COMPUTER CODES

Emissivity: A Program for Atomic Transition Calculations[†]

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Abstract. In this article we report the release of a new program for calculating emissivity and other physical parameters in atomic transition processes. The program, which can be downloaded with its documentation and a sample of input and output files from `www.scienceware.net/id1.html`, passed various rigorous tests and was used alongside R-matrix and Autostructure codes to generate theoretical data and analyze observational data. It is particularly useful for investigating atomic transition lines in astronomical context as the program is capable of generating a huge amount of theoretical data and comparing it to observational line list. A number of atomic transition algorithms and analytical techniques are implemented within the program and can be very useful in various situations. The program can be described as fast and efficient. Moreover, it requires modest computational resources.

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1 Introduction

The importance of atomic transition calculations cannot be overestimated as many scientific and technological applications rely upon them. For example they are extremely vital for astrophysical investigation and astronomical modeling. In laboratory-based studies,

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[†]The computer program associated with this paper is available at the journal's homepage with the link `www.global-sci.com/code/v7-1118-c101.cpp`. It can be freely downloaded.
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they can be used to probe the conditions of laser induced plasmas and provide essential information required for analyzing fusion conditions. An important physical parameter in atomic transition processes is emissivity which is a measure of the power radiated by an emitting object. Various physical parameters and indicators associated with emissivity are usually computed during emissivity calculations.

There are two main methods for performing emissivity calculations. The first is by the use of a well-structured atomic database built for this purpose such as CHIANTI [1]. The other is by performing *ab initio* calculations by solving capture-decay equations based on user-prepared raw atomic data. Although the first method is more convenient, it cannot replace the other. One reason is the limitation of databases and the nature of their contents. These limitations include availability of particular data, quality of data, method of production, type of atomic target in atomic scattering calculations, coupling scheme under which the data was produced, and so on. In this article we present a computer code 'Emissivity' that performs emissivity calculations based on the second method. Despite the name 'Emissivity' which is attached to the program for historical reasons, the program can perform other atomic transition calculations, as well as emissivity, and hence it is useful in several situations where atomic database tools are of limited use.

2   Theoretical background

In a thermodynamic equilibrium situation an excited atomic state is populated by recombination and radiative cascade from higher states, and depopulated by autoionization and radiative decay to lower states. Many recombination lines arise from radiative decay and subsequent cascade of strongly autoionizing resonance states near the ionization limit. These lines are dominated by low temperature dielectronic recombination which is a two step process that involves the capture of a colliding continuum electron by an ion to form a doubly excited state. These excited autoionizing atomic systems give rise to resonances in the photoionization cross sections. The populations of such resonance states are determined by the balance between autoionization and radiative decay. When autoionization dominates, the populations are then given by the Saha equation for thermodynamic equilibrium

$$N_{X_{(n-1)+}} = N_e N_{X_{n+}} \frac{g_{X_{(n-1)+}}}{2g_{X_{n+}}} \left(\frac{h^2}{2\pi m_e k T_e} \right)^{3/2} e^{-\Delta E_t / k T_e}, \tag{2.1}$$

where ΔE_t is the energy of the recombined electron in the $X_{(n-1)+}$ state relative to the ionization threshold, and the other symbols have their usual meaning as given in Nomenclature Section 6.

The Saha equation, which describes the ratio of different stages of ionization, is based on the assumption of Local Thermodynamic Equilibrium (LTE) in a gas where collision dominates other physical processes. Consequently, the local velocity and energy distributions of particles are given by the Maxwell and Boltzmann distributions respectively

and a temperature can be defined locally. The Saha equation is therefore strictly applicable only if elastic collisions are responsible for establishing the energetic distribution of particles. In many practical cases, however, atomic processes such as radiative transitions or dynamic effects are more important than elastic collisions and the assumption of LTE is not justified within the whole energy range. In these cases explicit detailed equilibrium calculations are required to determine the velocity and energy distributions of particles over the various energy levels [2].

To measure the departure of the state from thermodynamic equilibrium a departure coefficient, b_u, is defined as the ratio of autoionization probability to the sum of radiative and autoionization probabilities. The value of this coefficient is between 0 for radiative domination and 1 for thermodynamic equilibrium. A large value of b_u ($\simeq 1$) is then required to justify the assumption of a thermodynamic equilibrium and apply the relevant physics.

