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MICROWAVE RADIATION TRANSITIONS BETWEEN TRIPLET RYDBERG STATES OF ALKALINE-EARTH-LIKE ELEMENTS OF GROUP IIB IIB (Zn, Cd, Hg) AND YTTERBIUM Yb

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Abstract. Numerical values of quantum defects us ed for calculations of frequencies and matrix elements of dipole radiation transitions in the microwave range between triplet Rydberg states n^3S_1, n^3P_1, n^3D_2 and n^3F_3 series of Group IIb atoms with large principal quantum numbers have been determined $n > 20$. The calculation results within semi-empirical methods of quantum defect theory and Fues model potential are approximated by quadratic polynomials. The polynomial coefficients are tabulated along with numerical values of frequencies and matrix elements and can be used for measuring field strengths through microwave-induced splitting of electromagnetically induced transparency resonance, for development and planning of studies of microwave radiation characteristics using Rydberg atoms.

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1. INTRODUCTION

Precise measurement of electric field strength of microwave (μw) radiation based on measuring spectroscopic characteristics of radiative transitions between Rydberg states of atoms with large principal quantum numbers n has become a thoroughly studied theoretical and experimentally developed research area in modern atomic and molecular spectroscopy [1–13]. In this same μw spectral region, the frequencies of radiative transitions between Rydberg states of atoms are localized. Along with the frequencies of radiative transitions, they rapidly decrease proportionally to $n^{-\alpha}$, where $\alpha \geq 3$, and the widths of Rydberg energy levels [14]. Due to the practically infinite set of Rydberg states in any atom with distinctly expressed series of single-electron bound states, there is always a possibility to find such Rydberg levels where the transition frequency between them strictly coincides with a given μw radiation frequency ω_{Ryd}. Under the influence of the resonant field, Rydberg levels split proportionally to the Rabi $\Omega = F\mathcal{R}$ frequency is the product of μw electric field strength F and the matrix element $\mathcal{R}$ of radiative transition [10-13, 15]. Such splitting, transformed into resonance splitting for electromagnetically induced transparency (EIT) effect of strongly absorbed radiation probing the resonant transition from the ground to the first excited state, can be measured with high precision (see Fig. 1).

Thus, measuring the electric field strength of microwave radiation (microwave, millimeter, centimeter, radio frequency) can be based on measuring the frequency splitting of the EIT resonance effect of the optically absorbed wave by atoms. This effect, well-studied and effectively used

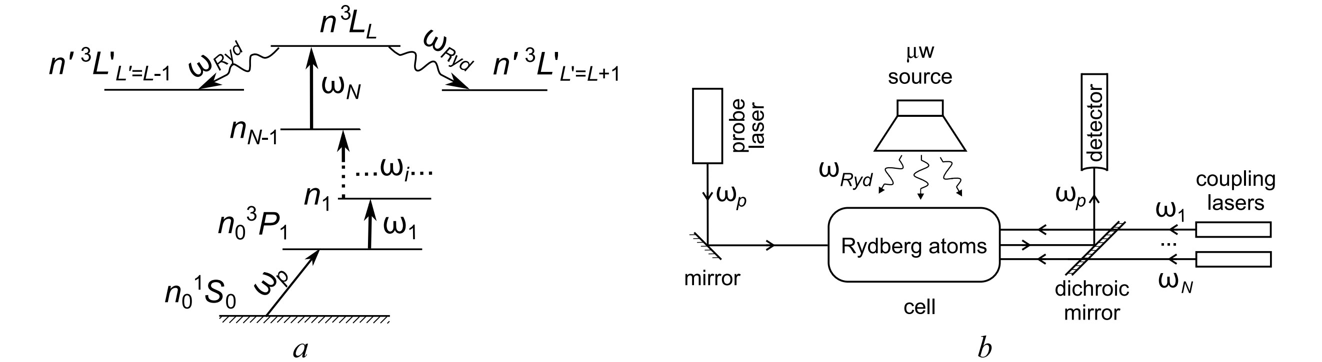

Fig. 1. *a* — Energy levels for N-photon excitation of triplet Rydberg nL-state and EIT resonance splitting by μw radiation resonant to transition $nL \to n'L'$ ($L' = L \pm 1$). *b* — Probe laser radiation (ω_p), coupling radiation beams (at frequencies $\omega_1, ..., \omega_N$) and μw radiation (ω_{Ryd})

for metrology of microwave fields in alkali elements of group I [1–11], can also be observed in divalent atoms of alkaline earth and alkaline earth-like elements of groups IIa and IIb. To date, detailed calculations of matrix elements of electric dipole radiation transitions between doublet states of alkali metal atoms [10,11], as well as between singlet states of alkaline earth-like atoms have been performed [12, 13].

