used to extend the quantum defect values to higher-energy levels, which are missing in tables of level energies. One can find in the literature lots of different equations with three and more terms approximating quantum defects for high-energy states. All approximations are based on rather smooth dependence on energy of the quantum defect, tending to a constant value at the ionization threshold, in each series with fixed spin-orbital quantum numbers. We have tested a number of such equations and come to a most efficient four-term equation, which provides accurate values of quantum defects for arbitrary high energy levels of S-, P-, D- and F-series of bound states in singly ionized atoms of the group II elements. The corresponding numerical values of coefficients in this equation are presented in tables (see section 2, tables 1 and 2).

To confirm applicability of the FMP approach, we give below extended tables of calculated lifetimes for each ion of the group II in order to present comparison with the most of data, currently existing and available from the literature. Naturally, being a single-electron approach to describing optical properties of many-electron atoms and ions, the FMP may not claim to be the highest-precision method for determining the lifetimes of excited states. Nevertheless, via the use of precise data on the energy levels, this semiempirical method accounts for the influence of all significant details of internal atomic structure on the outermost (valence) electron, which is responsible for interaction with photons emitted by excited ion in transition to lower energy levels. Therefore, the uncertainty of numerical data obtained in the FMP approximation, in majority of cases does not exceed 10% at most. It is worth of notice that the similar and yet higher ranges of uncertainty, 10-20% and above, are usually prescribed to the most of tabulated data of the literature on transition rates (see for example section 10 and specifically, table 10.5 of ref. [32]).

Since the role of non-Coulomb part of the atomic potential gradually decreases with the growth of the principal and orbital quantum numbers of optical-electron bound states, the semiempirical FMP wavefunctions reproduce the exact atomic wavefunctions more and more accurately with the growth of energy of highly excited states. Therefore the precision of the FMP data on the lifetimes of excited states also gradually increases with the increase of the level energy. The simplicity of equations derived in the FMP approach and presented in this paper for amplitudes of optical transitions, enable rather simple and accurate determination of lifetimes for arbitrary excited states. Together with calculated data, the tables include the most reliable data which elucidate numerically the validity of different existing in the literature approximations to the lifetimes of excited levels in the group II ions. Note, that the tables presented in this article, do not aim at any completeness of presentation of all existing so far numerical data. They only give a comparative illustration of precision and applicability of the FMP calculations to evaluating lifetimes of states which are not known so far. So, the principal goal of this paper is to present a method for rather simple and sufficiently precise calculations of lifetimes for arbitrary excited states in ions of the group II elements.

In section 1, the basic formulas are presented in the single-electron approximation for transition rates and lifetimes of excited levels. Section 2 gives analytical equations for the dipole transition amplitudes, based on analytical presentation of radial wavefunctions in the FMP method. The parameters for asymptotic presentation of quantum defects for arbitrary energy levels in S-, P-, D- and F-series of states in the group II ions are given in tables 1, 2. In section 3, the results of calculations, presented in tables 3 — 10, are discussed in comparison with the data available from the literature.

Atomic units e=m=$\hbar$=1, with the speed of light equal to the inverse fine-structure constant c=1/α=137.036, are used throughout the paper, unless otherwise specified.

1. RADIATION DECAY AND LIFETIME OF AN EXCITED STATE

The natural width of excited energy level is determined by the total rate of spontaneous radiation transitions to all lower levels and may be presented as

$$A_{nlj} = \sum_{n'}^{E_{n'l'j'}<E_{nlj}} A_{nn'} = \frac{4}{3c^3} \sum_{n'}^{E_{n'l'j'}<E_{nlj}} \omega_{nn'}^3 \mid M_{nn'} \mid^2, \tag{1}$$

where $A_{nn'}$, $\omega_{nn'} = E_{nlj} - E_{n'l'j'}$ and $M_{nn'} = \langle nlj|\mathbf{D}|n'l'j'\rangle$ are the rate, frequency and dipole matrix element of the radiation transition (with account of the fine-structure splitting between $|nl\rangle$-state sublevels with different total momenta j). $\mathbf{D} = -\mathbf{r}$ is the dipole moment in the single-electron approximation, where $\mathbf{r}$ is the valence-electron position vector. The summation over n' involves all states with energies $E_{n'l'j'}$ below E_{nlj}. Only states with orbital momenta $l' = l \pm 1$ and total momenta $j' = j, j \pm 1$ contribute to A_{nl} in the dipole approximation.

After integration over angular variables of the valence electron, averaging over magnetic quantum numbers of initial states and summation over final states with the use of standard methods of quantum theory of angular momentum [33], the matrix element $M_{nn'}$ may be presented as

$$|M_{nn'}|^2 = l_>(2j'+1)\left\{\begin{array}{ccc} 1 & l & l' \\ S & j' & j \end{array}\right\}^2 |\langle n'l'j'|r|nlj\rangle|^2, \qquad (2)$$

where S is the total spin, $l_> = (l+l'+1)/2$ is the greater value of the orbital quantum numbers l and l'.

Thus, the basic problem in determining the lifetimes of excited states is the numerical evaluation of the radial matrix elements $\langle n'l'j'|r|nlj\rangle$. The FMP seems a good candidate for this purpose, since it has demonstrated a good accuracy in similar calculations for Rydberg states in alkali-metal atoms [34], [35]. Similar to alkali atoms, the outermost shells of singly ionized atoms of the group II elements in their ground states consist of a single valence electron in a doublet $n_0s\,^2S_{1/2}$ state, where $n_0 = 2$ for Be$^+$, $n_0 = 3$ for Mg$^+$, $n_0 = 4$ for Ca$^+$ and Zn$^+$, $n_0 = 5$ for Sr$^+$ and Cd$^+$, $n_0 = 6$ for Ba$^+$ and Hg$^+$. The lifetimes of excited states with the valence electron in nl-states with orbital momenta $l = 0, 1, 2\ldots$ may be estimated in the single-electron approximation, similar to the estimations for alkali atoms.

In some cases, the fine structure of single-electron excited states in ions of the group II atoms may be neglected together with the dependence of the radial matrix element on the total momenta j and j', i.e. $\langle n'l'j'|r|nlj\rangle \approx \langle n'l'|r|nl\rangle$. Then the summation over j' may be performed analytically [33], giving:

$$\sum_{j'} |M_{nn'}|^2 = \frac{l_>}{2l+1}|\langle n'l'|r|nl\rangle|^2. \qquad (3)$$

Evidently, this approximation is well justified for highly excited Rydberg states where the fine-structure splitting rapidly vanishes with the growth of the principal quantum number, according to the law [36]

$$\Delta E_{jj'} = |E_{nlj} - E_{nlj'}| \propto n^{-3}.$$

For ions of alkaline-earth (group IIa) elements approximation (3) gives rather accurate results and the fine structure of all excited levels may be neglected. Quite different situation appears for the group IIb ions, where the fine-structure splitting of lower levels is essential and the summation (3) may not be performed without introducing significant errors into the result. Taking into account that the principal contribution into the sum (1) comes from transitions to the lowest states, the doublet structure of all states will be taken into account for ions Zn$^+$, Cd$^+$ and Hg$^+$.

2. MATRIX ELEMENTS OF RADIATION DECAY IN THE FMP APPROACH

By the analogy with the well-known quantum defect method (QDM), the FMP is based on determination of the effective principal ν_{nl} and orbital λ_{nl} quantum numbers of an atomic state from its energy, related by a usual hydrogen-like equation:

$$E_{nl} = -\frac{Z^2}{2\nu_{nl}^2}, \quad \nu_{nl} = n_r + \lambda_{nl} + 1, \qquad (4)$$

where Z is the charge of residual ion ($Z = 1$ for neutral atoms, $Z = 2$ for singly ionized atoms), n_r is the radial quantum number, which in a given series of bound states with a fixed orbital momentum l runs from zero for the lowest state to infinity for states in a close vicinity of continuum.