In thermodynamic equilibrium the rate of radiationless capture equals the rate of autoionization, giving [3]

$$N_e N_i \varrho_c = N_u^S \Gamma_u^a,\tag{2.2}$$

where N_e and N_i are the number density of electrons and ions respectively, ϱ_c is the recombination coefficient for the capture process, N_u^S is the Saha population of the doubly-excited state and Γ_u^a is the autoionization transition probability of that state. In non thermodynamic equilibrium situation, the balance is given by

$$N_e N_i \varrho_c = N_u (\Gamma_u^a + \Gamma_u^r),\tag{2.3}$$

where N_u is the non thermodynamic equilibrium population of the doubly-excited state and Γ_u^r is the radiative transition probability of that state. The departure coefficient b_u is a measure of the departure from thermodynamic equilibrium, and hence is the ratio of the non thermodynamic equilibrium population to the Saha population. Comparing Eqs. (2.2) and (2.3) gives

$$b_u = \frac{N_u}{N_u^S} = \frac{\Gamma_u^a}{\Gamma_u^a + \Gamma_u^r}.\tag{2.4}$$

3   Program description

'Emissivity' is a computer code that was developed to implement an atomic transition model. Some technical details of 'Emissivity' are presented in Table 1. The main functionality of the code is to find the transition lines from electronic recombination and cascade decay all the way down to the ground or a metastable state (that is all free-free, free-bound and bound-bound transitions) and calculate their emissivity. Other functionalities include finding the decay routes and performing analysis and comparison between the generated theoretical transitions and an observational list of lines. The program was compiled successfully with no errors or warnings using several compilers on different

Table 1: Technical details of 'Emissivity' code.

Feature	Description
Title	Emissivity
Type	Command line
Language	C++
Methodology	Hybrid of procedural and object oriented
Number of Lines	About 3000 including test blocks
Platform	Any computer with standard C++ compiler
Memory required	Case-dependent ($\sim$ few tens of megabytes)
Speed of execution	Case-, compiler- and platform-dependent ($\sim$ few seconds)
Vectorized?	Yes
Parallelized?	No
Platforms tested	Linux (RedHat and Fedora 32- and 64-bit), Windows XP, and Cygwin on Windows XP
Compilers tested	g++ (Linux and Cygwin), Dev-C++ (Windows), and Visual Studio 6.0 (Windows)

platforms. Systematic checks were performed throughout all stages of writing and debugging 'Emissivity' code and producing the results. These checks include:

• Using code fragments, which are limited in size and complexity and hence are less susceptible to bugs, throughout the code development to test various functions for possible bugs or defects.

• The atomic model on which the code is based was partially implemented within spreadsheets and the results were compared to the code predictions. The results of these two different implementations were identical.

• Extensive and systematic manual calculations were carried out throughout all stages of writing and debugging the code to check the code results. These include some limiting cases where the results are known in advance.

• The results from different compilers and platforms were compared and found to be identical apart from trivial formatting issues.

• Two rigorous physical tests, presented in Section 3, to check the physical sensibility of the results were also implemented within the 'Emissivity' code and all emissivity calculations passed these tests.

The program reads from plain text input files and writes the results to a main plain text output file. Other secondary output files can also be produced for particular purposes when required. The necessary input files are:

• The main file to pass the parameters and inform the program of the required calculations. The main parameters in this file will be outlined in Section 4.1.

• A file for passing the free-states data and oscillator strengths (f-values) for free-free and free-bound transitions with photon energies. The free-states data include an index

identifying the resonance, its energy position, width, configuration, term, 2*J*, parity, and a flag marking the energy position data as experimental or theoretical.

• A file containing the bound-states data. These data include an index identifying the state, its energy, effective quantum number, configuration, term, and a flag marking the energy data as experimental or theoretical.

• A file containing the oscillator strengths for the bound-bound transitions.

The last file is imported from the **R**-matrix code output while the rest are user made. Two other input data files are also required if comparison and analysis of observational data are needed. One of these is a data file that contains astronomical observations while the other includes mapping information of observational lines to their theoretical counterparts. The astronomical data file contains data such as observed wavelength, observed flux before and after correcting for reddening and dust extinction, ionic identification, laboratory wavelength, multiplet number, lower and upper spectral terms of transition, and statistical weights of lower and upper levels. The user can put the astronomical data in the desired format as long as the number of entries in each line of data is observed, possibly by using void strings (e.g. 'XXX') to fill vacancies. The mapping file contains the indices of the observational lines and their theoretical counterparts.

