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Photoionization of the $3s^23p^3nd$ Rydberg series of Cl^+ ion using the Screening constant by unit nuclear charge method

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ABSTRACT

We report calculations of accurate high lying resonance energies of the $[3s^23p^3(^2D^{\circ}_{5/2})]nd$ and $[3s^23p^3(^2P^{\circ}_{3/2})]nd$ Rydberg series originating from the ground $3s^23p^4\ ^3P_2$ and from the $3s^23p^4\ ^3P_{1,0}$ metastable states of Cl^+ along with the $[3s^23p^3(^2P^{\circ}_{1/2})]nd$ Rydberg series originating from the $3s^23p^4\ ^1S_0$ metastable state of the Cl^+ ion. Calculations are performed using the Screening Constant by Unit Nuclear Charge (SCUNC) method up to $n = 40$. The results obtained are compared with the existing Dirac – Coulomb *R*-matrix (DCR) calculations (McLaughlin, 2017) and Advanced Light Source (ALS) measurements (Hernández et al., 2015). Analysis of the present results is achieved in the framework of the standard quantum-defect theory and of the SCUNC-procedure based on the calculation of the effective charge. It is shown that the SCUNC-method agree very well the ALS measurements up to $n = 13$. New high lying accurate resonance energies ($n = 14$–40) are tabulated as benchmarked data for the atomic physics community in connection with the modeling of plasma and astrophysical systems.

1. Introduction

It is well known that visible matter in the Universe is almost in the plasma state and most observational data about the distant universe are conveyed through interstellar space by photons. Some of these photons are sufficiently energetic to induce the photoionization of atoms and ions according to the single process

$$\text{hn} + X^{q+} \rightarrow X^{(q+m)+} + me^-. \quad (1)$$

Photoionization of atoms and ions is then a fundamental process of importance in many astrophysical systems such as stars and nebulae. Of great important ions interesting to investigate are sulphur-like ions such as Cl^+ in connection with their abundances in photoionized astrophysical objects. In the past, various studies have indicated the great importance of S-like Cl^+ ion abundances for understanding extragalactic HII regions (Garnett, 1989). In addition, emission lines of S-like Cl^+ ion have been observed in the spectra of the Io torus (Küppers and Schneider, 2000) and in the optical spectra of planetary nebulae NGC 6741 and IC 5117 (Keenan et al., 2003). The ground state configuration of the Cl^+ ions is $3s^23p^4\ ^3P$ in the *LS* coupling scheme. For the ^3P term, the total spin $S = 1$ and the orbital momentum quantum number $L = 1$. As a result, the total angular momentum quantum number J takes the values $|L + S|$ up to $|L - S|$, that means $J = 2$, 1 and 0. Due to spin-orbit interaction, the $Cl^+ - 3s^23p^4\ ^3P$ configuration splits into three subshells namely the $3s^23p^4\ ^3P_2$ ground state and the $3s^23p^4\ ^3P_{1,0}$ metastable states. In the works of Ralchenko et al. (2014), the energy differences between the $3s^23p^4\ ^3P_2$ and $3s^23p^4\ ^3P_1$ states and between the $3s^23p^4\ ^3P_2$ and $3s^23p^4\ ^3P_0$ states are respectively equal to 86.3 meV and 123.5 meV. Then, according to the magnitude of the photon energy, the $3s^23p^4\ ^3P_2$ ground state and the $3s^23p^4\ ^3P_{1,0}$ metastable states of the Cl^+ ion can be photoionized. So, two photoionization processes originating from the ground and metastable states of this sulphur-like ion can be observed. Using Eq. (1), the two possible photoexcitation processes are the following

$$h\nu + Cl^+ (3s^23p^4\ ^3P_2) \rightarrow Cl^+ [3s^23p^3 (^3L_J)]\ nl. \quad (2)$$

$$h\nu + Cl^+ (3s^23p^4\ ^3P_{1,0}) \rightarrow Cl^+ [3s^23p^3 (^3L'_{J'})]\ n'l'. \quad (3)$$

These two processes can finally decay by single electron emission

$$Cl^+ [3s^23p^3 (^3L_J)]\ nl \rightarrow Cl^{2+} [3s^23p^3 (^3L_J)] + e^-. \quad (4)$$

$$Cl^+ [3s^23p^3 (^3L'_{J'})]\ n'l' \rightarrow Cl^{2+} [3s^23p^3 (^3L'_{J'})] + e^-. \quad (5)$$

