K-shell photoionization of Be-like and Li-like ions of atomic nitrogen: experiment and theory

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Abstract

Absolute cross sections for the K-shell photoionization of Be-like and Li-like atomic nitrogen ions were measured by employing the ion–photon merged-beam technique at the SOLEIL synchrotron radiation facility in Saint-Aubin, France. High-resolution spectroscopy at nominal resolutions of 38, 56, 111, 133 meV full width at half maximum (FWHM) for Be-like and 125 meV FWHM for Li-like atomic nitrogen ions was achieved for the photon energies ranging from 410 up to 460 eV. The experimental measurements are compared with theoretical estimates from the multi-configuration Dirac–Fock, R-matrix and an empirical method. The interplay between experiment and theory enabled the identification and characterization of the strong 1s → 2p resonances features observed in the K-shell spectra of each ion and the region around 460 eV for the 1s → 3p resonance of the N3+ ion yielding suitable agreement with experiment.

(Some figures may appear in colour only in the online journal)

1. Introduction

Photoabsorption and photoionization (PI) are fundamental atomic processes that play important roles in many physical systems, including a broad range of astrophysical objects as diverse as quasi-stellar objects, the atmosphere of hot stars, protoplanetary nebula, HII regions, novae and supernovae. Satellites Chandra and XMM-Newton currently provide a wealth of x-ray spectra of astronomical objects; the lack of high-quality atomic data hammers the interpretation of these spectra [1–5]. Studies recently carried out on carbon and its ions showed it was necessary to have good quality data to model the observations in the x-ray spectrum of the bright blazar Mkn 421 observed by the Chandra LETG+HRC-S [6].
Spectroscopy in the soft x-ray region (5–45 Å) including K-shell transitions of C, N, O, Ne, S and Si, in neutral, and low stages of ionization, L-shell transitions of Fe and Ni, provide a valuable tool for investigating the extreme environments in active galactic nuclei, binary systems, cataclysmic variable stars and Wolf–Rayet Stars [7] as well as the interstellar media (ISM) [8]. One may expect similar results concerning the chemical composition of the ISM if accurate data are available on neutral [2, 5, 9, 10], and various charge stages of ionization of atomic nitrogen K-edge cross sections [9, 11]. PI models of the brightest knot of star formation in the blue compact dwarf galaxy Mrk 209 required abundances for ions of oxygen and nitrogen [12]. Therefore PI cross section data and abundances for carbon, nitrogen, and oxygen in their various stages of ionization are essential for PI models applied to the plasma modelling in a variety of planetary nebulae [13]. Nitrogen abundance in particular plays a fundamental role in η Car studies, because it is a key tracer of CNO processing [14]. Li-like atomic nitrogen ions (N V) are used in the determination of PI structures of pressure-supported gas clouds in gravitationally dominant dark matter mini-halos in the extended Galactic halo or local group environment [15] with the modelling code CLOUDY [16, 17].

X-ray spectra obtained by Chandra from sources such as Capella, Procyon, and HR 1099 are used as standards to benchmark plasma spectral modelling codes. He-like nitrogen (N VI) lines have been observed with Chandra and XMM-Newton in the x-ray spectra of Capella and Procyon [18, 19], the M dwarf binary YY Gem [20], and the recorded outburst of the recurrent nova RS Oph [21], in the wavelengths region 28.7–29.6 Å (420 eV) that are attributed to 1s → 2ℓ transitions. XMM-Newton observations of the fast classical nova V2491 Cyg [22] have also indicated the N VI, Kα, and Kβ lines are present at about 28.78 and 24.90 Å. The He-like series lines of N VI and O VII are detected up to 1s → 5p, and for O VII, the recombination/ionization continuum at 16.77 Å (739.3 eV) is present between 16.6–16.8 Å. He-like N VI has also been observed in the Chandra-LETGS x-ray spectroscopy of NGC 5548 [23].

In the x-ray community, electron-beam-ion-trap (EBIT) measurements (used for calibrating resonance energies), have been carried out for the inner-shell 1s → 2ℓ transitions in He-like and Li-like nitrogen ions [24] (used in plasma modelling to determine impurity transport properties [25]). He-like and Li-like x-ray lines energies of atomic nitrogen have been measured at the Lawrence Livermore National Laboratory EBIT [24]. In EBIT experiments, the spectrum is contaminated and blended with ions in multiple stages of ionization, making spectral interpretation fraught with difficulties, unlike the cleaner higher-resolution spectra obtained from third generation synchrotron radiation facilities such as the Advanced Light Source, BESSY II, SOLEIL, ASTRID II and Petra III.

PI cross sections used for the modelling of astrophysical phenomena have mainly been provided by theoretical methods, due to limited experimental data being available. As a consequence, significant effort has been put into improving the quality of calculated data using state-of-the-art theoretical methods. Recent advances in the determination of atomic parameters for modelling K lines in cosmically abundant elements have been reviewed by Quinet and co-workers [4]. Until recently, many of these calculations have not been severely tested by experiment, and this remains an urgent task [26]. Experimental K-shell PI cross section measurements have been made by various groups on a variety of atoms and ions of astrophysical interest; He-like Li+ [27–29], Li atoms [30], Li-like B2+ [31], C3+ [32], Be-like B+ [33], C2+ [34], Li-like N+ [35], C-like N5+ [11], N-like O+ [36], F-like Ne+ [37], neutral nitrogen [10] and oxygen [38–41], valence shell studies on B-like ions, N2+, O3+ and F4+ [26]. Cℓ-like Ar+ [42], Mg-like Fe24+ [43], As-like Se+ [44–46] and Br-like Kr+ [47–49]. All this experimental data has been compared with various modern theoretical methods.

