

RADIATIVE TRANSITIONS BETWEEN LOWEST AUTOIONIZING STATES IN SODIUM

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The wavelengths and radiative transition probabilities for the transitions $2p^5 3s 3p \text{ } LSJ \rightarrow 2p^5 3s^2 \text{ } ^2P_{1/2,3/2}$ and $2p^5 3s 3p \text{ } LSJ \rightarrow 2p^6 3p \text{ } ^2P_{1/2,3/2}$ in Na atoms are calculated by using large scale configuration interaction approximation. The autoionization probabilities and electron impact excitation cross-sections for the $2p^5 3s 3p \text{ } LSJ$ levels are also calculated in single configuration intermediate coupling approach. The obtained results are used for evaluation of the role of radiative cascade transitions from the $2p^5 3s 3p \text{ } LSJ$ doublets in population of the $2p^5 3s^2 \text{ } ^2P_{1/2,3/2}$ lowest autoionizing levels.

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1. Introduction

In ejected-electron excitation functions for the lowest $2p^5 3s^2 \text{ } ^2P_{3/2}$ and $^2P_{1/2}$ autoionizing states in sodium [1], a strong resonance structure was revealed in the impact energy regions of 32–33 and 36.5–40.0 eV. However, recent *R*-matrix (close-coupling) calculations [2] did not confirm the existence of negative ion resonances at these energies. Another process, which may cause the observed structure, is the cascade population of the $2p^5 3s^2$ levels by the radiative transitions from the high-lying doublets. Earlier such a transition ($\lambda = 434.3$ nm) was found between the $2p^5 3s(^1P)3p \text{ } ^2P_{3/2}$ and $2p^5 3s^2 \text{ } ^2P_{3/2}$ autoionizing states in beam-foil excitation spectra [3]. In order to evaluate the real role of the radiative cascades in excitation of the lowest autoionizing doublet levels in sodium, the data on excitation and decay parameters for the $2p^5 3s np$, $2p^5 3p nd$, $2p^5 3d np$, and $2p^5 4s np$ even configurations are needed.

For the investigation of core-excited autoionizing states of Na, a number of experimental [1, 4–11] and theoretical [12, 13] works was devoted. The absorption spectrum was registered by Wolf et al [4], Connerade et al [5], Sugar et al [6], and Baig et al [7]. The ejected-electron spectra were also studied by different experimental methods [1, 8–10]. The radiative decay

of the $2p^5 3s 3p$ autoionizing states was studied by Zhenjak et al [11] in electron–atom collisions. Energy levels and lifetimes for some core-excited quartet states of Na were calculated by applying multiconfiguration Hartree–Fock (MCHF) approximation [12]. The systematic studies of the Na $2p^5 3s nl$ autoionizing (AI) states were performed by Zatsarinny and Bandurina [13]. They have used the configuration interaction (CI) approach. The set of radial orbitals was obtained from Hartree–Fock calculation of $2p^5 nl$ states of Na^+ within the fixed-core average energy approximation. These orbitals were used to make up the basis sets for the CI calculations of autoionizing states as described in [14, 15]. To achieve a better agreement between the calculated and experimental energies of AI levels, the radial orbitals of valence nl electrons were obtained by using a model potential with adjustable parameters. The data obtained were accurate enough to extend and clarify considerably the classification of lines in existing photoabsorption [4–7] and ejected-electron spectra [9].

The aim of the present work was an examination of the role of radiative transitions from the $2p^5 3s 3p \text{ } LSJ$ doublet states in electron impact excitation of the $2p^5 3s^2 \text{ } ^2P_{1/2,3/2}$ lowest autoionizing states. The second aim was a pure theoretical *ab initio* investigation of the lowest autoionizing states in sodium avoid-

ing the semi-empirical corrections. We have calculated the wavelengths and radiative transition probabilities for the transitions $2p^5 3s 3p \text{ } LSJ \rightarrow 2p^5 3s^2 \text{ } ^2P_{1/2,3/2}$ and $2p^5 3s 3p \text{ } LSJ \rightarrow 2p^6 3p \text{ } ^2P_{1/2,3/2}$ as well as the autoionization probabilities and electron impact excitation cross-sections for the $2p^5 3s 3p \text{ } LSJ$ levels. The description of methods used for the calculations is presented in the second section. The results of calculations are discussed in the third section.

