2000 Workshop on Atomic and Molecular Physics

Synchrotron Radiation Center
Stoughton, WI
October 28, 2000
Workshop Chair: Ralf Wehlitz
Introduction

Welcome to the University of Wisconsin and the Synchrotron Radiation Center (SRC) in Stoughton. In connection with the Users Group Meeting, the SRC is hosting an annual Workshop on Saturday, Oct. 28, 2000. This year’s Workshop focuses on various aspects of atomic and molecular physics using synchrotron radiation. Speakers have been invited to give presentations in the fields of absolute oscillator-strength measurements, limitations in the applicability of the dipole approximation, SR experiments combined with laser radiation, spin-orbit interactions, photoionization of ions, fragmentation dynamics of molecules, and related subjects. Workshop participants are encouraged to present a poster and to submit a one- to two-page summary of their presentation. This Workshop is also a great opportunity to learn more about the research possibilities at the Synchrotron Radiation Center!

Location

This Workshop takes place on the Kegonsa Research Campus which comprises the Physical Sciences Laboratory (PSL), the Center for Nano Technologies (CNTech), and the Synchrotron Radiation Center (SRC). All talks will be given in the Lecture Room (large conference room) of the PSL located near the SRC; 3725 Schneider Dr., Stoughton, WI-53589. The posters will be displayed in the PSL Lecture Room. Beverages and snacks will be served during the coffee breaks in the PSL Library adjacent to the Lecture Room.

Accommodation and Transportation

The invited speakers are accommodated in the Sheraton Inn – Madison, (706 John Nolen Drive, Madison, Wisconsin 53713, Tel: (608) 251-2300, Fax: (608) 251-1189). The hotel is about 10 miles (approx. 20 min.) from the Workshop site. Other Workshop participants can stay in this hotel at a discount rate. A shuttle bus service from and to the airport will be provided by the hotel. Furthermore, a shuttle bus will take Workshop participants from the Sheraton Inn to the PSL and back. Transportation to the Workshop dinner will also be provided.

Meals

All Workshop participants are invited to join the Friday night (Oct. 27) cookout of the SRC Users Meeting which takes place at the PSL. On Saturday morning, a breakfast will be provided in the PSL Library adjacent to the Lecture Room. Beverages and snacks will be served during the coffee breaks in the PSL Library. Also, a buffet-style lunch will be provided in the PSL Library.

In the evening we will have a dinner at “Halverson’s” on the shores of Lake Kegonsa (Stoughton), a restaurant with tradition since 1927.
Talks and Posters

All presentations will be given in the Lecture Room of the PSL. The talks will be given in plenary sessions (no parallel talks). The total time for each talk (including discussion!) will be 40 minutes, therefore speakers are asked to finish their presentation after 30–35 minutes to allow time for discussion.
Poster boards (36” wide, 48” high) for registered posters are available in the PSL Lecture Room. Posters can be put on the boards in the morning of the Workshop or during one of the coffee breaks and can be discussed in the coffee breaks or during the poster-session scheduled for the afternoon.
All submitted abstracts of talks as well as posters are available to Workshop participants in a booklet and on CD-ROM at the beginning of the Workshop.

Contact Information

<table>
<thead>
<tr>
<th>Pamela Layton (Secretary)</th>
<th>Ralf Wehlitz (Workshop Chair)</th>
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Web: http://www.src.wisc.edu

Acknowledgements

I wish to thank the SRC staff, in particular Pam Layton, Michelle Kirch, and Chris Moore, for helping me with the organization of this Workshop.
This Workshop is supported by NSF Grant No. DMR-9531009. The Synchrotron Radiation Center is funded by the National Science Foundation (Grant No. DMR-9531009) and operated by the Graduate School of the University of Wisconsin-Madison.
Historical Background of the Synchrotron Radiation Center (SRC)
(excerpt from An Invitation to See the Light, SRC, UW–Madison)

The Wisconsin Synchrotron Radiation Center (SRC) was originally built around Tantalus, a 240 MeV electron storage ring, which was a legacy of the Midwestern Universities Research Association (MURA) laboratory. Tantalus was planned to be a test bed for advanced accelerator concepts. However, after construction began in 1965, interest in the use of synchrotron radiation (SR) for research increased rapidly in both the United States and Europe. A sub-committee of the Solid State Science Panel of the National Research Council was given the responsibility to examine this development and make recommendations. Two Illinois members of this subcommittee, P.G. Kruger (former Director of MURA) and F.C. Brown, suggested the use of Tantalus as a source of synchrotron radiation for solid-state research. Minor alterations of the vacuum chamber were made to accommodate, first F.C. Brown and, shortly thereafter, H. Fritzche of Chicago and D. Lynch of Iowa State.

Interestingly, when Tantalus was commissioned in 1968, no funds were available for operation as a test bed. Thus, a decision was made to use it as the first dedicated source of synchrotron radiation. This decision, taken perhaps rather lightly at the time, was to have far-reaching effects on the future of synchrotron radiation research throughout the world. It was at SRC that the superiority of the electron storage ring as a source of SR was first demonstrated. Many subsequent innovations implemented at SRC have had considerable impact on the development of other SR facilities. Among these are: the use of a wiggler to extend the spectral capabilities of an SR source; the application of the microtron as an inexpensive injector for storage rings; the demonstration of the advantages of an intermediate energy (0.7-1.0 GeV), with respect to a high energy ring, for vacuum ultraviolet (VUV) and soft x-ray (sxr) research; and many innovations in VUV and SXR optics. Among the latter are the Toroidal Grating Monochromator (TGM), and the Grasshopper and Extended Range Grasshopper (ERG) monochromators.