It should be noted that the calculated sets of radiation transition frequencies in all atoms from the above groups, as well as corresponding matrix elements, provide necessary information not only for selection but also for evaluating the effectiveness of using the selected transition in a specific metrological task.

Along with singlet states, all divalent elements also possess triplet states, providing additional to singlet sets of radiation transition frequencies in the microwave range [16]. Furthermore, the first excited state of a divalent atom $n_0sn_0p(^3P_1)$, providing resonant absorption of probe laser radiation at the frequency of intercombination transition from the ground state $n_0s^2(^1S_0)$, is triplet. The radiation frequency of such partially forbidden transition by total electron shell spin in almost all atoms of groups IIa and IIb is approximately one and a half times lower than the frequency of fully allowed transition with excitation of singlet state $n_0sn_0p(^1P_1)$ (see the last rows of Table 1). In this regard, the results of numerical calculations of frequencies and amplitudes of radiation transitions between triplet Rydberg states of group IIb atoms, presented in this work, significantly complement the information obtained in [10–13], necessary for developing optical methods for precise measurement of microwave radiation characteristics.

Along with the tasks of metrology of microwave radiation characteristics, the calculated values of frequencies and amplitudes of radiation transitions between Rydberg states of atoms can be valuable in the development and optimization of digital information and radio-frequency communication systems based on Rydberg atoms [7, 9].

The paper is structured as follows.

Section 2 presents calculated numerical values of quantum defects for series n^3S_1, n^3P_1, n^3D_2, n^3F_3 triplet Rydberg states based on available literature data for energy levels of alkaline-earth-like atoms of group elements IIb (Zn, Cd, Hg) and ytterbium Yb. The numerical calculation results are consistent with the available data from modern literature.

Section 3 presents tables of frequencies for dipole transitions between the closest energy states.

Section 4 provides analytical expressions for the amplitudes of dipole-allowed radiation transitions between triplet Rydberg states in terms of radial matrix elements.

Section 5 discusses calculation methods and presents tables of numerical values for radial matrix elements of electric dipole transitions between Rydberg states.

Discussion of the obtained results and concluding remarks are presented in Section 6.

2. QUANTUM DEFECTS OF TRIPLET RYDBERG STATES OF GROUP IIB ATOMS AND YTTERBIUM

Currently, there are extensive databases containing numerical values of atomic state energies [17, 18], necessary for calculating frequencies of

Table 1. Numerical values of constants μ_{2q} in the Rydberg-Ritz formula (2) for triplet Rydberg states of Group IIb atoms and ytterbium. The values of the Rydberg constant Ry_A for the atom A, ionization potential Ip_A, excitation energy of resonance $^1P_1$ and metastable $^3P_1$ states are also indicated Excp_A

Series n^3L_J	$2\mu_{2q}$	Atom (ground state)			
		Zn ($3d^{10}4s^2$)	Cd ($4d^{10}5s^2$)	Hg ($6s^2$)	Yb ($6s^2$)
n^3S_1	μ_0	2.716551	3.65762	4.69743	4.44242
	μ_2	0.052543	0.221535	0.192163	0.249107
	μ_4	3.45004	0.908956	1.77218	1.98376
n^3P_1	μ_0	2.19734	3.1352	4.21193	3.95192
	μ_2	0.18688	0.791835	−1.17647	−2.16689
	μ_4	8.7502	14.1379	43.8889	11.6313
n^3D_2	μ_0	1.09071	2.08441	3.06532	2.75098
	μ_2	−0.246526	−0.081925	−0.939772	−0.70516
	μ_4	3.56537	4.48705	24.1838	37.3111
n^3F_3	μ_0	0.022242	0.0357423	1.08904	1.06520
	μ_2	0.31213	0.154961	−11.0497	0.304355
	μ_4	−9.51844	−7.15522	397.922	7.92697
Ry_A, cm^{-1}		109736.3949	109736.7802	109737.0156	109736.9677
Ip_A, cm^{-1}		75769.31	72540.05	84184.15	50443.0704
Excp_A, cm^{-1}	$^3P_1$	32501.399	30656.087	39412.237	17992.007
	$^1P_1$	46745.4032	43692.384	54068.6829	25068.222

radiative microwave transitions between Rydberg levels. Modern laser facilities allow obtaining such highly excited states using multi-photon transition spectroscopy methods [19, 20]. States n^3F_3, n^3D_2, n^3P_1 and n^3S_1 are the most suitable for observing microwave transitions in alkaline earth-like metals. Near the point of energy state condensation n^3L_J it is always possible to find such states $n'^3L'_{J'}$, for which transition frequencies $nL \to n'L'$ lie in the tera-, giga-, and megahertz range. They are determined in accordance with $\omega_{Ryd} = E_{nL} - E_{n'L'}$, where E_{nL} is the binding energy of the Rydberg state n^3L_J, which is conveniently represented by the relation [21–23]

