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 2S 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 3P and 1P thresholds on each other is found in each of the 2S, 2P and 2D 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-shell 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 1s2s2p63s23p5 3P states of Cl+, have been examined in detail. Since the initial (ground) state of the Cl atom is 1s2s2p63s23p5 3P, there are three possible symmetries for its final state continua, namely 2S, 2P, and 2D. The dominant resonance, shown in Fig. 1, is the 1s→3p, which can only be 2S owing to the angular momentum coupling, and is allowed because the 3p subshell of atomic chlorine is an open subshell.

For the higher resonances, for each principal quantum number, n, there are six resonances, one converging to the 3P threshold and one converging to the 1P threshold, in each of the 2S, 2P and 2D 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

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

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

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