2. Method of calculations

The theoretical investigation of the energies and radiative transition probabilities in Na atom is performed by using the method fully described and successfully applied in our previous papers [16–23]. While calculating the energy spectra, the relativistic effects were taken into account within the traditional Breit–Pauli approximation, i. e. the spin–orbit and other relativistic one- and two-electron interactions accurate up to the square of the fine structure constant were included.

The correlation corrections were taken into account by the CI technique. The basis set of non-relativistic radial orbitals was constructed as follows. The radial orbitals of electrons with $n \leq 3$ were determined by solving the Hartree–Fock equations [24]. For describing the excitations into the virtual states with a higher principal quantum number the transformed radial orbitals with a variable parameter (TROs) [17] were employed. Our experience in the application of this method to different atoms and ions (see Refs. [18–23]) reveals that the employment of such radial orbitals enables one to take into account the correlation corrections within the CI method quite efficiently. We study all the configurations of an odd parity (or those of an even parity) simultaneously; in fact, the levels of these configurations are located comparatively close and the improvement of the levels of one configuration has an influence on the locations of the levels of configurations with the same parity. Such approach allows us to take into account not only one- and two-electron virtual excitations according to the two-electron Hamiltonian used, but also the excitations of a higher order. We must note that such an approach is very important for the calculation of the oscillator strengths and transition probabilities of the forbidden one-electron transitions, as well as for the determination of characteristics of the two-electron transitions.

TROs with $n \leq 13$ and $l \leq 10$ are used in the calculations of Na I energy spectra. It is easy to get a wide basis set of radial orbitals obtained by the method described

in [17] and to generate many admixed configurations by a virtual excitation of one or two electrons from $2l$ and $3l$ shells, but then the rank of the energy operator matrix becomes very high, too. The total number of the admixed configurations is 13241 for odd configurations $2p^5 3s^2$, $2p^6 3p$, $2p^5 3s 3d$, and $2p^5 3p^2$, and 9500 for even configurations $2p^6 3s$, $2p^5 3s 3p$, and $2p^6 3d$. It is necessary to reduce the number of admixed configurations, because the accounting of a great number of admixed configurations exceeds the possibilities of a single computer (the PC) that we use, and not all of the admixed configurations are important. In this calculation the admixed configurations were selected according to their contribution to the wavefunction of the adjusted configurations. These contributions were evaluated in the second order of the perturbation theory as described in papers [25, 26]. These methods are based on the use of the second-order perturbation theory and the analytical expressions for sums of squares of the interconfigurational matrix elements and for the averaged energy differences between the adjusted and admixed configurations as well. They provide the balance of the accounted correlation corrections when the same selection criteria for each configuration are used. All configurations with the averaged weights higher than $2.0 \cdot 10^{-8}$ are included into the set of admixed configurations. For the odd configurations the number of admixed configurations is 2174, for the even configurations it is 2000. As it is shown in [27], such selection criterion is sufficient for the accurate calculations. The selection of the admixed configurations is performed by using the program SELECTCONF [28].

The total number of the configuration state functions (CSFs) for each configuration parity was found to be very large; these numbers were greater than 10^6 for even configurations and greater than 79000 for odd ones. The reduction of this number was achieved in the way described in [29] and used in our previous calculations. As a result, 62657 CSFs were obtained for two even adjusted configurations ($2p^6 3s$, $2p^5 3s 3p$) and 29997 CSFs for two odd ones ($2p^5 3s^2$, $2p^6 3p$). The virtually excited electrons were placed at the beginning of the list of the active shells and some restrictions were put on their intermediate and final LS momenta. This method is realized in program ATOTERM [30].

The multiconfiguration wave functions obtained by diagonalizing the matrix of the energy operator were used to compute the matrix elements of the electron transition operator and, correspondingly, oscillator strengths and probabilities of the electric dipole transitions.

Table 1. Calculated and experimental energies E (in eV) with respect to the ground state of Na, and autoionization probabilities A (in s^{-1}) for the $2p^5 3s^2 {}^2P_J$ and $2p^5 3s(L_1 S_1)3p {}^L S J$ states.