Theoretical K-shell PI cross sections for the iso-nuclear C I–C IV ions assembled recently to model the Chandra x-ray absorption spectrum of the blazar Mkn 421 [6] were found to be in excellent agreement with the astrophysical observations. Additionally, K-shell PI cross sections calculations on neutral nitrogen showed excellent accord with high resolution measurements made at the Advanced Light Source radiation facility in Berkeley, California [10] as have similar cross section calculations on singly and doubly ionized atomic nitrogen when compared with measurements from the SOLEIL synchrotron facility in Saint-Aubin, France [11, 50]. In fact, the majority of the high-resolution experimental studies from the third generation light sources have been shown to be in excellent agreement with detailed theoretical calculations performed using the state-of-the-art R-matrix method [51, 52] and with other theoretical approaches.

The present experimental and theoretical work on the prototype Be-like and Li-like atomic nitrogen ions provides cross section data for the PI of x-rays in the vicinity of the K-edge, where strong n = 2 inner-shell resonance states are observed. This work follows our earlier successful work on K-shell investigations for singly and doubly ionized atomic nitrogen [11, 50]. To our knowledge, there would appear to be limited experimental studies for resonance Auger energies reported to date on either Be-like or Li-like atomic nitrogen ions [24, 53, 54] for photon energies in the vicinity of the K-edge region. For Be-like atomic nitrogen, previous experimental and theoretical studies have been made in the valence region and in the near threshold region [26, 43, 55, 56] where it was necessary to include both the ground state and metastable excited states in the theoretical work in order to achieve suitable agreement with experiment. We follow a similar prescription here in the vicinity of the K-shell energy region as the Be-like (N27+) atomic nitrogen ions produced in the SOLEIL synchrotron radiation experiments are not purely in their ground state. Theoretical studies are an essential ingredient in order to determine the metastable constituents in the beam. In the case of Li-like atomic nitrogen ions one only needs to consider the case of the ground state as no metastable states are present in the parent beam.

K-shell PI when followed by Auger decay couples three or more ionization stages rather than two in the usual equations of ionization equilibrium [57]. The 1s → np photo-excitation
processes involved in the interaction of a photon with the 1s^22s^2 1S ground state of the Be-like nitrogen ion is:

\[ h\nu + N^+(1s^22s^21S) \rightarrow N^{+\ast}(1s2s2p^1P^\pm) \]

\[ N^{+\ast}(1s^22s^2S) + e^-(k_f^0) \text{ or } N^{+\ast}(1s^2np^2S) + e^-(k_f^0), \]

where \( n = 2, 3 \), and \( k_f^0 \) is the outgoing energy of the continuum electron with angular momentum \( t \). The strongest Auger decay channels being the spectator KLL channels where the Rydberg, np electron does not participate in the Auger decay.

Experimental studies on Be-like atomic nitrogen ions, in their ground state 1s^22s 1S, are contaminated by the presence of metastable states. In the SOLEIL experiments, N^+ ions are produced in the gas-phase from an electron-cyclotron-resonance-ion-source (ECRIS) therefore metastable states 1s^22p^3P may be present in the parent ion beam. The 1s^22p^3P metastable state, autoionization processes from the 1s \( \rightarrow \) 2p photo-excitation process are:

\[ h\nu + N^+(1s^22s2p^3P) \]

\[ N^+(1s2s[1S]2p^1P,1D,1S)1s^2S,3P^\pm) \]

For the case of Li-like ions, the strongest excitation processes in the interaction of a photon with the 1s^22s^2S_1/2 ground state of the Li-like nitrogen ion is the 1s \( \rightarrow \) 2p photo-excitation process:

\[ h\nu + N^{+\ast}(1s^22s^2S_{1/2}) \rightarrow N^{+\ast\ast}(1s2s2p^1P^\pm)2P_{1/2,3/2} \]

\[ N^{5+}(1s^21S_0) + e^-(k_f^0). \]

Detailed experimental PI measurements have been performed for the first time on these prototype Be-like and Li-like systems in the photon energy region of the K-edge.

In our previous publication on K-shell PI of N^+ ions [11] we highlighted the limitations of central fields calculations using Harte–Slater of Dirac–Slater potentials [58–62]. We stress again that results derived from these methods used in spectral modelling should be treated with caution.

For Be-like atomic nitrogen ions, state-of-the-art ab initio calculations for Auger inner-shell processes were carried out by Petrini and de Araújo [57] and by Berrington and co-workers [63] using the R-matrix method [51] and followed a similar procedure to the work on K-shell studies for the Be-like B^+ ion [64]. Petrini and co-workers [65] noted that once the 1s-hole was created in the ions, by single PI, with simultaneous shake-up and shake-off processes, Auger decay populates directly excited states of the residual ions, which then produces UV lines. Similarly, for Li-like atomic nitrogen ions, Charro and co-workers [66] performed R-matrix calculations in LS-coupling for PI cross sections and compared and contrasted their results with previous central field and R-matrix methods as only limited experimental data was available. However, no attempt was made in their calculations at determining resonance parameters.