It is worth drawing attention to the papers [12], [15], where the idea, completely equivalent to the FMP, was used to introduce non-integer orbital momenta into the radial wave functions of alkaline-earth ions. The papers appeared more than 20 years after the FMP was proposed by Simons for atomic calculations on the basis of the pseudopotential theory [24]. In every case the convenience of the FMP was used, which consisted in a simple analytical presentation of the radial wave functions in terms of generalized Laguerre polynomials $L_k^\alpha(x)$ or the confluent hypergeometric functions ${}_1F_1(-k;\alpha+1;x) = k!L_k^\alpha(x)/(\alpha+1)_k$,

$$R_{nl}(r) = \frac{2Z^{3/2}}{\nu^2}\sqrt{\frac{(2\lambda+2)_{n_r}}{n_r!\Gamma(2\lambda+2)}} \times \exp\left(-\frac{Zr}{\nu}\right)\left(\frac{2Zr}{\nu}\right)^{\lambda} {}_1F_1\left(-n_r;2\lambda+2;\frac{2Zr}{\nu}\right), \tag{5}$$

where $\Gamma(x)$ and $(x)_k = \Gamma(x+k)/\Gamma(x) = x(x+1)...(x+k-1)$ are the usual notations for the gamma-function and Pochhammer symbol [37].

The integral over radial variable r with FMP wavefunctions (5) may be calculated analytically and the radial matrix element is then presented in terms of the generalized hypergeometric function of two variables F_2 [37]:

$$\langle n'l'|r|nl\rangle = \frac{1}{4Z}\frac{\Gamma(a)}{\sqrt{\Gamma(c)\Gamma(c')}}\sqrt{\frac{(c)_{n_r}}{n_r!}\frac{(c')_{n'_r}}{n'_r!}}\,(x)^{\lambda+2}\left(x'\right)^{\lambda'+2}F_2\left(a;-n_r,-n'_r;c,c';x,x'\right). \tag{6}$$

where $a = \lambda+\lambda'+4$ is the mutual upper parameter of the two-fold series F_2, $c = 2\lambda+2$ and $c' = 2\lambda'+2$ are the lower parameters, $x = 2\nu'/(\nu'+\nu)$ and $x' = 2\nu/(\nu'+\nu)$ are the arguments of the hypergeometric function. The upper integer negative parameters, $-n_r$ and $-n'_r$ turn the infinite series into the two-fold polynomial with sign-alternating terms.

The general rule (4) allows for some modifications, which may be rather important for the behaviour of the wave-function (5) near the origin. Numerical calculations demonstrate that the wave functions of states with the lowest orbital momenta (mainly S- and P-states) are better approximated by a function with a shifted radial quantum number, i.e. n_r replaced by n_r+1 [38]. Evidently, this replacement is accompanied by the replacement of λ by $\lambda-1$ in order that the relation (4) continues to hold. In a few cases, an opposite replacement $n_r \to n_r-1$ $(\lambda \to \lambda+1)$ allows to improve the wave functions of D-states.

Evidently, the substitution of $\{n_r+1, \lambda-1\}$ for $\{n_r, \lambda\}$, reduces the power of the radial variable by unity, thus strengthening the role of the small-distance regions in the wave function and enhancing the contribution of small-r regions into transition matrix elements (2). Simultaneously, the role of the large-r regions may also be enhanced by the normalization factor $\sqrt{(\nu+\lambda)/(\nu-\lambda)}$, which is maximal for the lowest state of the series with a given orbital momentum. Nevertheless, the additional node in the wave function may cause cancellations between positive and negative contributions to the radial integral, which finally reduce the matrix element. Therefore, it is rather difficult to predict the variation of the matrix element caused by the indicated substitution, but in most cases it improves the agreement with the most reliable data of the literature.

It is worth of notice that the modifications tend to make the value of the model-potential parameter λ more close to the corresponding value of the orbital momentum l, when the absolute value of the difference $|\lambda - l|$ exceeds 0.5. In other words, in calculating radial matrix elements (6), the traditional rule for the choice of the radial quantum number n_r, which determines the number of nodes in the radial wavefunction, should be modified in agreement with an empirical rule so, as to minimize the absolute value of difference between the model-potential parameter λ and the corresponding orbital momentum quantum number l. This rule was reflected e.g. in an empirical integer parameter $I(l)$, introduced in [12] into the relation between λ, l and the quantum defect

$\delta_{nl} = n - \nu_{nl}$. This modification concerns mainly S-states, which have the largest quantum defects and enumeration of states with $l = 0$ should start from $n_r = 1$ instead of $n_r = 0$ [38]. In heavy ions this rule may be applicable also to P-states, and the replacement of $\{n_r, \lambda\}$ by $\{n_r{+}1, \lambda{-}1\}$ seems worthwhile, if

$$\lambda = \nu_{nP} - n_r - 1 = n - \delta_{nP} - n_r - 1 = n_0 - \delta_{nP} - 1 > 1.5.$$

Here $n_0 = n - n_r$ is the principal quantum number of the lowest-energy nP-state.

An opposite situation may appear for single-electron D-state excitations. Due to rather low energies, the orbital parameter of D-states in heavy atoms may take on values below 1.5 if the traditional method of prescribing $n_r = 0$ to the lowest level is used. In this case the repulsive centrifugal potential is not taken into account correctly. To account correctly for the centrifugal repulsion, the modification $\{n_r, \lambda\} \to \{n_r - 1, \lambda + 1\}$ should be introduced into the radial wave functions, with $n_r = 0, \lambda = \nu_{n_0 D}$ and $n_r = 0, \lambda = \nu_{n_0+1\,D} - 1$ for two lowest D-states, $|n_0 D\rangle$ and $|n_0{+}1D\rangle$. For the rest of the wavefunctions in the D-state subspace, the radial quantum number runs from 1 to infinity with λ determined in agreement with the relation (4).

In any case, all necessary empirical data for FMP are concentrated in the structure of energy levels which may be found in existing tables for atoms and ions [16], [17]. A smooth dependence of the orbital parameters λ and λ' on the principal quantum numbers in all single-electron nl-series of the group II ions returns nearly constant n-independent values for states with $n > 10$. To extrapolate the quantum defect to higher energy levels, not included in the tables, the asymptotic expansion may be used [12]

$$\delta_{nl} = a_0 + \frac{a_1}{m^2} + \frac{a_2}{m^4} + \frac{a_3}{m^6}, \tag{7}$$

where $m = n - d_0$. Numerical calculations demonstrate, that equation (7) with $d_0 = n_0 - 1$ gives the best fitting of the data taken from existing tables of energy levels. The value of d_0 grows with the growth of the atomic number, in consistency with the data of paper [12]. The coefficients a_k, $k = 0, 1, 2, 3$ may be determined from the standard curve fitting polynomial procedure. For the third-order extrapolation polynomial $y(x)$ four values of the function $y_i = y(x_i)$ are sufficient $(i = 1, 2, 3, 4)$, according to equation:

$$y(x) = \sum_{i=1}^{4} y_i \prod_{j=1,\, j\neq i}^{4} \frac{x - x_j}{x_i - x_j} = \sum_{k=0}^{3} a_k x^k. \tag{8}$$

In our case, $x = m^{-2}$ and $y(x) = \delta_{nl}(m^{-2})$. The values $y_i = \delta_{nl}(m_i^{-2})$, $m_i = n_i - d_0$, $i = 1, 2, 3, 4$ correspond to 4 different states from tables of energy levels (it is not mandatory to include the lowest-energy state $|n_0 l\rangle$ into this list, if the number of tabulated states exceeds 4).

