

Energy levels and characteristic features in photoionization of Cl III using the R-matrix method

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Abstract

We report study of Cl III for its large number of fine structure bound levels, 890, with $n \le 10$ and $l \le 9$, and $1/2 \le j \le 10$ 19/2 of even and odd parities with spectroscopic designation and photoionization cross sections ($\sigma_{\rm Pl}$) of the levels revealing various characteristic features. Various resonant structures and the shapes of the background, and their interference in $\sigma_{\rm PI}$ are illustrated for the ground, excited equivalent electron, low and high lying excited levels with single valence electron, and effects of fine structure couplings. $\sigma_{\rm PI}$ of the ground level shows Rydberg series of resonances on smooth background, and of equivalent electron levels producing strong closely spaced Rydberg series of resonances belonging to the low lying core ion excitation thresholds. They will impact applications in low temperature plasma. For the single valence electron excited levels, we find that $\sigma_{\rm PI}$ of low lying excited states are dominated by Rydberg series of resonances and of high lying excited states exhibit prominent broad feature of Seaton resonances. Partial photoionization cross sections of the ground level for leaving the core ion in the ground and various excited levels are also presented for applications in plasma modeling. The study was carried out in relativistic Breit-Pauli R-matrix method using a large close coupling wave function expansion of 45 levels of the core ion configurations $3s^23p^2$, $3s3p^3$, $3s^23p3d$, $3s^23p4s$, $3s3p^23d$, and $3p^4$ with closed 1s, 2s, 2p orbitals. They belong to the optimized set of 13 configurations of Cl IV, 3s²3p², 3s3p³, 3s²3p3d, 3s²3p4s, 3s²3p4d, 3s3p²3d, 3s3p²4s, 3s3p²4p, 3p⁴, 3p⁴, $3p^33d$, $3p^34s$, and $3p^34p$. Cl III energies are in good agreement with measured values. $\sigma_{\rm PI}$ features of low lying levels were benchmark with observation carried out at Advanced Light Source at LBNL with very good agreement. The present set of high accuracy data should complete for any practical applications.

Key words: Cl III, energy levels, characteristic features of photoionization, Rydberg and Seaton resonances, excitation to n = 10

1. Introduction

Chlorine, a highly reactive element, is known for its wide variety of applications, e.g., in cleaning water, bleaching, snow melting salt, etc. However, like other elements of odd number of protons, it is less abundant in astronomical objects. Hence, it is one less studied element and the Opacity Project (OP) [1], which studied radiative processes systematically of all astrophysically abundant atoms and ions did not include it. However, its presence is known in astronomical objects, such as, in low ionization stage in planetary nebula, for example, in NGC2818 [2], Jupiter moon Io (e.g., ref. [3]), in the solar flare [4], etc. Recently Cl III has been observed in NGC 5515 by SDSS (K. Arellano-Córdova, private communication). There are 83 observed energy levels Cl III available at the National Institute of Standards and Technology (NIST) compilation web table [5], which were measured by Martin et al. [6] (unpublished) as reported by NIST. Analysis of the spectral lines to obtain various diagnostics of the environmental plasma, chemical evolution require data of underlying science of photon-ion interaction. Photoionization is one important process among them. Study of features in the process help in identification of the element and modeling for various applications.

The present work reports obtaining 890 bound fine structure energy levels with $n \leq 10$ of Cl III from Breit–Pauli Rmatrix (BPRM) method developed under the OP [1] and the Iron Project (IP) [7] and identified spectroscopically using an algorithm developed by Nahar [8–10]. Photoionization cross sections have been obtained for all of these levels. The earlier work on photoionization of Cl III was carried out to benchmark the features of ground and low lying excited levels with good agreement between the theoretical and measured cross sections [11]. In contrast, the present work reports photoionization cross sections in detail with resonant features of the ground and many excited levels with n < 10 and l < 9 needed for complete astrophysical modeling for all practical applications, presents features of excited levels with Rydberg and Seaton resonances, partial cross sections for photoionization into various excited levels of the ion core not studied before but are needed for cascade and various other applications, relativistic effects, etc. The present study implements the same wavefunction expansion for Cl III as used in Nahar et al. [11].



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The work is carried out under the IP [7] that aims in solving astrophysical problems using high precision data of the atomic processes commonly take place in the plasma. IP is the follow-up of the OP [1] with the similar objectives.

2. Theory

Photoionization of an ion, e.g., Cl III, can be direct as in the following:

$$h\nu + \text{Cl III} \rightarrow e^- + \text{Cl IV}$$
 (1)

which produces the background cross section, $h\nu$ represents the photon, or through a two-step process when an intermediate doubly excited autoionizing state is formed in the continuum before ionization at an energy belonging to a state of a Rydberg series,

$$\text{Cl III} + h\nu \rightleftharpoons (\text{Cl III})^{**} \rightleftharpoons \text{Cl IV} + e^{-}$$
(2)

The Rydberg series of autoionizing states, $S_iL_iJ_i\pi_i\nu_l\ell$, where $S_iL_iJ_i\pi_i$ is an excited core ion state, and ν_l is the effective quantum number of the electron, lie above the ionization threshold but below the excited core ion state and converge on to the excited core ion state $S_iL_iJ_i\pi_i$. The energy position of an autoionizing Rydberg, E_r , belonging to the core ion threshold E_c is given by $E_r = E_c - z^2/\nu^2$, where z is the charge of the core ion. An autoionizing state introduces a Rydberg resonance in the cross section. Formation of resonances in photoionization is the reason for various features and structures in the process. The effective quantum number ν changes approximately by unity between any two consecutive resonances.

The other type of prominent resonance that appears in photoionization of single valence electron excited states is the Seaton resonance. This resonance is formed as manifestation of the process when the incoming photon, instead of causing a doubly excited state, is absorbed by the core ion for a dipole allowed transition of the ground state while the outer electron remains as a spectator in an excited orbital [12]. The excited state breaks into photoionization as the core ion drops down to the ground level. Typically a Seaton resonance is formed by the photo-excitation-of-the-core (PEC) of the ground state. However, a Seaton resonance can also form via a dipole allowed transition of a low lying excited state close to the ground state. Since the resonance depends on the core ion absorption for excitation only, the energy position of a Seaton resonance remains the same at the exact photon energy of excitation irrespective of the ionization threshold energy of the ion state. In interference with Rydberg resonances, a Seaton resonance can form a wide resonance with a background enhanced by orders of magnitude. Seaton resonances become more prominent, particularly the ones at higher energies, with higher excited state of the ion.