About a decade later this work was further extended by Garcia and co-workers [9], using the optical potential method within the Breit–Pauli R-matrix formalism [51, 52, 67, 68]. PI from the ground state, along the nitrogen iso-nuclear sequence was investigated, in the photon energy region of the K-edge. We note that for K-shell PI, the cross section calculations of Garcia and co-workers [9] included both radiation and Auger damping, which cause the smearing of the K-edge. Due to the lack of experimental data being available at that time a comparison with previous theoretical results (of lower calibre) were only possible. Garcia and co-workers [9] pointed out these earlier central field calculations do not take account of the resonance features that dominate the cross sections near the K-edge. In the present study we compare our theoretical results from the multi-configuration Dirac Fock (MCDF) and the R-matrix with pseudo states methods (RMPS), an empirical fitting approximation [69] (derived from previous experimental measurements on resonance energies and Auger widths of the iso-electronic sequence), prior theoretical results [9, 70, 71] and current experimental measurements made at the SOLEIL synchrotron radiation facility.

In this paper detailed theoretical calculations and experimental measurements are presented for the K-shell single photon ionization cross sections of Be-like atomic nitrogen ions (410–415 eV and 460–460.4 eV) and Li-like atomic nitrogen ions, (420–426 eV). Our theoretical predictions from the MCDF and R-matrix methods enabled identification of the 1s \( \rightarrow \) 2p resonances and their parameters, observed in the Be-like and Li-like nitrogen spectra and the 1s \( \rightarrow \) 3p resonance around 460 eV in Be-like nitrogen. The present investigation provides absolute values (experimental and theoretical) for cross sections along with the resonance strengths, for a photon colliding with the 1s^22s^2S ground state, autoionization processes from the 1s \( \rightarrow \) 2p photo-excitation process;
photon beam by using electrostatic deflectors and einzel lenses to focus the beam. After the interaction region between the photon and the ion beams, another dipole magnet separates the primary beam and the beam of ions which have gained one (or several) charge(s) in the interaction, the so-called photo-
ions. The primary ions are collected in a Faraday cup and the photon-ions are detected by multi-channel plates detector. The photon current is measured by a calibrated photodiode. Ions with the same charge as the photo-ions can also be produced by collisions between the primary ions and the residual gas or stripping on the walls in the interaction region. This background signal is subtracted by chopping the photon beam, collecting the data with and without photons for 20 s accumulation time.

For the absolute measurements of the PI cross sections, a −1000 V bias is applied on the 50 cm long interaction region and the data are collected with 30 meV photon energy steps. The overlap of the two beams and the density distributions of the interacted particles is determined in three dimensions by using two sets of three scanning slits. The cross sections obtained have an estimated systematic uncertainty of 15%. In another spectroscopy mode, no bias is applied to the interaction region allowing the photon and ion beams to interact over about 1 m and to scan the photon energy with a finer step. In this mode, only relative cross sections can be measured. They are later normalized on the cross sections determined in the absolute mode assuming the area under the resonances to be the same. Table 1 gives typical experimental parameters used to evaluate absolute cross sections for N\(^{3+}\) ions at a photon energy of 412.5 eV. The energy and band width of the photon beam are calibrated separately using a gas cell and N\(^2\) (1s\(^{-1}\)) PI lines, located at 400.87 eV [74] and Ar 2p\(_{3/2}\) 1.48 eV at 244.39 eV [75]. The photon energy, once corrected for Doppler shift, has an uncertainty of approximately 30 meV. Outstanding possibilities in terms of spectral resolution and flux at the N\(_2\) (1s\(^{-1}\)) K-edge have been discussed recently by Miron and co-workers [76, 77].

### 3. Theory

3.1. SCUNC: Li-like and Be-like nitrogen

In the framework of the screening constant by unit nuclear charge (SCUNC) formalism [69, 78, 79], the total energy of the core-excited states is expressed in the form given by,

\[
E(Nn\ell\ell',2S+1L^J) = -Z^2 \left[ \frac{1}{N^2} + \frac{1}{\ell^2} \left[ 1 - \beta (Nn\ell\ell',2S+1L^J; Z) \right]^2 \right],
\]

where \(E(Nn\ell\ell',2S+1L^J)\) is in Rydberg units. In this equation, the principal quantum numbers \(N\) and \(\ell\) are respectively for the inner and the outer electron of the He-like iso-electronic series. The \(\beta\)-parameters are screening constants by unit nuclear charge expanded in inverse powers of \(Z\) and are given by the expression,

\[
\beta (Nn\ell\ell',2S+1L^J) = \sum_{k=1}^{q} f_k \left( \frac{1}{Z} \right)^k
\]

where \(f_k (Nn\ell\ell',2S+1L^J)\) are parameters to be evaluated empirically from a previous experimental measurements. Similarly, one may get the Auger widths \(\Gamma\) in Rydbergs (1 Rydberg = 13.605 698 eV) from the formula

\[
\Gamma(Ry) = Z^2 \left[ 1 - \frac{f_1}{Z} \times \frac{Z}{Z_0} - \frac{f_1}{Z^2} \times \left( \frac{Z - Z_0}{Z_0} \right)^2 \right].
\]

The experiment measurements of Müller and co-workers on Be-like carbon and Li-like carbon and boron [31, 32, 34] were used to determine all the appropriate empirical parameters. For Be-like carbon, we note the labelling of the 1s2s2p\(^{2}P^0\) and 1s2s2p\(^{2}P^2\) states of Müller and co-workers [34] should be reversed as pointed out in our recent calculations on the carbon iso-nuclear sequence [6] used to model the x-ray spectra of the bright Blazar Mkn 421 observed by the Chandra satellite.