A smooth dependence on the principal quantum numbers (on the energy) of the quantum defect seen in equation (7) for $n \gg n_0$, transforms into a smooth dependence for the effective orbital momentums $\lambda = n_0 - I(l) - \delta_{nl}$ and $\lambda' = n_0' - I(l') - \delta_{n'l'}$ in equation (6). The integer number $I(l)$ is usually taken to be equal to 1, in a modified case it may equal 2 for S-states in all ions and for P-states in Ca$^+$, Sr$^+$ and Ba$^+$ (see tables 1, 2). So λ turn into practically invariable constant values

$$\lambda \to \lambda_0 = n_0 - I(l) - a_0$$

for all states with $n > 10$ in every particular nl-series of the group II ions.

3. RESULTS AND DISCUSSIONS

In table 1, the numerical values of constant coefficients a_k, as derived in the curve fitting polynomial procedure from the database for energy levels [17], are presented for S-, P-, D- and F-series with total momentum $j = l + 1/2$, together with the principal quantum numbers n_0 of the lowest states $|n_0 l\rangle$ and recommended values of the integer number $I(l)$ for singly ionized atoms of the group IIa (alkaline-earth) elements. The values of $I(l)$ are recommended on the basis of the rule minimizing the absolute value of the difference $\lambda_{nl} - l$.

Table 1. *Numerical values of the principal quantum number of the lowest-energy state* $|n_0 l\rangle$*, recommended values of the integer number* $I(l)$ *and coefficients* a_k *of equation (7) for* nS-*,* nP-*,* nD- *and* nF-*states in ions of the group IIa (alkaline-earth) elements.*

Ion	Series	n_0	$I(l)$	a_0	a_1	a_2	a_3
Be^+	nS	2	2	0.260183	0.02158	−0.02217	0.01176
	nP	2	1	0.050160	0.008877	0.0106746	−0.006045
	nD	3	1	0.0024040	−0.001472	0.000975	−0.0001059
	nF	4	1	0.0003635	−0.0009495	0.006352	−0.005512
Mg^+	nS	3	2(1)	1.0679	0.061945	−0.072216	0.039842
	nP	3	1	0.69684	0.089236	−0.12158	0.069798
	nD	3	1	0.045283	−0.049353	0.087641	−0.053106
	nF	4	1	0.0033624	−0.0036361	0.0072364	−0.0044965
Ca^+	nS	4	2	1.8041	0.12310	−0.15650	0.08818
	nP	4	2	1.4376	0.16326	−0.23682	0.13789
	nD	3	1	0.62709	0.06012	−0.03308	0.03280
	nF	4	1	0.02807	−0.03896	0.08081	−0.05104
Sr^+	nS	5	2	2.7076	0.16667	−0.22804	0.13253
	nP	5	2	2.3226	0.12494	−0.11006	0.05279
	nD	4	1	1.4523	0.20857	0.41452	0.61624
	nF	4	1	0.066685	−0.27168	1.4847	−1.2409
Ba^+	nS	6	2	3.5772	0.26100	−0.64229	0.47174
	nP	6	2	3.1679	0.52012	2.3678	1.9460
	nD	5	1	2.3716	0.39853	−0.94459	0.75546
	nF	4	1	0.85197	−0.72598	−1.4431	3.6026

An alternative possibility to take $I(0) = 1$ instead of $I(0) = 2$ for S-states in magnesium ions is mentioned in parentheses on the basis of comparison with the most reliable data of the literature for the lifetimes of nS- and nP-states (see table 4). Here an overestimate of the nS-state lifetimes, if we replace $\{n_r, \lambda\}$ by $\{n_r{+}1, \lambda{-}1\}$, is caused by an additional node in the wavefunction $|nS\rangle$ reducing the matrix element $\langle 3P|r|nS\rangle$. Quite more significant underestimate of the nP-state lifetimes is caused by an enhancement of the matrix element $|\langle 3S|r|nP\rangle|^2$ by a factor $2\nu_{3S} - 1 \approx 3$, caused by the substitution of $I(0){=}2$ for $I(0){=}1$ (see section 2). Therefore, the choice $I(0) = 1$ may be preferable, although the S-state effective orbital momentum in Mg^+ ions is more close to 1 than to 0. This fact corresponds to the priority of "Pauli repulsive forces", approximated by the positive centrifugal part of the FMP with $\lambda > 0$, over attractive polarization forces, approximated by the negative centripetal potential with $\lambda < 0$. Specifically, this priority is the most important in the ground state $3\,^2S_{1/2}$ providing the main contribution to the rate (1) of the nP-state spontaneous decays in Mg^+ ions.

The coefficients a_0, determining asymptotic values of quantum defects nearly coincide with those presented in [12], where equation (7) was used with somewhat different values of the constant d_0. Our choice $d_0 = n_0 - 1$, based on the best fitting the data for energy levels available from tables, provides also the smallest values of coefficients a_1, a_2, a_3, thus reducing to minimum the deviations of δ_{nl} from their exact values in tabulated states and from the asymptotic value $\delta_{nl} \approx a_0$ for states with rather high $n \gg n_0$.

Table 2. *Numerical values of the principal quantum number of the lowest-energy state $|n_0 l\rangle$, recommended values of the integer number $I(l)$ and coefficients a_k of equation (7) for nS-, nP-, nD- and nF-states in ions of the group IIb elements.*

Ion	Series	n_0	$I(l)$	a_0	a_1	a_2	a_3
Zn^+	$n\,^2S_{1/2}$	4	2	2.1890	0.090148	0.071230	−0.090932
	$n\,^2P_{1/2}$	4	1	1.85498	0.68633	2.7752	−2.0776
	$n\,^2P_{3/2}$	4	1	1.9566	−2.1788	7.9156	−5.8369
	$n\,^2D_{3/2}$	4	1	0.95116	0.068771	−0.12786	0.083365
	$n\,^2D_{5/2}$	4	1	0.94876	0.083137	−0.22714	0.16909
	$n\,^2F_{5/2}$	4	1	0.011614	0.18830	−0.81131	0.62549
	$n\,^2F_{7/2}$	4	1	0.024771	−0.15861	0.67638	−0.52840
Cd^+	$n\,^2S_{1/2}$	5	2	3.09648	0.17819	−0.15844	0.089701
	$n\,^2P_{1/2}$	5	1	2.7261	−0.14294	1.2832	−1.0478
	$n\,^2P_{3/2}$	5	1	2.6891	0.36168	−1.4486	1.1864
	$n\,^2D_{3/2}$	5	1	1.8825	0.15002	−0.24203	0.14320
	$n\,^2D_{5/2}$	5	1	1.8763	0.15352	−0.25442	0.15319
	$n\,^2F_{5/2}$	4	1	0.059023	−0.12964	0.21103	−0.10294
	$n\,^2F_{7/2}$	4	1	0.095894	−.63455	2.2614	−1.6861
Hg^+	$n\,^2S_{1/2}$	6	2	4.1526	0.02284	1.242	−2.9747
	$n\,^2P_{1/2}$	6	1	3.5461	2.6936	−8.0750	5.7381
	$n\,^2P_{3/2}$	6	1	3.6598	0.3260	−1.7050	1.5189
	$n\,^2D_{3/2}$	6	1	2.8406	1.4566	−26.658	148.055
	$n\,^2D_{5/2}$	6	1	2.8449	−0.1795	4.9416	−22.231
	$n\,^2F_{5/2}$	5	1	1.0872	−0.2588	0.7725	−0.5693
	$n\,^2F_{7/2}$	5	1	1.0836	−0.1374	0.2769	−0.1732

In table 2, the values of a_k, n_0 and recommended values of the integer number $I(l)$ are given for the fine-structure components of S-, P-, D- and F-series with the total angular momenta $j = l \pm 1/2$ in ions of the group IIb elements. The numerical data of tables 1 and 2 are useful for determining quantum defects of states, which are not presented in existing tables of energy levels.

