Fine-structure resolved photoionization of metastable Be-like ions C III, N IV, and O V

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Abstract. High-resolution photoionization experiments were carried out with beams of C III, N IV, and O V containing roughly equal amounts of ground-state and metastable ions. The energy scales of the experiments are calibrated with uncertainties of 1 to 10 meV depending on photon energy. These data favorably compare with state-of-the-art R-matrix calculations carried out on an energy grid with a spacing of 13.6 μeV.

1. Introduction

Berylliumlike ions are among the most important probe species in the diagnostics of technical and astrophysical plasmas. Moreover, Be-like ions with their two loosely bound electrons in the L-shell and two tightly bound K-shell electrons are almost perfect objects for investigating two-electron effects. Detailed knowledge of their structure and behaviour in atomic interactions is thus essential both for applications and for the fundamental understanding of many-electron phenomena. Previous work has already provided absolute cross section functions up to the (2pnl) resonance-series limits for photoionization of B⁺ ions with an energy resolution of 25 meV at around 30 eV photon energy [1], for photoionization of C²⁺ with an energy resolution of 30 meV at around 50 eV photon energy [2], for photoionization of N³⁺ with an energy resolution of 230 meV at around 70 eV photon energy [3], and for photoionization of O⁴⁺ with an energy resolution of 250 meV at around 110 eV photon energy [3]. For selected resonances in the photoionization of C²⁺ ions, measurements with energy spreads as low as 7.5 meV have been reported [4].

The present work aims at the investigation of state-selective photoexcitation of autoionizing levels of C²⁺, N³⁺, and O⁴⁺ ions. All these Be-like ions feature long lived 2s2p ³P states which can be easily populated in hot ion sources. Lifetimes range between 470 μs for O⁴⁺(2s2p ³P₁) [5] to essentially ∞ for the ³P₀ states. As a result, practically none of the possible beam components can decay during the few-μs flight times of the ions between the source and the photon-ion interaction region. The high-resolution high-flux photon beams of the Advanced Light Source (ALS) in Berkeley can be exploited to separate individual contributions to the photoionization of the ³P₀, ³P₁, and ³P₂ states of C III, N IV and O V. On the basis of high-precision experimental data, state-of-the-art R-matrix calculations for photoionization can be
tested at a new unprecedented level of detail.

2. Experimental and theoretical techniques
The Be-like target ions were produced with an all-permanent-magnet 10 GHz electron cyclotron resonance (ECR) ion source. A magnetically analyzed, well collimated ion beam was exposed under ultra-high-vacuum conditions to a counter-propagating photon beam at the ALS. Behind a second magnetic analyzer the photoionization products were detected by a single-particle detector. The parent ions were collected in a Faraday cup and the photon flux was monitored by a calibrated silicon X-ray photodiode. The experimental procedures of these experiments have been comprehensively described previously [6].

In the present experiments relative energy-scan measurements were carried out at different photon beam energy resolutions. The measurements were pushed to the practical limits of resolution which were mainly determined by limitations in the signal-to-background ratios acceptable for the experiments. The scan data were then normalized to absolute measurements available from the previous work [2, 3]. The total systematic uncertainty of the cross sections thus determined is about ±20%. Additional uncertainty arises from the presence of unknown fractions of metastable and ground-state ions in the parent beam. The energy scales of the experiments are calibrated with uncertainties of 1 to 10 meV depending on photon energy. Energy resolutions \(E/\Delta E\) of more than 20000 were reached.

R-matrix calculations were performed using the semi-relativistic Breit-Pauli approximation. Nine \(LS\) states were employed associated with \((1s^2nl)\) orbitals (with orbital quantum numbers up to \(n = 4\)) of the target ion core, that were retained in the close-coupling expansions for both the \(^1S\) ground and the \((2s2p\,^3P)\) metastable initial states of the Be-like parent ions. All the 9 states of the Li-like product ions were represented by multi-configuration interaction wave functions. The Breit-Pauli R-matrix approach was utilized to calculate the 15 \((LSJ)\) target ion state energies which arise from the 9 \(LS\) states. Photoionization cross sections for both the \(^1S\) ground and \((2s2p\,^3P)\) metastable initial states were determined in intermediate coupling \((LSJ)\) using the International R-Matrix/Opacity, Iron Project and RmaX Project programs [7, 8] with the scattering wave functions generated by allowing all possible three-electron promotions out of the base \(1s^22s^2\) configuration of the parent ion into the orbital set employed. The calculations were restricted to dipole allowed transitions. The calculations were carried out on an energy grid with a spacing of \(10^{-7}\) Ryd, which was essential to collect the full resonance strengths also of very narrow resonances.

