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On spectroscopic classification of autoionizing levels in Rb atoms

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Synopsis Large scale configuration interaction calculations of energy levels, autoionization probabilities and electron-impact excitation cross sections of the autoionizing states $4p^5nln'l'$ (nl =5s,4d,4f,n'l'=$4d, 5s, 5p, 5d, 5f, 5g, 6s, 6p, 6d, 7s, 7p$) of Rb up to 19.6 eV were performed for the first time. The relativistic effects were taken into account in the Dirac-Fock-Slater approximation. The calculated data were used for the novel classification of the lines in an experimental ejected-electron spectrum.

The energy spectra of the autoionizing states of alkali metal atoms were investigated in many experiments by registering ejected-electron (e.g. [1, 2] and references in [2]) or radiation (e.g. [3, 4]) spectra. The purpose of the present work was to perform more accurate calculations of the excitation energies for $4p^5nln'l'LSJ$ states of Rb by using large scale CI approximation in the basis of relativistic Dirac-Fock-Slater [5] radial orbitals and apply the theoretical values of them for the assignment of experimental ejected-electron spectrum [1]. As the spectra in [1] were presented for electrons ejected at the polar angle of 75^o with respect to the incident electron beam, the influence of the asymmetry of the angular distribution of Auger electrons were taken into account in the comparative analysis of calculated and experimental [1] relative intensities of lines for identification of autoionizing states in Rb atoms.

The calculations of energies, autoionization probabilities and electron impact excitation cross sections were performed in the basis of mixed relativistic configurations by using FAC computer code [5]. The radial orbitals for the construction of basis state wave functions were derived from a modified self-consisted Dirac-Fock-Slater iteration on the fictitious mean configuration with fractional occupation numbers representing the average electron cloud of the configurations included in the calculation. In order to optimize the local central potential including the approximated exchange part, the configurations $4p^6nl$, $n = 5, ..., 12$, $l = 0, 1, 2$ and nl =4f,...,10f, 5g,...,10g were used. The following 4p-core excited configurations were used to take into account the correlation effects as well: $4p^5nln'l'$, nl =5s,...,8s; 5p,...,8p; 5d,...,7d; 4f,5f; $n'l'$ =5s,...,10s; 5p,...,10p; 4d,...,10d; 4f,...,7f; 5g,...,7g. The same basis set was used to calculate cross sections and autoionization probabilities. The final state $4p^6\ ^1S_0$ of Rb^+ was obtained in a single configuration approximation.

The excitation cross sections were calculated in a relativistic distorted wave approximation [5]. The autoionization probabilities were calculated in relativistic distorted wave and isolated resonance approximations.

Theoretical classification of the levels was performed by assigning the quantum numbers of the term with the largest expansion coefficient. But, in the energy interval between 15.258 eV and 19.410 eV, the quantum numbers of the smaller expansion term were attributed to 15 levels. The identification of experimental spectrum is more reliable if it is possible to make the comparison of the intensities of calculated and measured spectra. The intensities of spectral lines are proportional to the electron-impact excitation cross sections. The influence of the asymmetry of the angular distribution was taken into account performing the novel identification of the ejected electron spectrum [1].

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