In 1977 SRC began construction of its own facility focusing on a new and much larger SR source, Aladdin. Ten years later, with Aladdin fully operational, Tantalus was decommissioned. The birthplace of SR research has not been lost, however. The man most responsible for its creation, the late Ed Rowe, contacted The Smithsonian National Museum of American History and convinced them of the historical significance of Tantalus. While awaiting display at the museum, Tantalus will share storage space with such distinguished innovations as the Carnegie Van de Graaff Accelerator and Ed McMillan’s Electron Synchrotron.
# Program

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<td>8:30</td>
<td><strong>D.W. Lindle</strong> (U of Nevada - Las Vegas) <em>Nondipole Effects in Molecular Photoemission</em></td>
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<td>9:10</td>
<td><strong>J.J. Neville</strong> (U of New Brunswick, Canada) <em>Ionic Fragmentation of Inner-Shell Excited Molecules</em></td>
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<td>9:50</td>
<td><strong>U. Becker</strong> (FHI der MPG, Germany) <em>Coherence and Interference Phenomena in Atomic and Molecular Photoemission</em></td>
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<td>10:45</td>
<td><strong>J.A. Fedchak</strong> (U of Wisconsin - Madison) <em>Absolute UV and VUV Resonance Oscillator Strengths of Astrophysical Interest</em></td>
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<td>11:25</td>
<td><strong>S.B. Whitfield</strong> (U of Wisconsin - Eau Claire) <em>Recent Results from the Photoionization of Open-Shell Atoms</em></td>
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<td>12:05</td>
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<td>12:55</td>
<td><strong>D.H. Jaecks</strong> (U of Nebraska - Lincoln) <em>Quantitative Measurements and Effects of Relativistic Interactions in Multielectron Photoprocesses</em></td>
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<td>13:35</td>
<td><strong>N. Berrah</strong> (Western Michigan U - Kalamazoo) <em>Orientation of the Ar 2p−1, Kr 3d−1, and Xe 4d−1 Hole States and Spin Polarization in the Resonant Auger Decay of Argon</em></td>
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<td><strong>Y. Azuma</strong> (Photon Factory, KEK, Japan) <em>Dominance of Doublet-to-Quartet Intercombination Transitions in the 3s Photoexcitation Spectrum of Potassium</em></td>
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<td><strong>P. Zimmermann</strong> (Technische Univ. Berlin, Germany) <em>Photoelectron Spectroscopy of Laser-Polarized Atoms</em></td>
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<td><strong>I.A. Sellin</strong> (U of Tennessee - Knoxville) <em>Novel Ion Traps</em></td>
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<td><strong>J.B. West</strong> (CLRC Daresbury Laboratory, UK) <em>Absolute Photoionization Cross Sections of Atomic Ions</em></td>
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<td>17:25</td>
<td>Poster Session</td>
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Invited Talks
Dominance of Doublet-to-Quartet Intercombination Transitions in the 3s Photoexcitation Spectrum of Potassium

Y. AZUMA
Photon Factory, KEK, Tsukuba, Ibaraki 305, Japan

The partial charge yield measurements of potassium 3s photoexcitation has been made at the Photon Factory. The spectrum shows broad window-like features due to 3s→np photoexcitation resonances. Comparison with Multi-Configuration Dirac-Fock calculations as well as some features in the K\(^{++}\) spectrum suggest an interpretation that the most prominent feature in the K\(^{+}\) spectrum (and total photoion yield) is due to a nominally forbidden doublet-to-quartet intercombination transition, while less prominent features due to doublet-to-doublet transitions also show. The comparative size of the intercombination features shed light on the structure and time-evolution of the continua. The implication of this result to the interpretation of the 3s photoexcitation spectra of neighboring atoms in the periodic table would also be discussed.
The properties of photoelectrons are determined basically by the character of the coherent superposition of its $l$-dependent partial waves. Over the last two decades, the aim of angle and spin resolved photoemission studies has primarily been the analysis of these properties with respect to the disentanglement of this coherent superposition. More recently, a different type of coherence properties of photoelectron emission started to attract rapidly increasing interest: the coherence of different electron waves being either emitted from one site at different times or, in case of a molecule, from two different sites. The coherent superposition of these independent electron waves gives rise to interference phenomena, which are characteristic for each process. This will be illustrated by three examples, each highlighting a different kind of coherent superposition in photoelectron emission.

(i) Coherence between photo and Auger electrons showing up in a characteristic line shape interference pattern when they have exactly the same kinetic energy. An example for this behavior is Xe 4d photoemission with subsequent NOO Auger decay [1].

(ii) Coherence between directly emitted photoelectrons and those scattered from different atomic sites of a molecule. Such coherent superposition gives rise to characteristic interference pattern also known as photoelectron diffraction pattern. These geometry-dependent patterns may be observed in dependence from photoelectron momenta $k$ varying either in magnitude or direction. Showcase example is CO:C(1s) photoemission from fixed-in-space CO molecules [2].

(iii) Coherence between photoelectrons being directly emitted from two different sites of a molecule. This type of coherence would be a direct proof of the delocalized nature of electrons in a molecular environment, even applying to deep electrons. The direct proof of this coherence effect has not yet been experimentally verified, but indirect proofs are presently under way. The showcase example for this is the N$_2$:N(1s) photoemission if fixed-in-space N$_2$ molecules. Coherent or non-coherent emission depends on the time scales in which Auger decay occurs and the photoelectron leaves the molecular environment. For near-threshold N$_2$:N(1s) photoemission a high degree of coherence is expected [3]. First results of studying this coherence effect are reported.

References
Orientation of the Ar 2p\(^{-1}\), Kr 3d\(^{-1}\) and Xe 4d\(^{-1}\) hole states and Spin Polarization in the Resonant Auger Decay of Argon *

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The photoionization process can be described by transition amplitudes and relative phase shifts of the outgoing electron waves. The number of parameters needed is model dependent. However, even for the simplest model - the LS-coupling - the determination of partial cross section and angular distribution values is not sufficient to derive such amplitudes and phase shifts. In many cases, additional information can be retrieved from the analysis of the alignment or orientation of the remaining ion [1,2]. While alignment can be created by any kind of particle or photon impact, orientation requires excitation by polarized particles or circularly polarized photons. We have performed such an experiment by carrying out spin polarization measurements of Auger lines following the Ar 2p, Kr 3d and Xe 4d photoionization. These measurements were carried out at the new elliptical polarization undulator (EPU) beamline of the Advanced Light Source (ALS) using the 1st harmonic of the undulator without a monochromator. Using the \(^1\)S\(_0\) Auger lines we could derive the orientation parameter \(A_{10}\) of the Ar 2p\(^{-1}\), Kr 3d\(^{-1}\) and Xe 4d\(^{-1}\) hole states over a broad photon energy range. The results will be compared to various theoretical calculations and complementary measurements of the alignment or the spin polarization of the photolines.