In tables 3–10, the comparison is given between the data calculated in the FMP approximation and the data available from the literature for the lifetimes of nS, nP, nD and nF states in Be^+, Mg^+, Ca^+, Sr^+, Ba^+, Zn^+, Cd^+ and Hg^+. As is seen from the tables, the data of the FMP approach gives values of the natural lifetimes in a satisfactory agreement with existing recommended data,

Table 3. *The FMP data for numerical values of natural lifetimes τ_{nl} (in nanoseconds) of the lowest nS-, nP-, nD and nF-states in Be^+ ions, in comparison with the values presented in the data base [17], the values calculated in ref. [13] within the Coulomb approximation with a Hartree-Slater core approach and the values determined on the basis of relativistic many-body calculation in ref. [10].*

State	FMP	[17]	[13]	[10]
$3S$	2.460	2.5	2.473	2.451
$4S$	4.200	4.3	4.196	4.174
$5S$	7.235	7.3	7.213	7.194
$6S$	11.75	12	11.70	11.673
$7S$	18.02	18.5	18.02	17.918
$8S$	26.33	26.5	26.22	26.17
$9S$	36.98	37.5	36.81	36.78
$10S$	50.26	51	50.02	49.89
$2P$	8.503	8.9	8.930	8.850
$3P$	5.521	5.6	5.431	5.417
$4P$	8.231	8.3	8.030	8.086
$5P$	13.15	13.5	12.76	12.918
$6P$	20.39	20.5	19.71	20.05
$7P$	30.28	30.5	29.19	29.78
$8P$	43.24	43.5	41.57	42.66
$9P$	59.67	60.1	57.25	58.86
$10P$	80.00	80.5	76.66	78.6
$3D$	0.8620	0.9	0.9110	0.901
$4D$	1.991	2.1	2.081	2.066
$5D$	3.816	3.9	3.971	3.938
$6D$	6.506	6.7	6.754	6.700
$7D$	10.23	10.5	10.61	10.518
$8D$	15.16	15.5	15.71	15.58
$9D$	21.46	22	22.22	22.01
$10D$	29.31	–	30.33	—
$4F$	4.510	4.5	4.522	4.525
$5F$	8.722	8.8	8.739	8.734
$6F$	14.91	15	14.93	14.948
$7F$	23.45	23.6	23.49	23.60
$8F$	34.72	35	34.77	35.03
$9F$	49.11	49.3	49.18	49.73
$10F$	66.98	67	67.08	—

the most complete and reliable of which are accumulated in the database [17]. The numerical data of different articles in the literature deal with a small amount of ions and with a small number of levels in them. An extended information is presented in references [12] and [14] in terms of interpolation functions of the principal quantum number n

$$\tau_{nl} = \tau_0 n^{\alpha}. \tag{9}$$

The constant factors τ_0 and exponents α were determined in [14] on the basis of the compiled data of the literature for S-, P-, D-, F- and G-states in both group IIa and IIb ions. In [12] the values of τ and α were determined on the basis of analytical calculations with the use of extrapolated quantum defects for same states of the group IIa ions. The magnitude of the departure of exponents from their asymptotic value α=3 in [12] does not exceed 0.17, whereas in [14] it achieves 0.6 for F-states in Cd$^+$ and yet more for P-states in Zn$^+$. The regions of validity for the interpolations are rather narrow (only from 4 to 12 in [14], and from 10 to 30 in [12]), and the difference between the values of the factors τ_0, presented for identical states, achieves one order of magnitude and even more. So the data of equation (9) with parameters from [12] and [14] may also differ by one order and more, as is seen in tables. Moreover, some particular numerical data, compiled from different sources and presented in [14] as "recommended values", do not match the results given by the interpolation equation. The results given by (9) with parameters from [12] also depart significantly from those of the data base [17].

As could be expected, the best agreement of the FMP results with recommended data of [17] is observed for Be$^+$, the simplest ion of the group II elements, where the fractional departure from the recommended data [17], from the data of the article [13] and from the data of the latest relativistic many-body calculations [10] does not exceed 1 to 3% (see table 3). The approximation equations of [14] overestimate the values of the lifetimes by a factor 6 to 8, although the data compiled from the literature in [14], agree satisfactorily with the recommended data of [17]. The approximation equations from [12] overestimate the recommended data by 2 orders of magnitude for all states, including the indicated in [12] region of validity $10 \leqslant n \leqslant 30$ for approximation (9).

More detailed information compiled from the literature is given in [14] as recommended data for magnesium ions. These data are presented in table 4 together with the results derived from approximation equations of [14] and [12], which are in evident disagreement with the recommended data and with each other. The results of calculations in the FMP approach for the lifetimes of S- and P-states corresponding to two choices of the integer number $I(0)$ are significantly closer to the recommended data, especially for $I(0) = 1$. The data of equation (9) with constant parameters τ_0 and α from [14] exceed by about one order the recommended data, presented both in [17] and in [14]. The parameters taken from [12] overestimate lifetimes of S and F-states by 2 orders, provide nearly coincidence with recommended data for D-states and underestimate the lifetimes of P-states, nearly coinciding with the FMP data corresponding to $I(0)$=2.

For ions Ca$^+$ the FMP data with $I(0)$=$I(1)$=2 slightly underestimate the lifetimes of S and F-states, providing good agreement with recommended data for P and D-states. The parameters of the paper [14] in approximation (9) overestimate by one order and more all the recommended data, whereas those of [12] underestimate the lifetimes of P-states (nearly factor one half) and overestimate those of S (twice), D (two orders) and F-states (one order and more).

The agreement of FMP with recommended data for Sr$^+$ holds to within 10–20%. The parameters of [12] in equation (9) give data with almost the same departure from the recommended values, while the parameters from [14] overestimate the lifetimes of all states by one order and more.

The similar agreement of FMP with recommended data for Ba$^+$ ions and overestimation of lifetimes by (9) with parameters of [14] is seen in table 7, with exception of S-states where the data of [12] gives lifetime values close to those recommended in [17].

Table 4. *Numerical values of lifetimes (in nanoseconds) of nS-, nP-, nD- and nF-states in magnesium ions* Mg^+ *for two different values of integer number* $I(0)$, *in comparison with recommended values of data base [17], the results of model potential (MP) calculations [15] and Hartree-Fock (HF) data also taken from [15] (these data was presented there as results published by C.F. Fisher et al. At. Data Nucl.Data Tables* ***92****, 607 (2006)), and the values calculated from approximation equations of [14] and [12]. The numbers in parentheses were presented in ref. [14] as "recommended values of radiation lifetimes". The FMP data for D- and F-states, presented in a single column, are independent of* $I(0)$.