3.2. MCDF: Li-like and Be-like nitrogen

MCDF calculations were performed based on a full intermediate-coupling regime in a \(jj\)-basis using the code developed by Bruneau [80]. Photo-excitation cross sections have been carried out for both Li-like and Be-like atomic nitrogen ions in the region of their respective K-edges. Only electric dipole transitions have been computed using the Babushkin gauge. For Be-like atomic nitrogen ion the following initial configurations have been considered: 1s\(^2\)\(^2S\), 1s\(^2\)\(^2P\) and 1s\(^2\)\(^2P\). Where the bar over the orbital is to indicate that they are different for the initial and final states. In order to describe the correlation and relaxation effects, multiple orbitals with the same quantum number have been used. Then, the following final configurations have been considered: 1s2s\(^2\)\(^2P\), 1s2s\(^2\)\(^2P\), 1s2p\(^3\)\(^1S\) and 1s2p\(^3\)\(^3P\). Such notation means that radial functions for \(n = 2\) orbitals are not the same for initial and final configurations. The wavefunctions have been calculated minimizing the following energy functional:

\[
E = \frac{\sum_{\alpha} (2J_\alpha + 1)E_\alpha}{2\sum_{\alpha} (2J_\alpha + 1)} + \frac{\sum_{\beta} (2J_\beta + 1)E_\beta}{2\sum_{\beta} (2J_\beta + 1)}
\]

where \(\alpha\) and \(\beta\) run over all the initial and final states, respectively.

Synthetic spectrum has been constructed as a weighted sum of photo-excitation cross sections from both the ground state levels 1s\(^2\)\(^2S\)(\(^1S\)) and the metastable state levels 1s\(^2\)\(^2P\)(\(^3P_{0,1,2}\)). Each electric dipole transition has been dressed by a Lorentzian profile, assuming a full width at half maximum (FWHM) equal respectively to 66 meV and
80 meV for the 1s-2p and 1s-3p transitions in Be-like atomic nitrogen. Such FWHM values have been deduced from the MDCC calculations that were performed separately. A mixture of 60% ground and 40% metastable states has been used to fit the experimental results. In order to compare directly with the Be-like experimental data, the synthetic spectrum has been convoluted with a Gaussian profile to simulate the experimental resolution. A similar procedure has been used for the Li-like atomic nitrogen ion, except that (i) the following configurations have been considered: 1s22s2, 1s22s2p, and 1s22p3p, and (ii) a Lorentzian FWHM equal to 45 meV and 60 meV has been used respectively for the 1s-2p and 1s-3p transitions in Li-like atomic nitrogen. It should not be pointed out that for the Li-like atomic nitrogen ion, only the ground state contribution has been retained to compare with experimental data.

3.3. R-matrix: Be-like nitrogen

The R-matrix method [51, 52, 67, 68], using a version of the codes implemented on parallel architectures [44, 48, 81] determined the necessary cross sections. For Be-like ions both the initial 1S ground state and the 3P determined the necessary cross sections. For Be-like ions the codes implemented on parallel architectures [44, 48, 81] were required. Cross section calculations were carried out in LS-coupling with 390-levels retained in the close-coupling expansion using the RMPS. The Hartree–Fock 1s, 2s and 2p tabulated orbitals of Clementi and Roetti [82] were used with n = 3 physical and n = 4 pseudo orbitals of the residual N4+ ion. The n = 4 pseudo-orbitals were determined by energy optimization on the ground state of the N4+ ion, with the atomic-structure code CIV3 [83]. The n = 4 pseudo-orbitals are used to account for core relaxation and electron correlation effects, in the multi-configuration interaction target wavefunctions. The N4+ residual 390 ion states used multi-configuration interaction target wavefunctions. The non-relativistic R-matrix method determined the energies of the N4+ bound states and all the appropriate cross sections. We determined PI cross sections for the 1s22s2 1S ground state and the 1s2s2p3P metastable state.

For the electron–ion collision work we allowed three-electron promotions out of selected base configurations of N4+. The collision work was carried out with 20 continuum functions and a boundary radius of 8.2 Bohr radii. From our RMPS calculations, the 1S ground state gave a bound state ionization potential of 5.69195 Rydbergs compared to the experimental value of 5.69420 Rydbergs. In the case of the 3P metastable state, the ionization potential from the RMPS calculations gave 5.08202 Rydbergs, compared to the experimental value of 5.08200 Rydbergs. A discrepancy respectively of approximately 31 meV for the ground state and 0.3 meV for the metastable state. It is seen that both RMPS theoretical results are in excellent agreement with the experimental values from the NIST tabulations [84].

For the 1S ground state and the 3P metastable state, the outer region electron–ion collision problem was solved by selecting an appropriately fine energy mesh of 2 × 10−7 Rydbergs (∼2.72 µeV) in order to delineate all the resonance features in the cross sections. Radiation and Auger damping were also included in the R-matrix calculations.

For a direct comparison with the SOLEIL experimental measurements (performed at the various energy resolutions), the R-matrix results were convoluted with an appropriate Gaussian function of FWHM and an admixture of 60% ground state and 40% metastable state was used to simulate experiment. The peaks found in the theoretical PI cross section spectrum were fitted to Fano profiles for overlapping resonances [85–91] instead of the energy derivative of the eigenphase sum method [92–94].

