K-shell Excitation in the Photoionization of the Open-shell Cl Atom

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Synopsis Calculations of the photoionization of atomic chlorine have been performed using the Belfast R-matrix methodology in the vicinity of the two lowest 1s ionization thresholds with the emphasis on the resonances converging to these thresholds. The results show the dominance of the 1s→3p ^{2}S resonance which occurs owing to the open 3p subshell atomic chlorine. In addition, the effects of interaction of the two series converging to each of the ^{3}P and ^{1}P thresholds on each other is found in each of the ^{2}S, ^{2}P and ^{2}D final-state manifolds.

The theoretical study of the photoionization of open-shell atoms is far more complicated than closed-shell owing to the various angular-momentum coupling engendered by the open-shall nature of the system. Building on previous theoretical work on atomic chlorine [1], the photoionization cross section is studied in the vicinity of the 1s threshold using the Belfast R-matrix method. Specifically, the cross sections and the resonances leading up to the first two 1s ionization thresholds, the $1s2s^22p^63s^23p^5$ ^{3,1}P states of Cl^+, have been examined in detail. Since the initial (ground) state of the Cl atom is $1s^22s^22p^63s^23p^5$ ^{2}P, there are three possible symmetries for its final state continua, namely ^{2}S, ^{2}P and ^{2}D. The dominant resonance, shown in Fig. 1, is the 1s→3p, which can only be ^{2}S owing to the angular momentum coupling, and is allowed because the 3p subshell of atomic chlorine is an open subshell.

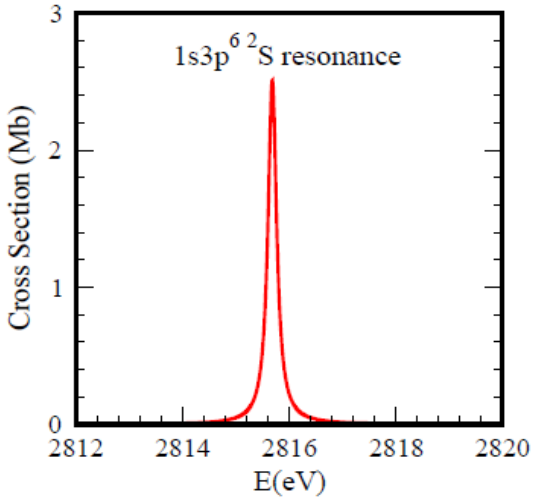

Figure 1: Calculated 1s→3p ^{2}S resonance in the photoionization cross section of atomic chlorine.

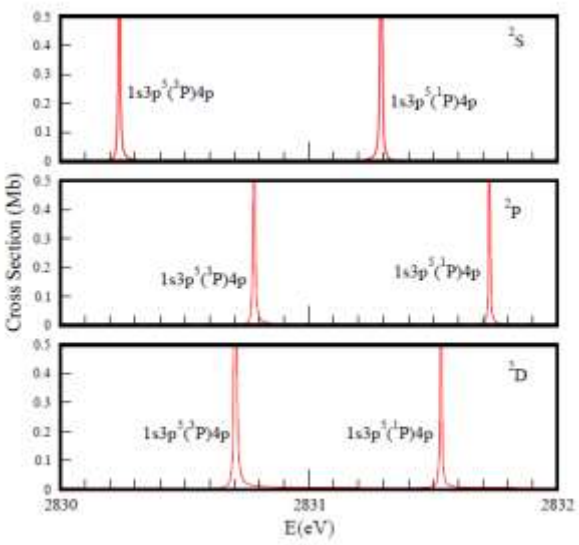

Figure 2: Calculated 1s→4p resonances in atomic chlorine converging to each of the ^{3}P and ^{1}P ionization thresholds for ^{2}S, ^{2}P and ^{2}D final states.

For the higher resonances, for each principal quantum number, n, there are six resonances, one converging to the ^{3}P threshold and one converging to the ^{1}P threshold, in each of the ^{2}S, ^{2}P and ^{2}D final states of the system. The six n=4 resonances are shown in Fig. 2 where it is evident that their energies are very dependent upon the details of the angular momentum coupling; the positions vary considerably with the angular momentum of the final state. In addition, the separation of the pair of resonances in each of the final-state manifolds differs considerably, as seen from Fig. 2.

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Reference

[1] W. C. Stolte, *et al*, Phys. Rev. A **88**, 053425 (2013).

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