The autoionizing states can be incorporated theoretically for generating resonances automatically using the ab initio close coupling (CC) approximation and the R-matrix method. In CC approximation, the core ion excitation are included in the wave function expansion where the atomic system is represented as a (N + 1) number of electrons, N is the number of electron in the core ion interacting with the (N + 1)th electron. This makes it possible to form a doubly excited autoionizing state. The (N + 1)th electron can be bound or in the continuum depending on its negative or positive energy (E). The total (e + ion) wave function, Ψ_E , in a symmetry $SL\pi$ is expressed by an expansion as (e.g., ref. [13])

$$\Psi_E (\mathbf{e} + \mathbf{ion}) = A \sum_i \chi_i (\mathbf{ion}) \theta_i + \sum_j c_j \Phi_j$$
(3)

where χ_i is the core ion eigenfunction at the ground and various excited levels and the sum is over the number of levels considered. θ_i is the (N + 1)th electron wave function with kinetic energy k_i^2 in a channel coupled with the core ion labeled as $S_i L_i (J_i) \pi_i k_i^2 \ell_i [SL(J) \pi]$. A is the antisymmetrization operator. In the second term (basically part of the first term), the Φ_j s are bound channel functions of the (N + 1)-electrons system that provides the orthogonality between the continuum and the bound electron orbitals and account for short range correlation. Substitution of $\Psi_E(e + ion)$ in the Schrodinger equation

$$H_{N+1}^{BP}\Psi_E = E\Psi_E \tag{4}$$

introduces a set of coupled equations that are solved by the Rmatrix method. The R-matrix method divides the space into inner region of a sphere containing the ion at the center and effects of all short range potential, and outer region from the sphere to infinity where all short range interactions have diminished except the Coulomb and higher order pole potentials. The details of the R-matrix method in the CC approximation can be found in, e.g., refs. [13–17]. The relativistic effects are included through Breit–Pauli approximation (e.g., ref. [17]) where the Hamiltonian, as adopted under the IP [7], is given by

$$H_{N+1}^{BP} = \sum_{i=1}^{N+1} \left\{ -\nabla_i^2 - \frac{2Z}{r_i} + \sum_{j>i}^{N+1} \frac{2}{r_{ij}} \right\} + H_{N+1}^{mass} + H_{N+1}^{Dar} + H_{N+1}^{so}$$
(5)

in Rydberg unit. The first curly bracketed term is the nonrelativistic Hamiltonian and the other three terms are relativistic corrections, mass correction, $H^{\text{mass}} = -\frac{\alpha^2}{4} \sum_i p_i^4$, Darwin, $H^{\text{Dar}} = \frac{Z\alpha^2}{4} \sum_i \nabla^2 \left(\frac{1}{r_i}\right)$, and spin-orbit interaction, $H^{\text{so}} = Z\alpha^2 \sum_i \frac{1}{r_i^3} \mathbf{l}_i \mathbf{.s}_i$ where *i* represents an electron. The BPRM approximation under the IP [7] includes all these terms and part of two-body interaction terms, such as the ones without the momentum operators [17]. In BPRM method the set of $SL\pi$ is recoupled to $J\pi$ levels of the (e + ion) system in intermediate coupling which is followed by diagonalization of the Hamiltonian.

The solution is a continuum wave function, Ψ_F with a positive energy (E > 0) for the electron and bound state, Ψ_B with a negative energy ($E \le 0$). The complex resonant structures in photoionization are produced from couplings between continuum channels that are open ($k_i^2 > 0$), and bound channels that are closed ($k_i^2 < 0$), at electron energies k_i^2 matching those of autoionizing Rydberg states, $S_i L_i J_i \pi_i \nu \ell$ belonging to excited core threshold $S_i L_i J_i \pi_i$. Photoionization cross section (σ_{PI}) of a bound level with statistical weight factor g_i being ionized by a photon of energy ω is given by (e.g., ref. [17])

$$\sigma_{\rm PI} = \frac{4\pi^2}{3c} \frac{1}{g_i} \omega \mathbf{S} \tag{6}$$

where **S** is the generalized line strength given by the expression

$$\mathbf{S} = |\langle \Psi_f || \mathbf{D}_L || \Psi_i \rangle |^2 = \left| \left\langle \psi_f | \sum_{j=1}^{N+1} r_j |\psi_i \right\rangle \right|^2$$
(7)

Here \mathbf{D}_L is the dipole operator in length form representing the ion-photon interaction, and Ψ_i and Ψ_f are the initial and final state wave functions.

The energies of an ion are calculated in STGB of the Rmatrix package of codes. In the R-matrix method, the energies are scanned through the poles in the Hamiltonian matrix. However, unlike atomic structure codes, the spectroscopic identification of the energies are not determined. A theoretical algorithm developed by Nahar in refs. [9, 18, 19] is used for the purpose. It is based on quantum defect analysis which indicates effective quantum number of Rydberg series of levels differ approximately by unity, percentage of channels contributed to a particular level, and angular momenta algebra for the possible states.

3. Computations

Computations using BPRM method involves a number of stages using the R-matrix package of codes [16, 20, 21]. The program for the first stage, STG1, starts with the wave function of the core ion, e.g., Cl IV in the present case, as the initial input. The Cl IV wave function expansion was obtained from atomic structure calculations using program SUPERSTRUC-TURE (SS) [22, 23]. SS represents the electron–electron interaction by Thomas–Fermi–Dirac–Amaldi potential and includes relativistic effects in Breit–Pauli approximation. SS computes the radial wavefunction of all orbitals which remain the same while the energies of states change with change the angular momenta of the states.

