Photoionization cross section calculations for the halogen-like ions Kr\(^+\) and Xe\(^+\)

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Abstract

Photoionization cross section calculations on the halogen-like ions; Kr\(^+\) and Xe\(^+\) have been performed for a photon energy range from each ion threshold to 15 eV, using large-scale close-coupling calculations within the Dirac–Coulomb \(R\)-matrix approximation. The results from our theoretical work are compared with recent measurements made at the ASTRID merged-beam set-up at the University of Aarhus in Denmark and from the Fourier transform ion cyclotron resonance trap method at the SOLEIL synchrotron radiation facility in Saint-Aubin, France Bizau \textit{et al} (2011 J. Phys. B: At. Mol. Opt. Phys. 44 055205) and the advanced light source Müller (2012 private communication), Aguilar \textit{et al} (2012 J. Phys.: Conf. Ser. at press). For each of these complex ions our theoretical cross section results over the photon energy range investigated are seen to be in excellent agreement with experiment. Resonance energy positions and quantum defects of the prominent Rydberg resonances series identified in the spectra are compared with experiment for these complex halogen-like ions.

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

1. Introduction

Most of the known matter in the Universe is in a plasma state and our information about the Universe is carried by photons, which are dispersed and detected for example by the orbiting Chandra x-ray observatory. While photons travel through stellar atmospheres and planetary nebulae, they are likely to interact with matter and therefore with ions. This makes the study of photoionization (PI) of atoms, molecules and their positive ions very important for astrophysicists, helping them to interpret stellar data.

PI cross sections of heavy atomic elements, in low stages of ionization, are currently of interest both experimentally and theoretically and for applications in astrophysics. The data from such processes have many applications in planetary nebulae, where they are of use in identifying weak emission lines of \(n\)-capture elements in NGC 3242. For example, the relative abundances of Xenon (Xe) and Krypton (Kr) can be used to determine key physical characteristics of \(s\)-process nucleosynthesis, such as the neutron exposure experienced by Fe-peak seed nuclei [4–7].

Xe and Kr ions are also of importance in man-made plasmas such as XUV light sources for semiconductor lithography [8], ion thrusters for space craft propulsion [9], and nuclear fusion plasmas [10]. Xe and Kr ions have also been detected in cosmic objects, e.g., in several planetary nebulae and in the ejected envelopes of low- and intermediate-mass stars [5, 7, 11–13]. For a profound understanding of these plasmas accurate cross sections are required for ionization and recombination processes that govern the charge balance of ions in plasmas. Kr and Xe ions are of particular importance in tokamak plasmas. Injection of high-Z gases, essentially Kr and Xe, has been proposed as a technique to mitigate disruption [14, 15], i.e. the uncontrolled and sudden loss of tokamak plasma current and energy. Disruption can produce severe damage on the vessel wall. The situation becomes more critical for large machines such as the International Thermonuclear Experimental Reactor, where incident-loading energy may reach several GW m\(^{-2}\) [16, 17].
After injection of the gases, highly charged Kr and Xe ions are dominant in the core of the plasma, and low-charged and singly charged ions are abundant near the edge.

Over the past decade, experimentally, PI data on ionic targets have been obtained using mainly two techniques: dual laser produced plasma and merged beam in synchrotron radiation facilities. While the former technique measures photoabsorption spectra [18], the latter provides absolute single and multiple PI cross sections [19, 20]. As indicated by Bizau et al [1] in recent studies on Kr+ and Xe+ ions, in the valence region, only the K-shell PI of the Kr+ ion has been reported on [21]. The bulk of the studies on the Xe+ ion have focused primarily on the region of 4d inner-shell excitation and ionization using the merged-beam technique [22–26]. The recent work on Xe+ of Bizau et al [1] together with the ongoing high resolution studies at the advanced light source (ALS) [2, 3], in the threshold region, make it pertinent to have suitable theoretical results available to compare with. As pointed out in the recent work of Bizau et al [1], no studies using the above experimental techniques have been published on the Kr+ ion or on the Xe+ ion in any other energy range and, in particular, close to the thresholds, where strong resonance features dominate the respective cross sections. Furthermore, no theoretical results on the PI processes are available for these ions outside the region of 4d inner-shell excitation in the Xe+ ion. In order to address these limitations, particularly for astrophysical applications, we have carried out large-scale PI cross section calculations in the threshold region for both singly ionized ions of Kr and Xe. Where possible we have benchmarked our theoretical work with the available experimental data in order to provide confidence in our work for applications.