$$E_{nL} = \mathrm{Ip}_A - \frac{\mathrm{Ry}_A}{(n-\mu_{nL})^2}. \tag{1}$$

Here Ip_A and Ry_A are respectively the ionization energy of the atom's ground state and the Rydberg constant accounting for the finite mass of the atom M_A; $\mathrm{Ry}_A = \mathrm{Ry}_\infty / (1 + M_A^{-1})$, $\mathrm{Ry}_\infty = 109737.315685$ cm^{-1} is the universal Rydberg constant (for $M_A = \infty$), μ_{nL} is the quantum defect of state n^3L_J. In this work, we consider states $n^3L_{J=L}$ $(L > 0)$ and $n^3S_{J=1}$.

The accuracy of energy values for the series E_{nL} in the energy level databases [17, 18] is limited to eight-nine decimal places. As n increases, the distance between adjacent levels decreases proportionally to n^{-3}. Therefore, the accuracy of ω_{Ryd} decreases to 3–4 digits due to mutual cancellation of higher orders during subtraction. For extrapolation of tabular data, this problem is solved by parameterizing the quantum defect μ_{nL} with the Rydberg-Ritz formula [21–23]

$$\mu_{nL} = \sum_{q=0}^{q_{max}} \frac{\mu_{2q}}{(n-\mu_0)^{2q}}, \tag{2}$$

where constants μ_{2q} are obtained by interpolating values μ_{nL}, calculated from tabular energies E_{nL} according to (1). In practice, typically, $q_{max} \le 2$.

A significant number of theoretical and experimental studies have been devoted to determining the constants Ip_A, Ry_A and μ_{2q} providing the energies of bound states of alkaline earth-like atoms. Table 1 shows the most reliable values of parameters for formulas (1), (2), calculated from the numerical values of energies of corresponding triplet state series presented in databases [17, 18]. Quantum defects are calculated using formula (1), and constants μ_{2q} are obtained through standard polynomial interpolation methods. As follows from the numerical values of parameters μ_{2q}, at $n > 15$ the main contribution to the sum (2) comes from terms with small values of q, mainly with $q = 0, 1$.

Along with the ionization energy Ip_A, the last row of Table 1 shows the energies of the first excited states Excp_A: triplet $^3P_1$ and singlet $^1P_1$, which determine the frequencies of radiation resonantly absorbed by normal atoms. These frequencies can be selected as the frequency of the probe radiation ω_p for measuring the electric field strength of microwave radiation by splitting the EIT effect resonance (see also Fig. 1). Moreover, the lower frequencies of triplet state excitations may prove to be more accessible and convenient for probing resonant transitions than the frequencies of singlet state excitations.

3. FREQUENCIES OF RADIATION MICROWAVE TRANSITIONS BETWEEN TRIPLET RYDBERG STATES OF GROUP IIb ATOMS AND YTTERBIUM

The data from Table 1 allow calculating using formula (1) the frequencies of resonant microwave transitions between triplet Rydberg states of the onsidered atoms with infinitely large values of principal quantum numbers. For the transition frequency $n^3L_J \to n'^3L'_{J'}$ according to (1), the dependence on effective principal quantum numbers of initial $\nu_{nL} = n - \mu_{nL}$ and final $\nu_{n'L'} = n' - \mu_{n'L'}$ Rydberg states can be written as

$$\Delta E_{nLL'} \equiv E_{nL} - E_{n'L'} = \\ = \mathrm{Ry}_A \frac{(\nu_{nL} - \nu_{n'L'})(\nu_{nL} + \nu_{n'L'})}{\nu_{nL}^2 \nu_{n'L'}^2}. \quad (3)$$

Principal quantum numbers n and n' may coincide or differ from each other by one or two units: $n' = n + \delta$, $\delta = 0, \pm 1, \pm 2$ (see Tables 2–5). The values of quantum defects μ_{nL} and $\mu_{n'L'}$ are calculated according to (2) using data from Table 1.

The frequencies of certain transitions between triplet Rydberg states of atoms Zn, Cd, Hg and Yb are given in Tables 2–5. Using polynomial interpolation of the calculated frequency values, one can obtain an asymptotic approximation formula for the transition frequency as a function of the principal quantum number n in the form

$$\Delta E_n = \frac{d_0}{n^3}\left(1 + \frac{d_1}{n} + \frac{d_2}{n^2}\right). \quad (4)$$

The values of coefficients d_0, d_1 and d_2, derived from the interpolation of the calculated frequencies (3) for transitions between states with $n = 20, 60, 120$, are also presented in Tables 2–5.