We have also made the first measurement of spin polarization of resonant Auger electrons emitted from the decay of the Ar 2p\(^{-1}\) → 4s and 2p\(^{-1}\) → 3d excited states. We used monochromated, circularly and linearly polarized light of 244 eV photon energy from the new elliptical polarization undulator (EPU) beamline of the Advanced Light Source (ALS) to carry out the experiment. Some of the Auger lines show a high degree of polarization, which will possibly enable the determination of Coulomb matrix elements


*Work supported by the Department of Energy, Office of Science, Basic Energy Sciences, Chemical Sciences Division.
ABSOLUTE UV AND VUV RESONANCE OSCILLATOR STRENGTHS OF ASTROPHYSICAL INTEREST

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A High Sensitivity Absorption Experiment (HSA) has been developed by the University of Wisconsin to measure UV and VUV oscillator strengths of both atoms and ions. Our HSA experiment incorporates the basic elements of a classic absorption spectroscopy experiment: a source of continuum radiation, an absorbing sample, and a spectrometer/detector system. Unlike most traditional absorption spectroscopy systems, the HSA experiment uses the Aladdin ring at the Synchrotron Radiation Center as a source of continuum UV and VUV radiation, a hollow cathode discharge (HCD) as an absorbing sample of ions or atoms, and a 3 m focal length vacuum echelle grating spectrometer equipped with a back-thinned deep UV sensitive CCD array as detector. This spectroscopy system can achieve a resolving power of better than 300,000 and is sensitive to fractional absorptions smaller than 1% at VUV wavelengths. To date, the HSA experiment has been used to measure oscillator strengths at wavelengths down to 145 nm.

The primary motivation for developing the HSA experiment is to measure UV and VUV resonance absorption oscillator strengths observed in spectra taken in the cold neutral hydrogen regions of the interstellar medium (ISM), using the Goddard High Resolution Spectrograph (GHRS) and its successor instrument the Space Telescope Imaging System (STIS) on the Hubble Space Telescope (HST). In this region of the ISM, most elements tend to be singly ionized and in the ground fine structure state. Accurate, absolute oscillator strengths are required to interpret the HST data and determine various properties of the ISM such as elemental abundances and cloud structure. Of particular importance are key resonance lines of the iron group elements. We have successfully measured absolute oscillator strengths of Fe II, Co II, Ni II, and Ti II using the HSA experiment.

The HSA experiment will be the primary subject of this presentation; however other present or future spectroscopy experiments in the University of Wisconsin laboratory astrophysics program will also be discussed.

This work is supported by NASA under grants NAG 5-4295 and NAG 5-6833 and by the NSF under grant DMR-95-31009 to the Synchrotron Radiation Center.
QUANTITATIVE MEASUREMENTS AND EFFECTS OF RELATIVISTIC INTERACTIONS IN MULTIELECTRON PHOTOPROCESSES

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We have developed new experimental techniques and analyses to characterize the manifestations of relativistic, spin-orbit interactions in the photoionization of Ar over an extended energy range. This has been accomplished by an articulation of the partitioning of the one unit of angular momentum brought to the Ar system by circularly polarized-ionizing photons with energies of 35 – 37 eV. The initial photon angular momentum is converted to orbital and spin angular momentum of the residual ion and free electron during the photo process. Since photons interact only with the spatial coordinates of a single electron, any net spin change in the system, when transforming the Ar atom to the residual ion plus free electron, must result from relativistic interactions in the photo process. Since the total spin of Ar is zero this concept can be expressed by the relation

\[ <M_S(\text{ion})> + <m_s(\text{free})> \neq 0. \]  

The Z components of the spins of the residual ion \( <M_S(\text{ion})> \) and free electron \( <m_s(\text{free})> \) can be determined if one uses circularly polarized ionizing radiation.

Using circularly polarized photons is advantageous because they have an intrinsic angular momentum in a direction parallel or antiparallel to the Z axis, the direction of propagation. Conservation of angular momentum tells us that when an isolated system like Ar absorbs a circularly polarized photon, the expectation value of the Z component of the total angular momentum of the system must be equal to that of the ionizing photon. If the residual ion is excited and fluoresces in a convenient wave length region, one can determine the Z component of the total angular momentum of the ion \( <J_z(\text{ion})> \) by measuring the linear and circular polarization of this radiation. When the ionizing photon angular momentum is in the direction of propagation, conservation of angular momentum can be expressed as

\[ <J_z(\text{ion})> + <j_z(\text{free})> = 1 \]  

where \( <j_z(\text{free})> \) is the Z component of the total angular momentum carried away by the ionized electron. A specific example of a photo process we have studied using circularly polarized radiation of right handed helicity is given by the reaction

\[ \text{hv} + \text{Ar} \rightarrow \text{Ar}^+ [3p^4 (3P) 4p] ^2P_{1/2} + \text{e}_{\text{free}}. \]

By measuring the degree of helicity \( P_3 \) of the radiation at a wave length \( \lambda = 465.8 \) nm, from the \( ^2P_{1/2} \) to \( ^2P_{3/2} \) transition emitted in the direction of the initial ionizing radiation, one can determine \( <J_z(\text{ion})> \). The value of \( <J_z(\text{ion})> \) can readily be found from the relationship,

\[ <J_z(\text{ion})> = - \frac{2J(J+1) P_3}{3 \hbar (1) \cos \theta} \]  

where \( \hbar (1) \) is a constant depending on the particular transition. The value of \( P_3 \) is the difference between the measured intensities of left handed and right handed helicity, of the fluorescent radiation emitted in a direction \( \theta \) relative to the direction of propagation of the ionizing radiation. \( P_3 = (I_{LHH} - I_{RHH}) / (I_{LHH} + I_{RHH}). \)

Equation (3) can be understood by noting that the intensities \( I_{LHH} \) and \( I_{RHH} \) have their angular momentum vectors pointing antiparallel and parallel to the direction of propagation. The difference is related to the angular momentum carried away by the fluorescent photon which in
turn is related to $<J_z(\text{ion})>$ through the dipole selection rules. When observing the fluorescence along the ionizing beam axis, the selection rules are $\Delta M_J = \pm 1$ for the emission of circularly polarized light. For the present measurements the fluorescent detectors for measuring $P_3$ are placed at an angle of $\theta = 30^\circ$ for experimental convenience.