The layout of this paper is as follows. Section 2 presents a brief outline of the theoretical work. Section 3 details the results obtained. Section 4 presents a discussion and a comparison of the results obtained between experiment and theory. Finally in section 5 conclusions are drawn from the present investigation.

2. Theory

Recent modifications to the Dirac-Atomic-R-matrix-Codes (DARC) [27] has now made it feasible to study PI of heavy complex systems of prime interest to astrophysics and plasma applications by including hundreds of target levels in the close-coupling calculations. This enables PI calculations on complex ions such as singly ionized ions of Kr and Xe, the focus of the current investigation to be carried out at the same degree of accuracy as those for electron impact excitation. Such extensions to the DARC codes have allowed us recently to address the complex problem of trans-iron element single photon ionization of Se+ ions. In this study we apply this suite of DARC codes to calculate detailed PI cross sections on the halogen-like ions, Kr+ and Xe+. Recent experimental measurements [1] have been made on these systems but limited theoretical work is available to compare with. PI cross sections on these halogen-like ions are performed for the ground and the excited metastable levels associated with the ns2np5 configuration (n = 4 and 5, respectively, for Kr+ and Xe+ ions) in order to benchmark our theoretical results with recent high resolution experimental measurements [1].

For both the ground and metastable initial states, the outer region electron–ion collision problem for each ion was solved (in the resonance region below and between all thresholds) using a suitably chosen fine energy mesh of 5 × 10−8 Rydbergs (≈ 0.68 μeV) to fully resolve all the extremely narrow resonance structure in the appropriate PI cross sections. The jj-coupled Hamiltonian diagonal matrices were adjusted so that the theoretical term energies matched the recommended experimental values of NIST [28]. We note that this energy adjustment ensures better positioning of resonances relative to all thresholds included in the calculation. In the energy region considered here we can see from tables 1 and 2 the shift to the 1D2 and 1S0 thresholds is minimal. For this reason in tables 3–5 we only include experimental series limits.

In order to compare directly with the available experimental measurements for each of these ions, we have convoluted the theoretical PI cross sections with a Gaussian function of the appropriate full width half maximum (FWHM) and statistically averaged the results for the ground and metastable states.
Table 3. Principal quantum number \( n \), resonance energies \( E \) (eV) and quantum defect \( \mu \) from experimental measurements of \( \text{Kr}^+ \) [1] compared with present theoretical estimates from the QB method. The Rydberg series \( 4s^24p^5\left( ^1D_2 \right) \) nd originating from the \( ^2P_{3/2} \) ground state and the \( ^2P_{1/2} \) metastable state of \( \text{Kr}^+ \) due to \( 4p \rightarrow nd \) transitions are tabulated.

| \( n \) | \( E \) (eV) | \( \mu \) | \( n \) | \( E \) (eV) | \( \mu \) |
|-------|----------------|---------|-------|----------------|---------|
| 6     | 24.579          | 0.16    | 6     | 24.562          | 0.19    |
| 7     | 25.002          | 0.19    | 7     | 24.989          | 0.23    |
| 8     | 25.284          | 0.19    | 8     | 25.280          | 0.20    |
| 9     | 25.473          | 0.20    | 9     | 25.475          | 0.19    |
| 10    | 25.603          | 0.25    | 10    | 25.605          | 0.23    |
| 11    | 25.713          | 0.16    | 11    | 25.710          | 0.19    |
| 12    | 25.786          | 0.18    | 12    | 25.785          | 0.19    |
| 13    | 25.844          | 0.19    | 13    | 25.842          | 0.23    |
| 14    | 25.890          | 0.19    |       |                 |         |
| 15    | 25.927          | 0.19    |       |                 |         |
|       | \( \infty \) 26.176\(^a\) | \( \infty \) 26.176\(^a\) |       |                 |         |

Table 4. Principal quantum number \( n \), resonance energies \( E \) (eV) and quantum defect \( \mu \) from experimental measurements of \( \text{Kr}^+ \) [1] compared with present theoretical estimates from the QB method. The Rydberg series \( 4s^24p^5\left( ^1S_0 \right) \) nd originating from the \( ^2P_{3/2} \) ground state and the \( ^2P_{1/2} \) metastable state of \( \text{Kr}^+ \) due to \( 4p \rightarrow nd \) transitions are tabulated.

