CHIANTI

An Astrophysical Database for Emission Line Spectroscopy

CHIANTI TECHNICAL REPORT No. 20

Level-resolved recombination and ionization rates

Version 1.0, 6 March 2019, Peter Young

1 Overview

This document describes how level-resolved ionization and recombination are included in the CHIANTI level balance solving routine (pop_solver). These processes were first included in CHIANTI 5 (Landi et al., 2006), and a major change occurred with CHIANTI 9 (Dere et al., 2019).

The data are only available for a small number of the total CHIANTI ions, and the coverage is given in Sect. 2.

Prior to the release of CHIANTI 9, the processes were included within the framework of the CHIANTI single ion model. The processes were not included directly in the level balance equations, but instead a "correction" was applied to the level populations. This method is described in Sect. 4. CHIANTI 9 has begun to replace this method with a new one whereby recombination rates (but not ionization rates) are directly incorporated into the level balance equations using new two-ion atomic models, and this is described in Sect. 3.

Unlike the electron and proton excitation data in CHIANTI, the ionization and recombination data are only defined over a specific temperature range (varying with the ion). Sect. 5 discusses how extrapolation is performed beyond this range.

2 Ion coverage

2.1 Recombination rates

As of CHIANTI 9, level-resolved recombination rates are only available for the H-like, He-like and Li-like isoelectronic sequences, and the ions Fe XVII–XXIII (Table 1). Note that coverage for the Li-like ions means that there is data for, e.g., O VII recombining to O VI, with the data stored in the O VI CHIANTI directory. Generally data are only available for the more abundant elements

Note that *either* a `reclvl` file *or* a `rrlvl` is available for an ion, but not both.

Table 1: Summary of ions for which level-resolved ionization or recombination data are available.

File type	Sequence	Ions
rrlvl	He	C, N, O, Ne, Mg, Al, Si, S, Ar, Ca, Fe, Ni, Zn
	Li	C, N, O, Ne, Mg, Al, Si, S, Ar, Ca, Fe, Ni, Zn
	Other	Fe XVIII, Fe XIX, Fe XX, Fe XXI, Fe XXII, Fe XXIII
reclvl	H	C, N, O, Na, Mg, Al, Si, S, Ar, Ca, Fe, Ni
	He	Na
	Other	Fe XVII
cilvl	Other	Fe XVII, Fe XVIII, Fe XIX, Fe XX, Fe XXI, Fe XXII

2.2 Ionization rates

These are only available for Fe XVII–XXII (Table 1). The data are taken from Gu (2003).

3 Direct radiative recombination rates (rrlvl files)

These are rates for the process of an electron being captured to produce a bound state of the recombining ion (i.e., radiative recombination). This serves as a population process for the bound state. The atomic data are mostly taken from Badnell (2006), and are stored in `.rrlvl` files. See CHIANTI Technical Report No. 24 for the format of these data files.

Unlike the earlier treatment of recombination (through the `reclvl` files), the rates are directly incorporated into the level balance equations by using a two-ion model. That is, the CHIANTI model for the recombining ion is added to the model for the recombined ion, thus allowing for the relative populations of the two ions to be correctly accounted for.

A feature of the software is that the `rrlvl` data are only included in the CHIANTI models if there also exists autoionization data for the ion.

For the 2-ion models, it is important that the relative ion populations obtained from the level balance calculations match those found in the ionization equilibrium file (`chianti.ioneq`). To do this, in addition to the level-resolved recombination rates, there must also be a ground-to-ground recombination rate. This rate is defined as the total radiative recombination rate (obtained with the routine `recomb_rate` with the `/radiative` keyword set) *minus* the sum of the individual level-resolved rates (this sum needs to omit the "1–1" transition from the `rrlvl` file).

For example, the CHIANTI 9 model of O VI has 923 levels and the O VII model has 49 levels. The 2-ion model has 972 levels, with the ground level of O VII becoming level 924. The level-resolved rates correspond to transitions from level 924 to the 63 bound levels of O VI. The rates from level 924 to levels 2–63 are summed, and then the rate from level 924 to 1 is defined as the total radiative recombination rate (from `recomb_rate`) minus this sum.

4 The population "correction" method (reclvl and cilvl files)

Unlike the method described in Sect. 3, this method is applied to the standard single ion CHIANTI models. The level-resolved ionization rates are stored in `.cilvl` files, and the recombination rates are stored in `.reclvl` files. The formats of these files are described in CHIANTI Technical Report No. 21.

The basic assumption is that the ion that receives population from ionization and recombination does not have any metastable levels. Only the ground level has significant population. In this scenario, the population of any excited level, i, is given by

$$n_i = \frac{\alpha_{\mathrm{in},i}}{\alpha_{\mathrm{out},i}} \tag{1}$$

where α is the total rate for all atomic processes that send population into or out of the level. To add a new atomic process, we can simply modify α to include these processes.

For recombination and ionization, only the "in" rates are affected and they become

$$\alpha^*_{\mathrm{in},i} = \alpha_{\mathrm{in},i} + N_{\mathrm{e}} R_i / f_0 \tag{2}$$

where f_0 is the fractional population of the ion of interest and R_i is the combined ionization and recombination rate into level i and is given by

$$R_j = f_- Q_j(T) + f_+ A_j(T) \tag{3}$$

where Q is the ionization rate, A is the recombination rate, and f_- and f_+ are the fractional populations of the ionizing and recombining ions, respectively.