We can test for the presence of relativistic interactions using the concepts expressed in (1), subject to the constraints of the angular momentum quantities in (2), from standard angular momentum coupling rules. We note that the total angular momentum $J = +1J$ (for right handed helicity) can be related to $J$ of the ion and $j_e$ of the free electron. Since there may be relativistic interactions in the photo process, we use $J-j_e$ coupling to describe the ion-free electron interaction. Since $j_e = \ell_e + s_e$ we can write the total wave function of the ion-free electron system as

$$\psi = \sum_{J, M_J} \sum_{j_e} \langle J M_J | j_e m_{j_e} \rangle \langle \ell_e m_{\ell_e} s_e m_s | j_e m_{j_e} \rangle \langle J_M_J | \ell_e m_{\ell_e} \rangle s_e m_s$$  \hspace{1cm} (5)

where $a_{J, j_e}$ is the probability amplitude for forming either the $j_e = 1/2$ or $3/2$ state of the free electron.

For Ar$^+$, the radiating ionic “state” designated by $^2P^O_{1/2}$ is a mixture of pure LS coupled states having the same $J$ value but different values of $L$ and $S$, with the $^2P^O_{1/2}$ being the largest component. When we replace $|J M_J\rangle$ with a sum over pure LS coupled states $|\psi\rangle$ becomes:

$$|\psi\rangle = \sum_{J, M_J} \sum_{j_e} \sum_{\ell, s} c_i \langle J M_J | j_e m_{j_e} \rangle \langle \ell_e m_{\ell_e} s_e m_s | j_e m_{j_e} \rangle \langle L^{(i)} M_L^{(i)} S^{(i)} | \ell_e m_{\ell_e} \rangle S_{s} m_s$$ \hspace{1cm} (6)

where $L^{(1)} = L^{(3)}$ and $L^{(2)} = 0$, and the $c_i$ are the mixing coefficients of the pure LS coupled states that form the radiating ionic “state”. With this form for the total wave function of the ion plus free electron, the two quantities in equation (1) can found by projecting $M_S(\text{ion})$ and $m_s(\text{free})$ onto the total wave function of the system as given in (6) while integrating over all electron emission angles.

$$\langle M_S(\text{ion}) \rangle = \sum_{M_S} M_S |\langle M_S | \psi \rangle|^2, \hspace{1cm} \langle m_s(\text{free}) \rangle = \sum_{m_s} m_s |\langle m_s | \psi \rangle|^2$$  \hspace{1cm} (7)

By inserting the known values of the expansion coefficients and $c_i$ into (6) to determine the values of the spin expectation values of the final state components given in (7), we can calculate their sum in terms of the measured circular polarization $P_3$ on the fluorescent 465.8 nm radiation.

$$\langle M_S(\text{ion}) \rangle + \langle m_s(\text{free}) \rangle = 1.03 P_3$$  \hspace{1cm} (8)

The measured circularly polarization $P_3$ over the entire energy range of the ionizing radiation that will be presented is nonzero except where transitions from positive to negative values occur. We conclude that relativistic spin orbit interactions are important over the entire energy range. Both terms in (8) are also nonzero over the entire energy range indicating that a measurement of the spin of the free electron would in be nonzero.

Parity and angular momentum conservation limits the number of partial waves of the free electron in the above case to $\ell = 0$ and 2. Since spin orbit interactions are significant we must designate the partial waves by their total angular momentum $j_e = 1/2$ and $3/2$.

We will describe other methods, with supporting experimental data that provide additional tests for relativistic interactions in the photo process.
The dipole approximation (DA) is a zeroth-order description of the angular distribution of photoelectrons which provides a simple well-known expression for the differential photoionization cross section for randomly oriented molecules. Within the DA, a single parameter, $\beta$, completely describes the angular distribution of photoelectrons with respect to a single axis, the light polarization in synchrotron-radiation experiments. Until our recent experiments at the Advanced Light Source (ALS), the DA was routinely adopted for measurements at photon energies below a few keV. First-order corrections to the DA, equivalent to including cross terms between the electric-quadrupole and electric-dipole interactions (i.e., pure quadrupole interactions are not included), lead primarily to forward/backward asymmetries, with respect to the photon-propagation direction, in photoelectron angular distributions. In the first experiments to probe the breakdown of the DA in photoionization of free molecules, we have discovered large nondipole effects at energies very close to core-level thresholds and at photon energies well below 1 keV. In several cases, these effects produce forward/backward asymmetries of a factor of two or more. These findings suggest many applications of angle-resolved photoemission need to be reconsidered in light of these important nondipole effects. In addition to an overview of these new results from the ALS, brief updates on theoretical developments and measurements of nondipole effects in fixed-in-space molecules will be presented.
IONIC FRAGMENTATION OF INNER-SHELL EXCITED MOLECULES

John J. Neville
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Box 45222, Fredericton, NB, Canada E3B 6E2

Absorption of a soft x-ray photon by a polyatomic molecule can initiate a complex
unimolecular dissociation reaction involving multiple bond-breaking and producing both
charged and neutral fragments. In a step-wise model, the process is initiated by the reso-
nant excitation or ionisation of an inner-shell electron to produce an intermediate core-hole
state with a lifetime on the order of $10^{-15}$ s. Relaxation by non-radiative processes (i.e.,
normal or resonant Auger decay) dominates for core-hole states of light atoms, resulting in a
singly or multiply ionised molecule, possibly also with an electron in an anti-bonding molec-
ular orbital. Finally, the resulting valence-ionised states are often dissociative and molecular
fragmentation occurs.

![Graph of F+ ion flight time](image)

**Figure 1.** Variation of F+ time-of-flight peak shape as a function of the second ionic frag-
ment detected in coincidence for P 2p ionisa-
tion of PF$_3$ at 160 eV photon energy.

Time-of-flight mass spectrometry provides
an effective method of studying such ionic frag-
mentation processes [1]. The flight time of an
ion is determined to first order by its mass-to-
charge ratio, but is modulated by the kinematics
of the molecular fragmentation process, as
is illustrated in Figure 1 for ionic fragmenta-
tion of PF$_3$ following P 2p ionisation at 160 eV
photon energy. Ion time-of-flight peak shapes
therefore provide a means of investigating the
mechanism of the molecular dissociation reac-
tion. In particular, the correlations between
flight times of multiple ionic fragments pro-
duced from dissociation of a single molecule
can allow determination of the mechanism of the
dissociation process. These concepts will
be illustrated using examples from recent ex-
periments performed at the Canadian Syn-
chrotron Radiation Facility at the Synchrotron Radiation Center, University of Wisconsin-
Madison. Results from inner-shell excitation studies of series of chemically related molecules
will be presented to demonstrate how changes in chemical and electronic structure are re-
lected in the inner-shell spectroscopy and the consequent fragmentation dynamics.

