Experimental photoionization cross-section measurements in the ground and metastable state threshold region of Se$^+$

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Abstract

Absolute photoionization cross-section measurements are reported for Se$^+$ in the photon energy range 18.0–31.0 eV, which spans the ionization thresholds of the $^4S_3/2$ ground state and the low-lying $^2P_{3/2}$, $^2P_{1/2}$ and $^2D_{5/2}$, $^2D_{3/2}$ metastable states. The measurements were performed using the Advanced Light Source synchrotron radiation facility. Strong photoexcitation–autoionization resonances due to $4p \rightarrow n^d$ transitions are seen in the cross-section spectrum and identified with a quantum-defect analysis.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Photoionization is an important process in determining the ionization balance and hence the abundances of elements in astrophysical nebulae. In the last few years, it has become possible to detect neutron($n$)-capture elements (atomic number $Z > 30$) in a large number of ionized nebulae [1, 2]. These elements are produced by slow or rapid $n$-capture nucleosynthesis (the ‘$s$-process’ and ‘$r$-process’, respectively). Measuring the abundances of these elements can reveal their dominant production sites in the Universe, as well as details of stellar structure, mixing and nucleosynthesis [3–9]. These astrophysical observations provide an impetus to determine the photoionization and recombination properties of $n$-capture elements.

Various $n$-capture elements have been detected in the spectra of planetary nebulae [2, 10–12], the photoionized ejecta of evolved low- and intermediate-mass stars (1–8 solar masses). Planetary nebula progenitor stars may experience $s$-process nucleosynthesis [5, 9, 13, 14], in which case their nebulae will exhibit enhanced abundances of trans-iron elements. The level of $s$-process enrichment for individual elements is strongly sensitive to the physical conditions and mixing processes in the stellar interior [5, 7, 9].

The principal difficulty in studying $s$-process enrichments in planetary nebulae is the large uncertainties (factors of 2–3) of $n$-capture element abundances derived from the observational data. There are two root causes for these uncertainties. First, due in part to their low cosmic abundances, only one or two ions of a given $n$-capture element can be detected in individual planetary nebulae. To derive elemental abundances, corrections must be applied for the abundances of unobserved ionization stages. These corrections can be large and uncertain when the unobserved ions constitute a significant fraction of an element’s overall abundance. Second, while robust ionization corrections can be derived from numerical simulations of nebulae [15, 16], this method relies on the availability of accurate atomic data for processes that affect the ionization equilibrium of each element. In photoionized nebulae, these atomic data include photoionization cross...
sections and rate coefficients for radiative and dielectronic recombination and charge exchange reactions. These data are unknown for the overwhelming majority of \( n \)-capture element ions. Uncertainties in the photoionization and recombination data of \( n \)-capture element ions can result in elemental abundance uncertainties of a factor of 2 or more [1].

The present work is part of a larger study to determine the photoionization and recombination properties of \( n \)-capture element ions [17], motivated by the astrophysical detection of these species and the importance of measuring their elemental abundances accurately to test theories of nucleosynthesis and stellar structure. The ultimate goal of this effort is to produce atomic data suitable for incorporation into codes that numerically simulate the thermal and ionization structure of nebulae, enabling significantly more accurate abundance determinations of trans-iron elements in astrophysical nebulae than are presently achievable. Determining these data over the range of energies and temperatures encountered in astrophysical environments necessitates a predominantly theoretical approach. However, experimental measurements are needed to constrain and establish the veracity of such calculations, particularly in the case of complex systems such as low-charge states of trans-iron elements.

Se was chosen as the first element of our investigation because it has been detected in nearly twice as many planetary nebulae as any other trans-iron element [2]. Experimental photoionization studies of other astrophysically observed \( n \)-capture elements have already been conducted by other groups for select Kr [18, 19] and Xe ions [20, 21].

This paper presents experimental determinations of the absolute Se\(^+\) photoionization cross section near the ground-state ionization threshold, and is the first in a series of papers on the photoionization of low-charge Se ions (up to five times ionized). In section 2, the experimental procedure for our photoionization cross-section measurements is described in detail. The results and analysis of the data are presented in section 3, and in section 4 we summarize our work.

2. Experiment

High-resolution measurements of the Se\(^+\) photoionization cross section have been carried out at the Advanced Light Source (ALS) synchrotron radiation facility at Lawrence Berkeley National Laboratory in California. This experiment used the merged beams technique [22] with the Ion Photon Beamline (IPB) apparatus located at undulator beamline 10.0.1 of the ALS. A detailed description of the IPB apparatus is available in Covington et al [23]. The IPB endstation has been used for photoionization cross-section measurements of a variety of singly and multiply charged ions [24–29].