3.4. R-matrix: Li-like nitrogen

For this Li-like system intermediate-coupling PI cross section calculations were performed using the semi-relativistic Breit–Pauli approximation which allows for relativistic effects to be included in a similar manner to our previous work on Li-like, boron [31] and carbon [32] ions. As in our previous work, radiation-damping [67] effects were also included within the confines of the R-matrix approach [51, 52] for completeness [51, 67, 98]. An appropriate number of N5+ residual ion states (19 LS, 31 LSJ levels) were included in our intermediate-coupling calculations. The n = 4 basis set of N5+ orbitals obtained from the atomic-structure code CIV3 [83] were used to represent the wavefunctions. PI cross section calculations were then performed in intermediate coupling for the 1s22s2s1S1/2 initial state of the N5+ ion in order to incorporate relativistic effects via the semi-relativistic Breit–Pauli approximation.

For cross section calculations He-like LS states were retained: 1s2 1S, 1s1s1S, 1snp1S, 1snp1P, 1snp1D, and 1snp1F, n ≤ 4, of the N5+ ion core giving rise to 31 LSJ states in the intermediate close-coupling expansions for the J = 1/2 initial scattering symmetry of the Li-like N4+ ion. The n = 4 pseudo states are included in an attempt to account for core relaxation, electron correlations effects and the infinite number of states (bound and continuum) left out by the truncation of the close-coupling expansion in our work. For the structure calculations of the residual N5+ ion, all n = 3 physical orbitals and n = 4 correlation orbitals were included in the multi-configuration interaction target wavefunctions expansions used to describe the states.

The Hartree–Fock 1s and 2s orbitals of Clementi and Roetti [82] together with the n = 3 orbitals were determined by energy optimization on the appropriate spectroscopic state using the atomic-structure code CIV3 [83]. The n = 4 correlation (pseudo) orbitals were determined by energy optimization on the ground state of this ion. All the states of the N5+ ion were then represented by using multi-configuration interaction wavefunctions. The Breit–Pauli R-matrix approach was used to calculate the energies of the N5+(LSJ) bound states and the subsequent PI cross sections. A minor shift (<0.1%) of the theoretical energies for the N5+ ion core states to experimental values [84] was made so that they would be in agreement with available experimental thresholds. Both double and triple promotion models for the scattering wavefunctions were investigated. The accuracy of the bound initial state wavefunction is more difficult to assess. Earlier LS-coupling calculations of Charro and co-workers.
and intermediate coupling. In previous LS all the PI cross sections for the initial ground state in on Li-like boron [31] and Li-like carbon [32] ions, two experimental measurements. We illustrate only the found here when compared with the high resolution SOLEIL employed yielding similar results. A similar tendency is and three-electron promotions scattering models were both results from the triple-promotion scattering model with the radii. For the 2S1 20 continuum functions and a boundary radius of 6.8 Bohr.

Figure 1. Photoionization cross sections for Be-like atomic nitrogen (N3+) ions measured with a 111 meV band pass at the SOLEIL radiation facility. Solid circles: total photoionization recorded in the relative mode. The error bars represent the statistical uncertainty. The absolute measurements (open triangles) total photoionization cross sections have been obtained with a larger energy step. The error bars give the total uncertainty of the experimental data. The MCDF (solid green line) and R-matrix (solid red line) calculations shown are convolution with a Gaussian profile of 111 meV FWHM and an appropriate weighting of the ground and metastable states (see text for details) to simulate the measurements. For the metastable 3P state, the MCDF calculations have been shifted up by +1.46 eV in order to match experiment. Table 2 gives the designation of the resonances 1–3 and their parameters.

[66] gave a value of 7.1909 Rydbergs, for the 1s22s 2S1/2 bound state. From our R-matrix calculation we obtain values of 7.19301 Rydbergs (double electron promotions), and 7.19332 Rydbergs (triple electron promotions) compared to a value of 7.19479 Rydbergs from the NIST tabulation [84]. A discrepancy of 24 meV and 20 meV respectively with experiment. PI cross sections out of the Li-like nitrogen ion N2+ (1s22s 2S1/2) ground state were then obtained for total angular momentum scattering symmetries of J = 1/2 and J = 3/2, odd parity, that contribute to the total.

The R-matrix method [51, 52, 67] was used to determine all the PI cross sections for the initial ground state in LS and intermediate coupling. In previous R-matrix work on Li-like boron [31] and Li-like carbon [32] ions, two and three-electron promotions scattering models were both employed yielding similar results. A similar tendency is found here when compared with the high resolution SOLEIL experimental measurements. We illustrate only the R-matrix results from the triple-promotion scattering model with the SOLEIL experimental measurements.

The electron–ion collision work was carried out with twenty continuum functions and a boundary radius of 6.8 Bohr radii. For the 2S1/2 initial state the outer region electron–ion collision problem was solved using an appropriate fine energy mesh of 2.0 × 10−7 Rydbergs (≈2.72 μeV) to delineate the resonance features in the cross sections.

For Li-like atomic nitrogen, the QB technique (applicable to atomic and molecular complexes) of Berrington and co-workers [92–94] was used to determine the resonance parameters and averaging was performed over final total angular momentum J values. All the resonance parameters for the Li-like atomic nitrogen ion are presented in table 3.

Finally, in order to compare directly with experiment, the theoretical cross section was convoluted with a Gaussian function of appropriate FWHM (125 meV) to simulate the energy resolution of the measurements. The experimental and theoretical results for this Li-like atomic nitrogen ion are presented in figure 5.