Configuration	J	E	E^a	E^b	E^c	A	A^d	A^a
$2p^5 3s^2 {}^2P$	3/2	30.494	30.853	30.768	30.77	$2.58 + 12$	$7.91 + 12$	$5.50 + 12$
$2p^5 3s^2 {}^2P$	1/2	30.647	31.022	30.934	30.94	$2.58 + 12$	$7.91 + 12$	$5.53 + 12$
$2p^5 3s({}^3P)3p {}^4S$	3/2	32.478	32.756	32.703	32.75	$2.49 + 06$	0.0	$7.84 + 05$
$2p^5 3s({}^3P)3p {}^4D$	7/2	32.776	33.084	33.056		0.0	0.0	0.0
$2p^5 3s({}^3P)3p {}^4D$	5/2	32.819	33.129	33.099	33.08	$5.07 + 10$	$1.18 + 11$	$4.21 + 10$
$2p^5 3s({}^3P)3p {}^4D$	3/2	32.861	33.172	33.142	33.15	$6.11 + 10$	$1.49 + 11$	$4.81 + 10$
$2p^5 3s({}^3P)3p {}^4D$	1/2	32.896	33.209	33.179		$5.94 + 08$	$2.00 + 09$	$3.01 + 09$
$2p^5 3s({}^3P)3p {}^4P$	5/2	32.989	33.336	33.295		$1.38 + 11$	$3.34 + 11$	$1.23 + 11$
$2p^5 3s({}^3P)3p {}^4P$	3/2	33.036	33.384	33.343	33.33	$1.67 + 11$	$4.56 + 11$	$1.68 + 11$
$2p^5 3s({}^3P)3p {}^4P$	1/2	33.061	33.409	33.366	33.42	$4.45 + 10$	$1.48 + 11$	$8.99 + 11$
$2p^5 3s({}^1P)3p {}^2D$	3/2	33.135	33.487	33.442	33.44	$1.65 + 12$	$3.36 + 12$	$1.30 + 12$
$2p^5 3s({}^1P)3p {}^2D$	5/2	33.191	33.544	33.499	33.50	$1.73 + 12$	$3.55 + 12$	$1.33 + 12$
$2p^5 3s({}^1P)3p {}^2P$	1/2	33.234	33.602	33.548	33.56	$2.32 + 10$	$5.60 + 10$	$3.96 + 11$
$2p^5 3s({}^1P)3p {}^2P$	3/2	33.269	33.638	33.584	33.63	$4.56 + 10$	$1.08 + 11$	$2.07 + 10$
$2p^5 3s({}^1P)3p {}^2S$	1/2	33.657	33.926	33.877	33.89	$5.44 + 12$	$1.42 + 13$	$5.05 + 13$
$2p^5 3s({}^3P)3p {}^2D$	5/2	34.922	34.840	34.788		$4.82 + 09$	$1.51 + 13$	$2.30 + 12$
$2p^5 3s({}^3P)3p {}^2S$	1/2	34.976	34.858	34.812	34.82	$2.72 + 12$	$2.96 + 12$	$1.97 + 13$
$2p^5 3s({}^3P)3p {}^2P$	3/2	34.968	34.878	34.842		$1.35 + 09$	$6.05 + 12$	$6.28 + 11$
$2p^5 3s({}^3P)3p {}^2D$	3/2	35.075	35.018	34.972	35.01	$2.70 + 09$	$8.99 + 12$	$1.64 + 12$
$2p^5 3s({}^3P)3p {}^2P$	1/2	35.135	35.048	35.005	35.22	$1.54 + 12$	$2.10 + 12$	$7.01 + 12$

^a Calculated data [13].^b Optical data [4, 6, 37].^c Ejected-electron data [9].^d Present calculations with Cowan code [34].

The electric dipole transitions were evaluated using two forms of the transition operator: ‘length’ (L) and ‘velocity’ (V). The radiative lifetimes are presented in both forms and that enables one to compare the results obtained using different forms. As it is known, the coincidence of the results obtained with these two forms of the operator serves as a reliability criterion for the data obtained by CI, when the basis of the admixed configuration included into configuration interaction is large. In the computations, along with our own computer codes, we also employed the program [31] for calculating the angular parts of the energy operator matrix elements and the programs [32, 33] for evaluating the characteristics of electronic transitions.