A question of considerable interest in the field of inner-shell spectroscopy of molecules is
the extent to which the highly localised nature of the initial inner-shell hole is reflected in the
ionic fragmentation process. A goal is to develop the ability to direct the bond dissociation
process by selection of the appropriate inner-shell excitation. However, the majority of the
research reported to date suggests that there tends to be little or no “memory” of the site
of the inner-shell hole in the molecular fragmentation. Exceptions to this trend will be
highlighted and conditions favouring site-specific fragmentation will be discussed. Partial
ion yield spectra of SPF$_3$ exhibiting significant fragmentation selectivity are compared in Figure 2 with the total ion yield spectrum.

This work is based upon research conducted at the Synchrotron Radiation Center, Univ. of Wisconsin–Madison, which is supported by the NSF under Award No. DMR-95-31009.

References

Figure 2: Selected ion yields of SPF$_3$ in the vicinity of the P 2p and S 2p ionisation thresholds.
Absolute measurements of photoionization cross sections of gas phase species are fraught with many problems, the most serious of which is the determination of the sample density. Apart from the rare gases and a few metal vapour atoms for which heat pipes can be used effectively, there are few reliable measurements for atomic species, leading to reliance on normalization methods such as oscillator strength sum rules, or calculations. For atomic ions the sample density problem is overcome because the charged particles can be detected using a Faraday cup or calibrated electron multiplier, but the beam density is now six orders of magnitude lower than it would be in a vapour cell, so the measurements are limited to species with high cross sections, $>10^{-19}$ cm$^2$. The low beam density can be offset to some extent by using the merged beam method, in which the ion and photon beams are merged over a path length of several centimetres, thereby increasing the size of the interaction region. For this a parallel beam for the incident radiation is required, ideally synchrotron radiation, and this was the method used by Lyon et al [1] at the Daresbury Synchrotron Radiation Source (SRS) who made the first measurements of this kind.

The measurements at the SRS were limited by the photon flux to cross sections $\sim 10^{-17}$ cm$^2$ and therefore to regions of the spectrum dominated by autoionization. Further developments had to await access to undulator radiation from the next generation of synchrotron radiation sources. At the present time facilities are being or have been set up in Japan at the Photon Factory and the SPring-8 facility, Super-ACO in France, the ALS at Berkeley and at the University of Aarhus in Denmark, all using the merged beam method. At Aarhus the focus has been on absolute measurements on ions of astrophysical interest, with the aims of testing current theoretical calculations and providing reliable identifications for the structure seen. These measurements will be the subject of this report.

In figure 1 the experimental layout is shown; a complete description has been given by Kjeldsen et al [2]. There are four main differences from that used previously at the SRS:
• access to an undulator and a more efficient optical system yields an increase in photon flux of two orders of magnitude;
• the interaction path length (IC) is 50 cm compared with the 10cm used originally;
• an extended photon energy range up to 180eV, compared to 40 eV at the SRS, is available;
• a facility for measuring triply and quadruply charged ions is included.

The Faraday cup (FC) was used to measure the intensity of the incident ion beam, and Johnston multipliers for the species resulting from ionization of that beam. The density of the target species was therefore known, and the overlap between the ion and photon beams was measured with slit-type beam scanners. Uncertainty in the overlap integral and in the calibration of the photodiode, together with an imprecise knowledge of the higher order content in the photon beam limit the accuracy of the cross sections obtained to 10%.

At Aarhus measurements have been completed on the singly charged ions of C[3], K[2], Mg[4], Al, I[5], and the doubly charged ions of Al, I[5] and Ne. The data have been useful for making comparisons with calculations carried out for the Opacity [6] and Iron [7] projects, and have also been used to clarify identifications of spectral features through the use of the experimental values of the oscillator strengths for the transitions concerned. An example is the absolute cross section for Mg$^+$ ions [4], where the prominent features around 61 eV, to be associated with excitation of the 2p electrons followed by autoionization, have been the subject of controversy in the literature. A comparison between the theoretical and measured values of the oscillator strengths of these lines suggest that they should be assigned to 2p — 3d transitions rather than 2p — 4s as previously thought. A second example is measurements on I$^+$ and I$^{++}$ ions [5], which help to resolve the factor of three discrepancy between theory and experiment for the cross section of iodine atoms in the region of the 4d "shape" resonance.

Acknowledgments
I am indebted to my colleagues at Aarhus University, Henrik Kjeldsen, Finn Folkmann, Helge Knudsen and Torkild Andersen for their enthusiasm in installing this project on the ASTRID storage ring and their hard work in making it successful.

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[6] The Opacity Project I995, Institute of Physics (Bristol, UK) vol. I
RECENT RESULTS FROM THE PHOTOIONIZATION OF OPEN-SHELL ATOMS

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The utilization of electron spectrometry in conjunction with synchrotron radiation has engendered a continuing interest in the study of the dynamics of atomic photoionization for nearly 30 years. Yet despite this rich history [1-4], the vast majority of experimental and theoretical work has focused on those atoms which have an isotropic charge distribution in the ground state, i.e. closed-shell atoms. Chief among these are the rare gases where extensive experimental and theoretical work abound [1,4]. Experimentally, this is largely due to the ease of using rare gases as an atomic target. In contrast, corresponding studies of open-shell atoms which generally have anisotropic charge distributions in the ground state are relatively scarce. This is most likely due to the inherent difficulty associated with producing a useful atomic beam of open-shell atoms. Despite this difficulty, there have been a number of significant and important experimental studies done on open-shell atoms [2,5], but not to the degree that has been carried out for closed-shell atoms. In other words, systematic and wide ranging experimental studies of open-shell atoms are still largely lacking. From a theoretical point of view, experimental studies of open-shell atoms will provide an invaluable guide as to what theoretical methods must be applied in order to give a correct description of the dynamics of the photoionization process for these atoms. At this workshop I will discuss some of our recent experimental results on atomic chlorine, atomic scandium and atomic iron as outlined below.

