Electron impact excitation of fine-structure levels in Cl II

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Abstract. The B-spline basis has been used in the R-matrix approach to calculate electron impact excitation collision strengths for transitions between the 3s3p43P0,1,2, 1D2 and 1S0 levels and from these levels to the fine-structure levels of the excited 3s3p, 3s3p44s, 3s3p43d, 3s3p43p and 3s3p4d configurations of Cl II. We considered 23 LS states 3s3p43P, 1D, 1S, 3s3p43P, 3s3p43S4P, 3s3p43S4D, 3s3p43S4D, 3s3p43S4D, 3s3p43S4D, 3s3p43S4D, 3s3p43S4D, 3s3p43S4D, 3s3p43S4D, 3s3p43S4D, 3s3p43S4D, 3s3p43S4D, 3s3p43S4D, 3s3p43S4D, 3s3p43S4D, 3s3p43S4D, 3s3p43S4D, 3s3p43S4D, 3s3p43S4D, 3s3p43S4D, and 3s3p43S4D in the close-coupling expansion that give rise to 51 fine-structure levels. The non-orthogonal orbitals are used for an accurate representation of both the target wavefunctions and the R-matrix basis functions. The collision strengths for transitions between fine-structure levels are calculated by transforming the LS-coupled K-matrices to K-matrices in an intermediate coupling scheme. The Rydberg series of resonances converging to excited state thresholds make substantial contributions to collision strengths. The thermally averaged collision strengths have been obtained by integrating collision strengths over a Maxwellian distribution of electron energies and these are listed in Table 2 for log T from 3.3 to 5.6 K.

Key words. atomic data – atomic processes – line: formation

1. Introduction

The fine-structure transitions among the levels of ground 3s23p configuration in Cl II give rise to spectral lines in the infrared and visible part of the spectrum and transitions from the ground configuration to excited 3s3p, 3s3p44s, 3s3p43d, 3s3p43p and 3s3p4d configurations occur in the ultraviolet (UV), far-ultraviolet (FUV) and extreme ultraviolet (EUV) wavelength regions. Emission lines of collisionally excited Cl II have been detected in the spectra of the Io torus from the ground-based observations (Küppers & Schneider 2000) as well as from the space-based observations by the Far-Ultraviolet Spectroscopic Explorer (FUSE) (Feldman et al. 2001). Electron-ion collision processes play an important role in the understanding of energy balance in various types of plasmas. Accurate electron impact collision strengths of fine-structure transitions in Cl II are needed for the interpretation of observed spectra to understand the physical processes and conditions such as temperature, density and chlorine abundance in Io-torus-Jupiter system.

The strong mixing between a number of levels of the different Rydberg 3s23pnl series and the 3s3p5 perturber states is caused by configuration-interaction (Tayal 2003). The Cl II wavefunctions show strong term dependence of the one-electron orbitals and large correlation corrections. The term dependent non-orthogonal orbitals in the multiconfiguration Hartree-Fock approach (Froese Fischer 1991; Zatsarinny & Froese Fischer 1999) have been used to provide adequate treatment of large correlation corrections as well as the interactions between different Rydberg series and perturber states. These wavefunctions yield excitation energies of Cl II target states that are in excellent agreement with the experimental values. The B-spline R-matrix approach (Zatsarinny & Froese Fischer 1999; Zatsarinny & Tayal 2001) has been used to calculate electron impact excitation collision strengths and effective collision strengths for all dipole allowed, intercombination and forbidden transitions among the fine-structure levels. Our calculation included 23 spectroscopic bound states of Cl II in the close-coupling expansion. We included 15 states 3s3p33P, 1D, 1S, 3s3p33P, 3s3p33P, 3s3p33P, 3s3p33P, 3s3p33P, 3s3p33P, 3s3p33P, 3s3p33P, 3s3p33P, 3s3p33P, 3s3p33P, 3s3p33P, 3s3p33P, 3s3p33P, 3s3p33P, 3s3p33P, 3s3p33P, 3s3p33P, 3s3p33P, and eight higher-lying states 3s3p33P, 3s3p33P, 3s3p33P, 3s3p33P, 3s3p33P, 3s3p33P, 3s3p33P, and 3s3p33P which have strong dipole connection with the 3s3p configuration. A B-spline basis has been used for the description of continuum functions. No orthogonality constraint has been imposed on the continuum functions and atomic bound orbitals. This procedure leads to substantial reduction in pseudo-resonances in the electron collisional excitation strengths. The completeness of the B-spline ensures that no Butter correction to the R-matrix elements is required.