State	FMP		[17]	[15]		[14]	[12]
	$I(0) = 1$	$I(0) = 2$		MP	HF		
$4S$	2.78	4.61	2.8	2.95	2.90	14.1 (2.8)	217
$5S$	5.05	7.42	5.1	5.05	5.04	32.2	519
$6S$	8.95	12.4	9.4	8.18	8.76	60.9 (9.5)	1016
$7S$	14.8	19.8	16	12.9	14.2	102	1753
$8S$	22.9	30.0	25	19.3	21.8	158	2777
$9S$	33.6	43.4	36	27.9	31.7	231	4135
$10S$	47.4	60.6	53	—	—	322	5870
$3P$	5.17	4.0	4	3.61	3.81	58 (3.9)	2.69
$4P$	19.6	12.4	20	18.8	18.7	184(19.4)	8.1
$5P$	52.6	23.0	53	48.2	45.5	421	17.9
$6P$	114	39.0	110	108	87.8	808	33.2
$7P$	215	61.7	200	200	149	1382	55.5
$8P$	366	92.7	340	321	234	2184	85.9
$9P$	578	133	530	478	334	3252	126
$10P$	862	184	780	650	—	4627	176
$3D$	2.49		2.2	1.97	2.05	38.9 (2.1)	4.09
$4D$	7.44		8.1	7.35	7.46	101 (8.8)	9.71
$5D$	16.5		20	18.2	18.4	211 (18.5)	19.0
$6D$	30.4		41	35.8	36.4	387 (38.1)	33.0
$7D$	50.3		72	61.4	62.7	645	52.5
$8D$	76.8		110	96.1	97.8	1004	78.6
$9D$	111		170	70.6	119	1484	112
$10D$	154		—	198	—	2104	154
$4F$	4.196		4.2	4.28	4.41	32.5 (4.4)	398
$5F$	8.051		8.1	8.14	8.41	62.4 (8.4)	773
$6F$	13.69		14	13.6	14.3	106 (12.9)	1329
$7F$	21.47		22	21.2	22.5	166 (21.5)	2100
$8F$	31.72		32	31.2	33.2	246 (32.0)	3123
$9F$	44.78		45	44.0	39.7	346	4431
$10F$	61.02		61	58.4	—	470	6060

Table 5. *Numerical values of the lifetimes τ_{nl} (in nanoseconds) calculated within the FMP approach for nS-, nP-, nD- and nF-states in the ions of Ca$^+$, in comparison with the recommended values of the data base [17], the data of relativistic Hartree-Fock calculations [22], model-potential calculations by Theodosiou [39] and the data given by approximation equations of ref. [14] and [12]. The numbers in parentheses were presented in ref. [14] as "recommended values of radiation lifetimes".*

State	FMP	[17]	[22]	[39]	[14]	[12]
$5S$	2.85	4.5	3.91	4.15	20.8 (4.4)	3.84
$6S$	4.98	7.2	6.39	6.76	44.5 (6.8)	8.46
$7S$	8.60	12	10.63	11.26	80.9 (11.4)	15.8
$8S$	13.9	19	–	–	132.4	26.3
$9S$	21.1	28	–	–	201	40.6
$10S$	30.7	41	–	–	290	59.3
$11S$	42.9	—	–	–	400	82.9
$12S$	58.0	—	–	–	534	112
$4P$	6.62	6.4	6.69	6.85	93.4(6.7)	3.8
$5P$	29.3	29	35.35	34.8	265 (33.7)	10.4
$6P$	85.2	70	99.8	90	564	21.5
$7P$	192	130	–	–	1027	38.3
$8P$	364	220	–	–	1690	61.9
$9P$	615	330	–	–	2590	93.3
$10P$	951	470	–	–	3762	134
$11P$	1398	–	–	—	5242	184
$12P$	1952	–	–	—	7067	245
$4D$	4.09	2.9	2.85	2.89	22.7 (3.0)	299
$5D$	7.00	6.1	6.21	6.20	50.0 (5.2)	658
$6D$	11.9	11	–	–	92.9	1223
$7D$	18.9	19	–	–	155	2044
$8D$	28.5	30	–	–	241	3167
$9D$	41.0	44	–	–	352	4639
$10D$	56.9	61	–	–	494	6509
$11D$	76.4	83	–	–	670	8823
$12D$	99.8	110	–	–	883	11630
$4F$	1.43	3	3.54	3.90	17.9	34.3
$5F$	2.56	5.1	–	–	32.8	67.2
$6F$	4.22	8.1	–	–	53.7	117
$7F$	6.52	12	–	–	81.5	186
$8F$	9.57	18	–	–	117	279
$9F$	13.48	25	–	–	161	399
$10F$	18.34	34	–	–	214	549

Table 6. *Numerical values of the lifetimes* τ_{nl} *(in nanoseconds) calculated with the FMP approach for* nS-, nP-, nD- *and* nF*-states in the ions of* Sr^+*, in comparison with the recommended values of the data base [17], the relativistic Hartree-Fock calculations with account of 46 configurations [40] and the data given by approximation equations of the articles [14] and [12]. The number in parentheses was presented in ref. [14] as "recommended value of radiation lifetime".*

State	FMP	[17]	[40]	[14]	[12]
$6S$	3.518	5.2	4.97	24.7	2.13
$7S$	6.062	8.3	7.32	52.6	4.83
$8S$	10.34	14	11.76	95.1	9.15
$9S$	16.60	22	18.41	155	15.5
$10S$	25.15	32	22.44	234	24.2
$11S$	36.40	45	—	336	35.7
$12S$	50.46	65	—	462	50.3
$5P$	6.754	6.6	6.96	102 (6.4)	15.6
$6P$	25.65	28	33.80	301	40.9
$7P$	66.43	72	88.55	660	82.7
$8P$	135.7	140	170.6	1233	145
$9P$	244.0	—	442	2077	231
$10P$	389.9	—	649	3251	346
$11P$	575.5	—	—	4814	492
$12P$	805.8	—	—	6829	673
$5D$	4.930	3.8	3.85	23.7	2.89
$6D$	7.85	7.0	6.90	47.2	6.09
$7D$	12.7	12	11.70	81.2	11.0
$8D$	19.6	18	18.72	127	17.9
$9D$	28.8	28	25.58	187	27.2
$10D$	40.7	40	34.53	262	39.2
$11D$	55.6	55	–	353	54.2
$12D$	74.2	75	–	463	72.6
$4F$	1.65	3	3.23	32.9	3.10
$5F$	2.92	4.5	5.33	60.1	5.97
$6F$	4.82	7.1	8.52	98.6	10.2
$7F$	7.45	11	12.85	150	16.1
$8F$	10.93	15	18.67	215	23.8
$9F$	15.41	21	26.11	296	33.7
$10F$	21.0	28	35.31	395	46.0
$11F$	27.8	39	–	511	60.9
$12F$	35.9	50	–	647	78.7

Table 7. *Numerical values of the lifetimes* τ_{nl} *(in nanoseconds) calculated with the FMP approach for* nS-, $nP_{3/2}$-, $nD_{5/2}$- *and* $nF_{7/2}$*-states in the ions of* Ba^+, *in comparison with the recommended values of the data base [17] and the data given by approximation equations of the articles [14] and [12]. The numbers in parentheses were presented in ref. [14] as "recommended values of radiation lifetimes".*

State	FMP	[17]	[14]	[12]
$7S$	4.39	6.2	28.5 (6.7)	2.55
$8S$	7.30	9.8	57.9	5.54
$9S$	12.20	16	101	10.2
$10S$	19.3	25	160	16.8
$11S$	29.0	37	237	25.8
$12S$	41.6	52	334	37.5
$6P$	5.79	6.3	61.3 (6.4)	17.4
$7P$	19.4	19	174	47.6
$8P$	46.5	43	375	99.3
$9P$	91.2	79	691	179
$10P$	157	130	1152	293
$11P$	244	200	1790	448
$12P$	356	285	2634	649
$6D$	5.79	4.7	31.5 (4.7)	36.5
$7D$	9.34	8.9	64.2	76.8
$8D$	15.3	15	112	138
$9D$	23.9	25	178	224
$10D$	35.3	37	265	338
$11D$	50.1	53	374	486
$12D$	68.7	75	509	671
$4F$	1.63	2.8	34.7	20.0
$5F$	4.77	12	55.3	33.9
$6F$	14.75	34	92.6	60.7
$7F$	34.20	49	148	104
$8F$	65.70	62	224	165
$9F$	111.7	77	322	249
$10F$	173.5	98	444	358
$11F$	254.6	120	593	497
$12F$	353.3	160	770	669

