ENERGIES AND WIDTHS OF THE $2s2p^6nl$ AUGER STATES IN NA^+

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The interpretation of ejected-electron spectra of sodium is additionally complicated by the fact that the Auger lines, originated from autoionizing states of both Na and Na^+, lie in the same energy region. In our previous paper [1] we presented the systematic calculations of energies and decay rates for the $2p^53snl$ ($n\leq8$) core-excited states in Na. In the present study we calculated furthermore the energies and widths of the Na^+ states with the $2s2p^6nl$ configurations, thus providing a possibility for a complete classification of lines in the electron spectra. Another motivation for the present study is the recent investigation of L-shell ionization of laser excited Na atoms [2]. Energy splitting of observed Auger lines due to spin-orbit interaction in the final state in combination with the experimental resolution of the total orbital angular moment of the initial laser-excited atomic state provides a rare possibility to study experimentally the partial widths and to test critically the theoretical values.

In present study, the $2s2p^6nl$ states are considered as confined core $2s2p^6$ plus far removed and weakly interacted outer electron nl. Then the frozen-core Hartree-Fock approximation is expected to suit for description of such states as first approximation with two additional improvements. The first is to use the many-configuration wavefunction for description of the core itself to introduce the inner-core correlation. Adding to the Hartree-Fock $2s2p^6$ core as correlation configurations $2s^22p^43l$ (l=0,1,2) and minimizing again the total energies within the many-configurational scheme, the following configuration mixing is obtained: $\Psi(2s2p^6) = 0.9814\ 2s2p^6 + 0.1800\ 2s^22p^43d + 0.0667\ 2s^22p^43s$ + 3 minor terms due to $2s^22p^43p$. The second improvement is the introduction of the core-polarization potential for outer electron to simulate the core-valence correlation. Auotoionizing rates were obtained by the well-known golden-rule-like expression, with using the close-coupling approximation to describe the final continuum wavefunction of the system 'ion+electron'.

Comparison of the resulting energies with the Hartree-Fock values show that the maximum correlation corrections are 0.24, 0.15, 0.06 eV for the 3s, 3p and 3d states, respectively, and they are caused mainly by the core polarization. Analyses of the partial widths obtained shows that the main corrections are connected with the inner-core correlation (up to the factor of 2.5), whereas the influence of the core polarization is much smaller (<10%). The close-coupling corrections have the same order of magnitude (<5%), except for the $2p^5\varepsilon p\ ^1S$ widths, where the virtual trap of ejected electron on unfilled shell of the residual ion increases the width by a factor of 3. The close agreement between experiment [2] and theoretical shapes of Auger lines indicates qualitatively a good agreement of total widths, whereas the agreement between the relative intensities of lines indicates the quality of the obtained partial widths. The relative intensities calculated with both correlated core and polarization potential are in a close agreement with the experimental data. The ratio of the partial widths was proved to be very sensitive to the approximation used and clearly indicates the importance of various correlation corrections. The most of corrections is connected with the inner-core correlation. The core-polarization contribution is much smaller, but it also gives rise to detectable corrections exceeded the experimental uncertainty.

1. O. Zatsarinny and L. Bandurina // J.Phys.B:At.Mol.Opt.Phys. , 1993, v.26, p.3765.
2. A. Dorn et al // J.Phys.B:At.Mol.Opt.Phys.,1995, v.28, p.L225.