Recently, Wilson & Bell (2002) reported collision data for the 10 fine-structure transitions among the ground configuration levels 3s3p43P0,1,2, 1D2 and 1S0 of Cl II. They included lowest 12 LS states 3s3p43P, 1D, 1S, 3s3p53P, 3s3p43P, 3s3p43P, 3s3p43P, 3s3p43P, 3s3p43P, 3s3p43P, 3s3p43P, and 3s3p43P in the close-coupling expansion that give rise to 51 fine-structure levels.
the description of term-dependence of radial functions. The 3s 23p 4 and 3s 23p 3 \( ^1 S \) configurations at the boundary which are needed for construction of the R-matrix are simply given by the coefficient of the last spline. The completeness of the B-spline basis ensures that no Buttle correction to the R-matrix elements is required. The R-matrix calculations with inclusion of exchange were carried out for all partial waves with \( L \leq 20 \).

The LS-coupled K-matrices are calculated by matching the inner region solutions at \( r = a \) with asymptotic solutions in the outer region. The FARM program (Burke & Noble 1995) has been used to find the asymptotic solutions. The collision strengths between fine-structure levels are calculated by transforming the LS-coupled K-matrices to K-matrices in an intermediate coupling scheme. We have used the intermediate-coupling frame transformation (ICFT) method (Giffin et al. 1998). This method employs multi-channel quantum defect theory (MQDT) to generate unphysical K-matrices in LS coupling and these are transformed to intermediate coupling. The physical K-matrices are then obtained from the intermediate-coupled unphysical K-matrices. The higher partial wave contributions for the dipole-allowed and other transitions are calculated using a top-up procedure based on the geometric series approximation (Burgess et al. 1970).

In the asymptotic region, the collision strength follows a high energy limiting behavior which is determined by the type of transition. For optically allowed electric-dipole transitions

\[
\Omega_{ij}(E) \sim E^{\rightarrow \infty} d \ln(E),
\]

where \( \Phi_i \) are channel functions formed from the multi-configurational functions of the target states and \( u_j \) are the radial basis functions describing the motion of the scattering electron. The operator \( A \) antisymmetrizes the wave function and \( a_{ijk} \) and \( b_{ijk} \) are expansion coefficients determined by diagonalizing the \((N+1)\)-electron Hamiltonian. The functions \( \phi_j \) in Eq. (1) are of bound-state type and are included to allow for short-range correlation effect. In our R-matrix calculation, the radial functions \( u_j \) are expanded in the spline basis as

\[
u_j(r) = \sum_i a_{ij} B_i(r),
\]

and the coefficients \( a_{ij} \) (which now replace \( a_{ijk} \) in Eq. (1)) and \( b_{ijk} \) are determined by diagonalizing the \((N+1)\)-electron Hamiltonian inside the R-matrix box of radius \( a \) that contain all bound atomic orbitals used for the description of Cl II states. We used 96 continuum basis functions for each orbital angular momentum and a boundary radius \( a = 25 \) au. For an accurate determination of electron flux through the boundary, we do not impose any boundary condition on \( u_j \) functions at the outer edge of the box. The amplitudes of the wavefunctions at the boundary which are needed for construction of the R-matrix are simply given by the coefficient of the last spline. The completeness of the B-spline basis ensures that no Buttle correction to the R-matrix elements is required. The R-matrix calculations with inclusion of exchange were carried out for all partial waves with \( L \leq 20 \).