| \( n \) | \( E \) (eV) | \( \mu \) | \( n \) | \( E \) (eV) | \( \mu \) |
|-------|----------------|---------|-------|----------------|---------|
| 4     | 23.854          | 0.28    | 4     | 23.845          | 0.29    |
| 5     | 25.288          | 0.34    | 5     | 25.280          | 0.20    |
| 6     | 26.096          | 0.34    | 6     | 26.100          | 0.33    |
| 7     | 26.569          | 0.34    | 7     | 26.580          | 0.31    |
| 8     | 27.534          | 0.34    | 8     | 27.530          | 0.38    |
| 9     | 27.936          | 0.34    | 9     | 27.910          | 0.38    |
| 10    | 28.461          | 0.34    | 10    | \( \infty \) 28.461\(^a\) | \( \infty \) 28.461\(^a\) |

2.1. \( \text{Kr}^+ \)

PI cross section calculations on the \( \text{Kr}^+ \) complex were carried out retaining 326-levels in our close-coupling calculations with the DARC. In R-matrix theory, all PI cross section calculations require the generation of atomic orbitals based primarily on the atomic structure of the residual ion. The present theoretical work for the PI of the \( \text{Kr}^+ \) ion employs relativistic atomic orbitals up to \( n = 4 \) generated for the residual \( \text{Kr}^{2+} \) ion, which were calculated using the extended-optimized-level (EOL) procedure within the GRASP structure code [29–31]. The 1s–4s, 2p–4p and 3d–4d orbitals were obtained from an EOL calculation on the lowest 14 levels associated with the \( 4s^24p^4, 4s^24p^3 \) and \( 4s^24p^3d^2 \) configurations where the remaining four configurations; \( 4s^24p^3d^2, 4s^24p^2d^2, 4s^24p^4d^2 \) and \( 4p^54d^2 \) were included in the calculation. Table 1 illustrates a sample of our target energy levels for the residual \( \text{Kr} \) III ion compared to the NIST tabulation [28] for the lowest eight levels associated with the \( 4s^24p^4 \) and \( 4s^24p^5 \) configurations.

PI cross section calculations for this complex trans-iron element included all 326 levels arising from the seven configurations: \( 4s^24p^5, 4s^24p^4d, 4s^24p^3d^2, 4p^5, 4s^24p^4d^2 \) and \( 4p^54d^2 \) in the close-coupling expansion. PI cross section calculations with this 336-level model were performed in the Dirac–Coulomb approximation using the DARC codes.

The R-matrix boundary radius of 7.44 Bohr radii was sufficient to envelop the radial extent of all the atomic orbitals of the residual \( \text{Kr}^{2+} \) ion. A basis of 16 continuum orbitals was sufficient to span the incident experimental photon energy range from threshold up to 40 eV. The 326-state model produced a maximum of 1511 coupled channels in our scattering work with Hamiltonian matrices of dimension of the order of 24 354 by 24 354 in size. Due to dipole selection rules, for total ground-state PI we need only to consider the bound-free dipole moments, \( 2J^\pi = 3^o \rightarrow 2J^\pi = 1^e, 3^e, 5^e \) whereas...
for the excited metastable states only the $2\Sigma^+ = 1^+$ $→ 2\Sigma^+$ is required.

2.2. Xe$^+$

Similarly for PI cross section calculations on the Xe$^+$ system we retained 326 levels of the residual Xe$^{1+}$ ion in our close-coupling calculations performed with the DARC. Analogous PI calculations on the Kr$^+$ case, were made similarly for the Xe$^+$ ion. For the Xe$^+$ case we have employed relativistic $n = 5$ atomic orbitals generated for the residual Xe$^{1+}$ ion, which were obtained using the energy-average-level procedure within the GRASP structure code on the 14 lowest levels associated with the 5s$^2$5p$^4$, 5s5p$^5$ and 5s$^2$5p$^2$5d$^2$ configurations. Table 2 gives a sample of our results for the Xe III ion for the energies of the lowest eight levels associated with the 5s$^2$5p$^4$ and 5s5p$^5$ configurations compared with the NIST [28] tabulations. Here again for the PI cross section calculations on this complex trans-iron system we included all 326 levels arising from the seven configurations: 5s$^2$5p$^4$, 5s5p$^5$, 5s$^2$5p$^5$5d, 5s$^2$5p$^2$5d$^2$, 5p$^6$, 5s5p$^5$d and 5p$^5$5d$^2$ in the close-coupling expansion. PI cross section calculations with this 326-level model were then carried out in the Dirac–Coulomb approximation using the DARC codes for photon energies up to about 15 eV above the ion threshold.