The autoionization probabilities were calculated by using the Cowan code [34] and Kupliauskienė code [35]. The wave functions were obtained in a single-configuration intermediate coupling approximation with Breit–Pauli relativistic corrections by using a complex of computer programs [24]. The electron-impact excitation cross-sections were calculated in distorted wave (DW) with exchange approximation. The wave functions obtained in the intermediate coupling approximation with Breit–Pauli relativistic corrections from the complex of codes [22] were used for the calculation of cross-sections [36].

3. Results and discussions

The calculated energies E (in eV) of the $2p^5 3s^2 {}^2P_J$ and $2p^5 3s(L_1 S_1)3p {}^L S J$ states and experimental data [4, 6, 37] as well as theoretical values from [13] with respect to the ground state of Na are presented in Table 1. The autoionization probabilities A (in s^{-1}) calculated in the present work by using our own and Cowan [34] computer programs and those taken from [13] are also included in the Table 1. The results of Table 1 show that the energy spectrum calculated in the present work is a bit wider than that obtained including a model potential [13], therefore, the agreement between calculated and experimental spectra is better for upper levels. The ordering of the energy levels obtained coincides with that calculated in [13] and experimental one [4–6, 37], except for the $2p^5 3s({}^3P)3p {}^2S_{1/2}$, ${}^2P_{1/2}$ levels, which are obtained interchanged in our calculations. The experimental energies are in better agreement with those calculated in [13] than in the present work. They stand between the energies calculated in the present work and in [13].

An inspection of the autoionization probabilities from Table 1 leads to the conclusion that single-configuration intermediate coupling results of the present work are in better agreement with those of [13] than those calculated with Cowan program [34]. For the

Table 2. Wavelengths λ (in nm) and probabilities A (in s^{-1}) calculated in configuration interaction approximation (length L and velocity V forms), expected values of wavelengths λ_{exp} calculated by using experimental energies of levels [4, 6, 37], and fluorescence yields γ for the transition from $2p^5 3s(L_1 S_1)3p LSJ$ to $2p^5 3s^2 {}^2P_{J0}$ states in Na.

$(L_1 S_1)LS$	J	J_0	λ	λ_{exp}	A^L	A^V	γ
$({}^1P)^2S$	1/2	3/2	392.0	398.8	1.28 +7	1.01 +7	2.4 –4
	1/2	1/2	411.9	421.3	4.70 +6	3.73 +6	8.6 –5
$({}^1P)^2P$	1/2	1/2	479.3	474.3	3.79 +5	5.61 +5	1.5 –5
	1/2	3/2	452.5	446.0	5.62 +5	6.36 +5	2.3 –5
	3/2	1/2	472.9	467.9	9.07 +4	1.19 +5	1.9 –6
	3/2	3/2	446.7	440.3	9.92 +5	1.24 +6	2.1 –5
$({}^1P)^2D$	3/2	1/2	498.2	494.4	1.93 +5	3.22 +5	1.2 –7
	3/2	3/2	469.3	463.7	1.67 +4	2.82 +4	1.0 –8
	5/2	3/2	459.7	454.0	3.44 +5	5.15 +5	2.0 –7
$({}^3P)^2S$	1/2	1/2	286.4	319.7	1.89 +6	2.39 +6	6.9 –7
	1/2	3/2	276.6	306.6	5.70 +8	4.64 +8	2.1 –4
$({}^3P)^2P$	1/2	1/2	276.3	304.6	5.97 +8	4.72 +8	2.2 –4
	1/2	3/2	267.1	292.6	5.77 +6	3.41 +6	2.1 –6
	3/2	1/2	286.9	317.3	3.12 +7	2.31 +7	0.01
	3/2	3/2	277.1	304.3	5.24 +8	4.06 +8	0.48
$({}^3P)^2D$	3/2	1/2	280.0	307.0	4.67 +8	3.60 +8	0.1
	3/2	3/2	270.6	294.9	6.84 +7	5.37 +7	0.015
	5/2	3/2	280.0	308.4	4.82 +8	3.66 +8	3.1 –4
$({}^3P)^4S$	3/2	1/2	677.0	700.9	7.67 +1	1.54 +2	1.3 –5
	3/2	3/2	624.7	640.8	5.23 +2	9.12 +2	8.7 –5
$({}^3P)^4P$	5/2	3/2	496.8	490.6	1.93 +4	3.20 +4	1.4 –7
	3/2	3/2	487.6	481.5	7.01 +3	8.76 +3	4.2 –7
	3/2	1/2	518.9	514.7	3.84 +4	6.58 +4	2.3 –7
	1/2	3/2	483.0	477.2	2.65 +4	1.50 +4	1.6 –7
	1/2	1/2	513.6	509.8	3.01 +4	2.71 +4	1.8 –7
$({}^3P)^4D$	5/2	3/2	533.2	531.9	5.29 +3	1.01 +4	1.0 –7
	3/2	3/2	523.8	522.3	1.03 +4	1.63 +4	1.7 –7
	3/2	1/2	560.0	561.5	1.25 +3	2.99 +3	2.0 –8
	1/2	3/2	516.0	514.3	3.53 +3	5.77 +3	5.5 –6
	1/2	1/2	551.1	552.3	9.07 +3	1.36 +4	1.4 –5