One particularly interesting difference between the photoionization of closed- and open-shell atoms involves the s-subshell. The photoionization of a closed-shell atom (in the dipole approximation) involves only one ionization channel, i.e. one proceeds from a $1S \to 1P$ term. In the absence of relativistic effects, this leads to $\beta = 2$ independent of the energy of the ionizing radiation. In the open-shell atom there are typically three different ionization channels, i.e. one proceeds from $2S+1L \to 2S+1(L - 1)$, $2S+1L$, $2S+1(L + 1)$. Interference between these channels is likely, leading to (i) $\beta \neq 2$, (ii) term dependent $\beta$ values and (iii) photon-energy dependent $\beta$ values. While theoretical predictions of this behavior were first made more than 20 years ago for 3s-subshell photoionization of atomic chlorine [6] and later for other open-shell atoms [7], they were not experimentally verified until this year [8].

Atomic Sc with a lone 3d electron, [Ar]3d4s$^2$(2D$_3/2$), is the simplest open-shell transition metal atom. Nevertheless, an accurate description of the photoionization dynamics of this atom, particularly in the region of the $3p \to 3d$ giant resonance, entails a considerable theoretical effort [9]. In LS-coupling alone there are 9 final ionic-states and 32 channels involved in the photoionization of the $3p$, $3d$ and $4s$ subshells [9]. A comparison of recent calculations [9], to the first measurements of atomic Sc [2], show marginal agreement. Part of the discrepancy was thought to involve the rather low photon energy resolution of the experiment. In addition, the experiment was unable to resolve contributions from the two 4s mainlines, giving only the relative partial cross section of their sum as a function of photon energy. Our measurements, with considerably improved resolution in both the analyzer and the photon bandpass, confirm the earlier experimental results. They also provide separate partial cross
sections as a function of photon energy for both the $4s(^3D)$ and the $4s(^1D)$ photolines and the major photoelectron satellite lines. Our measurements of the main photoelectron lines of atomic Sc compared to theory [9], are shown in Fig. 1. The poor agreement evident in the figure clearly indicates that important details in the calculation are lacking.

Atomic Fe, [$Ar]3d^64s^2(5D_4)$, was also investigated in the region of the $3p \to 3d$ giant resonance. In contrast to atomic Sc where there is a myriad of structure in the region of the $3p \to 3d$ giant resonance, see Fig. 1, atomic Fe appears to have only two principle excitations in this region which are considerably broader than what we observe in Sc. Photoionization of the $3d$-subshell of atomic Fe leads to five main photolines with differing terms. We have determined their relative partial cross sections as a function of photon energy through the $3p \to 3d$ giant resonance. Our results, with better statistics and higher resolution, are in good agreement with earlier results [10]. In addition, we have also determined the relative partial cross sections of both main $4s$ photolines and the primary photoelectron satellites. In contrast to the mainlines, some of the satellites show enhancement at the higher lying Rydberg excitations consistent with a shakeup picture of autoionization.

Figure 1: Atomic Sc mainlines in the region of the $3p \to 3d$ giant resonance.

I would like to thank Denise Caldwell, Ken Kehoe, Manfred Krause and Ralf Wehlitz for their collaboration and assistance in these measurements. This work was supported in part by an internal research grant from the University of Wisconsin–Eau Claire.

References
PHOTOELECTRON SPECTROSCOPY WITH LASER-POLARIZED ATOMS

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The pioneering experiments of Wuilleumier et al. [1] with laser-excited sodium atoms showed the large potential of the combined use of laser and synchrotron radiation for photoelectron spectroscopy. Later the well-defined polarization of both radiation sources was used to study the angular distribution of the photoelectrons from polarized atoms in the laser-excited state [2]. By the polarization of the laser radiation, however, not only polarized atoms in the excited state are produced. The atomic polarization can also be transferred by the spontaneous decay from the excited state to the ground state. In this way the laser radiation can be used for the preparation of polarized target atoms in the ground state. In contrast to photoelectron spectra of laser-excited states as the prototype of a two-colour experiment the photoelectron spectra of laser-polarized atoms in the ground state obviously do not differ energetically from those of unpolarized atoms in the ground state. By the pumping process only the angular distribution is influenced. Therefore, a high degree of polarization must be obtained and the success of this method critically depends on the efficiency of the pumping process. On the other hand the target preparation of polarized atoms by laser pumping offers an elegant method for the manipulation of atomic polarization: One can easily change between aligned and oriented atoms by changing between linearly and circularly polarized laser radiation, one can easily change the atomic alignment by changing the angle of polarization of linearly polarized laser radiation or one can easily change the direction of the atomic orientation by switching between left and right handed circularly polarized laser radiation.

Easy manipulation of the atomic polarization is an important argument in connection with photoelectron studies from polarized atoms [4,5]. The reason can be found in the rather complex theoretical description of the angular distribution of the photoelectrons from polarized atoms [3]. A significant simplification of the corresponding formula can be obtained if the analysis is concentrated on the difference spectra of two angular distributions by varying the target polarization and/or the polarization of the synchrotron radiation. This is the well-known method of dichroism experiments in the solid phase. In the case of the MDAD experiments (Magnetic Dichroism in the Angular Distribution) in the solid phase the direction of the atomic orientation is reversed by the short pulse of an external magnetic field. Therefore, one can make a direct comparison of the MDAD experiments in the solid phase with the corresponding experiments of laser-oriented free atoms where the direction of orientation is reversed by changing between left and right handed circularly polarized laser radiation.

References


Posters
Oscillator strengths for transitions in CO have been obtained at the Synchrotron Radiation Center of the Univ. of Wisconsin-Madison. Our focus was on transitions that will be observed in interstellar spectra with the Far Ultraviolet Spectroscopic Explorer; these transitions are also important in studies of selective isotope photodissociation where fractionation among isotopomers can occur. Absorption from the ground state \( X^1\Sigma^+ (\nu'' = 0) \) to \( B^1\Sigma^+ (\nu' = 0, 1) \), \( C^1\Sigma^+ (\nu' = 0, 1) \), and \( E^1\Pi (\nu' = 0) \) was measured with the 4 m Normal Incidence Monochromator. As in our earlier experiment, fits to the \( A-X (5,0) \) band, whose oscillator strength is well known, yielded the necessary column density and excitation temperature. These parameters were used in the least-squares fit of the transitions of interest to extract their band oscillator strengths. The final results for each absorption band are summarized in Table 1. Also included in Table 1 are other experimental and theoretical results.