4. Results and discussion

Figures 1–4 compare our experimental cross sections (solid circles) with theoretical predictions made from the MCDF (green curve) and R-matrix (red curve) methods for Be-like atomic nitrogen (N3+). Similarly in figure 5 we present those for Li-like atomic nitrogen (N4+) ions. For the Be-like atomic nitrogen (N4+) ion, the experimental cross section has been recorded with different band widths, ranging from 38 to 133 meV, presented in figures 1–4 respectively. Each cross section is obtained from the weighted mean of several sweeps (from three to eight following increasing resolution). The assignment, resonance excitation energy, Auger width and strengths of all the n = 2 observed lines are summarized in tables 2 and 3. For the determination of the experimental widths, each individual sweep has been fitted separately by Voigt profiles to avoid any possible shift in the energy delivered by the monochromator. Then the final width of the Lorentzian component was obtained from the weighted mean of the individual Lorentzian width determined from each fit. For the N3+ ion, splitting of the J components of the initial state [84] was also taken into account, assuming a statistical distribution of the levels. The experimental and theoretical oscillator strengths were obtained from the area under the lines.
Figure 2. Photoionization cross sections for Be-like atomic nitrogen ($\text{N}^{3+}$) ions measured with a 56 meV band pass at the SOLEIL radiation facility. Solid circles: total photoionization. The error bars give the statistical uncertainty of the experimental data. The MCDF (solid green line) and $R$-matrix (solid red line) calculations shown are convolution with a Gaussian profile of 56 meV FWHM and an appropriate weighting of the ground and metastable states (see text for details) to simulate the measurements. For the metastable $^3P$ state, the MCDF calculations have been shifted up by +1.46 eV in order to match experiment. Table 2 gives the designation of the resonances $1^-3^-$ and their parameters.

Figure 3. Photoionization cross sections for Be-like atomic nitrogen ($\text{N}^{3+}$) ions measured with a 38 meV band pass at the SOLEIL radiation facility. Solid circles: total photoionization. The error bars give the statistical uncertainty of the experimental data. The MCDF (solid green line) and $R$-matrix (solid red line) calculations shown are convolution with a Gaussian profile of 38 meV FWHM and an appropriate weighting of the ground state and metastable state (see text for details) to simulate the measurements. For the metastable $^3P$ state, the MCDF calculations have been shifted up by +1.46 eV in order to match experiment. Table 2 gives the designation of the resonances $1^-2^-$ and their parameters.

For Be-like atomic nitrogen ions, three peaks were observed in the experimental spectrum in the photon energy range 412–415 eV investigated. Figure 1, shows the experimental and theoretical results obtained at a resolution of 111 meV, figure 2 illustrates the results at the higher resolution of 56 meV. The double peak around 412 eV is more visible at the higher resolution of 38 meV, see figure 3. Due to the presence of metastable states in the beam of ions for $\text{N}^{3+}$, in order to make a true comparison of theory with experiment, the theoretical cross sections were convoluted using a Gaussian profile function of the appropriate width and an admixture of 40% metastable and 60% ground state ions used to simulate experiment. From our results illustrated in figures 1–4 it is seen over the entire photon energy region...
investigated, excellent agreement is achieved with the present R-matrix calculation, both on the absolute cross sections scale and for resonance energies positions. The MCDF calculations show less favourable agreement, as the double peak resonances due to the 1s2s2p 3P° metastable state lies over 1.46 eV below the experimental locations. In figures 1–3, for Be-like nitrogen, we have shifted the MCDF cross section calculations for the 1s2s2p 3P° metastable up by 1.46 eV in order to match the experimental measurements. Table 3 gives the resonances 1–2 and their parameters.

Figure 4. Photoionization cross sections for Be-like atomic nitrogen (N3+) ions measured with a 133 meV band pass at the SOLEIL radiation facility for the 1s → 3p resonance. Solid circles: total photoionization. The error bars give the statistical uncertainty of the experimental data. The MCDF (solid green line) and R-matrix (solid red line) calculations shown are convolution with a Gaussian profile of 133 meV FWHM and an appropriate weighting of the ground and metastable states (see text for details) to simulate the measurements.

Figure 5. Photoionization cross sections for Li-like atomic nitrogen (N4+) ions measured with a 125 meV FWHM band pass at the SOLEIL radiation facility. Solid circles: absolute total photoionization cross sections. The error bars give the statistical uncertainty of the experimental data. R-matrix (solid red line, 31 levels) intermediate coupling, MCDF (solid green line), calculations shown are convolution with a Gaussian profile of 125 meV FWHM to simulate the measurements. Table 3 gives the resonances 1–2 and their parameters.
Table 2. Be-like nitrogen (N\(^{3+}\)), present experimental and theoretical results for the resonance energies \(E_{\text{res}}^{(n)}\) (eV), natural line-widths \(\Gamma\) (meV) and resonance strengths \(\sigma_{\text{PI}}\) (in Mb eV), for the dominant core photo-excited \(n = 2\) states of the N\(^{3+}\) ion, in the photon energy region 410 to 415 eV compared with previous investigations. The experimental error in the calibrated photon energy is estimated to be \(\pm 30\) meV for the resonance energies.