The wavefunction of Cl IV was obtained by optimization of a set of 13 spectroscopic configurations with orbitals up to the 4d, 3s²3p², 3s3p³, 3s²3p3d, 3s²3p4s, 3s²3p4p, 3s²3p4d, $3s3p^23d$, $3s3p^24s$, $3s3p^24p$, $3p^4$, $3p^33d$, $3p^34s$, and $3p^34p$. The Thomas-Fermi scaling parameters for the orbitals are 1.2(1s), 1.2(2s), 1.0(2p), 1.25(3s), 1.07(3p), 1.05(3d), 1.2(4s), 1.02(4p), 1.4(4d). The optimization for energies and wavefunctions was carried out through changing the number of configurations and varying the orbital wavefunctions to compress or expand by varying Thomas-Fermi scaling parameters systematically until a set of energies was obtained that compared well with the observed energies. The present set of energies was selected after a number of trials that achieved an overall agreement between the calculated and measured values of a larger set of energies instead of focusing on improving a smaller set at lower energy as the present work aimed at obtaining a large wavefunction expansion that will accommodate the impact of excitation at high energy. The optimized set of configurations also took consideration of manageable computation by the R-matrix codes while retaining all important physical characteristics of the atomic process. SS was not adjusted by using any observed values. The set produced 248 fine structure levels out of which the first 45 levels were included in the wave function expansion of Cl III as in ref. [11].

Table 1 presents the ground and the lowest 44 excited fine structure levels of Cl IV included for Cl III wave function expansion. The calculated energies obtained from SS are compared in Table 1 with measured values by Martin et al. [6], which are available in the compiled table at NIST website [5]. As Table 1 shows, not all calculated energies have been measured yet, and most of the measured levels are the low lying ones. Comparison of calculated energies with the available measured energies shows good agreement, within a few percent, in general. However, there are some larger differences too, such as, ¹D and ¹S of the ground configuration have large differences while the other levels of the ground configuration have low differences. The accuracy of results obtained by the R-matrix method is much higher than these of core ion energies since R-matrix method can consider a much larger set of configurations than an atomic structure calculation.

For the first term in the wave function, eq. (1), of Cl III, we included $0 \le \ell \le 14$ partial waves for the interacting electron to combine with the 45 core excitation to form the set of Cl III states and 14 terms for the R-matrix basis sets in the inner region. The R-matrix boundary of the inner region was chosen to be large enough, $12 a_0$, to accommodate the bound orbitals well inside the boundary and their amplitudes reduce to near zero at the boundary. The second term of the wave function, eq. (1), included 47 (N + 1)-particle configurations with electron occupancy in the orbitals varying from minimum to a maximum number as specified within parentheses of the orbitals, 1s(2-2), 2s(2-2), 2p (6-6), 3s(0-2), 3p(0-5), 3d(0-3), 4s(0-2), 4p(0-2), 4d(0-1). These contributed in reducing considerably the uncertainties existed in the core ion wavefunctions and the R-matrix computations resulted in good agreement between the theoretical and experimental $\sigma_{\rm PI}$ of Cl III [11].

Unlike atomic structure where all possible states are determined by the configurations provided, energies from Rmatrix calculations are sorted by scanning through the poles in the Hamiltonian matrix. Fine meshes of effective quantum number, 0.001 and 0.0005, were used to scan and find the energies of Cl III. They were then processed for spectroscopic identification using the algorithm explained in refs. [18, 19].

Computation of photoionization cross sections included the radiation damping effect of resonances [16, 21]. For precise positions of the resonances in σ_{PI} , the calculated core ion excitation energies were replaced by the available observed energies during diagonalization of the (N + 1)electron Hamiltonian. The narrow resonances of photoionization were delineated with a very fine energy mesh, particularly in the energy region near the ionization threshold. Total computation required over a thousand of hours on the high performance computers at the Ohio Supercomputer Center.