3. Results and discussions
In the present study, photoionization experiments on C\(^{2+}\) ions and O\(^{4+}\) ions were restricted to the threshold regions of metastable \((2s2p\,^3P)\) parent states. Measurements were carried out with an ultimate resolution characterized by a photon energy spread of 3 meV at about 44 eV for C\(^{2+}\) and with roughly 11 meV at about 106 eV for O\(^{4+}\). Further increase of the resolution by closing the slits of the photon monochromator was not practical because the photon flux became forbiddingly low. The present calculations reproduce the observed structures remarkably well with maximum deviations of theoretical resonance energies from experiment at a level of only about 10 meV. Relative sizes of resonance peaks are well explained by assuming statistical population of the metastable components of the parent beam. On an absolute scale the experimental and theoretical cross sections are in very good agreement under the assumption that about half of the parent ions are in a metastable state.

Particular emphasis was put on the photoionization spectrum of N\(^{3+}\) ions. An overview spectrum from 68 eV to 88 eV was measured with a 40 meV resolution which marks an improvement of almost a factor 6 compared to the previously existing data. The overview spectrum is almost perfectly reproduced by the calculations which again assume statistical
Figure 1. Measurement at the photoionization threshold of N\(^{3+}\) \((2s2p\ 3P)\) ions. The step function shows the spectroscopic threshold energies [9] of the \(3P_{2,1,0}\) states. It was generated by distributing the measured strength according to statistical weights of the individual states involved. The solid line is a representation of the data using the step function washed out by a variable experimental energy spread (determined to be 9.3 meV).

A detailed threshold energy scan with N\(^{4+}\) ions indicates that statistical weighting is indeed a reasonable assumption. Figure 1 shows the results of a 9.3 meV-resolution scan compared with a combination of three step functions associated with the known ionization thresholds of the \(3P_{2,1,0}\) states [9] with step heights following the ratios 5:3:1. The steps were convoluted with a gaussian of 9.3 meV full width at half maximum (FWHM) and the resulting line perfectly agrees with the observed threshold cross section.

Figure 2 shows a measurement of the \((2p5p)\) resonance group arising from metastable N\(^{3+}\) \((2s2p\ 3P)\) ions. This group was not resolved in the experiments of Bizau et al [3]. In the present experiment, at least 7 distinct resonance contributions become visible at a resolving power \(E/\Delta E = 70\text{eV}/0.0033\text{eV} \approx 21200\). The solid line shows the theoretical result shifted by \(-8\) meV. The agreement between theory and experiment is truly remarkable.

The present study shows that state-of-the-art R-matrix calculations reproduce fine details in the photoionization of Be-like ions even at the level of state-to-state resolved data. Apparently, theory is well capable of providing excellent predictions of cross sections for Be-like ions in low charge states. The experiments provide good evidence for a statistical population of metastable states within the \(3P_{0,1,2}\) fine-structure manifold in Be-like ions produced by an ECR ion source. The agreement between theory and experiment gives great confidence in the relative fractions of metastable and ground-state ions deduced from comparisons as the one shown in figure 2.
Figure 2. Cross sections for photoionization of N\(^{3+}\) ions produced by an ECR source. The experiment was carried out with a photon energy spread as low as 3.3 meV. The data were normalized to previous absolute measurements of Bizau et al [3]. The R-matrix calculations assume 50% population of the ground state and statistical population of the remaining beam fraction of \(^3\)P metastable states. The theoretical result was convoluted with a 3.3 meV gaussian to simulate the experiment.

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