Table 8. *Numerical values of the lifetimes τ_{nl} (in nanoseconds) calculated within the FMP approach for nS-, $nP_{3/2}$-, $nD_{5/2}$- and $nF_{7/2}$-states in the ions of Zn^+, in comparison with the recommended values of the data base [17], the upper and lower values of the theory and experiment, taken from ref. [42], and the data given by approximation equations of ref. [14] with the numbers in parentheses presented there as "recommended values of radiation lifetimes".*

State	FMP	[17]	$[42]_{th}$	$[42]_{exp}$	[14]
$5S$	3.24	1.7	1.8–2.5	1.6–3.9	5.8 (2.1)
$6S$	5.66	3.6	3.6–4.7	—	26.0
$7S$	9.89	7.3	—	—	49.4 (7.2)
$8S$	16.0	—	—	—	81.2
$4P$	2.04	2.6	1.9–3.0	1.8–3.5	85.3 (2.5)
$5P$	16.9	16.7	15.5–18.6	—	695.4 (16.4)
$6P$	55.0	46.9	46.8–67.9	—	2999 (67.4)
$7P$	64.6	—	—	—	8890
$4D$	1.43	1.5	1.21–1.39	1.32–1.55	11.8 (1.5)
$5D$	3.45	3.7	3.26–3.75	4.9–5.9	29.7 (3.8)
$6D$	6.73	8.9	6.92–7.85	8.0–9.8	60.3 (8.3)
$7D$	11.8	17	11.5	10.50–17.0	108 (12.6)
$8D$	18.6	—	—	—	176 (15.8)
$4F$	4.97	4.3	4.25–4.81	3.2–6.9	43.6 (5.0)
$5F$	9.91	9.4	8.5–10.5	—	87.1
$6F$	17.0	17.3	17.2–18.8	—	154 (15.9)
$7F$	27.2	—	—	—	248

The recommended data for ions of the group IIb elements, presented in [17], differs noticeably from those presented in [14]. The FMP results locate in close vicinity of the recommended data as is seen in tables 8–10. Equation (9) with parameters from [14] overestimates the recommended data up to one order of magnitude.

Of specific interest are the metastable $nd(\,^2D_j)$-states ($j = 3/2, 5/2$) in Ca$^+$ ($n = 3$), Sr$^+$ ($n = 4$) and Ba$^+$ ($n = 5$) ions, which have rather long lifetimes and therefore may be useful in different practical applications. Therefore, an essential number of works were dedicated to determining the lifetimes of these states (see, for example, [21], [40], [43], [44]). We used the FMP approach for evaluating the lifetimes of these states and verified good agreement with existing data of the literature. The rate of radiative decay to the ground state from these levels is determined by the amplitude of electric quadrupole transition with the radial matrix element quite similar to the dipole one (6), with the replacement of the radial operator r by r^2. The FMP data for lifetimes of all these states gives values between the upper and lower boundaries of the most reliable data from the literature, accumulated in above cited papers. Table 11 presents comparison of results of the FMP approach with the boundaries of numerical data taken from the literature.

4. CONCLUSIONS

As is seen in tables 3–11, the FMP results are very close to the most reliable data of the literature to within the limits of uncertainties currently prescribed to the data on the radiation transition rates in atoms and ions [32]. Therefore, the data of the FMP calculations for the lifetimes

Table 9. *Numerical values of the lifetimes τ_{nl} (in nanoseconds) calculated with the FMP approach for nS-, $nP_{3/2}$-, $nD_{5/2}$- and $nF_{7/2}$-states in the ions of Cd^+, in comparison with the recommended values of the data base [17] and the data of ref. [14] given by approximation equations and compiled from the literature and presented there as "recommended values of radiation lifetimes" (numbers in parentheses).*

State	FMP	[17]	[14]
$6S$	3.925	2.1	10.4 (2.4)
$7S$	6.782	4.1	26.8
$8S$	11.63	7.7	52.7
$9S$	18.80	12.2	90.8
$10S$	28.63	19	143
$5P$	2.17	2.5	(3.2)
$6P$	15.0	16.8	—
$7P$	66.8	30.6	—
$8P$	157.1	92.5	—
$5D$	1.67	1.7	18.5
$6D$	4.02	5.9	44.1 (5.9)
$7D$	7.87	10	85.4 (9.5)
$8D$	13.56	18.6	146
$9D$	21.44	31	231
$4F$	5.90	5.8	71.1 (5.9)
$5F$	12.68	11.7	158
$6F$	22.69	—	307 (25.9)
$7F$	38.54	—	533

of arbitrary states in considered ions seems sufficiently reliable. Meanwhile the data, calculated with approximation equation (9) using the constants from [14] and [12] in most cases give results in essential disagreement with one another and with other available data of the literature. Therefore the basic claim of this paper consists in demonstrating reliability together with simplicity of the FMP code in estimating the lifetimes of the group II ions. The regions of validity for the FMP calculations are not limited to any extent, neither for principal, nor for orbital quantum numbers. The only limitation for the use of FMP is the performance of computing facilities, which are practically unlimited at present.

So, the analytical equation for matrix elements (6) may be used to generate simple codes for rather simple and accurate estimates of the lifetimes of arbitrary states in neutral and ionized atoms. In particular, the FMP opens the way for generating numerical data for lifetimes of Rydberg states, for which the data are not available at present in any database and may not be presented in any kind of sufficiently complete tables, due to infinite number of Rydberg levels. Naturally, the principal result of this article is not reduced to the numerical data of tables given to demonstrate the capacity of the method to reproduce reliably the lifetime values for excited states of the group II ions. This reliability approves the use of equation (6) with parameters determined from (7) and tables 1,2 for calculations of the lifetimes. In addition, the tables also clarify the accuracy and reliability of different approximation equations and the data available from the literature.

Table 10. *Numerical values of the lifetimes τ_{nl} (in nanoseconds) calculated with the FMP approach for nS-, $nP_{3/2}$-, $nD_{5/2}$- and $nF_{7/2}$-states in the ions of Hg$^+$, in comparison with the recommended values of the data base [17], the lower and upper values of experiment, $[41]_{exp}$, and theory $[41]_{th}$, taken from ref. [41], the latest data of "all-order calculations" with estimated uncertainties from [23], and the data of ref. [14], given by approximation equations and compiled from the literature and presented there as "recommended values of radiation lifetimes" (numbers in parentheses). The total momenta of states $7D_{3/2}$ and $8D_{3/2}$ are indicated explicitly.*