| | | | | E(NIET) | E(SS) | | | | | | E/MICT) | E(SS) | |
|----|----------------------|-----------------------------|----|----------|---------|-------|----|----------------------|----------------|----|----------|---------|-------|
| | Config | SI – | 21 | E(INIST) | E(33) | %D;f | | Config | SI – | 21 | E(INIST) | E(33) | %D;f |
| | | 31л | ۷J | Ку | Ку | /oDII | | Conng | <u>ЗL</u> л | ۷J | Ку | Ку | /oDII |
| 1 | $3s^2 3p^2$ | 3P | 0 | 0.0 | 0.0 | 0. | 24 | 3s ² 3p3d | $^{3}D^{0}$ | 6 | 1.70722 | 1.81795 | 6.1 |
| 2 | $3s^2 3p^2$ | ³ P | 2 | 0.00448 | 0.00455 | 1.6 | 25 | $3s3p^3$ | $^{1}D^{o}$ | 4 | | 1.80655 | |
| 3 | $3s^2 3p^2$ | ³ P | 4 | 0.01223 | 0.01260 | 3.1 | 26 | 3s ² 3p3d | $^{1}F^{o}$ | 6 | | 1.98042 | |
| 4 | $3s^2 3p^2$ | ^{1}D | 4 | 0.12546 | 0.15362 | 22. | 27 | 3s ² 3p4s | ${}^{3}P^{o}$ | 0 | 1.95946 | 1.98730 | 1.4 |
| 5 | $3s^2 3p^2$ | ¹ S | 0 | 0.29660 | 0.35080 | 18. | 28 | $3s^2 3p 4s$ | ${}^{3}P^{o}$ | 2 | 1.96277 | 1.99167 | 1.4 |
| 6 | $3s3p^3$ | ⁵ S ^o | 4 | 0.59232 | 0.58742 | 2.7 | 29 | $3s^2 3p 4s$ | ${}^{3}P^{o}$ | 4 | 1.97260 | 1.99951 | 1.3 |
| 7 | $3s3p^3$ | $^{3}D^{o}$ | 2 | 0.93635 | 1.11670 | 2.7 | 30 | $3s^2 3p 4s$ | $^{1}P^{o}$ | 2 | 1.99981 | 1.97027 | |
| 8 | $3s3p^3$ | $^{3}D^{o}$ | 4 | 0.93666 | 0.91142 | 2.7 | 31 | $3s^23p3d$ | $^{1}P^{o}$ | 2 | | 2.08706 | |
| 9 | $3s3p^3$ | $^{3}D^{o}$ | 6 | 0.93741 | 0.91213 | 2.7 | 32 | $3s3p^23d$ | ⁵ F | 2 | | 2.11520 | |
| 10 | $3s3p^3$ | ${}^{3}P^{o}$ | 4 | 1.09585 | 1.09071 | 0.5 | 33 | $3s3p^23d$ | ${}^{5}F$ | 4 | | 2.11661 | |
| 11 | $3s3p^3$ | ${}^{3}P^{o}$ | 2 | 1.09602 | 1.09109 | 0.4 | 34 | $3s3p^23d$ | ${}^{5}F$ | 6 | | 2.11876 | |
| 12 | $3s3p^3$ | ${}^{3}P^{o}$ | 0 | 1.09625 | 1.09120 | 0.5 | 35 | $3s3p^23d$ | ${}^{5}F$ | 8 | | 2.12170 | |
| 13 | $3s^23p3d$ | $^{1}D^{o}$ | 4 | 1.17860 | 1.20101 | 1.9 | 36 | $3s3p^23d$ | ${}^{5}F$ | 10 | | 2.12546 | |
| 14 | $3s3p^3$ | ³ S ⁰ | 2 | 1.50100 | 1.50988 | 0.6 | 37 | $3p^4$ | ^{1}D | 4 | | 2.14770 | |
| 15 | 3s²3p3d | ${}^{3}F^{o}$ | 4 | | 1.48284 | | 38 | $3s3p^23d$ | ^{5}D | 0 | | 2.17418 | |
| 16 | 3s ² 3p3d | ${}^{3}F^{o}$ | 6 | | 1.48713 | | 39 | $3s3p^23d$ | ^{5}D | 2 | | 2.17456 | |
| 17 | 3s ² 3p3d | ${}^{3}F^{o}$ | 8 | | 1.49298 | | 40 | $3s3p^23d$ | ^{5}D | 4 | | 2.17534 | |
| 18 | $3s3p^3$ | ${}^{1}P^{o}$ | 2 | 1.51946 | 1.58977 | 4.4 | 41 | $3s3p^23d$ | ^{5}D | 6 | | 2.17652 | |
| 19 | 3s ² 3p3d | ${}^{3}P^{o}$ | 4 | 1.65525 | 1.77591 | 6.8 | 42 | $3s3p^23d$ | ^{5}D | 8 | | 2.17812 | |
| 20 | 3s ² 3p3d | ${}^{3}P^{o}$ | 2 | 1.65917 | 1.77979 | 6.8 | 43 | $3p^4$ | ^{3}P | 0 | | 2.04208 | |
| 21 | 3s ² 3p3d | ${}^{3}P^{o}$ | 0 | 1.66124 | 1.78175 | 6.8 | 44 | $3p^{4}$ | ^{3}P | 2 | | 2.03903 | |
| 22 | 3s ² 3p3d | $^{3}D^{o}$ | 2 | 1.70414 | 1.81481 | 6.1 | 45 | $3p^4$ | ³ P | 4 | | 2.03237 | |
| 23 | $3s^23n3d$ | ³ D ⁰ | 4 | 1,70565 | 1.81660 | 6.1 | | - | | | | | |

Table 1. The table contains 45 fine structure levels of core ion Cl IV that have been included in the CC wavefunction expansion for Cl III.

Note: The calculated energies obtained from SUPERSTRUCTURE (SS) are compared with the measured values [6] available in the compiled table of NIST [5].

4. Results and discussions

We present a large number of bound fine structure levels of P-like chlorine ion, Cl III, with $n \leq 10$ and the corresponding photoionization cross sections ($\sigma_{\rm Pl}$). As mentioned in the "Introduction" section, photoionization cross sections of Cl III for the ground and low lying excited levels were calculated earlier to benchmark the combined photoionization spectral features measured at ALS set-up at LBNL and good agreement was found between the theoretical and measured cross sections [11]. Here we present cross sections of all energies that we have computed to illustrate the general characteristic features of photoionization for various types of bound levels of Cl III which could not be done with a few levels.

4.1. Energy levels of Cl III

We have obtained 890 bound fine structure levels of Cl III with $n \le 10$ and $0 \le l \le 9$, $1/2 \le J \le 19/2$ of even and odd parities using the relativistic BPRM method. While in an atomic structure calculations, the number of possible states from the given list of configuration are predetermined and assigned the energy eigenvalues, in the R-matrix approach as mentioned in the computation section, the eigenvalues are obtained from the poles in the Hamiltonian matrix. The present scanning of poles was carried out using a fine energy mesh in effective quantum numbers, and then these levels were identified with spectroscopic designations. The energy values are

compared with the measured values of Martin et al. [6] available at NIST compilation table [5] in Table 2.

In the table, the comparison between the theoretical and observed energies shows that 79 levels of the 83 observed levels are in agreement within 5%. One exception is for the level $3s^2 3p^2({}^{3}P)4s^4P_{1/2}$ with absolute calculated energy of 1.34 Ry which has large difference from measured value of 1.576 Ry. A possible reason for it is misidentification of the measured energy level since thie other measured levels of the state agree very well with the calculated values. Some differences are introduced from reasons, such as, methodology to compute the energies, number of dominant configurations considered contributing to the levels, configuration mixing coefficient for the state. A mixed state has more than one possible designations and an approach for spectroscopic designation assigns the state with the leading mixing coefficient which can be different from another approach. To be consistent with the designations of the observed levels at NIST compiled table, the present work adopted the NIST identifications for the mixed states. However, identification of three levels in NIST table did not show comparable match with those in the present work. For them, we are using the designations instead of those of NIST. The present designations are (i) $3s^2 3p^2({}^{3}P)3d({}^{2}D_{7/2})$ at energy 1.54022 Ry instead of $3s^2 3p^2 ({}^3P) 3d ({}^4D_{7/2}),$ (ii) $3s^2 3p^2 ({}^1D) 3d ({}^2P_{5/2})$ at 1.28924 Ry instead of $3s^2 3p^2({}^1D)3d({}^4P_{5/2})$, and (iii) $3s^2p^2({}^3P)3d({}^2P_{1/2})$ at 1.11298 Ry instead of $3s3p^4({}^{3}P)({}^{2}P_{1/2})$.



