PHOTOIONIZATION OF CHLORINE, SULFUR, PHOSPHORUS AND A HYPOTHESIS TO QUENCH METASTABLE STATES

by Guillermo Hinojosa

The objective of our proposal is to study the photoionization of Chlorine, Sulfur, and Phosphorus ions using the unique high resolution capability of 10.0.1 beamline in the ALS. These species are relevant in astrophysics and as a benchmark for state of the art theoretical models of the quantum properties of ions. We also propose to test a technique to quench the metastable states from the ion-beam based on recent experimental evidence and on a well known technique in chemistry. The work of this proposal may lay the foundations for a definite solution to control the metastable component of the initial ion-beam.

We propose to study ions that originate from open-shell atoms. They are of relevance because the electron correlation and the inter channel coupling effects in these systems are very strong and, therefore, they are a natural benchmark for detailed comparisons of the LS and \( jj \) coupling model.\[^1\] For this reason and with the unique high resolution features of the ALS, data from the photoionization of these ions are expected to provide a great deal of details to compare with theory. From a computational point of view, the main challenge in the description of open shell systems is the inclusion of a large number of states. For this reasons we expect that these data will encourage the development of theory to a level that is becoming more and more available thanks to the continuous development of computer power.

In addition, accurate photoionization cross sections and high resolution spectra of ions of astrophysical interest are required to model a large variety of objects such as active galactic nuclei, IIII regions, planetary nebulae, novae, and supernovae. Photoionization of ions of Chlorine, Sulfur and Phosphorus have critical roles in interstellar chemistry. For instance, they happen to be very reactive with H\(_2\), forming hydrogenic molecular ions such as ClH\(_2\) which is the best tracer of optically thick H\(_2\) components in diffuse clouds.\[^2\]

There is one single line of ClIII that is identified and used in abundance determination models\[^3\]. In spectroscopy, a single line is rarely a definite proof of identification. We propose to measure, with high resolution, the absorption spectra of this particular species which is very important in astrophysical observations.

Sulfur and its ionic states have been discovered in the plasma of Jupiter’s satellite Io and spectroscopic lines of its ions are routinely detected in the Jovian auroras.\[^4\] A number of strong features due to Sulfur ions have been observed in the spectra of the Io plasma torus, of the Sun and in stellar transition regions.\[^5\] Cross sections and precise spectroscopic lines measured with the high accu-
racy of beamline 10.0.1 would be of great aid in the understanding of these environments and in the design of future spectrometer space satellites.

To our knowledge, there exist high resolution data on the isoelectronic series of Chlorine-like ions such as Ar$^+$ [9], Ca$^{3+}$ [7], Al$^{2+}$ [8] and Ar$^{5+}$ [9]. For the ions that we propose to investigate, just low resolution data for S$^+$ [10] are available. For the case of Chlorine, only the pioneering work on the atomic case of Rušćić and Berkowitz has been reported [11].

The only issue in terms of feasibility for the present proposal, is the production of a reliable beam of Chlorine. To show that it is possible to produce such an ion-beam, a Cl$^+$ beam was generated in our local laboratory with the following procedure: a small amount of Ferric Chloride (FeCl$_3$) was heated directly inside the chamber of a filament-type ion source. This compound is available commercially and is harmless. The results are very promising and demonstrate that it is possible to produce a stable beam of Cl$^{9+}$ by heating this compound with the insertion oven of the ECR ion source. There are similar recipes to generate beams of S$^{7+}$ and P$^9+$ [12].

In this technique, the main general problem for the measurement of the cross section is the presence of an undetermined amount of metastable initial states in the ion-beam. Basically, the initial state is composed of two electronic states that have different photoionization probabilities (cross sections). One is the ground state and the second is a metastable state that is created by collisions with electrons inside the ion source. Actual cross section measurements are an indeterminate combination of the two states. As a result, theoretical models have been forced to include an empirical factor to fit the experiment, literally ruining any detailed conclusive comparisons with theory.

An early attempt to circumvent this problem consisted in measuring the attenuation fraction of an O$^+$ beam in collisions with N$_2$ [13]. A recent effort consisted in combining the ion-trap and the merged-beam techniques [14]. What we propose here is a very simple method that has been overlooked and consists of producing a ground state ion-beam rather than normalizing to independent experimental measurements. In chemistry, it is well established that resonant collisions quench efficiently the metastable component of ions [15]; it is a fundamental effect that has to do with the way internal energy gets shared in collisions.

First, we present two pieces of evidence to show that with the actual ion-photon beam (IPB) end station in the ALS, it was possible to generate pure ground state beams when the ion-beam source was a hot-filament source type that induced resonant collisions: (1) Cross section data on the photoionization of Kr$^+$ [16] turned out to be in agreement with similar data that was corrected for the metastable contribution [14] (see Fig. 1) and (2) The photoionization of CO$^+$ [17] cross section that was significantly lower than that of a data set measured with an ECR ion source [18].

In the ECR ion source, electrons couple with the source’s radio frequency and collide with the injected gas forming ions that remain in the plasma until they are expelled out of the ion source by electrostatic repulsion. While inside the ion source, these ions may suffer collisions with the surrounding gas. To test this idea we propose to inject a combination of Xe plus CH$_4$ gases in the ECR to produce a Xe$^+$ ion-beam because it is well known that in this particular collision system, the metastable state of Xe$^+$ is completely quenched [19, 20]. The ECR would be operated at its lower power and at its higher pressure to enhance this effect. Similar “quenching” collision systems for other ions (including Cl, S and P ions) are tabulated in reference [21].

In conclusion, we propose to measure systems that are per se relevant in atomic physics and in astrophysics. Because of its open shell character, these measurements will take full advantage of the high resolution power of the ALS. In addition, we will test a simple-to-check method to control the metastable component of the ion-beam.

The present proposal would be carried out by a team of scientists from the Institute of Physical Sciences at the National University of Mexico. This is a multidisciplinary group with familiarity in the

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2For instance, for all noble gases $^2$P$_{3/2}$ is the ground state and $^2$P$_{1/2}$ is the metastable state (with the exception of He).

3Thermal collisions with atoms or molecules with similar masses.

4In its earliest stage the IPB had a filament-type ion source.
Figure 1: Log-log plot of the photoionization of Kr$^+$. To show that our team has the capability to carry out this proposal and to illustrate the unique high resolution feature of the IPB in BL 10.0.1, we show data measured in the ALS by a team with the same team leader as that of the current proposal’s group [16]. The data consist in the cross sections measurements for the photoionization of Kr$^+$ (open triangles) to which a broad photon energy scan taken at a resolution of 10 meV and steps of 1 meV has been normalized (black dots). To demonstrate that resonant collisions quench the metastable component, the ALS’ data are compared to pure ground state cross sections (gray dots) of Bizau et al. [14] (measured with lower resolution). When the metastable component is important, the cross section is expected to be higher, here both sets of data are comparable.

use of synchrotron radiation. Some of the members are experienced in the ion-photon end station in beam line 10.0.1:

[List of co-authors has been removed by the author.]

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