Table 1: \( f \)-values (\( \times 10^3 \)) from current work and comparison with other determinations

<table>
<thead>
<tr>
<th>Reference</th>
<th>( B-X(0,0) )</th>
<th>( B-X(1,0) )</th>
<th>( C-X(0,0) )</th>
<th>( C-X(1,0) )</th>
<th>( E-X(0,0) )</th>
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<tr>
<td>Present Results (^a)</td>
<td>( 6.6\pm0.2 )</td>
<td>( 0.75\pm0.03 )</td>
<td>( 123\pm7 )</td>
<td>( 3.0\pm0.2 )</td>
<td>( 68\pm1 )</td>
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<tr>
<td>Lassettre &amp; Skerbele 1972 (^b)</td>
<td>15\pm3</td>
<td>2.0\pm0.4</td>
<td>163\pm15</td>
<td>7.0\pm0.6</td>
<td>94\pm9</td>
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<td>Eidelsberg et al. 1991 (^a)</td>
<td>4.52\pm0.45</td>
<td>0.72\pm0.07</td>
<td>61.9\pm6.2</td>
<td>2.77\pm0.28</td>
<td>36.5\pm3.7</td>
</tr>
<tr>
<td>Stark et al. 1992 (^a)</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>Chan et al. 1993 (^b)</td>
<td>8.03</td>
<td>1.32</td>
<td>117.7</td>
<td>3.56</td>
<td>70.6</td>
</tr>
<tr>
<td>Kanik et al. 1995 (^c)</td>
<td>12\pm3</td>
<td>...</td>
<td>154\pm41</td>
<td>...</td>
<td>...</td>
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<tr>
<td>Ciocca et al. 1997 (^c)</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>70.8\pm18.4</td>
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<td>Zhong et al. 1997 (^b)</td>
<td>5.98\pm0.93</td>
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<td>114\pm14</td>
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<td>Stark et al. 1999 (^d)</td>
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<td>1.1\pm0.1</td>
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<td>...</td>
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<tr>
<td>Theory:</td>
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<td></td>
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<td>Kirby &amp; Cooper 1989</td>
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<td>0.3</td>
<td>118.1</td>
<td>1.8</td>
<td>49</td>
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<tr>
<td>Chantranupong et al. 1992</td>
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<td>4.9</td>
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<td>4.8</td>
<td>0.43</td>
<td>89</td>
<td>2.9</td>
<td>49</td>
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\(^a\) Synchrotron absorption; \(^b\) Electron energy loss; \(^c\) Electron impact excitation; \(^d\) Laser absorption.

Our results are in excellent agreement with the recent work of Ciocca et al. (1997), Zhong et al. (1997), and Stark et al. (1999). Good agreement with Chan et al. (1993) and Kanik et al. (1995) is also seen. For the \( (0,0) \) bands, earlier absorption work by Eidelsberg et al. (1991) and Stark et al. (1992) gave significantly smaller \( f \)-values, but the results of Eidelsberg et al. show consistency with the recent work for the relatively weak \( (1,0) \) bands. A systematic trend is seen in the results presented by Eidelsberg et al.: The discrepancy between their \( f \)-values and the more recent determinations increases with increasing band strength. This trend suggests optical depth effects were not adequately treated in their analysis of CO absorption. The results of Stark et al.
may be affected by this problem as well. Agreement with theoretical results is seen at the factor-of-two level. Rocha et al. (1998) showed that the differences between their oscillator strengths, those of Chantranupong et al. (1992), and those of Zhong et al. (1997) mainly arise from the differences in Generalized Oscillator Strength (GOS) for small $K^2$, the square of the transferred momentum. The fact that all experimental techniques now give oscillator strengths similar to the ones obtained by Zhong et al. indicates more theoretical work on the GOS at small $K^2$ is warranted.

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References
PHOTOEMISSION STUDY OF THE FE ATOM

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The aim of this work is to gain a broader understanding of many-electron effects (or electron
correlations). These effects, evident in both inner shell and outer shell photoionization are
now understood by and large in the case of closed-shell atoms, such as the rare gases, but
are understood insufficiently in the case of open-shell atoms, which comprise the majority
of the elements in the periodic table.

The iron atom, with 6 electrons in
the 3d subshell, offers itself as a suit-
able, and intriguing, candidate and was
already subject of recent investigations
[1]. Photoelectron spectra of the 3d, 4s, and associated satellite lines were
recorded at SRC’s PGM undulator beam
line [2] providing the necessary high pho-
ton flux with still high energy-resolution. The experimental setup and elec-
tron spectrometer used in this experi-
ment are described elsewhere [3].

The constant-ionic-state (CIS) spec-
tra show several resonances which de-
pend strongly on the final state of the
Fe ion. Our study is the first extensive investigation on how resonances are affected by the
final ionic state. The resonances are often closely spaced having a natural width that is too
broad to resolve individual resonances. However, since the strength of a resonance varies
strongly with the final ionic state, it may be possible to decompose the CIS spectra into
single resonances. These results may serve as a test bench for theoretical calculations which
are still at the beginning of modeling open-shell atoms.

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References
TESTING THE WANNIER THRESHOLD LAW BY ANGLE-RESOLVED
PHOTOELECTRON SPECTROMETRY

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We have tested the Wannier threshold law employing a new experimental approach taking
advantage of recent developments in high-flux high-resolution monochromators. The corre-
lated motion of two slow-moving electrons in a Coulomb field was described by Wannier [1]
almost 50 years ago. Since then, numerous experiments were performed to test Wannier’s
threshold law for double-electron ejection using different methods [2].

In particular, this threshold law predicts for the double photoionization cross-section
\( \sigma^{2+} \): \( \sigma^{2+}(E) \propto E^\alpha \), where \( E \) is the excess energy and \( \alpha \) is the Wannier exponent, which
is 1.056 in the case of double photoionization of helium. An ion-yield measurement [3]
confirmed this value [1.05(2)]. Since the energy-sharing of the ejected electrons is uniform
near threshold according to Wannier’s theory, not only ions but also electrons created in the
double photoionization process with any kinetic energy can be used to test the threshold
law.