4. DIPOLE MICROWAVE TRANSITION AMPLITUDE BETWEEN TRIPLET STATES OF A DIVALENT ATOM

The matrix element of a single-electron dipole transition between triplet Rydberg states $\mathcal{R}_{nL'L}^{(\tau,M)} = \langle n'^3L'_{J'M+\tau} \mid x_\tau \mid n^3L_{JM}\rangle$ can be calculated using standard methods of atomic spectroscopy [24, 25]. The magnetic quantum number M here defines the projection of the total angular momentum vector $\mathbf{J}$ on the axis z. Integration over angular variables can be performed using quantum angular momentum theory methods [24], resulting in the matrix element $\mathcal{R}_{nL'L}^{(\tau,M)}$ will be expressed in terms of the radial matrix element $R_{nLL'} = \langle n'L' \mid r \mid nL\rangle$ as follows (see [24], sec. 13.1, formula (40)):

$$\mathcal{R}_{nL'L}^{(\tau,M)} = (-1)^{J+L'}\sqrt{2J+1}\, C_{JM\,1\tau}^{J'M+\tau} \times \\ \times \begin{Bmatrix} 1 & L' & L \\ 1 & J & J' \end{Bmatrix} \langle L' \parallel C_1 \parallel L\rangle \langle n'L' \mid r \mid nL\rangle. \quad (5)$$

Here $\tau = 0$ for π-polarization, $\tau = \pm 1$ for σ-polarization of microwave radiation;

$$\langle L' \parallel C_1 \parallel L\rangle = \sqrt{2L+1}\, C_{L010}^{L'0} = \\ = \begin{cases} -\sqrt{L} & \text{при} \quad L' = L - 1, \\ \sqrt{L+1} & \text{при} \quad L' = L + 1 \end{cases}$$

— reduced matrix element of the modified spherical function [24]

$$C_{q\tau}(\hat{\mathbf{r}}) = \sqrt{\frac{4\pi}{2q+1}}\, Y_{q\tau}(\hat{\mathbf{r}}), \qquad \hat{\mathbf{r}} = \mathbf{r} / r.$$

In formula (5), standard notations for Clebsch-Gordan coefficients and 6j-symbols are used.

Table 2. Frequencies of electric dipole transitions (in GHz) between triplet Rydberg states in zinc atoms: $\Delta E_{nSP} = E_{n^3S_1} - E_{(n-1)^3P_1}$, $\Delta E_{nPS} = E_{n^3P_1} - E_{n^3S_1}$, $\Delta E_{nPD} = E_{(n+2)^3P_1} - E_{n^3D_2}$, $\Delta E_{nDP} = E_{n^3D_2} - E_{(n+1)^3P_1}$, $\Delta E_{nFD} = E_{(n-1)^3F_3} - E_{n^3D_2}$

n	ΔE_{nSP}	ΔE_{nPS}	ΔE_{nPD}	ΔE_{nDP}	ΔE_{nFD}
20	640.070	632.508	810.333	105.887	64.8614
50	30.3914	31.7879	48.8874	6.02658	3.82946
100	3.46163	3.68087	5.99304	0.726529	0.464693
150	0.995017	1.06362	1.76426	0.212746	0.136290
200	0.413501	0.443158	0.741898	0.0892297	0.0572019
	Parameters of interpolation formula (4)				
d_0, THz	3171.94	3420.87	5878.12	701.845	450.433
d_1	8.32284	7.09337	1.92939	3.35842	3.19838
d_2	79.2793	49.8018	2.55069	15.6123	−3.17404

Table 3. Same as in Table 2, but for cadmium atoms: $\Delta E_{nSP} = E_{n^3S_1} - E_{(n-1)^3P_1}$, $\Delta E_{nPS} = E_{n^3P_1} - E_{n^3S_1}$, $\Delta E_{nPD} = E_{(n+2)^3P_1} - E_{n^3D_2}$, $\Delta E_{nDP} = E_{n^3D_2} - E_{(n+1)^3P_1}$, $\Delta E_{nFD} = E_{(n-2)^3F_3} - E_{n^3D_2}$

n	ΔE_{nSP}	ΔE_{nPS}	ΔE_{nPD}	ΔE_{nDP}	ΔE_{nFD}
20	757.070	748.542	1002.97	61.6292	54.7512
50	32.0868	33.9455	55.1076	3.06556	2.90036
100	3.54073	3.81241	6.55676	0.356898	0.340679
150	1.00761	1.09086	1.91135	0.103396	0.0988761
200	0.416684	0.452312	0.799833	0.0431419	0.0412848
	Parameters of interpolation formula (4)				
d_0, THz	3165.27	3450.72	6247.51	335.243	320.377
d_1	10.1984	9.39231	4.76317	5.69431	6.08108
d_2	161.409	106.308	18.4637	74.3851	25.2472