Se ions were produced by gently heating solid selenium inside a resistive oven within an electron-cyclotron-resonance (ECR) ion source. These ions were accelerated to an energy of 6 keV, and a 60° analysing magnet selected Se\(^+\) from the accelerated ion beam. The Se\(^+\) ions were collimated with two sets of vertical and horizontal slits and focused by three electrostatic einzel lenses. The resulting collimated ion beam had a typical diameter of a few millimetres, and a current ranging from 20 to 200 nA. The ions were merged onto the axis of the counter-propagating photon beam by a pair of 90° spherical bending plates. In the merged beam path, an electrical potential of 1.4 kV was placed on the ‘interaction region’ to energy-label photoions produced in a well-defined volume, for the purpose of absolute photoionization cross-section measurements. The interaction region consists of an isolated stainless-steel mesh cylinder with entrance and exit apertures defining an effective length of 29.4 cm. Two-dimensional intensity distributions of the photon and ion beams were measured by commercial rotating-wire beam profile monitors installed on either side of the interaction region, and by three translating-slit scanners located within the cylinder. Downstream from the interaction region, the Se\(^{2+}\) product ions were separated from the parent Se\(^+\) ion beam with a 45° dipole demerger magnet. This directed the Se\(^+\) ions to a Faraday cup, while the photoions were steered by a spherical 90° electrostatic deflector onto a negatively biased stainless steel plate. The secondary electrons produced by the Se\(^{2+}\) collisions on this plate were recorded by a single-particle channeltron detector. The detection efficiency has been determined on several occasions by measuring a femtoampere ion current at the stainless steel plate and comparing with the count rate generated from the channeltron. These measurements have consistently shown 100% efficiency for this detection scheme.

Photons were produced by a 10 cm period undulator located in the 1.9 GeV electron storage ring of the ALS. A grazing-incidence spherical grating monochromator delivered a highly collimated photon beam of spatial width less than 1 mm and divergence less than 0.05°. The photon energies were selected and scanned by rotating the grating and translating the exit slit of the monochromator, while simultaneously adjusting the undulator gap to maximize the beam intensity. The spectral resolution of the photon beam was controlled with the entrance and exit slits of the monochromator. The photon flux was typically 3 \( \times 10^{13} \) photons s\(^{-1}\), as measured by a silicon x-ray photodiode (IRD, SXUV-100) that was referenced to two identical photodiodes absolutely calibrated by the National Institute of Standards and Technology (NIST) and by the National Synchrotron Light Source (NSLS). To calibrate the photon energy, the well-known doubly excited states of He [30] were measured in first, second and third order. These measurements indicated that the uncertainty in the photon energies of the reported cross sections can be conservatively estimated to be less than 10 meV. The photon beam was mechanically chopped to separate photoions from the background produced by collisions between the parent ion beam and residual gas inside the interaction region.

3. Results and discussion

The photoion yield for Se\(^+\) was measured from 18 to 31 eV at a photon energy resolution of 28 meV (figures 1 and 2). The actual resolution was determined by fitting Lorentzian profiles to isolated features across the scanned energy region, and taking the average value of the fitted resonance widths.
Figure 1. Absolute cross-section measurements of photoionization of Se$^+$ are shown from 18 to 31 eV, at 28 meV resolution. The ionization thresholds of the quartet ground state and the four doublet metastable states (from NIST [33]) are indicated by vertical dashed lines. The shaded region represents energy scan measurements which are normalized to absolute cross-section measurements at specific energies (solid circles with error bars).

Figure 2. Absolute photoionization cross-section measurements in the region of the ground and metastable state thresholds at an energy resolution of 28 meV. Resonances originating from the $^2P^o$ metastable state have been identified as members of three different Rydberg series (open and solid triangles, and half-filled pink triangles; see table 1). Two more Rydberg series from the $^2D^o$ metastable state have been distinguished (open and filled red triangles) and are listed in table 2. All these series converge to either the $^1D^o$ or the $^1S^o$ excited states of Se$^{2+}$ as indicated by thick vertical lines. One series originating from the $^4S_{1/2}$ ground state converging to the $^3P^o$ state of Se$^{2+}$ has also been identified and is indicated by half-filled purple triangles. The vertical dashed lines indicate the reported metastable and ground-state ionization thresholds from NIST [33].