In this section we summarize the theoretical background for the atomic transition model as implemented in the 'Emissivity' code:

• The program starts by obtaining the radiative transition probability Γ^r_{ul} for all free-free transitions as given by

$$\Gamma^r_{ul} = \frac{\alpha^3 E_p^2 g_l f_{ul}}{2 g_u \tau_o},\tag{3.1}$$

where the photon energy E_p is in Rydberg, and the other symbols are defined in Nomenclature Section6. This is followed by obtaining the radiative transition probability Γ^r_{ul} for all free-bound transitions, as in the case of free-free transitions.

• The total radiative transition probability Γ^r_u for all resonances is then found. This is the probability of radiative decay from an upper resonance state to all accessible lower resonances and bound states. This probability is found by summing up the individual probabilities Γ^r_{ul} over all lower free and bound states l for which a transition is possible according to the electric dipole rules; that is

$$\Gamma^r_u = \sum_l \Gamma^r_{ul}.\tag{3.2}$$

• The departure coefficient, b_u, for all resonances is then obtained

$$b_u = \frac{\Gamma^a_u}{\Gamma^a_u + \Gamma^r_u},\tag{3.3}$$

where Γ^a_u and Γ^r_u are the autoionization and radiative transition probabilities of state u, and Γ^a is given by

$$\Gamma^a = \frac{\Delta_r}{\hbar}.\tag{3.4}$$

• The next step is to calculate the population of resonances by summing up two components: the Saha capture, and the radiative decay from all upper levels. In thermodynamic equilibrium the rate of radiationless capture equals the rate of autoionization, giving

$$N_e N_i \varrho_c = N_l^S \Gamma_l^a, \tag{3.5}$$

where N_e and N_i are the number density of electrons and ions respectively, ϱ_c is the recombination coefficient for the capture process, N_l^S is the Saha population of the doubly-excited state and Γ_l^a is the autoionization transition probability of that state. In non thermodynamic equilibrium situation, the population and depopulation of the autoionizing state due to radiative decay from upper states and to lower states respectively should be included, and hence the balance is given by

$$N_e N_i \varrho_c + \sum_u N_u \Gamma_{ul}^r = N_l (\Gamma_l^a + \Gamma_l^r), \tag{3.6}$$

where N_l is the non thermodynamic equilibrium population of the doubly-excited state, Γ_l^r is the radiative transition probability of that state, Γ_{ul}^r is the radiative transition probability from an upper state u to the autoionizing state l, and the sum is over all upper states that can decay to the autoionizing state. Combining (3.5) and (3.6) yields

$$N_l^S \Gamma_l^a + \sum_u N_u \Gamma_{ul}^r = N_l (\Gamma_l^a + \Gamma_l^r). \tag{3.7}$$

On manipulating (3.7) the following relation can be obtained

$$
\begin{aligned}
N_l &= N_l^S \left(\frac{\Gamma_l^a}{\Gamma_l^a + \Gamma_l^r} \right) + \sum_u \frac{N_u \Gamma_{ul}^r}{\Gamma_l^r + \Gamma_l^a} \\
&= N_l^S b_l + \sum_u \frac{N_u \Gamma_{ul}^r}{\Gamma_l^r + \Gamma_l^a},
\end{aligned}
\tag{3.8}
$$

where b_l is the departure coefficient of the autoionizing state. This last relation is used in calculating the population.

• The next step is to calculate Γ_{ul}^r for the bound-bound transitions. In these calculations the f-values can be in length form or velocity form, though the length values are usually more reliable, and hence 'Emissivity' reads these values from the f-values file produced by the **R**-matrix code. This is followed by finding Γ_u^r for the bound states by summing up Γ_{ul}^r over all lower bound states l, as given earlier by (3.2) for the case of resonances.

• The population of the bound states is then obtained

$$N_l = \sum_u \frac{N_u \Gamma_{ul}^r}{\Gamma_l^r}, \tag{3.9}$$

where u includes all upper free and bound states.

• Finally, all possible free-free, free-bound and bound-bound transitions are found. The emissivity of all recombination lines that arise from a transition from an upper state u to a lower state l is then computed using the relation

$$\varepsilon_{ul} = N_u \Gamma_{ul}^r h\nu, \tag{3.10}$$

where ν is the frequency of the transition line.