$2p^5 3s({}^3P)3p {}^2D_{5/2,3/2}$ and ${}^2P_{3/2}$ levels an order of 2 discrepancy between our autoionization (AI) probabilities and those of [13] as well as calculated with Cowan program was obtained. The Coulomb autoionization of the $2p^5 3s3p {}^2P_J$ and $2p^5 3s3p {}^4L_J$ states is forbidden due to parity arguments. The non-zero values of AI probabilities for these levels are obtained due to admixture of the $2p^5 3s3p {}^2S_{1/2}$ and ${}^2D_{1/2,3/2}$ states. Therefore, the values of the AI probabilities from these states are smaller than those of allowed transitions (see Table 1). But the values of AI probabilities strongly depend on the coefficients of the intermediate expansion, and strong mixture of terms results in large values of calculated probabilities for the states the autoionization from which is forbidden in pure LS approximation.

The wavelengths and radiative decay probabilities for the transitions from $2p^5 3s(L_1 S_1)3p LSJ$ to $2p^5 3s^2 {}^2P_{J0}$ states and from $2p^5 3s(L_1 S_1)3p LSJ$ to $2p^6 3p {}^2P_{J0}$ states calculated in CI approximation (length L and velocity V forms) as well as fluorescence yields γ are presented in Tables 2 and 3, respectively. The AI states can decay via both radiative and autoionization transitions. The competition between these decay channels decreases the number of atoms populating the lower lying states under investigation. The probability of the radiative transition in this case is described by the ratio γ , called fluorescence yield, of the radiative transition probability between levels under investigation and the sum of the probabilities of all possible transitions (both radiative and autoionizing). For the decay of the

Table 3. Wavelengths λ (in nm) and probabilities A (in s^{-1}) calculated in configuration interaction approximation (length L and velocity V forms) and fluorescence yields γ for the transition from $2p^5 3s(L_1 S_1) 3p LSJ$ to $2p^6 3p^2 P_{J_0}$ states in Na.