In a very recent past, Hernández et al. (2015) measured at the Advanced Light Source at Lawrence Berkeley National Laboratory absolute photoionization cross-sections for the Cl^+ ion in its ground and metastable states, $3s^23p^4\ ^3P_{2,1,0}$ and $3s^23p^4\ ^1D_2$, $^1S_0$, using the merged beams photon–ion technique at a photon energy resolution of 15 meV in the energy range 19–28 eV. As stated by Covington et al. (2011), for comparison with high-resolution measurements such as from ALS experiments, state-of-the-art-theoretical methods are required using highly correlated wave functions. Relativistic effects are also required,

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since fine-structure effects can be resolved. Using the Dirac–Coulomb *R*-matrix (DCR) method, McLaughlin (2017) performed calculations in the energy range 19–28 eV as in the ALS experiments (Hernández et al., 2015) to assign and identify the resonance series in the ALS spectra of the Cl^+ ion. The $3s^23p^3nd$ states have been identified in the Cl^+ spectra as the prominent Rydberg series belonging to the $3p \to nd$ transitions. The weaker Rydberg series $3s^23p^3ns$, identified as $3p \to ns$ transitions and window resonances $3s3p^4$ (^4P) np features, due to $3s \to np$ transitions, have also been found in the spectra (McLaughlin, 2017). In the present work, we focus our study on the $3s^23p^3nd$ prominent Rydberg series identified in the Cl^+ spectra. The corresponding $3p \to nd$ transitions are deduced from Eqs. (2) and (3) as follows,

$$h\nu + Cl^+ (3s^23p^4\ ^3P_2) \xrightarrow{\text{and}} Cl^+ [3s^23p^3 (^3D_{5/2})]\ nd. \quad Cl^+ [3s^23p^3 (^3P_{3/2})]\ nd. \tag{6}$$

$$h\nu + Cl^+ (3s^23p^4\ ^3P_{1,0}) \xrightarrow{\text{and}} Cl^+ [3s^23p^3 (^3D_{5/2})]\ nd. \quad Cl^+ [3s^23p^3 (^3P_{3/2})]\ nd. \tag{7}$$

For the metastable states, $3s^23p^4\ ^1S_0$ and $3s^23p^4\ ^1D_2$ present in the parent ion beam of the ALS experiments, we obtain for the $3p \to nd$ transitions.

$$h\nu + Cl^+ (3s^23p^4\ ^1S_0) \to Cl^+ [3s^23p^3 (^2P_{1/2})]\ nd\cdot \tag{8}$$

$$h\nu + Cl^+ (3s^23p^4\ ^1D_2) \to Cl^+ [3s^23p^3 (^2D_{5/2})]\ nd\cdot \tag{9}$$

In both the ALS measurements (Hernández et al., 2015) and the DCR calculations (McLaughlin, 2017), the studies have been limited to $n = 13$. In addition, comparison have been done between the DCR calculations and the ALS uncertain resonance energies for the $3p \to nd$ transitions. Besides ALS measurements were absent for some transitions such as the $3s^23p^4\ ^3P_0 \to [3s^23p^3 (^2D_{5/2})]\ nd$ transitions where only the 24.219 eV precise data for the $[3s^23p^3 (^2D_{5/2})]\ 6d$ level and the uncertain value (25.000 eV) for the $[3s^23p^3 (^2D_{5/2})]\ 8d$ level have been quoted. In the energy range 19–28 eV, a huge of high lying resonance energies exist. These high lying Rydberg series are very useful data for the NIST database where many resonances are tabulated up to $n = 60$ for atomic systems such as Mg. The goal of the present study is to extend the previous ALS measurements (Hernández et al., 2015) and the DCR calculations (McLaughlin, 2017) to the high lying $3p \to nd$ transitions with $n = 6$– 40 and to tabulated accurate data to be compared with the ALS uncertain and absent resonance energies for the $3p \to nd$ transitions. Comparison with the DCR predictions is also aimed. For this purpose, we apply the Screening constant by unit nuclear charge (SCUNC) formalism (Goyal et al., 2016; Khatri et al., 2016; Sakho, 2016, 2017, 2018)very suitable in reproducing excellently experimental data. Analysis of the present results is achieved in the framework of the standard quantum-defect theory and of the SCUNC-procedure by calculating the effective charge. The present paper is organized as follows. Section 2 presents a brief outline of the theoretical part of the work. In Section 3, we present and discuss the results obtained compared with the existing ALS measurements (Hernández et al., 2015) and with the DCR calculations (McLaughlin, 2017). In Section 4, we summarize our study and draw conclusions.