| Resonance (Label) | SOLEIL (Experiment\(^a\)) | R-matrix (Theory) | MCDF/Others (Theory) |
|------------------|--------------------------|-------------------|----------------------|
| \(1s^22s^23P\) \(\rightarrow\) \(1s^22s2p^2[4P]3P\) \(\ddagger\) | 412.396 ± 0.03 | 412.358\(^b\) | 410.925\(^c\) |
| \(\Gamma\) | 85 ± 14 | 12\(^b\) | 25\(^b\) |
| \(\sigma_{\text{PI}}\) | 21.08 ± 4.3 | 11.18\(^b\) | 411.074\(^d\) |
| \(\Gamma\) | 46 ± 32 | 59\(^b\) | 22\(^d\) |
| \(\sigma_{\text{PI}}\) | 4.70 ± 2.8 | 6.4\(^b\) | 58\(^d\) |
| \(1s^22s^23S\) \(\rightarrow\) \(1s^22s2p^2[2D]3D\) \(\ddagger\) | 414.033 ± 0.03 | 414.043\(^b\) | 414.104\(^e\) |
| \(\Gamma\) | 93 ± 13 | 60\(^b\) | 27\(^d\) |
| \(\sigma_{\text{PI}}\) | 42.6 ± 6.45 | 34.3\(^b\) | 81\(^b\) |

\(^a\) SOLEIL, experimental work.
\(^b\) LS-coupling, R-matrix present work, R-matrix + Berrington and co-workers [63].
\(^c\) Multi-configuration Dirac–Fock (MCDF), present work.
\(^d\) MCDF, Chen and co-workers [71].
\(^e\) Saddle-point with complex-rotation method (SPM-CR) [95,96].
\(^f\) (SPM-CR)[97].
\(^g\) R-matrix, intermediate coupling, level averaged [9].
\(^h\) Screening constant by unit nuclear charge (SCUNC) approximation [69, 78, 79].

Estimates for the resonance energies, of Be-like nitrogen made using the screening constant by unit nuclear charge (SCUNC) empirical fitting approach [69] show satisfactory agreement with the more sophisticated theoretical methods and experiment. In the case of the Auger widths, apart from the first \(1s^22s2p^2[4P]3P\) resonance we see they are all in respectable agreement with experiment. We note that the more sophisticated theoretical methods such as R-matrix and the saddle point method consistently give values in agreement with each other and in general with experiment. We point out that in recent K-shell measurements for Be-like boron (e.g., B\(^{+}\) [33]) the Auger width for the \(1s^22s2p^2[4P]3P\) gave a value of \(\sim 10\) meV, consistent with theory. So we suspect that even higher resolution than the present work performed at SOLEIL would be required to fully resolve the double peak structure in the N\(^{3+}\) spectrum at about 412 eV.

Figure 4 shows the SOLEIL data taken in the region of the \(1s^22s^23S\) \(\rightarrow\) \(1s^22s2p^21P\) resonance located around 460 eV at an energy resolution of 133 meV. Due to the limited experimental data taken in this region (as illustrated in figure 4), it was not possible to fit the experimental data to extract a reliable Auger width. We find an experimental value for the energy of this resonance to be 460.280 ± 0.04 eV, a strength of 6.30 ± 2.6 which compares favourably with theoretical predictions from the RMPS value of 460.107 eV with a resonance strength of 6.59. Furthermore, the RMPS provides an Auger width of 72 meV for this \(1s^2\rightarrow\) 3p resonance. For the \(1s^2\rightarrow\) 3p resonance a position of 460.019 ± 0.045 eV with an Auger width of 87 meV was determined from the empirical fitting SCUNC approximation [69]. The optical potential R-matrix method ([9]) for this same resonance gave a value of 462.373 eV with an Auger width of 68 meV. The present MCDF work gave values of 460.189 eV for the position and 80 meV for the Auger width. No other values appear to be available in the literature. We note that numerical values of cross sections from previous R-matrix work [9] are available for only the ground state for this Be-like ion and as such similar comparisons cannot be made in figures 1–4.
Table 3. Li-like nitrogen (N$^{4+}$), present experimental and theoretical results for the resonance energies $E_{\text{ph}}^{(\text{res})}$ (eV), natural line-widths $\Gamma$ (meV) and resonance strengths $\sigma^{\text{PI}}$ (Mb eV) for the 1s$^2$2s$^2$S $\rightarrow$ 1s[2s2p $^3$P]$^2$P$^\circ$ core-excited states of the N$^{4+}$ ion, in the photon energy region 420 to 426 eV compared with previous investigations. The intermediate-coupling results have been averaged over the fine structure levels to compare with experiment and with other theoretical methods. The error in the calibrated photon energy is estimated to be $\pm$ 30 meV for the resonance energies and the experimental resolution was 125 meV determined from multi-function Voigt fits to the measurements.