Absolute photoionization cross sections were measured at discrete photon energies with the same resolution. The photoionization spectrum was multiplied by a polynomial function to normalize the spectroscopic data to all absolute cross-section measurements, which are indicated in figure 1 by solid circles with associated uncertainties. Absolute photoionization measurements with the IPB apparatus at the ALS typically are uncertain by $\sim$20% at a 90% confidence level estimates.
level [23, 31]. For a detailed discussion of uncertainty estimates for photoionization measurements with the IPB apparatus, see [23, 31]. Note that these uncertainties do not account for contamination from higher order radiation from the undulator at low photon energies. A previous experiment on Xe3+ [32] using the same beamline estimated the contamination of higher order radiation to be ∼2% near 40 eV. At lower photon energies, the contamination of higher order radiation is expected to be larger, but not by more than a factor of 2–3 compared to the contamination at 40 eV. The total experimental uncertainties of the absolute measurements are estimated to be 30%, which accounts for the possible contamination of the photon beam by higher order radiation. We note that the lowest energy absolute cross section values are estimated to be ±0.010 eV or less.

Table 1. Principal quantum numbers (n), resonance energies and quantum defects (δ) determined from the present measurements of photoionization of Se+. Two distinct Rydberg series are observed from the $^2P_{1/2}$ and one from the $^2P_{3/2}$ metastable states of Se+, all due to $4p \rightarrow ns$ transitions. The uncertainties in the experimental energies are estimated to be ±0.010 eV or less.

| Initial Se+ state: 4s$^2$4p$^3$ ($^2P_{1/2}$) | Rydberg series | Energy (eV) | δ |
|--------------------------------------------|----------------|-------------|---|
| $4s^24p^3(1D_2)nd$ | n  | 18.268 | 0.14 | 5 | 19.301 | 0.24 |
| 6 | 18.697 | 0.14 | 6 | 20.074 | 0.22 |
| 7 | 18.972 | 0.14 | 7 | 20.530 | 0.19 |
| 8 | 19.160 | 0.14 | 8 | 20.815 | 0.17 |
| 9 | 19.296 | 0.12 | 9 | 21.008 | 0.15 |
| 10 | 19.395 | 0.1 | 11 | 21.703 | – |
| ∞ | 19.853 | – | – | – | – |
| Initial Se+ state: 4s$^2$4p$^1$ ($^2P_{3/2}$) | Rydberg series | Energy (eV) | δ |
|--------------------------------------------|----------------|-------------|---|
| $4s^24p^1(1D_2)nd$ | n  | 18.354 | 0.17 | 6 | 18.788 | 0.17 |
| 7 | 18.970 | 0.16 | 8 | 19.262 | 0.14 |
| 9 | 19.298 | 0.12 | 10 | 19.955 | – |
| ∞ | 19.955 | – | – | – | – |
| $^a$ NIST tabulations [33];

Identifications for the observed Se+ structure (see figure 2) are made based on the O+ resonance identifications and the use of the quantum-defect form of the Rydberg formula

$$E_n = E_\infty - \frac{R(Z - N)^2}{(n - \delta_n^2)}$$

where $Z$ is the charge of the nucleus, $N$ is the number of core electrons, $n$ is the principal quantum number, $E_\infty$ is the series limit and $\delta_n$ is the dimensionless quantum defect parameter that indicates the departure of the energy level $E_n$ from the hydrogenic value. Two series from the $^2P_{3/2}$ metastable state and one from $^2P_{1/2}$ have been identified. The $4s^24p^3(1D)nd$ series converging to the $^1D$ series limit is shown in figure 2 by open blue triangles for resonances originating from the $^2P_{3/2}$ state, and by filled blue triangles for resonances from $^2P_{1/2}$. The $4s^24p^3(1S)nd$ series converging to the $^1S$ series limit originating from the $^2P_{3/2}$ state is depicted by half-filled pink triangles in figure 2. In addition, two other series from the $^2D_j^o$ ($j = 3/2, 5/2$) metastable states are indicated by inverted open and filled red triangles above the spectrum. These resonances correspond to the $4s^24p^3(1D)nd$ series converging to the $^1D$ limit. In the measured energy range, only one Rydberg series is observed from the $^4S_{3/2}$ ground state, whose first autoionizing member is $4s^24p^3(1P_{1/2})$d. The series is indicated with inverted open and filled red triangles just above the ground state threshold.

Tables 1–3 list the principal quantum numbers, resonance energies and quantum defects of the identified members of
Table 2. Principal quantum numbers \( (n) \), resonance energies and quantum defects \( (\delta) \) determined from the present measurements of photoionization of Se\(^+\). Two distinct Rydberg series are observed from the \( ^2\text{D}^\prime \) metastable state of Se\(^+\), due to \( 4p \to nd \) transitions. The uncertainties in the experimental energies are estimated to be \( \pm 0.010 \) eV or less.

