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Photoionization of magnesium near threshold

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The observation of structure in the photoionization cross section of magnesium in the vicinity of the 3*s* threshold is reported. The structure is the result of simultaneous (single photon) two-electron excitation followed by autoionization. The data are in excellent agreement with theory.

Photoionization of alkaline earth atoms is interesting because the autoionizing resonances that occur in the vicinity of the first-ionization-threshold result from simultaneous excitation of the two outer *ns* electrons. Because of this property, and, of course, their astrophysical importance, photoionization of both magnesium and calcium has been extensively studied. Two rather comprehensive theoretical treatments of photoionization of magnesium have been reported, one using the relativistic random-phase approximation[1] (RRPA), and the other the Fano continuum configuration interaction formalism.[2] This latter work included both autoionizing and continuum states. Experimental work on photoionization of magnesium near threshold has been performed only by photoabsorption and has been reported by Ditchburn and Marr,[3] Esteva, Mehlman-Balloffet, and Romand,[4] and Mehlman-Balloffet and Esteva.[5] The experiment of Ditchburn and Marr was restricted to wavelengths in the interval 1450–1650 Å which included neither the Cooper minimum[6] nor any autoionizing resonances. The other two experiments employed a wider range of wavelengths, but, because they were performed using a magnesium plasma, data analysis was complicated by large variable background signals.

The experiments reported here were designed to provide new data on photoionization of magnesium near threshold. Rather than examine photoabsorption as in the earlier work, we have chosen to make our measurements by directly detecting the product Mg^+ ions. The wavelength range included the 1622-Å 3*s* threshold (7.644 eV) and extended down to 1100 Å ($\sim$11.3 eV). Indeed, we observe both the Cooper minimum and two-electron excitations, the data being in excellent agreement with both the theoretical predictions of Ref. 2 and the earlier experiments.

Radiation from the National Synchrotron Light Source (NSLS) at Brookhaven National Laboratory was used in these experiments, which were performed at the Chemistry Department windowed beam line, U9A. After passing through the LiF window, which is opaque to wavelengths below $\sim$1100 Å, synchrotron light was dispersed using a 0.5-m Seya-Namioka normal-incidence grating spectrometer. After wavelength selection the light beam was directed into a reaction cell at which point it was intersected by a beam of magnesium atoms.[7] Ions formed at the intersection of the beams were electrostatically extracted from the cell in a direction perpendicular to the plane defined by the two beams; scattered light produced no observable effects. After extraction the ions were focused into a quadrupole mass filter and detected with a channeltron particle multiplier using conventional single-particle counting techniques. Data were acquired with the setting of the mass filter fixed at 24 amu, while the wavelength of the synchrotron light was varied stepwise. Ion counts were accumulated for a fixed time, typically 2 sec, at each wavelength setting, thus yielding an ion signal versus wavelength function. Variation of the photon flux as a function of wavelength was simultaneously measured using a sodium salicylate coated photomultiplier tube. This permitted us to correct the ion signal for variations of the incident photon flux with wavelength. Although the synchrotron radiation is delivered to the beam line in pulses, the rapid repetition rate, every 170 nsec in the single bunch mode, as compared with the dwell times, permitted the experiment to be carried out in a quasi-continuous-wave mode. Uncertainties in the absolute values of the photon flux and the magnesium atom density prevent us from reporting absolute cross sections at this time.

Figure 1 shows both the data, corrected for the wavelength dependence of the photon flux, and the theoret-

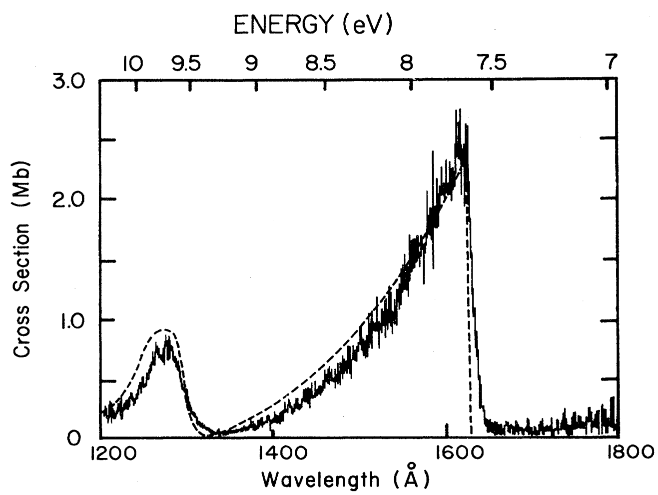

FIG. 1. Photoionization cross section as a function of wavelength. The bandwidth of the ionizing radiation was 16 Å FWHM. The dashed curve was taken from the theoretical treatment of Ref. 2. The data have been normalized to the theoretical value at threshold.

