Proceedings - Conference on Autoionization of Atoms and Small Molecules
Argonne National Laboratory, May 2-3, 1985

BNL 36406
BNL--36406

DE85 011812

PHOTOIONIZATION OF ALKALI AND ALKALINE EARTH ATOMS: Na AND Mg

Jack M. Preses
Department of Chemistry, Brookhaven National Laboratory,
Upton, NY 11973

C. E. Burkhardt, R. L. Corey, D. L. Earsom, T. L. Daulton,
W. P. Garver, J. J. Leventhal
Department of Physics, University of Missouri, St. Louis, MO 63121

A. Z. Msezane
Department of Physics, Atlanta University, Atlanta, GA 30314

S. T. Manson
Department of Physics and Astronomy, Georgia State University,
Atlanta, GA 30303

ABSTRACT

Determinations of the photoionization cross sections of ground state magnesium atoms and excited state sodium atoms have been made over a wide wavelength range. The ground state measurement in magnesium was performed using synchrotron radiation from the UV ring at the National Synchrotron Light Source. Several autoionizing resonances were observed. The photoionization cross section of excited sodium atoms was determined by irradiating laser-produced Na(3p) with synchrotron light. In both cases, agreement with theory is excellent. Future experiments will be directed toward examination of photoionization of laser excited alkaline earth metals; these experiments should yield a wealth of new data on autoionizing states.

INTRODUCTION

Theoretical calculations and experimental measurements of photoionization cross sections of atoms and molecules have been the subject of great interest in recent years.[1,2] The advent of intense laser sources in the visible and UV regions of the spectrum made such measurements much simpler than with other laboratory sources. However, these studies are subject to a number of restrictions. Photoionization thresholds of most atoms and molecules tend to lie in regions of the UV where laser sources are weak, not broadly tunable, and inconvenient to use. Inner shell ionizations are especially difficult to study for these reasons. In addition, molecular species, with large numbers of electrons in orbitals not of high symmetry do not lend themselves to simple theoretical treatments. In spite of these difficulties measurements have been made.[1,2,3] These determinations, however, have largely been done for ground state systems. Experiments designed to study photoionization of electronically excited systems are scarce,[3] especially over an appreciable range of ionizing energies. We have chosen to exploit the unique features of laser radiation (high intensity) together with those of synchrotron radiation (broadband tunability) in order to study the photoionization of atoms.

Alkaline earth atoms are especially interesting because they generally have autoionizing resonances near the first ionization threshold due to states populated by simultaneous excitation of the two outer ns electrons. Therefore, atoms from this group have attracted the interest of both experimentalists and theoreticians. There have been two theoretical treatments of photoionization in magnesium; one using the relativistic random-phase approximation,[4] and the other using the Fano contin um configuration interaction method.[5] Several measurements of the photoionization cross section of ground state magnesium near threshold have been reported,[6-8] but none of these represented a continuous determination over a wide wavelength range. We decided, therefore, to study photoionization of ground state magnesium atoms as our first experiment using the windowed line at the National Synchrotron Light Source.[9] This experiment is ideally suited to the windowed beam line.

EXPERIMENTAL

The relative cross section was measured over a wavelength range from threshold to about two eV above threshold. Synchrotron radiation, passed through a LiF window to isolate the apparatus from the ring, was dispersed through a 0.5 m Seya-Namioka monochromator (16.7 Å/mm, slit width 1.0 mm). The synchrotron light intersected an effusive beam of magnesium atoms at right angles. Ions were extracted electrostatically and were focused into a quadrupole mass filter set to pass 24 a.m.u. Ions were counted using a Channeltron, and spectra were accumulated in a LeCroy 3500 multichannel analyzer with a 3521A MCS module controlled by an external computer. Data were corrected for the variation of photon flux as a function of wavelength using a photomultiplier and sodium salicylate. Typically, 1024 samples were taken between 1200 and 1800 Å, with a dwell time of two seconds at each wavelength. The synchrotron produced 500 psec (FWHM) pulses every 180 nsec (single bunch mode); this high repetition rate permitted the experiment to operate in a quasi-CW mode. By collecting ion counts vs. wavelength, and subsequently correcting the shape of the curve thus obtained for photon flux, the shape of the photoionization cross section as a function of wavelength was obtained. One of the advantages of this method in which the photoionization signal is itself the (mass analyzed) photoions is that it eliminates spurious effects due to contaminants such as may occur in a photoabsorption experiment.

RESULTS

Figure 1 shows the data for magnesium corrected for the variation of the synchrotron photon flux. Also plotted is the theoretical prediction from reference 5. Since our data are relative, we have normalized the calculation and the experimental result at the threshold. When our data are thus normalized the agreement between experiment and theory is excellent. The minimum near 1341 Å is probably the Cooper minimum[4,5] predicted to lie near 10 eV. The feature near 1265 Å, and two additional peaks shown in Fig. 2 are autoionizing resonances arising from the 3p4s, 3p3d, and 3p5s doubly excited states of neutral magnesium. Because the photon flux on beam line U9A is very low at wavelengths shorter than 1200 Å, the data shown in Fig. 2 have not been corrected for photon flux. The wavelengths at which these resonances occur correspond to energies of the autoionizing states in excellent agreement with those predicted in the theoretical treatment of ref. 5. For our second experiment we wished to study photoionization of a laser excited atom. Because of our extensive experience with sodium, and because a CW laser that could provide the D-line wavelengths was available, we chose to study the photoionization of Na(3p). The apparatus used in these experiments was the same one used in the magnesium work with the addition of the laser, the beam from which intersected the sodium atom beam antiparallel to the dispersed synchrotron beam. Since the synchrotron radiation wavelengths available with the windowed line are not short enough for inner shell excitations, autoionizing resonances were not studied. Nevertheless the results are quite intriguing. The bandwidth of the synchrotron radiation was about 10 Å, and samples were taken every 2 Å with a dwell time of two seconds per sample. The quadrupole mass filter was, of course, set to 23 a.m.u. and the detector was a conventional Cu:Be particle multiplier.