| Initial Se\(^+\) state: \( 4s^24p^3 \left( ^2\text{D}^\prime_{3/2} \right) \) | Initial Se\(^+\) state: \( 4s^24p^3 \left( ^2\text{D}^\prime_{5/2} \right) \) |
|---|---|
| Rydberg series \( 4s^24p^2 \left( ^1\text{D}^2 \right) nd \) | Rydberg series \( 4s^24p^3 \left( ^1\text{D}^2 \right) nd \) |
| \( n \) | Energy (eV) | \( \delta \) | \( n \) | Energy (eV) | \( \delta \) |
| 6 | 19.499 | 0.17 | 6 | 19.575 | 0.17 |
| 7 | 19.933 | 0.17 | 7 | 20.009 | 0.17 |
| 8 | 20.212 | 0.17 | 8 | 20.288 | 0.17 |
| 9 | 20.402 | 0.17 | 9 | 20.478 | 0.17 |
| 10 | 20.537 | 0.17 | 10 | 20.613 | 0.17 |
| 11 | 20.637 | 0.16 | 11 | 20.713 | 0.16 |
| 12 | 20.712 | 0.16 | 12 | 20.788 | 0.16 |
| 13 | 20.770 | 0.15 | 13 | 20.846 | 0.15 |
| 14 | 20.816 | 0.15 | 14 | 20.895 | 0.15 |
| 15 | 20.853 | 0.15 | 15 | 20.929 | 0.15 |
| \( \infty \) | \( 21.100^a \) | \( \infty \) | \( 21.167^a \) | \( \infty \) |

\( ^a \) NIST tabulations [33].

Table 3. Principal quantum numbers \( (n) \), resonance energies and quantum defects \( (\delta) \) determined from the present measurements of photoionization of Se\(^+\). One distinct Rydberg series is observed from the \( ^4\text{S}\) metastable state of Se\(^+\), due to \( 4p \to nd \) transitions. The uncertainties in the experimental energies are estimated to be \( \pm 0.010 \) eV or less.

| Initial Se\(^+\) state: \( 4s^24p^3 \left( ^4\text{S}_{3/2} \right) \) | Rydberg series \( 4s^24p^2 \left( ^3\text{P}_2 \right) nd \) |
|---|---|
| \( n \) | Energy (eV) | \( \delta \) |
| 11 | 21.215 | 0.21 |
| 12 | 21.291 | 0.21 |
| 13 | 21.349 | 0.21 |
| 14 | 21.396 | 0.21 |
| 15 | 21.433 | 0.21 |
| 16 | 21.464 | 0.21 |
| 17 | 21.489 | 0.21 |
| 18 | 21.510 | 0.21 |
| 19 | 21.528 | 0.21 |
| 20 | 21.543 | 0.21 |
| \( \infty \) | \( 21.682 \) | \( \infty \) |

\( ^a \) NIST tabulations [33].

It is important to note that ECR ion sources are known to produce ions in the ground and metastable states in fractions that may differ from statistically weighted values. Therefore, the reported cross-section measurements correspond to an unknown admixture of metastable and ground state fractions. In the case of O\(^+\) [31] the metastable fractions were determined using the beam attenuation method \( (4S \ 43\%, \ 2D \ 42\% \text{ and } 3P \ 15\%) \), clearly differing from the statistically weighted values \( (4S \ 20\%, \ 2D \ 50\% \text{ and } 3P \ 30\%) \) but not as much as those reported using translational energy spectroscopy \( (4S \ 60\%, \ 2D \ 19\% \text{ and } 3P \ 21\%) \) [34]. Similarly, we do not expect statistically weighted metastable fractions in our Se\(^+\) measurements.

4. Summary

The absolute photoionization cross section of Se\(^+\) has been measured in the energy region of the ground state ionization threshold. The cross section exhibits a wealth of resonances that form a clear pattern of Rydberg series. The strongest resonances are identified as \( 4p \to nd \) transitions belonging to the \( 4s^24p^2 \left( ^1\text{D}^2 \right) nd \) and \( 4s^24p^3 \left( ^1\text{D}^2 \right) nd \) series originating from the \( ^4\text{S}^0 \) and \( ^2\text{D}^\prime \) metastable states. The sole series from the \( ^4\text{S}_{3/2} \) ground state is identified as \( 4s^24p^3 \left( ^3\text{P}_2 \right) nd \). The resonance positions and quantum defects are determined for the initial members of each of these series.

The photoionization cross sections from the present study (and for other low-charge Se ions, to be presented in forthcoming papers) will be used to calibrate a broader theoretical effort to determine the photoionization and recombination properties of astrophysically observed \( n \)-capture elements [17]. The resulting atomic data determinations will enable the abundances of trans-iron species in astrophysical nebulae to be derived to a much higher degree of accuracy than is currently possible, which bears implications for the nucleosynthetic sites and chemical evolution of Se and other trans-iron elements. Our absolute
cross sections for Se⁺ can be accessed via secure FTP at the IP address 131.243.76.25 (note that a username and password are required; these can be obtained by contacting AA at aaguilar@lbl.gov), or by contacting the authors NCS (sterling@pa.msu.edu) and AA.

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