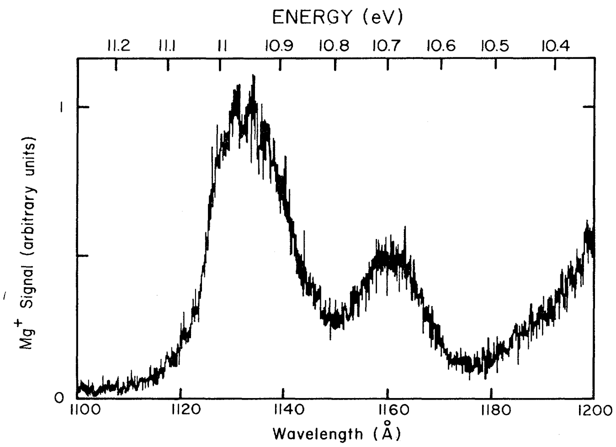

FIG. 2. Photoionization cross section in the wavelength range 1100–1200 Å. The bandwidth of the ionizing radiation was 4 Å FWHM. These data have not been corrected for the wavelength dependence of the photon flux.

ical photoionization cross section[2] in the wavelength range 1200–1800 Å. The bandwidth of the incident radiation was 16 Å full width at half maximum for this particular scan. Because we are unable to obtain abosolute cross sections, the data have been normalized to the theoretical value at threshold. The agreement between theory and experiment in this wavelength range is excellent. The minimum at ~1341 Å (9.25 eV), at which point the Mg^+ signal completely disappears, is probably the Cooper minimum, the location of which is predicted to within ~0.15 eV by Bates and Altick.[2] Deshmukh and Manson,[1] using the RRPA, predict an energy of 11.1 eV for the location of the Cooper minimum. The probable reason for the better agreement with Bates and Altick is that their calculation was performed with an explicit multiconfigurational wave function containing more of the correlations important in the threshold region than were included in the RRPA treatment.[8]

Because the threshold energy for inner-shell ionization is considerably higher than the photon energies available in these experiments, the peak in the photoionization cross section at ~1265 Å must result from autoionization of doubly excited MgI states embedded in the Mg^+ continuum. Here again the correlation between theory and experiment is striking. According to Bates and Altick[2] this peak is the result of simultaneous excitation of the two 3*s* electrons to a 3*p*4*s* state. In fact, although the photon flux below 1200 Å is quite low, we were able to observe two additional resonances at 1132 and 1160 Å. Figure 2 shows these data which, because of the low, but slowly varying photon flux, have not been corrected. The widths of the resonances, ~10 Å, are in excess of the 4-Å bandwidth of the ionizing radiation, and suggest autoionizing lifetimes of ~10^{-14} sec.

If the selection rules for LS coupling are strictly obeyed for these two electron excitations, the only states that can be produced by photoabsorption are those with $^1P^o$ designations. Although several doubly excited states lying in the Mg^+ continuum are known spectroscopically,[9,10] none are $^1P^o$, making it unlikely that these are the ones we are observing. The configuration interaction calculations of Bates and Altick[2] indicate that the two electron resonances observed here are the 3*p*4*s*, 3*p*3*d*, and 3*p*5*s* $^1P^o$ autoionizing states. Table I contains a listing of their calculated energies together with the energies as determined by absorption spectroscopy[4] and in this work. Comparison shows that, in addition to the satisfying agreement between our data and the theoretically determined wavelength dependence of the cross section, there is also excellent agreement in the absolute values of the energies of the autoionizing states. It is clear that at wavelengths shorter than that at which the Cooper minimum occurs the photoionization cross section is indeed dominated by the effects of autoionizing resonances as predicted by theory.[2]

TABLE I. Energies (in eV) of $^1P^o$ doubly excited states of MgI as determined by theory, absorption spectroscopy, and this work.

State	Theoretical[a]	Absorption[b]	This work
3*p*4*s*	10.0	9.85	9.76
3*p*3*d*	10.8	10.65	10.69
3*p*5*s*	11.1	10.93	10.95

[a] Reference 2. [b] Reference 5.

Further work on photoionization of magnesium is expected to clarify the nature of the two electron resonances. It would be desirable to investigate the possibility that additional structure in the ionization efficiency function is present, as is suggested by close examination of the peaks in our data. Such a study would require higher resolution (narrower bandwidth of the ionizing radiation) than that employed in the work reported here. It is also planned to extend the wavelength range to permit examination of higher-energy resonances by using the windowless beam line, U11. In fact, using the NSLS it should be possible to extend the wavelength range to the extreme ultraviolet so that inner-shell ionization of magnesium can also be studied.

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