Table 4. Same as in Table 2, but for mercury atoms: $\Delta E_{nSP} = E_{n^3S_1} - E_{(n-1)^3P_1}$, $\Delta E_{nPS} = E_{n^3P_1} - E_{n^3S_1}$, $\Delta E_{nPD} = E_{(n+2)^3P_1} - E_{n^3D_2}$, $\Delta E_{nDP} = E_{n^3D_2} - E_{(n+1)^3P_1}$, $\Delta E_{nFD} = E_{(n-1)^3F_3} - E_{n^3D_2}$

n	ΔE_{nSP}	ΔE_{nPS}	ΔE_{nPD}	ΔE_{nDP}	ΔE_{nFD}
20	983.938	859.032	1074.09	200.241	1247.37
50	36.9910	33.8576	52.8664	9.36689	60.5000
100	3.94162	3.66356	6.08440	1.06130	6.95468
150	1.10924	1.03623	1.75474	0.304517	2.00584
200	0.456198	0.427252	0.730418	0.126435	0.835038
	Parameters of interpolation formula (4)				
d_0, THz	3434.87	3232.04	5624.75	967.457	6438.80
d_1	11.8590	10.9580	7.56225	8.82170	7.24673
d_2	279.478	231.357	59.8187	85.8910	74.99121

Table 5. Same as in Table 2, but for ytterbium atoms: $\Delta E_{nSP} = E_{n^3S_1} - E_{(n-1)^3P_1}$, $\Delta E_{nPS} = E_{n^3P_1} - E_{n^3S_1}$, $\Delta E_{nDP} = E_{n^3D_2} - E_{(n+1)^3P_1}$, $\Delta E_{nDF} = E_{n^3D_2} - E_{(n-2)^3F_3}$, $\Delta E_{nFD} = E_{(n-1)^3F_3} - E_{n^3D_2}$

n	ΔE_{nSP}	ΔE_{nPS}	ΔE_{nDP}	ΔE_{nDF}	ΔE_{nFD}
20	916.114	833.140	254.977	418.199	825.765
50	35.9728	33.6656	12.5720	19.8255	41.8361
100	3.87086	3.67235	1.44086	2.25963	4.85389
150	1.09252	1.04147	0.414816	0.649735	1.40338
200	0.449955	0.429974	0.172507	0.270064	0.584881
	Parameters of interpolation formula (4)				
d_0, THz	3387.35	3261.28	1322.76	2073.50	4517.44
d_1	11.9367	10.4479	8.44738	8.12900	6.98857
d_2	226.710	208.528	47.8908	82.8190	45.1730

The amplitude of the microwave transition (5) can be conveniently represented as a product of the angular factor $({}^3L'_{J'M+\tau}|{}^3L_{JM})$ and the radial matrix element:

$$\mathcal{R}^{(\tau,M)}_{nL'L} = ({}^3L'_{J'M+\tau}|{}^3L_{JM})R_{nLL'}. \tag{6}$$

In particular, when $L, L' > 0$, $J = L$, $J' = L'$ in the case of π-transitions ($\tau = 0$)

$$({}^3L'_{J'M}|{}^3L_{JM}) = \\ = A_{L'L}\sqrt{L'(L'+1)+L(L+1)-2M^2};$$

in the case of σ-transitions ($\tau = \pm 1$)

$$({}^3L'_{J'M\pm1}|{}^3L_{JM}) = A_{L'L}(L'-L)\times \\ \times\sqrt{[L' \pm M(L'-L)][L'+1 \pm M(L'-L)]}.$$

Here

$$A_{L'L} = \frac{L'(L'+1)+L(L+1)-2}{\sqrt{8L'L(L'+1)(L+1)(2L'+1)(2L+1)}}, \\ L' = L \pm 1.$$

However, in the case of $L = 0$, $M = 0, \pm 1$, $J' = L' = 1$ the results differ only in signs. For π-transitions

$$({}^3P_{1M}|{}^3S_{1M}) = -\mathrm{sign}(M)/\sqrt{6};$$

for σ-transitions

$$({}^3P_{1M\pm1}|{}^3S_{1M}) = \pm 1/\sqrt{6}.$$

Note that at $|M| > J$ or at $|M+\tau| > J'$ the angular factor becomes zero.