Table 2. Comparison between the present theoretical BPRM and observed energies of Cl III [6] available at NIST [5].

Table 2. (concluded).

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| | 0 | | | - [- | * |
|------------------------------|------------------|----------------|----------------|------------|----------------|
| Level | | $J:I_J$ | E(Ry,BPRM) | E(Ry,NIST) | %Dif |
| 3s23p3 | $^{4}S^{o}$ | 1.5 1 | 2.925 | 3.057 | 4.53 |
| 3s23p3 | $^{2}D^{o}$ | 2.5 1 | 2.760 | 2.879 | 4.32 |
| 3s23p3 | $^{2}D^{o}$ | 1.5 2 | 2.760 | 2.880 | 4.32 |
| 3s23p3 | ${}^{2}P^{0}$ | 1.5 3 | 2.652 | 2.753 | 3.79 |
| 3s23p3 | ${}^{2}P^{o}$ | 0.5 1 | 2.653 | 2.754 | 3.78 |
| 3s3p4(3P) | ^{4}P | 2.5 1 | 2.027 | 2.114 | 4.31 |
| 3s3p4(3P) | ^{4}P | 1.5 1 | 2.022 | 2.109 | 4.32 |
| 3s3p4(3P) | ^{4}P | 0.5 1 | 2.018 | 2.106 | 4.33 |
| 3s3p4(1D) | ^{2}D | 2.5 2 | 1.812 | 1.884 | 4.00 |
| 3s3p4(1D) | ^{2}D | 1.5 2 | 1.812 | 1.884 | 4.00 |
| 3s23p2(3P)3d | ${}^{4}F$ | 4.5 1 | 1.581 | 1.645 | 4.08 |
| 3s23p2(3P)3d | ${}^{4}F$ | 3.5 2 | 1.585 | 1.609 | 1.51 |
| 3s23p2(3P)3d | ${}^{4}F$ | 2.5 4 | 1.588 | 1.610 | 1.41 |
| 3s23v2(3P)3d | ^{4}F | 1.5 4 | 1.590 | 1.654 | 4.04 |
| 3s23p2(3P)3d | ^{2}D | 3.5 3 | 1.540 | 1.530 | 0.65 |
| 3s23n2(3P)3d | 4D | 2.5 5 | 1.541 | 1.536 | 0.32 |
| 3s23n2(3P)3d | 4D | 155 | 1.541 | 1 611 | 4.55 |
| 352322(31)34 | ע 4 ח | 054 | 1.540 | 1.011 | 4.55 |
| 3523µ2(3F)30 3573n7(3D)Ac | 4 D | 256 | 1.340 | 1.012 | -1.04 0 0 0 |
| 3023µ2(31)43 | г 4 р | 4.00 156 | 1.004 | 1.047 | 1.00 |
| 3523µ2(31)45 | ґ 4 р | 1.50 | 1.00ð 1.040 | 1.332 | 1.03 |
| 3323p2(3P)45 | -1' 2 n | 0.55 | 1.342 | 1.3/6 | 1/.49 |
| 3\$23p2(3P)4\$ | 2P 2D | 1.5 7 | 1.293 | 1.307 | 1.10 |
| 3s23p2(3P)4s | 2°P | 0.56 | 1.299 | 1.356 | 4.53 |
| 3s23p2(1D)3d | 4P | 2.5 7 | 1.289 | 1.282 | 0.56 |
| 3s23p2(3P)3d | *₽ 4- | 1.5 8 | 1.288 | 1.280 | 0.60 |
| 3s23p2(3P)3d | *P | 0.5 7 | 1.287 | 1.314 | 2.10 |
| 3s23p2(3P)3d | ² D | 2.5 8 | 1.257 | 1.226 | 2.42 |
| 3s23p2(3P)3d | ² D | 1.5 9 | 1.266 | 1.235 | 2.43 |
| 3s23p2(1D)3d | ² P | 1.5 10 | 1.231 | 1.219 | 1.02 |
| 3s23p2(1D)3d | ² P | 0.5 8 | 1.228 | 1.214 | 1.16 |
| 3s23p2(1D)4s | ^{2}D | 2.5 9 | 1.208 | 1.207 | 0.06 |
| 3s23p2(1D)4s | ^{2}D | 1.5 11 | 1.208 | 1.207 | 0.06 |
| 3s23p2(1D)3d | ^{2}D | 2.5 10 | 1.148 | 1.125 | 2.03 |
| 3s23p2(1D)3d | ^{2}D | 1.5 12 | 1.145 | 1.123 | 1.94 |
| 3s23p2(1D)3d! | ^{2}F | 3.5 5 | 1.137 | 1.115 | 1.94 |
| 3s23p2(3P)3d | ^{2}F | 2.5 11 | 1.138 | 1.116 | 1.94 |
| 3s23p2(3p)3d! | ^{2}P | 1.5 13 | 1.112 | 1.082 | 2.56 |
| 3s2p2(3P)3d | ^{2}P | 0.5 9 | 1.113 | 1.085 | 2.53 |
| 3s23p2(3P)4p | $^4D^o$ | 3.5 1 | 1.081 | 1.086 | 0.50 |
| 3s23p2(3P)4p | $^4D^o$ | 2.5 2 | 1.086 | 1.092 | 0.50 |
| 3s23p2(3P)4p | $^4D^o$ | 1.5 4 | 1.090 | 1.096 | 0.50 |
| 3s23p2(3P)4v | $^4D^o$ | 0.5 2 | 1.093 | 1.131 | 3.51 |
| 3s23n2(3P)4n | $^{4}P^{0}$ | 2.5 3 | 1.061 | 1.065 | 0.40 |
| 3s23n2(3P)4n | 4 P ⁰ | 1.5.5 | 1.065 | 1.069 | 0.44 |
| 3s23n2(3P)4n | 4 p0 | 0.5.3 | 1.000 | 1 098 | 3.03 |
| 3s23n2(3P)4n | 1 0م2 | 254 | 1 048 | 1.050 | 0.00 |
| 3323µ2(31)4µ 3323µ2(3D)4µ | ں 100° | 2.J 4 1 5 6 | 1.040 | 1.049 | 0.09 |
| 3023µ2(31)4µ | 4 00 | 1.00 | 1.020 | 1.057 | 0.09 |
| 3323µ2(31)4p | -3° 2 m | 1.5 / | 1.048 | 1.055 | 0.01 |
| 3\$23p2(3P)4p | -P° 2.50 | 1.5 9 | 1.019 | 1.018 | 0.08 |
| 3s23p2(3P)4p | ~P° 2~ | 0.54 | 1.020 | 1.070 | 4.95 |
| 3s23p2(1D)4p | ≁F⁰ 2∽∽ | 3.5 3 | 9.501E-01 | 9.266E-01j | 2.47 |
| 3s23p2(1D)4p | 4F0 250 | 2.5 6 | 9.518E-01 | 9.281E-01 | 2.48 |
| 3s23p2(1D)4p | $^{2}D^{o}$ | 2.5 7 | 9.397E-01 | 9.214E-01 | 1.94 |