• Apart from the normal debugging and testing of the program components to verify that they do what they are supposed to do, two physical tests are incorporated within the program to validate its functionality and confirm that no serious errors have occurred in processing and generating the data. These tests are the population-balance test and the metastable test. The first test relies on the fact that the population of each state should equal the depopulation. This balance is given by the relation

$$\sum_{j>i} N_j \Gamma_{ji}^r = N_i \sum_{k<i} \Gamma_{ik}^r. \tag{3.11}$$

The second test is based on the fact that the total number of electrons leaving the resonances in radiative decay should equal the total number arriving at the metastable states. This balance is given by the relation

$$\sum_{\forall j} N_j \Gamma_j^r = \sum_{\forall i, k>i} N_k \Gamma_{ki}^r, \tag{3.12}$$

where i is an index for metastable states and j is an index for resonances.

4 Input and output

The detailed technical description of the program input and output files is given in the program documentation which can be obtained from the 'Emissivity' web page. However, in this section we give a general description of the nature of the input parameters and the expected output data so that the user can decide if the program is relevant for the required purpose.

4.1 Input

Various physical and computational parameters are required for successful run. Some of these are optional and only required for obtaining particular data. The main input parameters are:

• The temperature in K and the number densities of electrons and ions in m^{-3}. The program uses a temperature vector to generate data for various temperatures. These values can be regularly or irregularly spaced.

- The residual charge of the ion, which is required for scaling some of the data obtained from the **R**-matrix code output files.

- Boolean flag for reading and processing observational astronomical data obtained from an external input data file. A mapping file is also required for this process. If the user chooses to read astronomical data, the data lines will be inserted between the theoretical lines in the main output file (i.e. 'Transitions') according to their observed wavelength. By inserting the observational lines where they belong, i.e. closest to their theoretical counterparts according to their wavelength, the observational lines can be easily identified according to their atomic designation (i.e. their upper and lower levels and so on).

- Boolean flag to run the aforementioned physical tests.

- Parameters for generating and writing normalization emissivity data for theoretical and observational lines to the main output file alongside the original emissivity data. The normalization can be internal using the emissivity of one of the transition lines produced by the program. It can also be with respect to an outside set of emissivity values corresponding to the input temperatures. Another possibility is to normalize with respect to an outside set of emissivity data in the form of effective recombination coefficients corresponding to the specified input temperatures. In this case the wavelength of the line to be normalized to is required. The effective recombination coefficient $\varrho_f(\lambda)$ is defined such that the emissivity $\varepsilon(\lambda)$ of a transition line with wavelength λ is

$$\varepsilon(\lambda) = N_e N_i \varrho_f(\lambda) \frac{hc}{\lambda}. \tag{4.1}$$

Another choice for normalization is to be with respect to an outside set of emissivity data in the form of effective recombination coefficients corresponding to a set of temperatures that may be different from those used in the input. In this case, the recombination coefficients corresponding to the input temperature values are obtained by interpolation or extrapolation using a polynomial interpolation routine.

- Parameters to control the production and writing of the effective recombination coefficients, ϱ_f, which are equivalent to the given emissivities. Vacuum wavelength of the transition lines will be used due to the restriction on the air wavelength formula ($\lambda \geq 2000$Å).

- Parameters to control the algorithm for minimizing the sum of least square deviations of emissivity between the observational lines and their theoretical counterparts over the input temperature range. This sum is given by

$$S = \sum_{\forall \text{lines}} \left(\varepsilon_o^N - \varepsilon_t^N \right)^2, \tag{4.2}$$

where ε_o^N and ε_t^N are the normalized observational and theoretical emissivities respectively. This algorithm also offers the possibility of computing the temperature confidence

interval and its relevant parameters. The individual square differences for each one of the least squares and their percentage difference which is given by

$$\left(\frac{\varepsilon_o^N - \varepsilon_t^N}{\varepsilon_o^N}\right) \times 100 \tag{4.3}$$

can also be written to the main output file. The confidence interval for the goodness-of-fit index χ^2 can also be found if required by providing the degrees of freedom η and the change in the goodness-of-fit index $\Delta\chi^2$. This algorithm is to be used for analyzing the theoretical transitions and comparing them to a list of observational lines, as will be clarified in Section 5. The parameters in this algorithm follow the general statistics convention.

• Parameters to run and control an algorithm for finding the decay routes to a particular state, bound or free, from all upper states. As the number of decay routes can be very large (millions and even billions) especially for the low bound states, a parameter is used to control the maximum number of detected routes. The results (number of decay routes and the routes themselves grouped in complete and non-complete) are written to an output file other than the main one. The states of each decay route are identified by their configuration, term and $2J$. For resonances, the Saha capture term and the radiative decay term are also given when relevant. These temperature-dependent data are given for a single temperature, that is the first value in the input temperature vector.