The LS-coupled K-matrices are calculated by matching the inner region solutions at \( r = a \) with asymptotic solutions in the outer region. The FARM program (Burke & Noble 1995) has been used to find the asymptotic solutions. The collision strengths between fine-structure levels are calculated by transforming the LS-coupled K-matrices to K-matrices in an intermediate coupling scheme. We have used the intermediate-coupling frame transformation (ICFT) method (Giffin et al. 1998). This method employs multi-channel quantum defect theory (MQDT) to generate unphysical K-matrices in LS coupling and these are transformed to intermediate coupling. The physical K-matrices are then obtained from the intermediate-coupled unphysical K-matrices. The higher partial wave contributions for the dipole-allowed and other transitions are calculated using a top-up procedure based on the geometric series approximation (Burgess et al. 1970).

In the asymptotic region, the collision strength follows a high energy limiting behavior which is determined by the type of transition. For optically allowed electric-dipole transitions

\[
\Omega_{ij}(E) \sim E^{\rightarrow \infty} d \ln(E),
\]

where the parameter \( d \) is proportional to the oscillator strength. In the case of the multipole optically forbidden transitions such as electric quadrupole or magnetic dipole transitions

\[
\Omega_{ij}(E) \sim E^{\rightarrow \infty} constant,
\]

where the value of constant can be obtained from the Bethe approximation. The intercombination transitions have the asymptotic form

\[
\Omega_{ij}(E) \sim E^{\rightarrow \infty} \frac{1}{E^2}.
\]
The rapid decrease of collision strengths with incident electron energies in the case of intercombination transitions is due to the fact that these transitions can only occur through electron exchange. In many applications it is convenient to use excitation rate coefficients or thermally averaged collision strengths as a function of electron temperature. The electron excitation rates are obtained by averaging total collision strengths over a Maxwellian distribution of electron energies. The excitation rate coefficient for a transition from state $i$ to state $f$ at electron temperature $T_e$ is given by

$$C_{if} = \frac{8.629 \times 10^{-6}}{g_if f} \gamma_{if}(T_e) \exp\left(-\frac{\Delta E_{if}}{kT_e}\right) \text{ cm}^3\text{s}^{-1},$$

where $g_i$ is the statistical weight of the lower level $i$, $\Delta E_{if} = E_f - E_i$ is the excitation energy, and $\gamma_{if}$ is a dimensionless quantity called effective collision strength and is given by

$$\gamma_{if}(T_e) = \int_0^\infty \Omega_{if}(E_f) \exp\left(-\frac{E_f}{kT_e}\right) \frac{dE_f}{kT_e},$$

where $\Omega_{if}$ is the total collision strength for transitions between levels $i$ and $f$, $k$ is the Boltzmann constant, and $E_f$ is the energy of incident electron with respect to the upper level $f$. If the collision strength is assumed to be independent of the incident electron energy, we have $\gamma_{if} = \Omega_{if}$.

The effective collision strengths are calculated by integrating collision strengths for fine-structure levels over a Maxwellian distribution of electron energies.

### 3. Results and discussion

Our target wavefunctions correctly represent the main correlation corrections and the interaction between different Rydberg series and perturbers as indicated by excellent agreement between the calculated excitation energies and experimental values. Excitation energies of the 23 LS CI II target states relative to the ground state are presented in Table 1 where our calculated results are compared with the experimental values from the National Institute of Standard and Technology (NIST) (http://physics.nist.gov) and the calculations of Wilson & Bell (2002) and Berrington & Nakazaki (2002). Wilson & Bell (2002) calculated wavefunctions for the 12 LS CI II states and Berrington & Nakazaki (2002) used R-matrix method (Berrington et al. 1995) to obtain radiative data for a large number of CI II terms. Our calculation shows very good agreement with the calculation of Berrington & Nakazaki (2002) except for the assignments of the lowest $1\text{P}^0$ and third lowest $1\text{P}^0$ states. In our calculation these $1\text{P}^0$ states belong to the 3s3p$^3$ and 3s$^2$3p$^3(2D)^4$ configurations which agree with the NIST compilation. The labeling of these two states from the NIST compilation differ from the assignments in our calculation. Our calculation is in better agreement with the measured values for most states than the calculation of Wilson & Bell (2002). The 3s3p$^3 1\text{P}^0$ state in our calculation is slightly over correlated compared to the ground state.