5. RADIAL MATRIX ELEMENTS OF ELECTRIC DIPOLE TRANSITIONS BETWEEN TRIPLET RYDBERG STATES OF GROUP IIb IIB ATOMS AND YTTERBIUM

The main contribution to the numerical value of the radial matrix element $R_{nLL'}$ in the amplitude of the electric dipole transition (6) is determined by the dipole transition of the Rydberg electron between states with close values of principal quantum numbers $n' = n + \delta$, $\delta = 0, \pm 1, \pm 2$ and adjacent values of orbital quantum numbers $L' = L \pm 1$. For describing the initial and final states of the Rydberg electron, the most effective and convenient are the Coulomb-like wave functions of quantum defect theory (QDT) [21], as well as wave functions of the one-electron Fues model potential (FMP) [26]. In these methods, radial wave functions are expressed through polynomials of the radial variable of the Rydberg electron. Analytical expressions for wave

Table 6. Numerical values (in atomic units) and coefficients of the approximation polynomial (7) for radial matrix elements of electric dipole transitions between triplet Rydberg states in zinc atoms. The corresponding transition frequencies and designations are presented in Table 2

n	R_{nSP}	R_{nPS}	R_{nPD}	R_{nDP}	R_{nFD}
20	320.046	340.454	163.305	528.249	533.487
50	2484.06	2461.60	1134.41	3543.21	3579.62
100	10623.2	10311.1	4695.57	14489.5	14623.8
150	24427.9	23553.4	10685.1	32837.4	33127.3
200	43898.3	42188.4	19102.9	58586.9	59090.2
	Coefficients of the approximation polynomial (7)				
a_0	10.5604	4.91810	1.57102	−1.409802	−5.27257
a_1	−7.18628	−4.79438	−1.62659	−3.12398	−2.89512
a_2	1.13312	1.07856	0.485665	1.48033	1.49186

Table 7. Same as in Table 6, but for cadmium atoms. The corresponding transition frequencies are presented in Table 3

n	R_{nSP}	R_{nPS}	R_{nPD}	R_{nDP}	R_{nFD}
20	285.639	304.698	119.400	477.824	477.918
50	2394.24	2356.27	892.355	3432.88	3439.92
100	10458.6	10071.1	3780.19	14340.1	14360.0
150	24210.8	23155.4	8667.56	32724.9	32759.6
200	43650.8	41609.1	15554.5	58587.3	58638.5
	Coefficients of the approximation polynomial (7)				
a_0	17.6801	10.8922	4.06868	3.28447	−0.758824
a_1	−9.34697	−6.78693	−2.22971	−6.18416	−5.98064
a_2	1.13756	1.07389	0.399909	1.49552	1.49589

Table 8. Same as in Table 6, but for mercury atoms. The corresponding transition frequencies are presented in Table 4

n	R_{nSP}	R_{nPS}	R_{nPD}	R_{nDP}	R_{nFD}
20	239.404	277.727	147.26	419.321	121.457
50	2181.12	2356.78	1181.69	3226.76	860.164
100	9758.54	10328.6	5101.37	13757.7	3532.73
150	22762.9	23933.2	11765.3	31603.4	8003.65
200	41194.1	43170.7	21173.4	56763.9	14272.8
	Coefficients of the approximation polynomial (7)				
a_0	30.6019	17.8696	6.24588	10.6045	−14.0383
a_1	−11.2587	−9.55068	−3.93331	−8.82462	−0.499583
a_2	1.08538	1.12658	0.548845	1.46295	0.359672

Table 9. Same as in Table 6, but for ytterbium atoms. The corresponding transition frequencies are presented in Table 5

n	R_{nSP}	R_{nPS}	R_{nDP}	R_{nDF}	R_{nFD}
20	251.340	283.722	427.376	365.051	282.489
50	2222.69	2367.39	3202.00	2903.13	1936.43
100	9878.76	10318.7	13550.1	12473.0	7974.70
150	22997.8	23868.0	31052.8	28717.4	18115.45
200	41579.7	43015.1	55710.2	51636.4	32358.7
	Coefficients of the approximation polynomial (7)				
a_0	29.5584	13.9154	8.51495	7.89387	0.634271
a_1	−10.7667	−8.90942	−7.67661	−8.84123	−2.30882
a_2	1.09259	1.11958	1.43092	1.33492	0.820495

functions and radial matrix elements $R_{nLL'}$ in QDT and FMP approaches are given in [11]. The difference in numerical calculation results using QDT and FMP wave functions at $20 < n < 50$ does not exceed 1–3%, which is within the error margins of semi-empirical QDT and FMP methods based on using numerical values of atomic energy levels With increasing principal quantum numbers, the difference between QDT and FMP results rapidly decreases, reaching 0.1% at $n > 150$.