| Level | | $J : I_J$ | E(Ry,BPRM) | E(Ry,NIST) | %Dif |
|--------------|---------------|-----------|------------|------------|------|
| 3s23p2(1D)4p | $^{2}D^{o}$ | 1.5 10 | 9.391E-01 | 9.208E-01 | 1.95 |
| 3s23p2(1D)4p | ${}^{2}P^{0}$ | 1.5 11 | 9.010E-01 | 8.847E-01 | 1.81 |
| 3s23p2(1D)4p | ${}^{2}P^{0}$ | 0.5 7 | 9.031E-01 | 8.846E-01 | 2.06 |
| 3s23p2(3P)4d | ${}^{4}F$ | 4.5 3 | 7.327E-01 | 7.203E-01 | 1.69 |
| 3s23p2(3P)4d | ${}^{4}F$ | 3.5 6 | 7.372E-01 | 7.247E-01 | 1.70 |
| 3s23p2(3P)4d | ${}^{4}F$ | 2.5 13 | 7.403E-01 | 7.277E-01 | 1.71 |
| 3s23p2(3P)4d | ${}^{4}F$ | 1.5 15 | 7.424E-01 | 7.296E-01 | 1.72 |
| 3s23p2(3P)4d | 4D | 3.5 7 | 7.192E-01 | 7.058E-01 | 1.87 |
| 3s23p2(3P)4d | ^{4}D | 2.5 14 | 7.225E-01 | 7.084E-01 | 1.95 |
| 3s23p2(3P)4d | ^{4}D | 1.5 16 | 7.235E-01 | 7.093E-01 | 1.96 |
| 3s23p2(3P)4d | ^{4}D | 0.5 12 | 7.237E-01 | 7.097E-01 | 1.93 |
| 3s23p2(3P)4d | ^{4}P | 2.5 15 | 7.121E-01 | 6.939E-01 | 2.55 |
| 3s23p2(3P)4d | ^{4}P | 1.5 17 | 7.097E-01 | 6.948E-01 | 2.11 |
| 3s23p2(3P)4d | ^{4}P | 0.5 13 | 7.086E-01 | 6.895E-01 | 2.71 |
| 3s23p2(3P)4d | ^{2}F | 3.5 8 | 6.952E-01 | 6.748E-01 | 2.92 |
| 3s23p2(3P)4d | ^{2}F | 2.5 16 | 7.030E-01 | 6.827E-01 | 2.89 |
| 3s23p2(3P)5s | ^{4}P | 2.5 17 | 6.819E-01 | 6.676E-01 | 2.10 |
| 3s23p2(3P)5s | ^{4}P | 1.5 19 | 6.887E-01 | 6.744E-01 | 2.07 |
| 3s23p2(3P)5s | ^{4}P | 0.5 14 | 6.927E-01 | 6.886E-01 | 0.59 |
| 3s23p2(3P)4d | ^{2}D | 2.5 18 | 6.590E-01 | 6.329E-01 | 3.96 |
| 3s23p2(3P)4d | ^{2}D | 1.5 20 | 6.601E-01 | 6.544E-01 | 0.87 |
| 3s23p2(1D)4d | ^{2}D | 2.5 19 | 6.041E-01 | 5.665E-01 | 6.22 |
| 3s23p2(1D)4d | ^{2}D | 1.5 21 | 6.047E-01 | 6.342E-01 | 4.88 |
| 3s23p2(1D)4d | ^{2}F | 3.5 9 | 6.004E-01 | 5.710E-01 | 4.89 |
| 3s23p2(1D)4d | ^{2}F | 2.5 20 | 5.999E-01 | 5.524E-01 | 7.91 |
| 3s23p2(1D)5s | ^{2}D | $2.5\ 21$ | 5.658E-01 | 5.481E-01 | 3.13 |
| 3s23p2(1D)5s | ^{2}D | 1.5 22 | 5.657E-01 | 5.531E-01 | 2.23 |
| 3 <i>p</i> 5 | ${}^{2}P^{o}$ | 1.5 48 | 2.597E-01 | 2.529E-01 | 2.63 |
| 3 <i>p</i> 5 | ${}^{2}P^{o}$ | 0.5 32 | 2.500E-01 | 2.498E-01 | 0.05 |

Note: I_J is the calculated level index for its position in its $J\pi$ symmetry. Negative sign for the energies is omitted for convenience. NIST, National Institute of Standards and Technology.

The complete table of energies will be available at the NORAD-Atomic-Data database [24]. Since BPRM energies are computed by specifying the high angular momentum limit for the j-values of the levels, the set of fine structure levels belonging to an LS term, particularly with high angular momentum which may require even higher angular momenta levels, may not be complete. It may also be possible that a level is missing due to very narrow energy gaps in a j-symmetry where the effective quantum number mesh was not able detect the consequent levels in the Hamiltonian matrix.