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<th>BN</th>
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<td>1.5480</td>
<td>1.5718</td>
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$^a$ The labeling of these states from Berrington & Nakazaki (2002) are changed to match our assignments.

We chose a fine energy mesh (0.0002 Ryd) for collision strengths calculation in the thresholds energy region which allowed us to include resonance structures accurately. We calculated collision strengths at 8150 energy points in the thresholds region upto 1.60 Ryd and at 150 energy points in the above threshold region upto 16.6 Ryd. The collision strengths are displayed as a function of electron energy for the low-lying forbidden 3s$^2$3p$^4 3\text{P}^1–3s^23p^43\text{P}^2, 3s^23p^4 3\text{P}^1–3s^23p^4 3\text{D}^2$ and 3s$^23p^4 3\text{D}^2–3s^23p^4 3\text{S}^0$ transitions in Figs. 1–3 respectively in the thresholds energy region. Our results can be compared with 12-state R-matrix calculation of Wilson & Bell (2002) (not shown). Both calculations exhibit similar complicated resonance structure because of the interference and overlapping of several Rydberg series of resonances. Our calculation includes additional resonances converging to higher excited states above 1.15 Ryd because of the inclusion of additional 11 target states in the close-coupling expansion in our work that have thresholds between 1.172 Ryd and 1.598 Ryd. It is clear that these resonances converging to higher excited states make significant contributions. There seem to be some differences in the background collision strengths away from resonances from the two calculations. These differences can be clearly noted for
Fig. 1. Collision strength for the forbidden $3s^23p^4\,^3P_1-3s^23p^4\,^3P_2$ transition in Cl II as a function of electron energy (Ryd) in the thresholds energy region.

Fig. 2. Collision strength for the forbidden $3s^23p^4\,^3P_1-3s^23p^4\,^1D_2$ transition in Cl II as a function of electron energy (Ryd) in the thresholds energy region.
the $3s^23p^4\ ^1D_2\rightarrow3s^23p^3(^2D)4s\ ^4S_2$ transition shown in Fig. 3 of the present paper and Fig. 10 of their paper. The differences in background collision strengths are perhaps caused by the differences in the wavefunctions used in the two calculations.

We have plotted collision strengths as a function of electron energy in the above highest excitation threshold region from 1.6 Ryd to 16.6 Ryd in Fig. 4 for the allowed $3s^23p^4\ ^1D_2\rightarrow3s^23p^3(^2D)4s\ ^4D_2$ (solid curve), $3s^23p^4\ ^3P_1\rightarrow3s^23p^3(^4S)4s\ ^4S_2$ (long-dashed curve) and $3s^23p^4\ ^1D_2\rightarrow3s^23p^3(^2D)3d\ ^1P_1$ (short-dashed curve) transitions. The collision strengths in this energy region show smooth variation with energy. The collision strengths for allowed transitions show increasing trend with energy in the high energy region and depend on the oscillator strength of the transitions (Eq. (3)). It is clear from Fig. 4 that the $3s^23p^4\ ^1D_2\rightarrow3s^23p^3(^2D)4s\ ^4D_2$ transition is the strongest of the three allowed transitions.

The effective collision strengths are calculated by taking into account important resonance effects. These are obtained by integrating resonant collision strengths below the highest excitation threshold and smooth collision strengths above the highest threshold over a Maxwellian distribution of electron energies (Eq. (7)). In Table 2 we present effective collision strengths for all transitions between the $3s^23p^4\ ^3P_{0,1,2},\ ^1D_2$ and $^1S_0$ levels and from these levels to the 38 fine-structure levels of the excited configurations at electron temperatures from $\log T = 3.3$ to 6.0 K. The experimental wavelengths of transitions are also listed in Table 2. For many transitions the resonance effects in collision strengths enhance the effective collision strengths substantially in the lower temperature region. It may be noted that we presented effective collision
Fig. 5. Effective collision strength for the forbidden 3s\(^2\)3p\(^4\)\(^3\)P\(_0\)–
3s\(^2\)3p\(^4\)\(^3\)P\(_1\) transition in Cl II as a function of log \(T\) (K). Solid curve, present results; dashed-curve, Wilson & Bell.