The numerical values of radial matrix elements of dipole microwave transitions $R_{nLL'}$, found using QDT wave functions, for atoms of zinc, cadmium, mercury, and ytterbium are given in Tables 6–9 in the range of principal quantum numbers n from 20 to 200. The dependence $R_{nLL'}$ on n can be approximated by a quadratic polynomial of the form

$$R_{nLL'} = a_0 + a_1 n + a_2 n^2. \qquad (7)$$

Coefficients a_0, a_1 and a_2 of this polynomial, obtained by polynomial interpolation of the calculated matrix element values $R_{nLL'}$ at $n = 50$, 100, 150, are also given in Tables 6–9.

6. CONCLUSIONS

The calculated frequencies of radiative transitions between triplet Rydberg states of alkaline-earth-like elements of group IIb and ytterbium significantly expand the database on Rydberg atoms. Tables 2–5 for radiation transition frequencies provide new information about the possibilities of practical use of Rydberg atoms for research aimed at developing new methods for metrology of radio frequency and microwave range fields.

The results of calculations performed in this work for frequencies and amplitudes of radiative transitions between triplet Rydberg states of alkaline-earth-like elements of group IIb and ytterbium provide new information about the spectra of Rydberg states of these atoms. This information may be useful for future applications of Rydberg atoms not only in microwave radiation metrology but also for creating new information and communication systems based on micrometer, millimeter, and centimeter radiation sources operating at frequencies of radiative transitions between atomic Rydberg states. To evaluate the efficiency of such transitions, expression (7) with coefficients a_0, a_1 and a_2 from Tables 6–9, can be used, which reproduces the numerical values of radial matrix elements of radiative transitions in the region of principal quantum numbers n from 15 to 500 with a fractional uncertainty not exceeding 0.1%.

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REFERENCES

1. J. A. Sedlacek, A. Schwettmann, H. Kübler, R. Löw, T. Pfau, and J. P. Shaffer, *Microwave Electrometry with Rydberg Atoms in a Vapour Cell Using Bright Atomic Resonances*, Nat. Phys. **8**, 819 (2012).

2. C. L. Holloway, J. A. Gordon, S. Jefferts, A. Schwarzkopf, D. A. Anderson, S. A. Miller, N. Thaicharoen, and G. Raithel, *Broadband Rydberg Atom-Based Electric-Field Probe for SI-Traceable, Self-Calibrated Measurements*, IEEE Trans. Antennas Propag. **62**, 6169 (2014).

3. H. Fan, S. Kumar, J. Sedlacek, H. Kübler, Sh. Karimkashi, and J. P. Shaffer, *Atom Based RF Electric Field Sensing*, J. Phys. B: Atom. Mol. Opt. Phys. **48**, 202001 (2015).

4. C. L. Holloway, M. T. Simons, J. A. Gordon, J. A. Gordon, P. F. Wilson, C. M. Cooke, D. A. Anderson, and G. Raithel, *Atom-Based RF Electric Field Metrology: from Self-Calibrated Measurements to Subwavelength and Near-Field Imaging*, IEEE Trans. Electromagn. Compat. **59**, 717 (2017).

5. D. A. Anderson and G. Raithel, *Continuous Frequency Measurements of High-Intensity Microwave Electric Fields with Atomic Vapor Cells*, Appl. Phys. Lett. **111**, 053504 (2017).

6. Y. Jiao, L. Hao, X. Han, S. Bai, G. Raithel, J. Zhao, and S. Jia, *Atom-Based Radio-Frequency Field Calibration and Polarization Measurement Using Cesium nDJ Floquet States*, Phys. Rev. Appl. **8**, 014028 (2017).

7. Z. Song, Z. Feng, X. Liu, D. Li, H. Zhang, J. Liu, and L. Zhang, *Quantum-Based Determination of Antenna Finite Range Gain by Using Rydberg Atoms*, IEEE Antennas Wireless Propag. Lett. **16**, 1589 (2017).

8. M. T. Simons, J. A. Gordon, and C. L. Holloway, *Fiber-Coupled Vapor Cell for a Portable Rydberg Atom-Based Radio Frequency Electric Field Sensor*, Appl. Opt. **57**, 6456 (2018).

9. Z. Song, H. Liu, X. Liu, W. Zhang, H. Zou, J. Zhang, and J. Qu, *Rydberg-Atom-Based Digital Communication Using a Continuously Tunable Radio-Frequency Carrier*, Opt. Express **27**, 8848 (2019).

10. E. F. Stelmashenko, O. A. Klezovich, V. N. Baryshev, V. A. Tishchenko, I. Yu. Blinov, V. G. Palchikov, V. D. Ovsyannikov, *Measuring the Electric Field Strength of Microwave Radiation at the Frequency of the Radiation Transition between Rydberg States of Atoms ^{85}Rb*, Opt. Spectrosc. **128**, 1063 (2020) [E. F. Stelmashenko, O. A. Klezovich, V. N. Baryshev, V. A. Tishchenko, I. Yu. Blinov, V. G. Palchikov, and V. D. Ovsyannikov, *Measuring the Electric Field Strength of Microwave Radiation at the Frequency of the Radiation Transition between Rydberg States of Atoms ^{85}Rb*, Opt. Spectrosc. **128**, 1067 (2020)].