In contrast to previous experiments, which detected ‘zero-energy’ electrons
[4,5,6], we have measured the relative intensities of the \( \text{He}^+(n \ell) \) photoelectron satellite lines \( (n \leq 9) \) at several
photon energies near the double-photoionization threshold. From these relative intensities we
determined the relative differential cross sections \( d\sigma/dE \) \((h\nu)\) of the ‘high-energy’ electrons
created in the double-photoionization process. Using a least-squares fit (Fig. 1) we could
derive the Wannier exponent \( \alpha = 1.062(6) \) in reasonable agreement with theory.

However, it is noteworthy that most experimental values for \( \alpha \) determined
from electron measurements lie systematically higher than given by theory [2]. In a new
experiment performed at SRC’s PGM undulator beamline we tried to reduce the experimental
error for \( \alpha \) to tackle this problem. Moreover, our method of using non-zero kinetic-energy
electrons enables us to determine the angular distribution parameter \( \beta \) of electrons created
in the double-photoionization process right at threshold.

Figure 1: Differential ‘high-kinetic’ energy cross section \( d\sigma/dE \) \((E = h\nu - E_B^{2+})\) as a function of photon
ergy. The solid line is a fit curve to our data.
The extrapolation of the angular distribution parameter $\beta$ of zero-kinetic energy electrons can be done in two different ways: a) by determining the angular distribution of each photosatellite He$^+(n\ell)$ and extrapolating the $\beta$-values to $n \to \infty$; b) by extrapolating the cross section $d\sigma/dE(n)$ to ‘$n = \infty$’ for different angles and then deriving the angular distribution parameter from these extrapolated intensities.

It is worthwhile to mention that the intensities of the He$^+(n\ell)$ photosatellites do not follow a $1/n^3$ law at angles other than the magic angle because this law applies only to the partial but not differential cross section. However, we found a similar law with a different exponent for other emission angles.

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References
CREATING BARE LITHIUM AT HIGH PHOTON ENERGIES

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The investigation of multiple-ionization processes of atoms and molecules is of fundamental importance for understanding the interactions among charged particles in a Coulomb field. Not only the interaction itself but also the relative strength of multiple-ionization processes provide valuable information for, e.g., modeling conditions in astronomical objects. Although multiple ionization appears to be a simple process, even the interaction of only three charged particles cannot be described analytically [1]. In order to find a model that is able to describe the multiple ionization process, recent investigations have been focuses on a simple case, namely, the double photoionization of helium.

The established relationship between double ionization by photons and charged particles [2] has been useful for relating the results from both experimental techniques [3]. However, in contrast to charged particles, ionization by a single photon has a well-defined energy and angular momentum transfer from the projectile to the target, and provides a simpler testing ground for theoretical models.

Recently, measurements of the triple-to-single photoionization ratio and the triple photoionization cross section of atomic lithium were performed for energies up to 220 eV above the triple-ionization threshold [4,5]. The complete break-up of the Li atom into four particles can occur only by simultaneous ejection of all three electrons, i.e., Auger decay processes cannot contribute to the triple ionization cross section. Moreover, in contrast to other atoms, Li has only one triple-ionization threshold, which makes it well suited as a unique source of information on pure three-electron correlation, and corresponding theoretical calculations — when they become available — can be compared directly with experimental results. However, up to now, theoretical predictions of the triple-to-single photoionization ratio are available only for the high-energy limit [4,6,7]. Moreover, in contrast to the much debated double-to-single photoionization ratio in He, the triple-to-single photoionization ratio is expected to

Figure 1: The triple-to-single photoionization ratio of Lithium (top panel) and the triple-photoionization cross section (bottom panel). Circles: Refs. 4 and 5; square: this work; solid line: Ref. 9; dotted line: Ref. 10. The arrows at the top panel indicate calculated ratios at the high-energy limit [4,6,7].
show a larger dynamic, i.e., the ratio at the high energy limit is expected to be about 10 times lower than its maximal value while the double photoionization ratio changes only by a factor of 2.3 (not taking Compton scattering into account). Therefore, we have measured the triple-to-single photoionization ratio at an higher photon energy than heretofore namely 1050 eV above the triple-ionization threshold.

The experiment was conducted at the Multilayer beamline [8] at SRC using an ion time-of-flight spectrometer in pulsed extraction mode. The low-energetic stray light, inherently present at this beamline, was suppressed by a 1.2 µm-thick carbon filter.

Figure 1 shows our new data point at 1050 eV excess energy along with previously measured data [4,5]. Also included in the figure are two experimental curves in the attempt to model the energy dependence of the ratio and the triple-photoionization cross section since no theoretical prediction at finite energies is published yet. The solid curve is the double-to-single photoionization ratio and double photoionization cross section of He, respectively. Both curves were scaled arbitrarily in the ‘y’-direction to fit the data. The energy axis for both curves was compressed by a factor of 9/4 according to the notion that the energy axis for double ionization scales as $Z^2$ and that the triple-ionization process of Li can be approximated by the double-ionization of Li$^+$. This assumption is not true for lower photon energies because the interaction among all three electrons becomes important as can be seen in the Fig. 1. However, at higher energies this model seems to work well and the third electron does not influence the energy dependence at high energies.

The dotted curves are for electron-impact double-ionization of He. In this case, we have 3 outgoing electrons as in the case of triple photoionization of Li. However, the final ionic charge and the projectile are different. Again, these curves were scaled arbitrarily in ‘y’-direction to fit the data. In the upper panel of Fig. 1, this curve is slightly too high at low energies and high energies while it fits the data reasonably well at medium energies. In the lower panel of Fig. 1 this curves fits fairly well to the low-energy Li$^{3+}$ cross section but seems to be too high for higher energies.

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References
PHOTOELECTRON SPECTROMETRY OF ATOMIC SCANDIUM IN THE REGION OF THE $3p \rightarrow 3d$ GIANT RESONANCE

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A determination of the relative partial photoionization cross sections of the $3d$ and $4s$ main-lines and associated satellites of atomic scandium in the region of the $3p \rightarrow nd, ms$ excitations has been carried out using electron spectrometry in conjunction with monochromatized synchrotron radiation. The superior resolution inherent in these measurements has revealed additional structure not previously seen in earlier experimental work, highlighting the rich and complex structure of this relatively simple open-shell atom. A comparison with recent calculations in LS coupling shows marginal agreement at best, suggesting in part that LS coupling is inadequate to correctly describe the dynamics of the photoionization process of this atom.
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