4.2. Photoionization of the ground level

The ground level is the most stable level of any ion and hence plays an important role in all applications in plasma. Typically, $\sigma_{\rm PI}$ of the ground state of any ion shows feature of a smooth background cross section which decreases slowly with energy, and Rydberg series of resonances which are usually strong for low lying excitation of the core ion. However, photoionization cross section $\sigma_{\rm PI}$ of the ground state is not necessarily the most dominant one. Figure 1 presents $\sigma_{\rm PI}$ of

Fig. 1. Photoionization cross sections, σ_{PI} , of the ground $3s^2 3p^3 \left({}^4S^{\circ}_{3/2}\right)$ state of Cl III. The features are typical for a ground state where Rydberg series of resonances appear on a relatively smooth background which is decreasing slowly with energy. The arrows point to the excitation thresholds of the core ion Cl IV where Rydberg series of resonances converge.



the ground $3s^2 3p^3 \left({}^4S^o_{3/2}\right)$ state of Cl III. The Rydberg series of resonances can be seen converging on to various excitation thresholds (pointed by arrows) of the core ion. Some arrows at core ion excitation thresholds do not have resonances converging to. These core states either do not couple or have very weak coupling with the state being photoionized. It may be noted that with higher core ion excitation, the resonances becoming weaker and tend to converging on to the background.

4.3. Photoionization of excited equivalent electron levels

The energy levels of any ion typically has one or a few equivalent electron states. These states have more than one electron in the outer orbit. These equivalent electron states, particularly from an excited configuration, are found to show characteristic features of closely lying strong high peak resonances belonging to the low lying core ion excitation thresholds. Figure 2 presents $\sigma_{\rm PI}$ of two equivalent electron states, (a) $3s^2 3p^3 ({}^2D_{3/2}^0)$ of ground configuration and (b) $3s 3p^4 ({}^4P_{3/2})$ of an excited configuration. While the top panel (a) shows strong resonances in the lower energy region, the dominance of resonances does not extend over larger number of excited core ion states. In contrast, lower panel (b) shows strong resonances continuing converging on to the core ion states. The arrows indicate energy positions of various excitation thresholds of the core ion. These low energy features have significant contributions in applications such as recombination rate, photoionization rates, etc. at low temperature plasma. One arrow with the n = 3 indicates the last core ion excitation of complex n = 3. The ground configuration corresponds to the n = 3 complex. Beyond it, resonances become weaker. The background cross section of equivalent electron states also decreases slowly with energy making them important in the high temperature plasma applications.

4.4. Photoionization of excited levels with single valence electron

The features of photoionization of low and high lying single valence electron excited states have been seen to be characterized by dominance of the Rydberg and Seaton resonances. Low lying states are dominated by strong Rydberg resonances while Seaton resonances are more distinct in high lying excited states. Unlike the ground and equivalent electron levels, the background cross section of these levels decrease faster at high energy, but may enhanced again at core ion thresholds for dipole excitation.

Figure 3 presents photoionization cross section $\sigma_{\rm PI}$ of a low lying excited level, $3s^2 3p^2 3d({}^4F_{3/2})$. The figure illustrates the dominance of high peak Rydberg series of resonances. These resonances are typically narrow but usually with certain shape which is retained for a series converging to an excitation threshold of the core ion. The arrows in the figure indicate energy positions of various core ion excitation thresholds. Due to their closely lying positions the Rydberg series belong to them are overlapped.

Figure 4 presents photoionization cross sections $\sigma_{\rm PI}$ of three high lying single valence electron excited level (a) $3s^2 3p^2 4p \left({}^4P^o_{3/2} \right)$, (b) $3s^2 3p^2 4d ({}^4P_{5/2})$, and (c) $3s^2 3p^2 6g ({}^4H_{7/2})$ to illustrate certain features of these levels as the ionization threshold moves progressively toward lower energies. In addition to the narrow Rydberg resonances, these levels show broad resonant structures. These are Seaton resonances [12, 25] as explained in the theory section. The arrows indicate the exact photon energies for transition of the core ion ground level $3s^2 3p^2({}^{3}P_0)$ to various dipole allowed levels, that is the PEC positions, and hence the positions of the Seaton resonances as the core ion absorbs the photons. Since the transition energies remain the same irrespective of the ionization thresholds, Seaton resonances appear at the same energies for all excited levels. It is also the reason for the missing of the first Seaton resonance in panel (a) where the ionization **Fig. 2.** Photoionization cross sections σ_{PI} of two equivalent electron levels of Cl III: (*a*) $3s^2 3p^3 \left({}^2D_{3/2}^o\right)$ of ground configuration and (*b*) $3s 3p^4 ({}^4P_{3/2})$ of an excited configuration. The arrows indicate energy positions of various excitation thresholds of the core ion. One arrow shows the last energy of the n = 3 complex. Lower panel illustrates the dominance of strong high peak resonances belonging to various core ion excitation thresholds, especially for the lower ones belonging to n = 3 complex for the excited state. Presence of such closely lying strong resonances are usually seen for the equivalent states of excited configurations.



Fig. 3. Photoionization cross sections σ_{PI} of a low lying single valence electron excited level, $3s^2 3p^2 3d({}^4F_{3/2})$ of Cl III. The figure illustrates the dominance of Rydberg series of resonances for the level. But the series are overlapped by the closely lying excitation thresholds. The arrows indicate energy positions of various core ion excitation thresholds.



threshold of the level is higher than the PEC. Seaton resonances are more prominent when the transitions have high radiative decay rates (e.g., ref. [25]). The other characteristic of the Seaton resonances is that they are more prominent in $\sigma_{\rm PI}$ of higher excited levels. As seen in the figure that for the high-

est excited level (panel c), the background has the largest enhancement, a few orders of magnitude over the background.

