Doubly excited states in the photoionization of the ground state of Mg

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There has been great interest in the photoabsorption studies of atoms and ions with two valence electrons because of the relative simplicity of these atomic systems to understand electron correlation effects. Photoionization cross sections of magnesium are also needed for astrophysical applications. We studied photoionization of the ground $3s^2\ ^1S$ state of atomic magnesium in the energy region between the Mg^+(3s) and Mg^+(4p) thresholds using noniterative variational R-matrix method [1] combined with multichannel quantum defect theory at the R-matrix surface. The initial and final states are represented by configuration-interaction wave functions. The calculated ionization energies of the Mg^+(3s, 3p, 4s, 3d and 4p) states relative to the ground state of atomic magnesium show excellent agreement with the experimental values.

We calculated total and partial photoionization cross sections in both length and velocity formulations. There is excellent agreement between length and velocity gauges in our calculation. Most of the earlier studies focused on photoionization of the ground state of Mg in the energy region between the Mg^+(3s) and Mg^+(3p) thresholds where there is only one open channel. We calculated total and partial photoionization cross sections for photon energies up to the Mg^+(4p) threshold.

The photoelectron angular distribution asymmetry parameter β for leaving the ion in the Mg^+(3p) state is calculated for the first time. The angular distribution parameter varies with photon energy between the expected values of -1.0 and 2.0. The resonance features in the angular distribution asymmetry parameter show up more clearly than in the photoionization cross sections. In order to examine the doubly excited autoionizing levels below the Mg^+(4p) threshold, we performed a detailed variational R-matrix calculation to obtain position E_r, effective quantum number n^* and width Γ of the major levels of the 3pns, 3pnd and 4pns series of autoionizing resonances. Theoretical resonance parameters are calculated from the maximum derivative of the eigenphase sum δ which is the sum over the eigenphase in each channel. Our length photoionization cross sections (solid curve) in the energy region below the Mg^+(3p) threshold are compared with the Opacity Project [2] calculation (dotted curve) in Fig. 1. The shape of cross sections in the two calculations show excellent agreement. The resonance structure in the Opacity Project calculation is shifted by about 0.062 eV to higher energy side. Our results will be compared with other calculations and experiments.

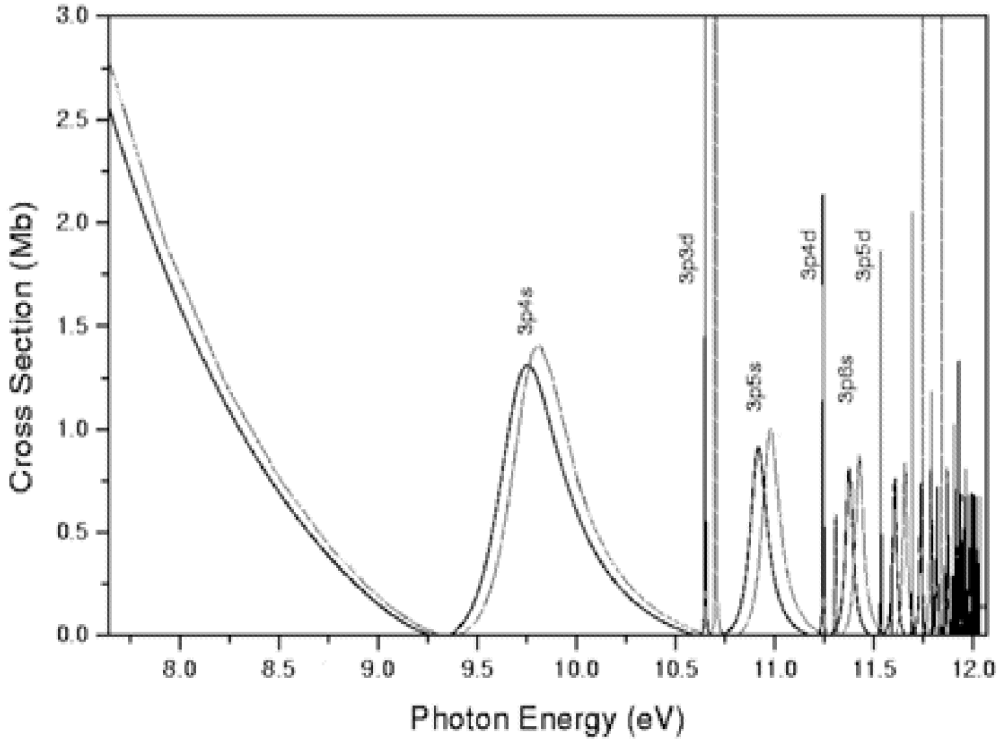

Figure 1: Total photoionization cross sections for ground state of Mg as a function of photon energy below the $Mg^+(3p)$ threshold. Present results: Solid curve; Opacity Project: dotted curve.

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