$(L_1 S_1) LS$	J	J_0	λ	A^L	A^V	γ
$(^1P)^2S$	1/2	1/2	39.38	9.08 +8	8.72 +8	1.7 –5
	1/2	3/2	39.39	1.40 +9	1.35 +9	2.4 –4
$(^1P)^2P$	1/2	1/2	39.92	8.61 +8	8.23 +8	0.035
	1/2	3/2	39.92	6.39 +8	5.98 +8	0.026
	3/2	1/2	39.87	4.40 +8	4.10 +8	9.4 –3
	3/2	3/2	39.88	1.04 +9	9.92 +8	0.022
$(^1P)^2D$	3/2	1/2	40.04	1.18 +9	1.05 +9	7.2 –4
	3/2	3/2	40.05	3.83 +8	3.47 +8	2.2 –4
	5/2	3/2	39.98	1.65 +9	1.47 +9	9.5 –4
$(^3P)^2S$	1/2	1/2	37.80	2.75 +8	2.25 +8	1.0 –4
	1/2	3/2	37.80	3.65 +7	3.64 +7	1.3 –5
$(^3P)^2P$	1/2	1/2	37.62	4.52 +8	4.00 +8	1.7 –4
	1/2	3/2	37.62	4.06 +8	3.22 +8	1.5 –4
	3/2	1/2	37.81	1.05 +9	6.03 +8	0.335
	3/2	3/2	37.81	1.77 +8	2.17 +8	0.057
$(^3P)^2D$	3/2	1/2	37.68	2.57 +8	7.41 +7	0.057
	3/2	3/2	37.69	9.94 +8	6.92 +8	0.221
	5/2	3/2	37.86	1.34 +9	6.24 +8	8.7 –4
$(^3P)^4S$	3/2	1/2	40.91	9.24 +5	9.19 +5	0.154
	3/2	3/2	40.92	4.31 +6	4.30 +6	0.718
$(^3P)^4P$	5/2	3/2	40.24	1.54 +8	1.39 +8	1.3 –3
	3/2	3/2	40.18	1.67 +8	1.55 +8	1.0 –4
	3/2	1/2	40.17	1.08 +8	9.46 +7	6.5 –4
	1/2	3/2	40.15	7.16 +6	4.84 +6	2.1 –4
	1/2	1/2	40.14	3.46 +7	2.98 +7	4.3 –5
$(^3P)^4D$	5/2	3/2	40.46	5.08 +7	4.63 +7	1.0 –3
	3/2	3/2	40.41	6.03 +5	7.56 +5	9.9 –6
	3/2	1/2	40.40	7.87 +7	7.24 +7	1.3 –3
	1/2	3/2	40.36	1.37 +7	1.36 +7	0.021
	1/2	1/2	40.36	3.41 +7	3.36 +7	0.053

$2p^5 3s 3p^2 L_J$ states one autoionization ($2p^6 \epsilon l, l = 0, 2$) and two radiative channels are possible. The calculated radiative transition wavelengths, probabilities, and fluorescence yields γ for the transitions $2p^5 3s 3p^2 L_J \rightarrow 2p^5 3s^2 {}^2P_{1/2,3/2}$ and $2p^5 3s 3p^2 L_J \rightarrow 2p^6 3p^2 P_{1/2,3/2}$ are presented in Tables 2 and 3, respectively. The accuracy of these calculations can be estimated by comparing the calculated and measured wavelengths and by comparing the calculated transition probabilities in the length and velocity forms of electric dipole operator. From the data presented in Tables 2 and 3 it is seen that the agreement between transition probabilities of the length and velocity forms is very good. Thus, we can conclude that the calculated transition probabilities are reliable and suitable for further applications. We do not know the measured values of wavelengths

for the transitions under investigation. For comparison, the expected wavelengths λ_{exp} (in nm) were calculated by using the experimental energy values [4, 6, 37] (see Table 1). The accuracy of calculated wavelengths is not high, as the differences between them and expected ones reach up to 10 nm. In [3], the wavelength of the transition $2p^5 3s({}^3P) 3p^2 P_{3/2} \rightarrow 2p^5 3s^2 {}^2P_{3/2}$ was $\lambda_{\text{exp}} = 434.3$ nm. The calculated value of the same transition in the present work is 446.7 nm, and that obtained by using the experimental energies of levels is 440.3 nm. Anyway, these values can be useful for the classification of future experimental data.

The data from Tables 1 and 2 can be used for the quantitative evaluation of the contribution made by radiative cascades from the $2p^5 3s 3p LSJ$ levels to the population of the $2p^5 3s^2 {}^2P_{1/2,3/2}$ levels. As can be seen from Table 2, the fluorescence yields indicating the probability of transitions $2p^5 3s 3p LSJ \rightarrow 2p^5 3s^2 {}^2P_{1/2,3/2}$ are very small except for transitions from the $2p^5 3s({}^3P) 3p^2 P_{3/2}$ and ${}^2D_{3/2}$ levels. The corresponding contributions to the excitation cross-sections could be seen in excitation functions of the $2p^5 3s^2 {}^2P_{1/2,3/2}$ levels at 34.97 and 35.08 eV energies of exciting electron. The population density of these levels can be evaluated with the help of expression