11. V. D. Ovsiannikov, V. G. Palchikov, and I. L. Glukhov, *Microwave Field Metrology Based on Rydberg States of Alkali-Metal Atoms*, Photonics **9**, 635 (2022).

12. I. L. Glukhov, A. A. Kamensky, V. D. Ovsyannikov, V. G. Palchikov, *Precision Spectroscopy of Rydberg States of Alkaline Earth Atoms for Measuring Microwave Radiation Characteristics*, JETP **164**, 193 (2023) [I. L. Glukhov, A. A. Kamenski, V. D. Ovsiannikov, and V. G. Pal'chikov, *Precision Spectroscopy of Rydberg States in Alkaline Earth Atoms for Millimeter-Wave Radiation Measurement*, JETP **137**, 169 (2023)].

13. I. L. Glukhov, A. A. Kamenski, V. D. Ovsiannikov, and V. G. Palchikov, *Precision Spectroscopy of Radiation Transitions between Singlet Rydberg States of the Group IIb and Yb Atoms*, Photonics **10**, 1153 (2023).

14. H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of One- and Two-Electron Atoms*, GIFML, Moscow (1960) [H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of One- and Two-Electron Atoms*, Springer-Verlag, Berlin – Göttingen Heidelberg, Germany (1957)].

15. L. D. Landau, E. M. Lifhitz, *Quantum Mechanics (Nonrelativistic Theory)*, Fizmatlit, Moscow (2021), §§ 39, 40 [L. D. Landau and E. M. Lifshitz, *Quantum Mechanics, Nonrelativistic Theory*, Pergamon Press, Oxford, UK (1989), Secs. 39, 40].

16. Y.-Li. Zhou, D. Yan, and W. Li, *Rydberg Electromagnetically Induced Transparency and Absorption of Strontium Triplet States in a Weak Microwave Field*, Phys. Rev. A **105**, 053714 (2022).

17. A. Kramida, Yu. Ralchenko, J. Reader, and NIST ASD Team (2023). NIST Atomic Spectra Database (ver. 5.11), [Online]. Available: https://physics.nist.gov/asd [2024, February 16]. National Institute of Standards and Technology, Gaithersburg, MD.

18. V. V. Kazakov, V. G. Kazakov, V. S. Kovalev, O. I. Meshkov, and A. S. Yatsenko, *Electronic Structure of Atoms: Atomic Spectroscopy Information System*, Phys. Scripta **92**, 105002 (2017).

19. A. K. Mohapatra, T. R. Jackson, and C. S. Adams, *Coherent Optical Detection of Highly Excited Rydberg States Using Electromagnetically Induced Transparency*, Phys. Rev. Lett. **98**, 113003 (2007).

20. F. B. Dunning, T. C. Killian, S. Yoshida, and J. Burgdörfer, *Recent Advances in Rydberg Physics Using Alkaline-Earth Atoms, J.* Phys. B: Atom. Mol. Opt. Phys. **49**, 112003 (2016).

21. M. J. Seaton, *Quantum Defect Theory*, Rep. Prog. Phys. **46**, 167 (1983).

22. W. C. Martin, *Series Formulas for the Spectrum of Atomic Sodium* (Na I), J. Opt. Soc. Amer. **70**, 784 (1980).

23. F. Robicheaux, *Calculations of Long Range Interactions for 8Sr Rydberg States, J.* Phys. B: Atom. Mol. Opt. Phys. **52**, 244001 (2019).

24. D. A. Varshalovich, A. N. Moskalev, and V. K. Khersonskii, *Quantum Theory of Angular Momentum*, Nauka, Leningrad (1975) [D. A. Varshalovich, A. N. Moskalev, and V. K. Khersonskii, *Quantum Theory of Angular Momentum: Irreducible Tensors, Spherical Harmonics, Vector Coupling Coefficients, 3nj Symbols*, World Scientific, Singapore (1988)].

25. I. I. Sobelman, *An Introduction to the Theory of Atomic Spectra*, GIFML, Moscow (1963) [I. I. Sobelman, *An Introduction to the Theory of Atomic Spectra*, Pergamon Press, London, UK (1972)].

26. N. L. Manakov, V. D. Ovsiannikov, and L. P. Rapoport, *Atoms in a Laser Field*, Phys. Rep. 141, 320 (1986).