There is one Seaton resonance at about 1.8 Rydberg (marked with a black arrow) which does not correspond to core ion group state to a dipole allowed transition. However, **Fig. 4.** Photoionization cross sections σ_{PI} of three high lying single valence electron levels with progressively lower ionization thresholds, (a) $3s^23p^24p\left({}^{4}P^{0}_{3/2}\right)$, (b) $3s^23p^24d({}^{4}P_{5/2})$, and (c) $3s^23p^26g({}^{4}H_{7/2})$). The arrows indicate exact photon energies of the core ion ground state to excite to various dipole allowed states. The black arrow corresponds to dipole allowed transition from three low lying excited levels. As the core ion goes through the excitation, known as PEC (photo-excitation-of-core), a Seaton resonance is introduced.



its position and strengths come from dipole allowed transitions from three low lying excited levels, (a) $3s^2 3p^2(^3P_1)$, (b) $3s^2 s 3p^2(^3P_2)$, and (c) $3s^2 3p^2(^1D_2)$ to $3s 3p^3(^1D_2^0)$.

4.5. Fine structure coupling features in photoionization

Inclusion of relativistic fine structure channels through BPRM method in calculating photoionization cross sections $\sigma_{\rm PI}$ increases the accuracy. Splitting of LS terms of the core ion into their fine structure levels results in larger number of excited core ion thresholds, and hence larger number of Rydberg series of resonances belonging to them. LS resonances are approximately the averaged of the fine structure series, but fine structure increases the accuracy as the resonances are more resolved and spread over somewhat larger energy region. However, the accuracy may not be significant when the resonances are statistically averaged to obtain integrated quantities for recombination rates or photoionization rates or plasma opacity at high temperature. Exceptions are noticeable for low energy and low temperature plasma when fine structure coupling creates resonant features, which are actually observed in experiments (e.g., refs. [26, 27]), but not allowed in LS coupling. The impact is always significant in applications for low temperature plasmas. In Fig. 5, the effect of coupling of relativistic fine structure channels on photoionization is illustrated for the ground $3s^2 3p^3 \left({}^4S^o_{3/2} \right)$ level of Cl III. The cross sections and structures of Rydberg series of resonances below the core ion excitation threshold $3s^23p^2(^3P_2)$ (pointed by arrow) are created by the coupling of fine structure channels, $3s^23p^2(^3P_1)(\epsilon s, \epsilon d)$ and $3s^23p^2(^3P_2)(\epsilon s, \epsilon d)$ which are not allowed to form in LS coupling. Ionization threshold has been lowered to $3s^23p^2(^3P_0)$ (pointed by arrow). The resonances will affect the recombination rates. It is not only the ground level, most of the excited levels show such resonant feature at and near the ionization threshold.

4.6. Partial photoionization cross sections of Cl III for leaving the core ion into various excited core ion levels

In close-coupling approximation, the total photoionization cross section of a level is obtained by summing the partial cross sections of channels that leave the ion in the ground and various excited levels of the core ion. Hence, for the present case with 45 core ion states, the total cross section corresponds to sum of contributions from 45 channels that leave ion ionized Cl III in various core ion states. These partial cross sections are needed for applications, such as, for recombination, cascading effect, determination of level populations. Figure 6 presents features in the eight lowest partial $\sigma_{\rm PI}$ of the ground level as Cl III photoionized leaving the residual ion Cl IV at eight lowest levels, specified in the panels. The total cross section of any level presented here is the sum of 45 partial cross sections leaving the residual ion in 45 different core ion levels. However, with higher excitation

Fig. 5. Near threshold photoionization cross sections, σ_{PI} , of the ground $3s^2 3p^3 \left({}^4S^{\circ}_{3/2}\right)$ of Cl III to illustrate the effect of coupling of fine structure channels on photoionization in the region between $3s^2 3p^2 ({}^3P_0)$ and $3s^2 3p^2 ({}^3P_2)$ filled with resonances and background enhancement at thresholds $3s^2 3p^2 ({}^3P_1)$ and $3s^2 3p^2 ({}^3P_2)$. These cannot be formed in LS coupling approximation.



Fig. 6. Partial photoionization cross sections, σ_{PI} , of the ground $3s^2 3p^3 \left({}^4S^o_{3/2}\right)$ level of Cl III leaving the residual ion Cl IV in (a) the ground and (b–h) seven excited levels, as specified in panels. Total cross section of any level is obtained from summing of 45 such partial cross sections. Forty five is the number of core ion levels considered for the present work.



of the residual ion, the partial cross sections become weaker and contribute negligibly to the total.

5. Conclusion

We present 890 levels with spectroscopic designation and the corresponding total photoionization cross sections of Cl III. Characteristic features in $\sigma_{\rm PI}$ corresponding to various types of bound levels are illustrated with the followings:

- The ground level shows typical features with Rydberg resonances belonging to low lying core ion excitation and a smooth slow decay background cross section at high energy.
- Strong Rydberg resonances, closely lying for levels of excited configuration, are characteristic of equivalent electron levels. They typically belong to the low lying core ion levels and contribute significantly in the low-temperature plasma but also remain significant at high temperature

- Single valence electron excited levels exhibit different features—Rydberg series of resonance dominate the low lying excited levels and Seaton resonances are prominent for high lying excited states. However, the background $\sigma_{\rm PI}$ of both types of levels decrease faster with higher energy.
- Photoionization cross sections also show the importance of fine structure coupling at near threshold low energy that reveal features that cannot be created in LS coupling approximation.
- We also present partial cross sections of the ground state leaving the core ion at various excitation thresholds.

Present data have already been benchmark with experiment [11]. Based on the benchmark and high accuracy in the energies, 79 of 83 observed levels agree within with 5% of the observed values, the present photoionization cross sections should be accurate with 10%. The large set of data should enable complete and precise plasma modelings and applications, such as, producing synthetic spectra, plasma opacities, and plasma diagnostics.

The complete set of data for photoionization cross sections and the energy levels are available online from NORAD-Atomic-Data website at: http://norad.astronomy.ohio-state. edu/.

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Data availability

All atomic data will be available online at NORAD-Atomic-Data database at The Ohio State University: https://norad.as tronomy.osu.edu/.

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Competing interests

There is no competing interest for the present work.

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