Fig. 6. Effective collision strength for the forbidden 3s\(^2\)3p\(^4\)\(^3\)P\(_1\)–
3s\(^2\)3p\(^4\)\(^1\)D\(_2\) transition in Cl II as a function of log \(T\) (K). Solid curve, present results; dashed-curve, Wilson & Bell.

Fig. 7. Effective collision strength for the forbidden 3s\(^2\)3p\(^4\)\(^3\)P\(_1\)–
3s\(^2\)3p\(^4\)\(^1\)S\(_0\) transition in Cl II as a function of log \(T\) (K). Solid curve, present results; dashed-curve, Wilson & Bell.

Fig. 8. Effective collision strength for the forbidden 3s\(^2\)3p\(^4\)\(^1\)D\(_2\)–
3s\(^2\)3p\(^4\)\(^1\)S\(_0\) transition in Cl II as a function of log \(T\) (K). Solid curve, present results; dashed-curve, Wilson & Bell.

strengths for 43 fine-structure levels because the results for higher excitation levels (44–51) may not be accurate. The transitions involving these higher excitation levels are less accurate because of the neglect of coupling to levels that lie below and above. The main purpose of these levels in our calculation is to account for their strong coupling with lower levels.

Wilson & Bell (2002) presented effective collision strengths for 10 fine-structure transitions among the ground 3s\(^2\)3p\(^4\) configuration levels that can be compared with our results. Their results are normally larger than the present results, particularly at lower temperatures. Our results for the forbidden 3s\(^2\)3p\(^4\)\(^1\)D\(_2\) and 3s\(^2\)3p\(^4\)\(^1\)S\(_0\) transitions are compared with their results in Figs. 5–8 respectively. Our results are shown by solid curve, while the results of Wilson & Bell (2002) are shown by the dashed curve. Our results are lower than Wilson & Bell (2002) at log \(T\) \(\leq\) 5.0 for the 3s\(^2\)3p\(^4\)\(^1\)D\(_2\) and 3s\(^2\)3p\(^4\)\(^1\)S\(_0\) transitions by up to 12%. The effective collision strengths from our calculation for the 3s\(^2\)3p\(^4\)\(^1\)D\(_2\)–3s\(^2\)3p\(^4\)\(^1\)S\(_0\) transition between the two calculations do not account for the large difference.

4. Summary

We have presented elaborate calculations of collision strengths and effective collision strengths for transitions between the 3s\(^2\)3p\(^3\)\(^3\)P\(_{0,1,2}\), 3s\(^2\)3p\(^4\)\(^1\)D\(_2\) and 3s\(^2\)3p\(^4\)\(^1\)S\(_0\) levels and from these levels to 38 excited levels of Cl II. Our results are presented over a wide
electron temperature range suitable for use in astrophysical plasma modeling. In our work we used non-orthogonal orbitals both for the representation of target wavefunctions and for the representation of scattering functions. The use of non-orthogonal orbitals considerably simplifies the structure of the bound part of the close-coupling expansion, that leads to substantial reduction in pseudo-resonances. We used ICFT method to transform LS-coupled K-matrices to K-matrices in intermediate coupling. This method should lead to improved accuracy compared to standard transformation method used by Wilson & Bell (2002) to calculate level-to-level electron impact excitation collision strengths. Our calculation should also be accurate because of the inclusion of additional 11 excited states in the close-coupling expansion to ensure convergence of results for fine-structure transitions presented in our work. Significant differences with earlier calculation (Wilson & Bell 2002) are noted for some transitions which may have important consequences for astrophysical plasma diagnostics.

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