2. Theory

2.1. Brief description of the SCUNC formalism

In the framework of the Screening Constant by Unit Nuclear Charge formalism, the total energy of the $(Nl,\ nl')\ ^{2S+1}L_\pi$ excited states is expressed in the form (in Rydberg)

$$E(Nl, nl';\ ^{2S+1}L_\pi) = -Z^2\left(\frac{1}{N^2} + \frac{1}{n^2}\left[1 - \beta(Nl, nl';\ ^{2S+1}L_\pi;\ Z)\right]^2\right). \tag{10}$$

In this equation, the principal quantum numbers N and n are respectively for the inner and the outer electron of the helium-isoelectronic series. The β-parameters are screening constants by unit nuclear charge expanded in inverse powers of Z and given by

$$\beta(Nl\ nl';\ ^{2S+1}L^\pi; Z) = \sum_{k=1}^{q} f_k\left(\frac{1}{Z}\right)^k. \tag{11}$$

where $f_k = f_k(Nl\ nl';\ ^{2S+1}L_\pi)$ are parameters to be evaluated empirically.

For a given Rydberg series originating from a-$^{2S+1}L_J$ state, we obtain using (Sakho, 2018)

$$E_n = E_\infty - \frac{Z^2}{n^2}\left[1 - \beta(nl; s; \mu, \nu;^{2S+1}L^\pi; Z)\right]^2. \tag{12}$$

In this equation, ν and μ ($\mu > \nu$) denote the principal quantum numbers of the $(^{2S+1}L_J)$ nl Rydberg series used in the empirical determination of the f_i - screening constants, s represents the spin of the nl-electron ($s = ½$), E_∞ is the energy value of the series limit, E_n denotes the resonance energy and Z stands for the atomic number. The β-parameters are screening constants by unit nuclear charge expanded in inverse powers of Z and given by

$$\beta\left(Z,\ ^{2S+1}L_J, n, s, \mu, \nu\right) = \sum_{k=1}^{q} f_k\left(\frac{1}{Z}\right)^k. \tag{13}$$

where $f_k = f_k(^{2S+1}L_J, n, s, \mu, \nu)$ are screening constants to be evaluated empirically. In Eq.(13), q stands for the number of terms in the expansion of the β–parameter. Generally, precise resonance energies are obtained for $q < 5$. The resonance energy are the in the form

$$E_n = E_\infty - \frac{Z^2}{n^2}\left\{1 - \frac{f_1(^{2S+1}L_J^\pi)}{Z(n-1)} - \frac{f_2(^{2S+1}L_J^\pi)}{Z} \pm \sum_{k=1}^{q}\sum_{k'=1}^{q'} f_1^{k'} F\left(n, \mu, \nu, s\right) \times \left(\frac{1}{Z}\right)^k\right\}^2. \tag{14}$$

The quantity $\pm \sum_{k=1}^{q}\sum_{k'=1}^{q'} f_1^{k'} F(n, \mu, \nu, s) \times \left(\frac{1}{Z}\right)^k$ is a corrective term introduced to stabilize the resonance energies with increasing the principal quantum number n. Besides, resonance energies are usually analyzed from the standard quantum-defect expansion formula

$$E_n = E_\infty - \frac{RZ_{core}^2}{(n-\delta)^2}. \tag{15}$$

In this equation, R is the Rydberg constant, E_∞ denotes the converging limit, Z_{core} represents the electric charge of the core ion, and δ means the quantum defect. In addition, theoretical and measured energy positions can be analyzed by calculating the Z^*-effective charge in the framework of the SCUNC-procedure

$$E_n = E_\infty - \frac{Z^{*2}}{n^2}R. \tag{16}$$

The relationship between Z^* and δ is in the form

$$Z^* = \frac{Z_{core}}{\left(1 - \frac{\delta}{n}\right)}. \tag{17}$$

According to this equation, each Rydberg series must satisfy the following conditions

$$\begin{cases} Z^* \geq Z_{core} & if\ \delta \geq 0 \\ Z^* \leq Z_{core} & if\ \delta \leq 0. \\ \lim Z^*_{n\to\infty} = Z_{core} \end{cases} \tag{18}$$