4.2 Output

The program produces a main output file which contains the essential emissivity data. The file starts with a number of text lines summarizing the input data used and the output results, followed by a few commentary lines explaining the symbols and units. This is followed by a number of data lines matching the number of transitions. The data for each transition include an index identifying the transition, status (FF, FB or BB transition), the experimental state of the energy data of the upper and lower levels, the attributes of the upper and lower levels (configuration, term, $2J$ and parity), wavelength in vacuum, wavelength in air for $\lambda \geq 2000$Å, the emissivities corresponding to the given temperatures, the normalized emissivities and the effective recombination coefficients corresponding to the given emissivities. Writing the normalized emissivities and the effective recombination coefficients is optional and can be turned off. As mentioned earlier, if the user chooses to read the astronomical data, the observational lines will be inserted between the theoretical lines in the main output file according to their lab wavelength.

There are other subsidiary output files. One of these is a file containing the results of the minimization algorithm. This file contains information on η, $\Delta\chi^2$, $\mathfrak{a}$, temperature at minimum χ^2, and the temperature limits for the confidence interval. This is followed by the temperature array with the corresponding least squares residuals, the $\mathfrak{a}\chi^2$ and the χ^2 arrays as functions of temperature. Another output file is one containing mapping data

used for testing purposes. A third output file is a decay routes file which was outlined previously.

5   Case study

In this section we outline a case study in which 'Emissivity' code was used to investigate the recombination lines in the spectra of planetary nebulae. The full details of this investigation are to be published elsewhere. Because the recombination rate is a function of electron temperature T_e and number density N_e, the observed variation of the lines intensity can be used in principle to determine the temperature and density of the line-emitting region. The study focuses on the recombination lines of C II, that is the emission lines produced by the following recombination process

$$C^{2+} + e^- \rightarrow C^+ \tag{5.1}$$

and the subsequent radiative cascade decay which continues until the atom reaches the ground or a metastable state. These lines are an important diagnostic tool that can provide valuable information on the physical conditions in various astrophysical environments such as planetary nebulae and interstellar medium.

In this investigation, two C III targets were prepared and used to generate theoretical atomic data. One of these targets contains 17 levels within 9 terms while the other contains 46 levels within 26 terms. For each one of these targets, 64 resonances and 142 bound states were theoretically found. All these levels were fully identified according to their atomic designation. On comparing these theoretical data to their experimental counterparts very good agreement in energy position and fine structure splitting was obtained. The main tools used in this theoretical investigation are the **R**-matrix suite [4, 5] which is an atomic scattering code based on the **R**-matrix formulation of the close coupling approximation, and Autostructure [5, 6] which is a general purpose automatic atomic structure code based on the Thomas-Fermi-Dirac formulation. All calculations were carried out in the intermediate coupling scheme and hence the results are generally more accurate and comprehensive than most of the previous analogous attempts which were performed in *LS*-coupling. The oscillator strengths, which are required for transition calculations, were obtained either directly or by integrating photoionization cross sections (FF directly from Autostructure, BB directly from **R**-matrix, and FB indirectly from **R**-matrix photoionization data).

The results of this theoretical investigation were then used to investigate and analyze the spectra of the planetary nebula NGC 7027. The main tool used in this analysis is the 'Emissivity' code which is the subject of this article. NGC 7027 is a compact, bright, young, high excitation planetary nebula with one of the hottest central stars known for a planetary nebula. Among the observed planetary nebulae, it has one of the richest lines emission which spans most parts of the electromagnetic spectrum and has been a challenge for observers as well as theoreticians. NGC 7027 is located about 0.9 kpc

from the sun in the direction of the constellation Cygnus in the Milky Way. It has been a reference object and the subject of several spectral surveys, and probably it is the best studied planetary nebula. There are several indications that the progenitor of NGC 7027 is a carbon-rich star [7,8].

The rich spectra of NGC 7027 was thoroughly examined by Zhang *et al.* [8]. The extensive line list presented in this study comprises over 1100 transition lines from many atoms and ions of various elements. This includes many recombination lines of carbon and its ions. Their list was used as the main source of observational data in our investigation. In total, 35 carbon lines were extracted from Zhang *et al.* [8] according to certain criteria and used in this investigation. These are the C II lines that come from transitions where at least one of the interacting states have an excited core and the lines are not blended with non-C II lines, although some may be blended with other C II lines. It is noteworthy that all these 35 observational lines were found and identified in our theoretical line list which is generated by 'Emissivity' code and contains 6187 optically-allowed (E1) transitions.

