Photoionization cross sections of Ar^+ ions

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The ground state photoionization of an initial Ar II ion containing 17 electrons can be described by the following process (A benchmark for comparison can be obtained in the literature [1]);

$$h\nu + \text{Ar II} \rightarrow \text{Ar III} + e^-.$$

The ground state of Ar II has electronic configuration $1s^2 2s^2 2p^6 3s^2 3p^5 (^2P^o)$ and the ion Ar III is left in a possible excited final target state with an ejected electron in the continuum. To compute any relevant atomic data, we implemented a fully relativistic Breit-Pauli R-matrix calculation [2, 3]. The R-matrix method [4, 5] deals with the division of configuration space into an internal and external region by a sphere of fixed radius $r_a = 16.6$ a.u. centered upon the nucleus of point mass. The photoionization cross sections σ, are obtained by matching the solutions at open and closed channel boundary conditions via the R-matrix at r_a and are defined in the following way,

$$\sigma = \frac{4}{3}\pi^2 a_o^2 \alpha \frac{\omega}{g_i} S.$$

Where a_o is the bohr radius, α the fine structure constant, ω the photon energy and g_i the statistical weight of the initial bound state. S is given as the generalized line-strength describing a transition between an initial bound state to a final free state comprised of either the dipole length or velocity approximations. These dipole approximations arise from the truncation of the wave function which results in minor discrepancies. The final scattering state is represented by the wavefunction of the residual ion plus the ejected continuum electron.

The present model has been established by implementing Hartree-Fock orbitals of 1s, 2s, 3s, 2p, 3p from the tables of Clementi and Roetti [6]. In order to extend the model, the orbitals 3d, 4s, 4p, 4d were optimized on the lowest lying energy levels observed by NIST [1] with the aid of CIV3 [7], whilst maintaining a closed $1s^2 2s^2 2p^6$ core. The addition of these optimized orbitals resulted in a total of 7 possible configurations and 64 LSπ target states. The possible 17-electron configurations are thus constructed from this orbital set. The partial wave contribution included L=0 to L=10 for both even and odd parities and in the external region a mesh of 80,000 energy points was chosen for the continuum electron to obtain convergence of the resonant structures.

In consideration with the $^2P^o$ initial ground state, we are primarily concerned with the dipole matrices describing the transitions of $^2P^o \rightarrow {}^2S^e, {}^2P^e, {}^2D^e$ in compliance with the selection rules. With this information we are able to obtain partial and total cross sections. Results will be presented at the conference for both LSπ transitions and Jπ fine-structure transitions. Also presented along with ground state photoionization will be excited state photoionization cross-section results.

References

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