The "corrected" level population is then

$$n^*_i = \xi n_i \tag{4}$$

where

$$\xi = 1 + \frac{N_{\mathrm{e}} R_i / f_0}{\alpha_{\mathrm{out},i}} \tag{5}$$

The CHIANTI routine that performs this correction is `correct_pops.pro`, which is called from `pop_solver.pro`.

For the ions for which this method is applied to (mostly the H-like sequence), the assumption that there are no metastable levels is correct up to densities of about 10^{13} cm^{-3}. This limit is rarely reached in hot coronal plasmas.

4.1 Zero ionization fractions

From Eq. 5 it can be seen that ξ is not defined if $f_0 = 0$. The software thus checks for temperatures where $f_0 = 0$ and sets all ionization and recombination rates to zero.

5 Extrapolation

The ionization and recombination rates are defined over particular temperature ranges in the data files. If the CHIANTI software requires rates outside of these ranges, then an extrapolation is required. The methods used for the different files are given below.

For **reclvl** files (recombination), extrapolation is performed by the IDL routine `ci_rec_interp`. The rates are set to zero *below* the temperature range. *Above* the temperature range a linear extrapolation of the two highest temperature points is performed. However, if the extrapolated point has a higher value than the rate at the highest temperature point, then it is set to this latter value (radiative recombination rates should decrease with temperature, so this should not happen).

For **rrlvl** files (recombination), extrapolation is performed within the IDL routine `ch_load_2ion_rates`. For temperatures below the data range, the rate is set to be the rate at the lowest temperature point of the range. For temperatures above the range, the rate is set to the rate at the highest temperature point of the range. [Author note: this over-estimates the rate. It is better to use a linear extrapolation.]

For **cilvl** files (ionization), extrapolation is performed by the IDL routine `ci_rec_interp`. The rates are set to zero *above* the temperature range. *Below* the temperature range a linear extrapolation of the two lowest temperature points is performed.

(Note that extrapolations are applied to the log values of the temperatures and rates.)

6 Unusual line ratio effects

The method for including level-resolved ionization rates leads to an unusual feature for some transitions. An example is shown in Fig. 1. The Fe XXI λ102.217/λ128.753 ratio rises abruptly below log $T = 6.2$ and falls again at log $T = 5.95$. Outside of this temperature range the ratio varies smoothly.

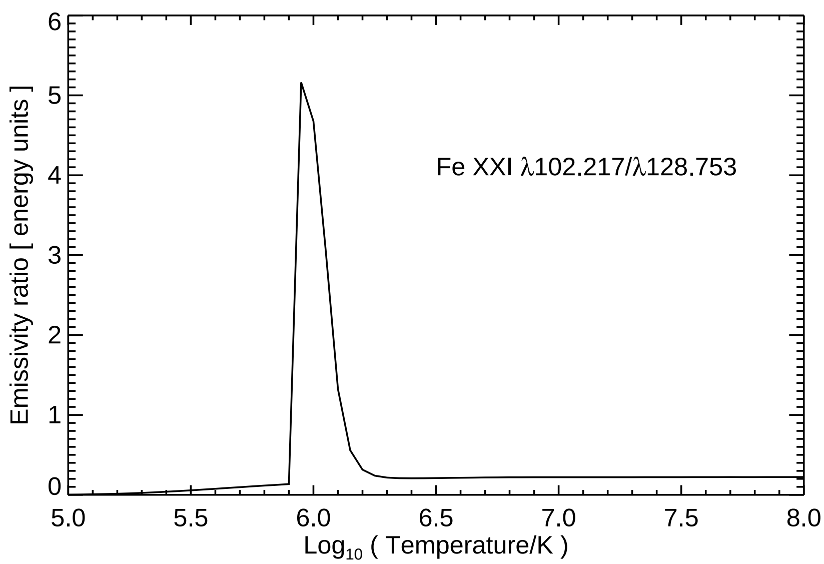

Figure 1: A ratio of emissivities for two Fe XXI lines. The prominent spike at log $T = 6.0$ arises because of the level-resolved ionization rates.

The cause of the spike lies in the ionization fractions for Fe XXI and Fe XX. From log $T = 6.20$ to 5.95, the ratio of Fe XX to Fe XXI varies from 10^5 to 2×10^9. At log $T = 5.90$ the ionization fraction of Fe XXI is zero. Thus for log $T \leq 5.90$ the level balance equations for Fe XXI are solved without any contribution from level-resolved ionization from Fe XX.

At log $T = 5.95$ the ionization rate coefficients into levels 7 and 13 (which give rise to λ128 and λ102, respectively) are 6–7 orders of magnitude smaller than the electron excitation rate coefficients. However, because the Fe XX ionization fraction is nine orders of magnitude larger than for Fe XXI, then the ionization rates dominate the electron excitation rates. The effect is greater for λ102 than for λ128, which is why the λ102/λ128 ratio rises abruptly. When the ionization fraction of Fe XXI falls to zero at log $T = 5.90$ then the ionization rates go to zero and we go back to an excitation-dominated regime, causing the λ102/λ128 ratio to fall abruptly.

Although the abrupt change in the ratio seems to suggest an error, this is not the case. It just reflects the cutoff in the tabulated ionization fraction values where, below a certain value, the fraction is set to zero. One should bear in mind that, although the spike in the line ratio plot is real, the ion fraction of the emitting ion is so low at these temperatures that the lines will be unobservable.

Note that this effect is due to the ionization rates and the treatment of these did not change in CHIANTI 9. In a later version it is expected to create 3-ion models that will allow ionization to be directly incorporated in the level balance equations, and this will get rid of these unusual ratio examples.

References

Badnell, N. R. 2006, ApJS, 167, 334

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A Document history

Version 1.0, 6-Mar-2019. First version created.