The synchrotron-based measurements yield the relative photoionization cross sections, but measurement of the absolute magnitude, at least for Na(3p) is more easily accomplished using two pulsed lasers, one tuned to a D line, and the other tuned to the Na(3p) threshold wavelength. This measurement, performed in the atomic physics laboratory at UMSL, yielded a threshold value of 8.5 Mb, remarkably close to the theoretical value. Scaling of the synchrotron data thus permitted the determination of the cross section over the entire range.

The cross section (Fig. 3) rises sharply at threshold, then drops monotonically as the photon energy increases. The rise at the high energy end of the plot is due to the onset of ground state (^2S) photoionization, and may be ignored for the purposes of the present discussion. Also shown in the figure are two calculations of the absolute cross section. The upper line is the result of a central field Hartree-Slater calculation.[11-13] The lower line is a Hartree-Fock calculation. The excellent agreement between the two calculations (and the experimental data) is a measure of the confidence one may place in the reliability of the calculations. In fact, the Hartree-Fock calculation shown is the average of the Hartree-Fock cross sections determined in the dipole-length and the dipole-velocity formulations. In this case, the two Hartree-Fock calculations produced results so close together, that they could not be plotted together clearly.

The wavelength range of the data shown in Fig. 3 does not include the Cooper minimum expected in 3p→εd transitions, about 10 eV above threshold in this system. It is expected that cross section calculations will be least accurate in such regions. However, the present results indicate that theoretical predictions of photoionization cross sections far from Cooper minima can be quite accurate.

It is our intention to perform additional experiments on excited atoms. We are particularly interested in extending our studies of ground state magnesium to investigate photoionization of Mg (3s3p, $^1P^o$). However, limitations associated with the expense of obtaining CW laser light at the 2852 Å resonance line of magnesium may make it necessary to study photoionization of Ba (6s6p $^1P^o$) next. In either case, we expect to obtain new information on autoionizing resonances.

ACKNOWLEDGEMENT

This research was carried out at Brookhaven National Laboratory under contract DE-AC02-76CH00016 with the U. S. Department of Energy and supported by its Division of Chemical Sciences, Office of Basic Energy Sciences.

REFERENCES

1. J. A. R. Samson, "Atomic Photoionization", Handbuch der Physik, (Springer-Verlag, Berlin, 1982), Vol. XXXI, p. 123.
2. J. Berkowitz, Photoabsorption, Photoionization and Photoelectron Spectroscopy (Academic Press, 1979).
3. H. T. Duong, J. Pinard, and J.-L. Valle, J. Phys. B 11, 797 (1978).
4. P. C. Deshmukh and S. T. Manson, Phys. Rev. A 28, 209 (1983).
5. G. N. Bates and P. L. Altick, J. Phys. B 6, 653 (1973).
6. R. W. Ditchburn and G. B. Marr, Proc. Phys. Soc. London, Sect. A 66, 655 (1953).
7. J. M. Esteva, G. Mehlman-Balloffet, and J. Romand, J. Quant. Spectrosc. Radiat. Transfer 12, 1291 (1972).
8. G. Mehlman-Balloffet and J. M. Esteva, Astrophys. J. 157, 945 (1969).
9. J. M. Preses, C. E. Burkhardt, W. P. Garver and J. J. Leventhal, Phys. Rev. A 29, 985 (1984).
10. C. E. Burkhardt, R. L. Corey, W. P. Garver, J. J. Leventhal, M. Allegrini and L. Moi, Phys. Rev. A (submitted; "Ionization of Rydberg Atoms").
11. A. F. Starace, "Theory of Atomic Photoionization", Handbuch der Physik, (Springer-Verlag, Berlin, 1982), Vol. XXXI, pp. 1-121.
12. S. T. Manson, Adv. Electronic Electron Phys. 41, 73 (1976).
13. A. Z. Msezane and S. T. Manson, Phys. Rev. A 30, 1795 (1984).

To be added in proof.

Fig. 1. Photoionization cross section of MgI as a function of wavelength. The dashed curve is from reference 5. Figure from reference 9.

To be added in proof.

Fig. 2. Photoionization cross section of MgI from 1100 - 1200 Å. Figure from reference 9.

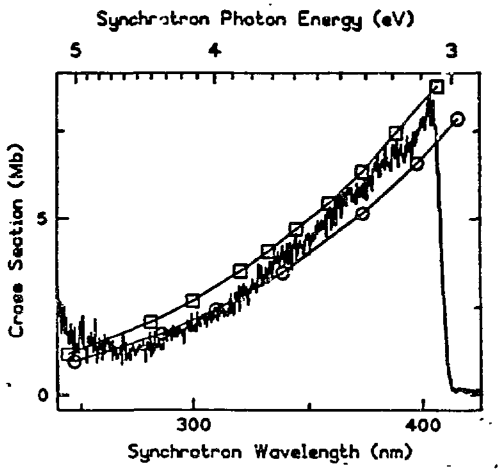

Fig. 3. The photoionization cross section of 3p sodium atoms from threshold to about 2 eV above threshold. The squares denote a Hartree-Slater calculation. The circles are the average of two Hartree-Fock calculations whose results are very close together (see text).