| Resonance (Label) | SOLEIL/others | $E_{\text{ph}}^{(\text{res})}$ (Theory) | $\Gamma$ (Theory) | MCDF/others | $\sigma^{\text{PI}}$ (Theory) |
|-------------------|---------------|----------------------------------------|------------------|-------------|-------------------------------|
| $1s^22s^2S \rightarrow 1s[2s2p ^3P]^2P^\circ$ |               | 421.472 ± 0.03$^a$ $^{1}$ 421.448$^b$ | 11 ± 8 $^c$ | 47.3 ± 7.4 $^e$             |
| | | $^{2}$ 421.521 ± 0.05$^c$ $^{2}$ 420.612$^a$ | | 60$^c$ | $^{3}$ 425.340$^i$           |
| | | $^{3}$ 421.228 ± 0.05$^c$ $^{3}$ 421.321$^b$ | | $^{4}$ 425.654$^c$           |
| | | $^{4}$ 421.120 ± 0.07$^d$ $^{4}$ 421.572$^a$ | | $^{5}$ 425.660$^c$           |
| | | $^{5}$ 411.482$^m$ | | $^{6}$ 425.666$^m$           |
| $1s^22s^2S \rightarrow 1s[2s2p ^1P]^2P^\circ$ |               | 425.449 ± 0.03$^a$ $^{1}$ 425.606$^e$ | $^{1}$ 424.823$^i$ | 7.3 ± 2.5 $^{1}$             |
| | | $^{2}$ 425.624 ± 0.40$^c$ $^{2}$ 426.020$^g$ | | $^{5}$ 425.850$^i$           |
| | | $^{3}$ 424.890 ± 0.15$^d$ $^{3}$ 425.421$^h$ | | $^{6}$ 425.660$^c$           |
| | | $^{4}$ 425.770$^i$ | | $^{7}$ 425.666$^m$           |
| | | $^{5}$ 425.530$^i$ | | $^{8}$ 425.666$^m$           |
| | | $^{6}$ 425.770$^i$ | | $^{9}$ 425.666$^m$           |

$^a$ SOLEIL, present measurements.
$^b$ EBIT, measurements [24].
$^c$ Laser produced plasmas (LPP), measurements [53].
$^d$ Electron spectroscopy in ion-atom collisions, measurements [54].
$^e$ R-matrix, intermediate-coupling (31 levels) present results, level averaged.
$^f$ Multi-configuration Dirac–Fock (MCDF) method, present work.
$^g$ MCDF [70, 99].
$^h$ Saddle-point method with complex-rotation (SPM-CR) [100].
$^i$ Intermediate-coupling, semi-relativistic method [101].
$^j$ R-matrix, intermediate coupling, results, level averaged [9].
$^k$ Complex scaled multi-reference configuration interaction method (CMR-CI) [102].
$^l$ Saddle-point method with R-matrix (SPM-RM). [103].
$^m$ Screening constant by unit nuclear charge (SCUNC) approximation [69, 78, 79].

Table 3 presents the resonance parameters for the two resonances observed in the Li-like atomic nitrogen experimental measurements illustrated in figure 5. We note that only the first narrow peak in the Li-like experimental spectrum located at 421.472 ± 0.03 eV was able to be properly fitted, giving a Auger line width of 11 ± 8 meV. Both the sophisticated R-matrix and Saddle point methods are in agreement with each other and the experimental value for the location of this resonance. Theoretical predictions from R-matrix calculations and other methods for the Auger width all lie within the experimental error estimate for this resonance. The second peak in the Li-like atomic nitrogen photoionization cross section, located at 425.449 ± 0.03 eV, had limited experimental data taken on the lower energy side of the peak and due to the rather large noise level (large scatter in the experimental cross section data) made it impossible to fit. The noise level was simply just too large to do a proper fit of this peak. For the natural line width of this 1s$^2$2s$^2$P$^\circ$ resonance, R-matrix calculations give a value of 42 meV, present MCDF estimates of 45 meV, and the Saddle point method 42 meV. From previous R-matrix work [9] we have extracted resonance positions and widths. For the first resonance we find an energy of 420.612 eV and for the second resonance an energy of 424.823 eV, a discrepancy of about 0.9 eV and 0.6 eV lower than the present experiment, with values of 6 meV and 53 meV for the respective widths.

It is also seen that the present R-matrix calculations yield a resonance strength of 6.5 Mb eV, MCDF estimates a value of 9 Mb eV and both theoretical values are in suitable agreement with the experimental measurement of 7.3 ± 2.5. For the positions of both resonances, the theoretical values from the RMPS calculations are in more favourable agreement with the SOLEIL synchrotron measurements than either the earlier EBIT [24], the laser produced plasmas (LPP) [53] or those determined from electron spectroscopy in ion-atom collisions.
5. Conclusions

K-shell photoionization for Be-like and Li-like atomic nitrogen ions, respectively N$^{1+}$ and N$^{2+}$, has been performed using state-of-the-art experimental and theoretical methods in the vicinity of their respective K-edges. To our knowledge this would appear to be the first time high-resolution spectroscopy has been performed (at a photon energy resolution of respectively, 38 meV, 56 meV, 111 meV, 133 meV FWHM for Be-like and 125 meV FWHM for Li-like atomic nitrogen ions). The measurements at the SOLEIL synchrotron radiation facility, in Saint-Aubin, France, cover the photon energy ranges 410–415 eV and 460–460.4 eV for Be-like and 420–426 eV for Li-like atomic nitrogen ions. The strong peaks found in the respective PI cross sections in the photon energy regions studied are identified as the 1s → 2p and 1s → 3p transitions in the Be-like and 1s → 2p transitions in the Li-like K-shell spectrum that are assigned spectroscopically. All the n = 2 resonance parameters have been tabulated in table 2 for Be-like and in table 3 for Li-like atomic nitrogen ions. For the observed peaks, respectable agreement is seen with the present theoretical and experimental results both on the photon-energy scale and the absolute cross section scale. Some differences are highlighted and discussed.

The strength of the present study is the high resolution of the spectra along with theoretical predictions made using state-of-the-art MCDF and R-matrix methods. The present results have been compared with high-resolution experimental measurements made at the SOLEIL synchrotron radiation facility and with other theoretical methods so would be suitable to be incorporated into astrophysical modelling codes like CLOUDY [16, 17], XSTAR [104] and AtomDB [105] used to numerically simulate the thermal and ionization structure of ionized astrophysical nebulae.

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