3. Results

Figures 1 and 2 presents our theoretical results from the 326-level model using the DARC suite of codes. In order to compare directly with the experimental results of Bizau et al [1] we have statistically averaged the results from the ground and metastable levels and convoluted respective cross sections with a Gaussian of 30 meV FWHM for Kr$^+$ ions and 25 meV for Xe$^+$ ions. In the near threshold region (cf figures 1(b) and 2(b)) we see clearly (from a comparison of the theoretical and experimental results of Bizau et al [1]) that the rich and complex resonance structure is better reproduced by the DARC calculations for Kr$^+$ than for Xe$^+$, which could be due to the limited resolution in those experiments. Figure 3 shows a comparison with recent ALS measurements for Xe$^+$ ions in the near threshold region taken at the ALS at a extremely high resolution of 4 meV [2]. Here we see that the experimental PI cross sections (apart from the region of the $n = 14$ member of the 5s$^2$5p$^4$ ($^3P_1$) nd series) are reproduced by our DARC calculations.

The multi-channel $R$-matrix eigenphase derivative (QB) technique (applicable to atomic and molecular complexes) of Berrington and co-workers [32–34] modified to cater for jj-coupling was used to determine the resonance parameters of the prominent series. The resonance width $\Gamma$ was determined from the inverse of the energy derivative of the eigenphase sum $\delta$ at the resonance energy $E_r$ via

$$
\Gamma = 2 \left( \frac{\delta \Gamma}{dE} \right)^{-1} \bigg|_{E=E_r} .
$$

The results for all the resonance parameters determined from the QB method are presented in tables 3 and 4 for Kr$^+$ ions and compared with the available experimentally determined ones. Table 5 give similar results for the corresponding Xe$^+$ ion.

4. Discussion

The hypothesis of statistical population is very reasonable since the life time is huge (0.34 s for the case of Kr$^+$) if compared to the beam transport times. Note also that the excited $^3P_{1/2}$ metastable Kr$^+$ ions produced either in an ion source or ion trap rarely collide with surfaces or residual gas before PI takes place. As a result, statistical population of the ions seems consistent with their measurements both using an ion source and an ion trap without delay [1]. For the case of Kr$^+$ ions studied here resonance positions and quantum defects are in excellent agreement with the available experimental measurements as can be seen from tables 3 and 4. The magnitude of the absolute cross sections are also in
exciting agreement with experimental values as illustrated in figure 1.

For Xe$^+$ ions the difference in the resolution between the Bizau et al [1] (25 meV) and current ALS measurements (2.2 meV) [2] and that taken at 4 meV shown in figure 3 [3] is over a factor of ten better. Bizau et al noted that, given their poor resolution, they do not attempt to obtain more detailed spectroscopic information: ‘Considering the moderate energy resolution chosen in this work to compensate for the low density of target ions, we have not attempted a detailed identification of the observed structures, which are most of the time composed of several unresolved lines’. In the near threshold region we do not fully reproduce the resonance strengths in the experimental data of Bizau et al [1] which could be due to the limited resolution in those experiments. We also note here there is a discrepancy in the quantum defects
for the Rydberg series in Xe$^+$ as given in table 5 with the experimental values of Bizau and co-workers [1]. The recent high resolution measurements (4 meV) see figure 3 made at the ALS by Muller and co-workers [3] have made possible spectroscopic studies of the Xe$^+$ PI spectrum in the near threshold region producing an average quantum defect for the 5s$^2$5p$^4$($^3$P$^1$) nd Rydberg series of 0.16 which are comparable values to our DARC estimates for the 5s$^2$5p$^4$($^1$D$^2$) nd series in table 5 [2, 3]. For Xe$^+$ ions a more stringent test with recent extremely high resolution experimental measurements made at the ALS at 4 meV indicate (in the near threshold region, apart from the $n = 14$ member of the Rydberg series) very good agreement giving us confidence in our theoretical results.

5. Conclusions

State-of-the-art theoretical methods were used to investigate photons interacting with the halogen-like ions, Kr$^+$ and Xe$^+$, in the energy region extending to about 15 eV beyond the ionization threshold. Given the complexity of these halogen-like ions, throughout the energy region investigated the agreement (on the photon-energy scale and on the absolute PI cross section scale) is better for Kr$^+$ ions than for Xe$^+$ ions with the recent experimental measurements of Bizau et al [1] and our DARC calculations. However our DARC calculations in the near threshold region are seen to reproduce most of the recent extremely high resolution ALS measurements on Xe$^+$ ions [2, 3]. It is seen that the photoionization cross section exhibits a wealth of resonances which theory is able to mostly reproduce. The prominent members of the Rydberg series are analysed and compared with experiment. We point out that the strength of this study is the benchmarking of our theoretical work with the available experimental data. Such detailed comparison between theory and experiment strengthens the validity of our results giving confidence in their use for astrophysical applications.