$$N_1 = \frac{N_0 N_e v}{A_{10} + A_1^a} (\sigma_{01} + \sigma_{02} \gamma_{21}) \quad (1)$$

obtained by using the balance equations for three-level system in [16]. In (1), N_1 and N_0 are the population densities of the levels $2p^5 3s 3p LSJ$ and $2p^6 3s^2 S_{1/2}$, respectively, N_e and v are the density and velocity of exciting electrons, σ_{01} and σ_{02} are the excitation cross-sections from the ground states to the $2p^5 3s^2 {}^2P_{J_0}$ and $2p^5 3s 3p LSJ$ levels, respectively, A_{10} and A_1^a are radiative and autoionization probabilities from the states $2p^5 3s^2 {}^2P_{J_0}$, respectively, and γ_{21} is the fluorescence yield of the transition $2p^5 3s 3p LSJ \rightarrow 2p^5 3s^2 {}^2P_{J_0}$. The cross-sections for the excitation $2p^6 3s^2 S_{1/2} \rightarrow 2p^5 3s^2 {}^2P_{J_0}$ are investigated both experimentally (e. g. [1, 38]) and theoretically [38]. The excitation cross-sections of the states $2p^5 3s 3p LSJ$ were calculated in the present work by applying DW with exchange approximation. For a number of selected energies, they are presented in Table 4. One can see from Table 4 that the excitation cross-sections of the $2p^5 3s({}^3P) 3p^2 S_{1/2}$, ${}^2P_{1/2,3/2}$, and ${}^2D_{3/2,5/2}$ states are by about two orders of magnitude greater than those of the $2p^5 3s^2$

Table 4. Excitation cross-sections (in cm^2) calculated in distorted wave with exchange approximation for the transitions $2p^6 3s^2 S_{1/2} \rightarrow 2p^5 3s(L_1 S_1) 3p LSJ$ in Na for selected electron impact energies E (in eV).

$(L_1 S_1) LS$	J	$E = 30$	$E = 40$	$E = 50$	$E = 70$
$(^1P)^2S$	1/2	3.8–22	2.5–21	2.9–21	1.6–21
$(^1P)^2P$	1/2	1.2–24	8.2–24	9.4–24	5.3–24
	3/2	7.0–26	2.5–25	2.8–25	1.7–24
$(^1P)^2D$	3/2	1.6–24	5.8–24	6.4–24	3.8–24
	5/2	3.1–24	1.1–23	1.3–23	7.4–24
$(^3P)^2S$	1/2	4.0–21	2.6–20	3.0–21	1.7–20
$(^3P)^2P$	1/2	2.5–21	1.74–20	2.0–20	1.1–20
	3/2	6.9–22	5.1–21	5.5–21	3.1–21
$(^3P)^2D$	3/2	7.1–22	2.5–21	2.9–21	1.7–21
	5/2	1.7–21	6.0–21	6.7–21	4.0–21
$(^3P)^4S$	3/2	3.7–30	1.4–29	1.5–29	8.9–30
$(^3P)^4P$	5/2	2.0–25	7.1–25	7.9–25	4.7–25
	3/2	1.6–25	5.6–25	6.2–25	3.7–25
	1/2	2.1–24	1.4–23	1.6–23	8.9–24
$(^3P)^4D$	5/2	7.9–26	2.9–25	3.2–25	1.9–25
	3/2	5.6–26	2.0–25	2.2–25	1.3–25
	1/2	1.5–26	9.8–26	1.1–25	6.3–26

$^2P_{J0}$ states. The contribution of the cascade populations $\Delta = \sigma_{02}\gamma_{21}$ can be obtained from (1) as follows:

$$\Delta(^2P_{3/2}) = 0.48 \sigma(2p^6 3s \rightarrow 2p^5 3s(^3P) 3p^2 P_{3/2}) + 0.015 \sigma(2p^6 3s \rightarrow 2p^5 3s(^3P) 3p^2 D_{3/2}), \quad (2)$$

$$\Delta(^2P_{1/2}) = 0.01 \sigma(2p^6 3s \rightarrow 2p^5 3s(^3P) 3p^2 P_{1/2}) + 0.1 \sigma(2p^6 3s \rightarrow 2p^5 3s(^3P) 3p^2 D_{3/2}). \quad (3)$$

