Low-energy outer-shell photodetachment of the negative ion of aluminum

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Synopsis The photodetachment of the negative ion of Al is investigated by employing the *B*-spline *R*-matrix method for photon energies ranging from threshold to 12 eV. Several prominent resonance features are predicted, thereby providing new challenges in the study of this highly correlated process.

The photodetachment of Al^- investigated in the present work is part of our systematic study of the photodetachment of negative ions from the IIIB group of the periodic system [1,2]. Negative ions in this group have the $(ns^2np^2)^3P$ ground state, and photoexcitation of the ns electron leads to prominent $nsnp^3$ resonances. The accurate description of these resonances is a major challenge for theory. As shown in our recent study of the photodetachment of B^- [1] and Ga^- [2], their interpretation is not trivial and has led to different assignments in various previous calculations.

The calculations were performed with the B-spline R-matrix code [3]. The multi-configuration Hartree-Fock method with non-orthogonal orbitals in connection with B-spline expansions was employed for an accurate representation of the target wave functions. The scattering model contained the lowest 10 bound states of aluminum up to the $3s^26s$ state, plus the 3s-excited states $(3s3p^2)^2S$ and $(3s3p^2)^2P$ that lie in the target continuum. The latter states were included to allow for a proper description of the 3s photodetachment.

Figure 1 exhibits our results for the total photodetachment cross section of Al^- from its ground $(3s^23p^2)^3P$ state, with affinity of 432 meV. The cross section shows a complicated energy dependence due to different partial-wave and resonance contributions. Details will be presented at the conference. In particular, the minimum at 3.87 eV is due to the $(3s3p^3)^3D^o$ window resonance, whereas the sharp peak at 3.69 eV is due to the $(3s^24s4p)^3P^o$ resonance. This finding is in close agreement with the experimental measurements [4].

The Al^- ion has an excited $(3s^23p^2)^1D$ bound state with a binding energy of 0.109 eV. The total photodetachment cross sections for the ^1D initial state is presented in Fig. 2. The cross sections exhibit prominent resonance-like structures, but not all peaks can be related to particular resonances: only the maximum around 6 eV is due to the combined contribution of two $(4s4p^3)$ ^1P and ^1D negative-ion states. All other structures reflect near-threshold maxima caused by the opening of new channels.

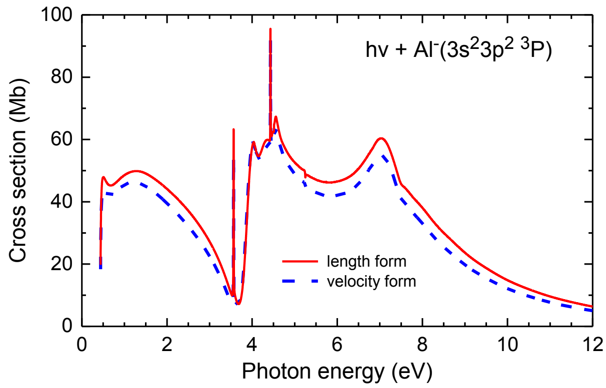

Figure 1. Total photodetachment cross sections of Al^- from the ground $(3s^23p^2)^3P$ state.

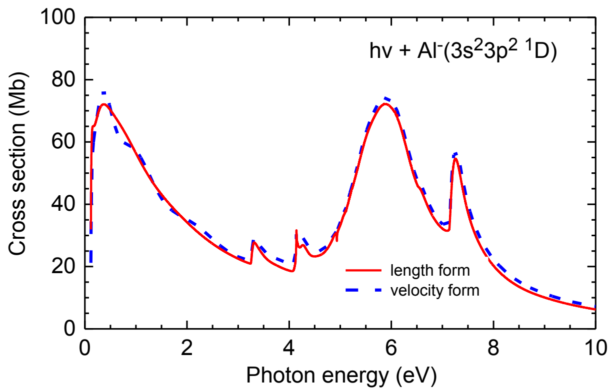

Figure 2. Total photodetachment cross sections of Al^- from the excited $(3s^23p^2)^1D$ state.

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References

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