State	FMP	[17]	$[41]_{exp}$	$[41]_{th}$	[23]	[14]
$7S$	3.52	1.99	1.7–2.1	1.93–3.06	1.889 ± 0.014	(2.4)
$8S$	6.67	3.9	–	3.9–5.34	3.85 ± 0.14	(4.8)
$9S$	11.86	7.5	7.1–11.5	8.77-9.22	7.10 ± 0.12	(8.8)
$10S$	19.76	3.8	3.4–4.2	14.45–20.2	11.62 ± 0.24	(16.6)
$6P$	1.17	1.8	1.8–2.04	0.9	1.594 ± 0.010	(1.9)
$7P$	4.72	3.1	2.9–3.3	2.82	9.56 ± 0.96	—
$8P$	22.1	33	—	—	32.8 ± 2.9	—
$9P$	60.5	92	—	—	92.0 ± 2.7	—
$10P$	128.2	—	—	—	—	—
$6D$	1.56	1.56	1.6–2.5	1.3	1.548 ± 0.020	(1.7)
$7D_{3/2}$	2.78	5	4.4–5.6	3.53–5.09	3.535 ± 0.058	12.2 (4.9)
$8D_{3/2}$	5.32	10.6	7.9–11.2	7.8–10.3	7.44 ± 0.15	21.8 (9.7)
$9D$	12.33	14.5	12.9–15.9	—	14.55 ± 0.62	37.3 (15.1)
$10D$	19.47	24.5	17.2–20.6	27.0–27.5	24.5 ± 1.6	58.6 (24.5)
$5F$	6.59	3.2	7.1–9.5	6.27–6.34	6.04 ± 0.04	(7.2)
$6F$	14.66	15	—	—	16.27 ± 0.69	—
$7F$	27.62	30	—	—	34.02 ± 0.87	—
$8F$	46.39	54	—	—	61.2 ± 2.2	—
$9F$	71.75	—	—	—	—	—

Table 11. *Numerical values of the lifetimes τ_{nl} (in seconds) calculated within the FMP approach for metastable $nD_{3/2}$- and $nD_{5/2}$-states in the ions of Ca$^+$, Sr$^+$ and Ba$^+$. The ranges of theoretical and experimental data accumulated in the literature are presented for comparison. For Ca$^+$ the data is taken from ref. [44], for Sr$^+$ from ref. [40] and the data for Ba$^+$ is taken from ref. [43].*

Ion	State	FMP	experiment	theory
Ca$^+$	$3d\,^2D_{3/2}$	1.40	$1.04 \div 1.23$	$1.05 \div 1.3$
	$3d\,^2D_{3/2}$	1.40	$0.72 \div 1.42$	$1.05 \div 1.25$
Sr$^+$	$4d\,^2D_{3/2}$	0.28	$0.391 \div 0.444$	$0.347 \div 0.484$
	$4d\,^2D_{5/2}$	0.28	$0.209 \div 0.405$	$0.311 \div 0.430$
Ba$^+$	$5d\,^2D_{3/2}$	64.9	$45.4 \div 83.7$	$17.1 \div 105$
	$5d\,^2D_{5/2}$	25.5	$27.4 \div 63$	$19.0 \div 36.5$

Comparison of general behaviour of numerical values for the lifetimes seen in tables 3–10 gives information on precision and uncertainties of possible future computations of lifetimes for excited states of the group II ions with arbitrary principal and orbital quantum numbers.

Taking into account strong and rapidly arising at present interest to Rydberg states with very high principal quantum numbers, the FMP approach seems worthwhile for rather accurate and simply reproducible estimations of the basic spectroscopic properties of the bound states with arbitrary quantum numbers in atoms and ions. Due to infinite number of ionic bound states, the formulas of the FMP approach may become a useful tool for obtaining new data, still absent in the literature.

ACKNOWLEDGEMENTS

This work was supported in part by the Russian Foundation for Basic Research (RFBR grant No 11-02-00152a).

REFERENCES

[1] Takamoto M. An optical lattice clock / M. Takamoto, F.-L. Hong, R. Hogashi and H. Katori // Nature — 2005 — Vol. 435 — P. 321–324.

[2] Ludlow A.D. Sr Lattice Clock at 1×10^{-16} Fractional Uncertainty by Remote Optical Evaluation with a Ca Clock / A. D. Ludlow, T. Zelevinsky, G. K. Campbell et al // Science — 2008 — Vol. 319 — P. 1805–1808.

[3] Yi L. Optical Lattice Trapping of ^{1}99Hg and Determination of the Magic Wavelength for the Ultraviolet $^1S_0$–$^3P_0$ Clock Transition / L. Yi, J. J. McFerran, Y. L. Coq and S. Bize // Phys. Rev. Lett. — 2011 — Vol. 106 — 073005.

[4] Zhang X.L. Fidelity of a Rydberg-blockade quantum gate from simulated quantum process tomography / X. L. Zhang, A. T. Gill, L. Isenhower, T. G. Walker, and M. Saffman // Pys. Rev. A — 2012 — Vol. 85 — 042310.

[5] Gorshkov A.V. Photon-Photon Interactions via Rydberg Blockade / A. V. Gorshkov, J. Otterbach, M. Fleischhauer, T. Pohl and M. D. Lukin // Phys. Rev. Lett. — 2011 — Vol. 107 — 133602.

[6] Saffman M. Quantum information with Rydberg atoms / M. Saffman, T. G. Walker and K. Mölmer // Rev. Mod. Phys. — 2010 — Vol. 82 — P. 2313.

[7] Häffner H. Quantum computing with trapped ions / H. Häffner, C. F. Roos and R. Blatt // Phys. Rep. — 2008 — Vol. 469 — P. 155.

[8] Benhelm J. Experimental quantum-information processing with ^{43}Ca$^+$ ions / J. Benhelm, G. Kirchmair, C. F. Roos and R. Blatt // Pys. Rev. A — 2008 — Vol. 77 — 062306.

[9] M. Muller M. Trapped Rydberg ions: from spin chains to fast quantum gates / M. Muller, L. Liang, I. Lesanovsky and P. Zoller // New J. Phys. — 2008 — Vol. 10 — 093009.

[10] Safronova U.I. Relativistic many-body calculation of energies, lifetimes, polarizabilities, and hyperpolarizabilities in Li-like Be$^+$ / U.I. Safronova and M.S. Safronova // Phys. Rev. A — 2013 — Vol. 87 — 032502.

[11] McQuillen P. Imaging the evolution of an ultracold strontium Rydberg gas / P. McQuillen, X. Zhang, T. Strickler, F. B. Dunning, and T. C. Killian // Phys. Rev. A — 2013 — Vol. 87 — 013407.

[12] Djerad M. T. Atomic parameters for transitions involving Rydberg states of singly ionized alkaline earths / M. T. Djerad // J. Physique II — 1991 — Vol. 1 — P. 1–9.

[13] Theodosiou C.E. Lifetimes of the Singly Excited Be II and Be III States with $n < 11$ / C.

E. Theodosiou // Phys. Scripta — 1992 — Vol. 45 — P. 450 – 453.

[14] Rykova O.V. Lifetimes of Rydberg states for ions of the group 2 elements / O. V. Rykova and Ya. F. Verolainen // Optics and Spectroscopy — 1994 — Vol. 76, Iss. 1 — P. 23.

[15] Celik G. Transition probabilities, oscillator strengths and lifetimes for singly ionized magnesium / G. Celik, S. Ates, S. Ozarslan and M. Taser // J. Quant. Spectr. and Radiation Transfer — 2011 — Vol. 112 — P. 2330–2334.

[16] Yu. Ralchenko, A. Kramida, J Reader and NIST ASD Team National Institute of Standards and Technology, Gaithersburg, MD 2011 NIST Atomic Spectra Database (version 4.1) Available: http://physics.nist.gov/asd

[17] Information system “Electronic structure of atoms” Novosibirsk State University Institute of Automation and Electrometry. Availiable at http://grotrian.nsu.ru/en

[18] Monroe C. Demonstration of a Fundamental Quantum Logic Gate / C. Monroe, D. M. Meekhof, B. E. King, W. M. Itano and D. J. Wineland // Phys. Rev. Lett. — 1995 — Vol. 75 — P. 4714.