'Emissivity' was then used to minimize the departure of the normalized theoretical emissivities from their observational counterparts using a least-squares procedure where the temperature plays the role of a fitting parameter. The purpose of this procedure is to find the optimal temperature that gives the best fit of the theoretical model to the observational data, and hence identifying the temperature of the line-emitting regions in the nebula. The results of this investigation from both atomic targets indicate an electron temperature of about 10200-10500 K which is typical for line-emitting regions in planetary nebulae. Moreover, it agrees very well with some previous results obtained from He I recombination lines of this nebula (e.g., Peimbert and Peimbert [9]).

6   Nomenclature and notation

6.1   Notation

α	fine structure constant $(=e^2/(\hbar c 4\pi\epsilon_o) \simeq 7.2973525376\times 10^{-3})$
Γ^a	autoionization transition probability (s^{-1})
Γ^r	radiative transition probability (s^{-1})
Γ^r_{ul}	radiative transition probability from upper state u to lower state l (s^{-1})
$\Delta\chi^2$	change in goodness-of-fit index
Δ_r	width of resonance (J)
ΔE	energy difference (J)
ϵ_o	permittivity of vacuum $(\simeq 8.854187817\times 10^{-12}\mathrm{F.m}^{-1})$
ε	emissivity of transition line $(\mathrm{J.s}^{-1}.\mathrm{m}^{-3})$
ε_{ul}	emissivity of transition line from state u to state l $(\mathrm{J.s}^{-1}.\mathrm{m}^{-3})$
ε_o^N	normalized observational emissivity
ε_t^N	normalized theoretical emissivity
η	number of degrees of freedom

λ	wavelength (m)
ν	frequency (s^{-1})
ϱ_c	recombination coefficient for capture process ($m^3.s^{-1}$)
ϱ_f	effective recombination coefficient ($m^3.s^{-1}$)
τ_o	atomic time unit ($=\hbar/E_h \simeq 2.418884326505 \times 10^{-17}$s)
χ^2	goodness-of-fit index
$\mathfrak{a}$	scaling parameter in χ^2 confidence interval procedure
Å	angstrom
b_l (b_u)	departure coefficient of state l (state u)
c	speed of light in vacuum (299792458 $m.s^{-1}$)
e	elementary charge ($\simeq 1.602176487 \times 10^{-19}$C)
e^-	electron
E	energy (J)
E_h	Hartree energy ($\simeq 4.35974394 \times 10^{-18}$J)
E_p	photon energy (J)
f	oscillator strength
f_{ul}	oscillator strength of transition between upper state u and lower state l
g	statistical weight in coupling schemes ($=2J+1$ for IC)
h	Planck's constant ($\simeq 6.6260693 \times 10^{-34}$ J.s)
$\hbar$	reduced Planck's constant ($=h/2\pi \simeq 1.0545717 \times 10^{-34}$ J.s)
J	total angular momentum quantum number
k	Boltzmann's constant ($\simeq 1.3806505 \times 10^{-23}$ J.K^{-1})
L	total orbital angular momentum quantum number
m_e	mass of electron ($\simeq 9.10938215 \times 10^{-31}$kg)
N	number density (m^{-3})
N_e	number density of electrons (m^{-3})
N_i	number density of ions (m^{-3})
N^S	Saha population (m^{-3})
R	resonance matrix in **R**-matrix theory
S	total spin angular momentum quantum number
T_e	electron temperature (K)
X_{n+}	ion of effective positive charge n
$X_{(n-1)+}$	bound state of recombined ion with effective positive charge $n-1$

6.2 Abbreviations

BB	Bound-Bound (transition between bound states)
C	Coulomb
F	Faraday
FB	Free-Bound (transition between auto-ionizing and bound states)
FF	Free-Free (transition between auto-ionizing states)
IC	Intermediate Coupling
J	Joule
K	Kelvin
kg	kilogram

LTE	Local Thermodynamic Equilibrium
$(.)_l$	lower
m	meter
s	second
$(.)_u$	upper
$(.)_{ul}$	upper to lower
$\forall$	for all

Note: units, when relevant, are given in the SI system. Some symbols may rely on the context for unambiguous identification. The physical constants are obtained from the National Institute of Standards and Technology (NIST) website [10]. It should be remarked that most subscripts (e.g. l and u) are dummy variables, and hence they are subject in their interpretation to the context and are not specific to the particular cases they are referring to.

Acknowledgments

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