By using the excitation cross-section values from Table 4, these contributions are obtained: $\Delta(^2P_{3/2}) = 3.3 \cdot 10^{-22} \text{ cm}^2$, $\Delta(^2P_{1/2}) = 7.3 \cdot 10^{-22} \text{ cm}^2$ and $\Delta(^2P_{3/2}) = 2.4 \cdot 10^{-21} \text{ cm}^2$, $\Delta(^2P_{1/2}) = 4.3 \cdot 10^{-22} \text{ cm}^2$ for the impact energies of 35 and 40 eV, respectively. Comparison of these data with the excitation cross-section of the $2p^5 3s^2 ^2P_{1/2,3/2}$ levels of about $1.5 \cdot 10^{-18} \text{ cm}^2$ shows that the radiative cascades themselves should not effect significantly the population of $2p^5 3s^2 ^2P_{1/2,3/2}$ states.

4. Conclusions

The energy spectra of $2p^5 3s^2 ^2P_{1/2,3/2}$ and $2p^5 3s 3p LSJ$ states are calculated by using highly accurate configuration interaction wavefunctions. The contributions

of all configurations with the average weights higher than $2.0 \cdot 10^{-8}$ from the set of 13241 and 9500 of admixed configurations is taken into account. Comparison of the calculated energies with other available data shows that experimental energy values stand between the present data and those obtained in [13]. The calculated autoionization and radiative decay probabilities for the $2p^5 3s 3p LSJ$ levels are used to obtain the fluorescence yields for the $2p^5 3s 3p LSJ \rightarrow 2p^6 3p ^2P_{1/2,3/2}$ radiative transitions. The evaluations based on these data and calculated excitation cross-sections allow us to come to a conclusion that the radiative cascades themselves should not effect significantly the population of the $2p^5 3s^2 ^2P_{1/2,3/2}$ states.

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RADIACINIAI ŠUOLIAI TARP ŽEMIAUSIŲ Na ATOMO AUTOJONIZACINIŲ BŪSENŲ

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Santrauka

Užregistruotame Na atomo sužadinimo į $2p^5 3s^2 \ ^2P_{1/2,3/2}$ būsenas skerspjūvyje ties 32–33 ir 36,5–40 eV žadinančio elektrono energijomis pastebėti maksimumai, kurių negalima paaiškinti $2p^5 3s 3p \ ^4S$ rezonansų susidarymu. Norint išsiaiškinti jų priežastį, atlikti labai tikslūs $2p^5 3s^2 \ ^2P_{1/2,3/2}$ ir $2p^5 3s 3p \ ^4S$ būsenų energijos spektrų ir radiacinių šuolių tarp jų tikimybių skaičiavimai. Sužadinimo į $2p^5 3s^2 \ ^2P_{1/2,3/2}$ skerspjūvio priedui dėl kaskadų iš $2p^5 3s 3p \ ^4S$ įvertinti taip pat apskaičiuotos $2p^5 3s^2 \ ^2P_{1/2,3/2}$ ir

$2p^5 3s 3p \ ^4S$ būsenų autojonizacijos tikimybės, fluorescencijos našumai ir sužadinimo į $2p^5 3s 3p \ ^4S$ skerspjūviai. Rasti 2 lygmenys $2p^5 3s(^3P)3p \ ^2P_{3/2}$ ir $^2D_{3/2}$, iš kurių fluorescencijos našumai dideli, ir būtų galima tikėtis pastebimo kaskadų indėlio. Atlikus įvertinimus, panaudojant apskaičiuotus sužadinimo skerspjūvius, tenka padaryti išvadą, kad šuolių iš $2p^5 3s 3p \ ^4S$ skerspjūvio priedas $2p^5 3s^2 \ ^2P_{1/2,3/2}$ sužadinimo skerspjūviui yra per mažas maksimumams eksperimentiniame spektre paaiškinti.