[19] Mukherjee R. Many-body physics with alkaline-earth Rydberg lattices / R. Mukherjee, J. Millen, R. Nath, M. P. A. Jones and T. Pohl // J. Phys. B — 2011 — Vol. 44 — 184010.

[20] Ovsiannikov V.D. Rydberg Spectroscopy in an Optical Lattice: Blackbody Thermometry for Atomic Clocks / V. D. Ovsiannikov, A. Derevianko and K. Gibble // Phys. Rev. Lett. — 2011 — Vol. 107 — 093003.

[21] Guet C. Relativistic many-body calculations of transition rates for Ca^+, Sr^+, and Ba^+ / C. Guet and W. R. Johnson // Phys. Rev. A — 1991 — Vol. 44, — P. 1531; see also Erratum in: Phys. Rev. A — 2007 — Vol. 76 — 039905(E).

[22] Safronova U.I. Excitation energies, E1, M1, and E2 transition rates, and lifetimes in Ca^+, Sr^+, Cd^+, Ba^+, and Hg^+ / U. I. Safronova and M. S. Safronova // Can. J. Phys. — 2011 — Vol. 89 — P. 465–472.

[23] Simmons M. Blackbody radiation shift, multipole polarizabilities, oscillator strengths, lifetimes, hyperfine constants, and excitation energies in Hg^+ / M.Simmons, U.I. Safronova and M.S. Safronova // Phys. Rev. A — 2011 — Vol. 84 — 052510.

[24] Simons G. New model potential for Pseudopotential calculations / G. Simons // J. Chem. Phys. — 1971 — Vol. 55 — P. 756.

[25] Simons G. New procedure for generating valence and Rydberg orbitals. I. Atomic oscillator strengths / G. Simons // J. Chem. Phys. — 1974 — Vol. 60 — P. 645.

[26] Manakov N.L. Atomic calculations using perturbation theory with a model potential / N. L. Manakov, V. D. Ovsiannikov and L. P. Rapoport // Optics and Spectroscopy — 1975 — Vol. 38, Iss. 2 — P. 115.

[27] Manakov N.L. The use of a model potential for the calculation of dynamic polarizabilities, dispersion forces and the light shifts of atomic levels / N. L. Manakov and V. D. Ovsiannikov // J. Phys. B — 1977 — Vol. 10 — P. 569–581.

[28] Manakov N.L. Atoms in a laser field / N. L. Manakov, V. D. Ovsiannikov and L. P. Rapoport // Phys. Rep. — 1986 — Vol. 141 — P. 319–433.

[29] Kostelecký V.A. Analytical wave functions for atomic quantum-defect theory / V. A. Kostelecký and M. M. Nieto // Phys. Rev. A — 1985 — Vol. 32 — P. 3243.

[30] Bates D.R. The Calculation of the Absolute Strengths of Spectral Lines / D. R. Bates and A. Damgaard // Phil. Trans. A — 1949 — Vol. 242 — P. 101.

[31] Klarsfeld S. Alternative forms of the Coulomb approximation for bound-bound multipole transitions / S. Klarsfeld // Phys. Rev. A — 1989 — Vol. 39 — P. 2324

[32] Springer handbook of Atomic, Molecular and Optical Physics. Section 10. Atomic Spectroscopy. / G. W. F. Drake (Ed.) — New York: Springer Science+Business Media, Inc., 2006.

[33] Varshalovich D.A. Quantum Theory of Angular Momentum / D. A. Varshalovich, A. N. Moskalev and V. K. Khersonskii — Singapore: World Scientific Publishing, 1988.

[34] Ovsiannikov V.D. Lifetime of Rydberg Atom / V. D. Ovsiannikov and I. L. Glukhov // Proceedings of Voronezh State University — 2006 — No 2 — P. 99–106.

[35] Ovsiannikov V.D. Rates of blackbody radiation-induced transitions from Rydberg states of alkali atoms / V. D. Ovsiannikov, I. L. Glukhov and E. A. Nekipelov // J. Phys. B — 2011 — Vol. 44 — 195010.

[36] Sobel'man I.I. Introduction to the Theory of Atomic Spectra / I. I. Sobel'man — New York: Pergamon Press, 1972.

[37] Bateman H. Higher Transcendental Functions. Vol. 1 / H. Bateman and A. Erdelyi — New York: McGraw-Hill Book Company, 1953.

[38] A. Derevianko Fine-structure effects in relativistic calculations of the static polarizability of the helium atom / A. Derevianko, W. R. Johnson, V. D. Ovsyannikov, V. G. Pal'chikov, D. R. Plante and G. von Oppen // J. Exp. Theor. Phys. — 1999 — Vol. 88, Iss. 2 — P. 272.

[39] Theodosiou C.E. Accurate calculation of the 4p lifetimes of Ca^+ / C. E. Theodosiou // Phys. Rev. A — 1980 — Vol. 39 — P. 4880.

[40] Biemont E. Lifetimes of metastable states in Sr II / E. Biemont, J. Lidberg, S. Mannervik, L.-O. Norlin, P. Royen, A. Schmitt, W. Shi and X. Tordoir // Eur. Phys. J. D — 2000 — Vol 11, No 3 — P. 355 — 365.

[41] Blagoev K. Radiative lifetimes of $5d10nl$ states of Hg^+ / K. Blagoev, P. Bogdanovich, N. Dimitrov and A. Momkauskaite // Phys. Rev. A — 1988 — Vol. 37 — P. 4679.

[42] Blagoev K.B. Radiative Lifetimes of Zn I, II Excited States / K.B. Blagoev, G. Malcheva, V. Penchev, E. Biémont, H.L. Xu, A. Persson and S. Svanberg // Phys. Scripta — 2004 — Vol. 69 — P. 433 – 440.

[43] Gurell J. Laser-probing measurements and calculations of lifetimes of the $5d^2D_{3/2}$ and $5d^2D_{5/2}$ metastable levels in Ba II / J. Gurell, E. Biémont, K. Blagoev et al. // Phys. Rev. A — 2007 — Vol. 75 — 052506.

[44] Kreuter A. Experimental and theoretical study of the $3d^2D$-level lifetimes of $^{40}\mathrm{Ca}^+$ / A. Kreuter, C. Becher, G.P.T. Lancaster, et al // Phys. Rev. A — 2005 — Vol. 71 — 032504.

Глухов Игорь Леонидович, кандидат физико-математических наук, ассистент кафедры экспериментальной физики физического факультета Воронежского государственного университета
E-mail: Glukhov@phys.vsu.ru
Тел.: +7(473)–220–86–25

Glukhov Igor, Candidate in Physics and Mathematics Sciences, teaching assistant, Experimental Physics department, Faculty of Physics, Voronezh State University
E-mail: Glukhov@phys.vsu.ru
Tel.: +7(473)–220–86–25

Никитина Елизавета Андреевна, аспирант кафедры теоретической физики физического факультета Воронежского государственного университета
E-mail: lis211290@mail.ru
Тел.: +7(950)–773–22–91

Nikitina Elizaveta, graduate student, Theoretical Physics department, Faculty of Physics, Voronezh State University
E-mail: lis211290@mail.ru
Tel.: +7(950)–773–22–91

Овсянников Виталий Дмитриевич, доктор физико-математических наук, профессор кафедры теоретической физики физического факультета Воронежского государственного университета
E-mail: OVD@phys.vsu.ru
Тел.: +7(473)–220–87–56

Ovsiannikov Vitaly, Doctor in Physics and Mathematics Sciences, professor, Theoretical Physics department, Faculty of Physics, Voronezh State University
E-mail: OVD@phys.vsu.ru
Tel.: +7(473)–220–87–56