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# CHIANTI

An Astrophysical Database for Emission Line Spectroscopy

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CHIANTI TECHNICAL REPORT No. 30

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The ionization equilibrium file (ioneq)

A basic assumption of CHIANTI is that the plasma is in ionization equilibrium. The distribution of charge states with temperature is stored in a file that has the extension “ioneq”. This document describes the format of this file and how it is created.

## 1 Background

It has been standard in astrophysics to use tables of ionization fractions that have been computed in the coronal (or zero-density) approximation, such that there is no dependence of the ionization fractions on density or pressure. Early versions of CHIANTI made use of ion fraction tables from Arnaud & Rothenflug (1985), Arnaud & Raymond (1992), Mazzotta et al. (1998) and Bryans et al. (2006, 2009). Generally, the most recent of these files was set to be the CHIANTI default ioneq file (see Section 6).

Beginning with CHIANTI 6 (Dere et al., 2009), software and data were introduced that enabled an ioneq file to be directly computed from ionization and recombination rates stored in the database. The resulting ioneq file was named `chianti.ioneq` and was set to be the default file for the database. With subsequent versions updated ionization and/or recombination rates have been introduced, leading to changes to the `chianti.ioneq` file.

A further change was introduced in CHIANTI 10 (Del Zanna et al., 2021), whereby a modified ioneq file could be computed by including the density-dependent dielectronic recombination (DR) suppression process. The default `chianti.ioneq` remained the same, but the user had the option of computing a modified ioneq file based on a specified pressure or density.

CHIANTI 11 (Dufresne et al., 2024) introduced new advanced ion models for several isonuclear sequences, whereby the default behavior is to compute density or pressure-dependent ion fractions on-the-fly as part of synthetic spectrum calculations, for example. The coronal approximation ioneq file continues to be computed and made available as the “default” file (Section 6).

## 2 Computing the ionization balance

An ioneq file is created with the routine `ch_calc_ioneq`. The example below computes the file for a density of  $10^{10} \text{ cm}^{-3}$  and temperatures  $\log T = 4.0$  to  $\log T = 8.0$  in 0.05 dex intervals:

```
IDL> d=ch_calc_ioneq(temp,dens=1e10,outname='chianti_d10.ioneq')
```

The output `d` is a 3D array containing all of the ion fractions as a function of temperature. The `pressure` keyword is available for computing the ion fractions at a fixed pressure.

To compute the coronal approximation ion fraction file, the call is:

```
IDL> d=ch_calc_ioneq(temp,advanced_model=0,outname='chianti.ioneq')
```

This file is equivalent to the `chianti.ioneq` file distributed with versions of CHIANTI prior to version 11.

For more details about `ch_calc_ioneq` and the advanced ion models, see CHIANTI Technical Report No. 32.

### 3 Reading an ioneq file

An ioneq file is read with the routine `read_ioneq`, and an example call is:

```
IDL> read_ioneq, ioneq_file, log_temp, ioneq
```

where `log_temp` gives the temperature array at which the ion fractions are tabulated, and `ioneq` gives the ion fractions. The latter is a 3D array, where the first dimension is temperature, the second dimension is the element atomic number, and the third dimension is the ion number (0 corresponds to the neutral atom).

### 4 Format of the ioneq file

The ioneq file is an ASCII format file, and the first line (format: 2i3) contains two integers. The first gives the number of elements of the temperature array, and the second gives the number of elements.

The second line gives the logarithm of the temperature array in the format Nf6.2, where N is the number of temperatures.

The remaining data lines give the ion fractions for each ion of each element. For example, the first of these lines will be for `h_1`, the second will be `h_2`, the third will be `he_1`, etc. The format of each line is (2i3,Ne10.3), where N is the number of temperatures. The integers give the atomic number and the ion number, respectively, and the remaining numbers give the ion fractions.

The end of the data is marked by a line containing '-1', which is followed by comments, and then a final '-1'.

### 5 Calculating the ion fractions

The ion fractions are calculated from the ionization and recombination rates. CHIANTI only includes rates between neighboring ions, which makes the calculations relatively simple.

For a given element and temperature, the routine computes the ratio of the ionization rate to the recombination rate for each ion. For example, the ionization rate from `o_1` to `o_2`, and the recombination rate from `o_2` to `o_1`. The ion for which this ratio is closest to one is set as the reference ion and assigned a population of 1. The code then works up and down from this ion computing the population of each ion iteratively based on the ionization-to-recombination ratios. If the reference ion is denoted by  $i$ , then the populations of  $i - 1$  and  $i + 1$  ions are given by:

$$N_{i-1} = \frac{R_i}{I_{i-1}} \quad (1)$$

$$N_{i+1} = \frac{I_i}{R_{i+1}} \quad (2)$$

where  $I_i$  is the ionization rate from ion  $i$  to  $i + 1$  and  $R_i$  is the recombination rate from ion  $i$  to ion  $i - 1$ . The populations are then normalized such that  $\sum N_i = 1$ .

## 6 The default ioneq file (!ioneq\_file)

Prior to CHIANTI 11, there was a single ioneq file computed from the ionization and recombination rates in CHIANTI that represented the recommended ionization equilibrium dataset. This file was called `chianti.ioneq` and was placed in the directory `!xuvtop/ioneq`. The system variable `!ioneq_file` pointed to this file, and so it could be read with

```
IDL> read_ioneq, !ioneq_file, log_temp, ioneq
```

for example.

For CHIANTI 11, this file continues to be distributed and is assigned to `!ioneq_file`. It should be noted, however, that routines such as `ch_synthetic` and `ch_ss` no longer use this file, but instead calculate the ion fraction data using `ch_calc_ioneq` using the specified density or pressure.

## References

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- Mazzotta, P., Mazzitelli, G., Colafrancesco, S., & Vittorio, N. 1998, A&AS, 133, 403, doi: <http://doi.org/10.1051/aas:199833010.1051/aas:1998330>

## A Document history

*Ver. 2.0, 25-Nov-2024.* Major rewrite of document for CHIANTI 11.

*Ver. 1.0, 30-May-2023.* First version of document.

## B The `make_ioneq_all` file

Prior to CHIANTI 11, the `ioneq` file was created with the routine `make_ioneq_all`. The default, coronal approximation file was created with:

```
IDL> make_ioneq_all,outname='chianti.ioneq'
```

The ion fractions are tabulated for temperatures from  $\log T = 4.0$  to  $\log T = 9.0$  in 0.05 dex intervals. All ions of all elements up to and including zinc are printed.

If a user requires a file computed for a different temperature regime, they can use the `temp=` input.

Density or pressure-dependent `ioneq` files that show the effects of DR suppression can be created with the following calls:

```
IDL> make_ioneq_all,density=1e10,outname='chianti_d10.ioneq'
```

```
IDL> make_ioneq_all,pressure=1e15,outname='chianti_p15.ioneq'
```

Further details are given in CHIANTI Technical Report No. 17. Note that this approach has been superseded by the advanced ion models introduced in CHIANTI 11.

The DR suppression `ioneq` files can be reproduced by `ch_calc_ioneq` with the following call:

```
IDL> d=ch_calc_ioneq(temp,adv=0,density=1e10,outname='chianti_d10.ioneq',/dr_supp)
```

which switches off the advanced models but switches on DR suppression.