The photoionization cross sections from this study are suitable to be included into state-of-the-art photoionization modelling codes Cloudy and XSTAR [35, 36] that are used to numerically simulate the thermal and ionization structure of ionized astrophysical nebulae.

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References

[1] Bizau J M et al 2011 J. Phys. B: At. Mol. Opt. Phys. 44 055205
[2] Müller A 2012 private communication
[3] Aguilar A et al 2012 J. Phys.: Conf. Ser. at press
[4] Sharpee B, Zhang Y, Williams R, Pellegrini E, Cavagnolo K, Baldwin J A, Phillips M and Liu X W 2007 Astrophys. J. 659 1265
[5] Sterling N C et al 2009 Publ. Astron. Soc. Aust. 26 339
[6] Karakas A I, van Raai M A, Lugaro M, Sterling N C and Dinerstein H L 2009 Astrophys. J. 690 1130
[7] Sterling N C, Dinerstein H L and Kallman T R 2007 Astrophys. J. Suppl. Ser. 169 37
[8] Kieft E R et al 2005 Phys. Rev. E 71 036402
[9] Lerner E J 2000 Ind. Phys. 6 16
[10] Skinner C H 1997 Phys. Scr. T 134 014022
[11] Sterling N C and Dinerstein H L 2005 An infrared survey of neutron-capture elements in planetary nebulae Cosmic Abundances as Records of Stellar Evolution and Nucleosynthesis (ASP Conf. Ser.) vol 336 ed T G Barnes, III and F N Bash (San Francisco, CA: Astronomical Society of the Pacific) p 367
[12] Sterling N C and Dinerstein H L 2008 Astrophys. J. Suppl. Ser. 174 157
[13] Yíce K, Castelli F and Hubrig S 2011 Astron. Astrophys. 528 A37
[14] Riccardo V et al 2002 Plasma Phys. Control. Fusion 44 905
[15] Nishida V et al 2002 Nucl. Fusion 42 1197
[16] Federici G et al 2002 Nucl. Fusion 41 1967
[17] ITER Physics Basis 1999 Nucl. Fusion 39 2137
[18] Carroll P K and Costello J 1986 Phys. Rev. Lett. 57 1581
[19] West J B 2001 J. Phys. B: At. Mol. Opt. Phys. 34 R45
[20] Kjeldsen H 2006 J. Phys. B: At. Mol. Opt. Phys. 39 R325
[21] Southworth S et al 2006 Phys. Rev. A 76 043421
[22] Sano M et al 1996 J. Phys. B: At. Mol. Opt. Phys. 29 5305
[23] Koizumi T et al 1997 Phys. Scr. T 73 131
[24] Andersen P et al 2001 J. Phys. B: At. Mol. Opt. Phys. 34 2009
[25] Itoh Y et al 2001 J. Phys. B: At. Mol. Opt. Phys. 34 2493
[26] Gottwald A, Gert C and Richter M 1999 Phys. Rev. Lett. 82 2068
[27] Fivet V, Bautista M A and Ballance C P 2012 J. Phys. B: At. Mol. Opt. Phys. 45 035201
[28] Ralchenko Y, Kramida A E, Reader J and NIST ASD Team 2011 NIST Atomic Spectra Database (version 4.0.1), National Institute of Standards and Technology, Gaithersburg, MD, USA, http://physics.nist.gov/asd

[29] Dyall K G, Grant I P, Johnson C T and Plummer E P 1989 Comput. Phys. Commun. 55 425

[30] Parpia F, Froese Fischer C and Grant I P 2006 Comput. Phys. Commun. 94 249

[31] Grant I P 2007 Quantum Theory of Atoms and Molecules: Theory and Computation (New York: Springer)

[32] Quigley L and Berrington K A 1996 J. Phys. B: At. Mol. Opt. Phys. 29 4529

[33] Quigley L, Berrington K A and Pelan J 1998 Comput. Phys. Commun. 114 225

[34] Ballance C P, Berrington K A and McLaughlin B M 1999 Phys. Rev. A 60 R4217

[35] Ferland G J, Korista K T, Verner D A, Ferguson J W, Kingdom J B and Verner E M 1998 Publ. Astron. Soc. Pac. 110 761

[36] Kallman T and Bautista M 2001 Astrophys. J. Suppl. Ser. 133 221