CHIANTI

An Astrophysical Database for Emission Line Spectroscopy

CHIANTI TECHNICAL REPORT No. 10

The CHIANTI radiative data files (wgfa)

Ver. 1.2, 22 February 2019, Peter Young
Ver. 1.1, 11 December 2017, Peter Young
Ver. 1.0, 14 Jul 2016, Peter Young

The CHIANTI wgfa file stores the radiative decay rates that, together with the electron collision strengths, are the two most critical data-sets for computing the level balance of an ion. The wgfa files are also used to store autoionization rates and two-photon transitions.

1 General information

In addition to the radiative decay rates, the wgfa file is used to store the two-photon transitions for hydrogen and helium-like ions. For helium-like ions this is the $1s^2\ ^1S_0 – 1s2s\ ^1S_0$ transition, and for hydrogen-like ions it is the $1s\ ^1S_{1/2} – 2s\ ^1S_{1/2}$ transition. The upper states decay by releasing two photons that combined have the energy of the transition. From an ensemble of particles the emission results in the two-photon continuum which is modeled using the CHIANTI two_photon.pro routine. However, it is also important to include the decay when computing the level populations of the ions, hence the decay rates are included in the wgfa file. Since the transitions are assigned a zero wavelength, then they do not give rise to an emission line and thus do not contribute to a synthetic spectrum (other than through the separately-computed two-photon continuum).

The wgfa file also stores autoionization rates for some ions. Atomic levels above the ionization threshold of an ion can decay to a bound state through radiative decay, but also by auto-ionizing, i.e., an electron is ejected giving a bound state of the next ionization state of the ion. The autoionization rates are represented as transitions to the ground state of the ion, and are assigned a zero wavelength since they do not give rise to any emission. Note that if an auto-ionizing state is able to radiatively decay to the ground state, then this transition will be represented twice in the wgfa file: one entry for the radiative decay, and one entry for the autoionization. The latter is distinguished through a zero value for the wavelength.

With CHIANTI 9 (released in 2019) the CHIANTI team have begun separating out the autoionization rates from the wgfa files into “auto” files (see CHIANTI Technical Report No. 8). This has been done for the lithium-like sequence, for example. There are no plans to remove the two-photon transitions from the wgfa files.

2 Computing the wavelengths

The wavelengths in the wgfa files are computed from the energy levels in the elvlc files (see CHIANTI Technical Report No. 1). The latter files contain two energy columns: one with observed energies, and the second with theoretical energies. Usually all levels will have a theoretical energy, but often only a fraction of the levels will have an observed energy.

If both levels for a transition have observed energies, then these are used to compute the wavelength. Similarly, if both levels only have theoretical energies, then these energies are used to compute the wavelength.

In the case where one level has an observed energy, but the other level only has a theoretical energy then the recommendation is to compute the wavelength with the two theoretical energies. Consider the example below of two levels from Ni XI (the elvlc entries are shown).

```
385     3s2 3p5 4d              3  D    1.0         -1.000    1650331.000
440     3s 3p6 4s               1  S    0.0    1629344.000    1688705.000
```

There is transition between these two levels, with an A-value of $9.17 \times 10^5\ s^{-1}$. There is a choice to use either the observed energy for level 440, or the theoretical energy. The wavelengths are 4764.9 Å with the observed energy and 2605.9 Å with the theoretical energy. Thus it is recommended that the 2605.9 wavelength goes into the wgfa file.

Why? Whereas the theoretical energy is generally not accurate (it’s 3.6% too high for level 440 above), the theoretical energy difference between levels 385 and 440 is probably quite accurate as the energy for level 385 is probably over-estimated by about 3.6% too. As you can see, the observed energy for level 440 is actually lower than the theoretical energy for 385, and it is highly unlikely that this is true in reality.

One exception is the case where a theoretical energy has been optimized in some way such that it is believed to very accurate. For example, if the level 385 energy above was believed to be accurate to, say, 0.01% then it is reasonable to derive the wavelength using the observed energy of level 440.

Irrespective of how the wavelength for transition 385-440 is derived, the wavelength should be given as a negative number in the wgfa file.

3 Data columns

There are five data columns and one free-format column, and each is described below. The format for the column is indicated by Fortran-style notation: *i7*, *a30*, etc.

The end of the data entries is marked by a line containing only '-1'. Comments are then entered in a free format, and the comments are terminated with a line containing only '-1'.

Column 1 – lower level index *i5*

This contains the level index of the energetically-lower level of the transition. The level indices are defined in the CHIANTI .elvlc file.

Column 2 – upper level index *i5*

The level index of the energetically-higher level of the transition. The level indices are defined in the CHIANTI .elvlc file.

Column 3 – wavelength *f15*

The wavelength of the transition in angstroms. A negative wavelength means that one or both of the levels do not have an experimental energy. A zero wavelength indicates that the transition is either a 2-photon transition (hydrogen or helium-like ions only), or that it is an autoionization rate. Generally wavelengths are given to three decimal places, with exceptions for very short and very long wavelength transitions. The CHIANTI data assessor will generally compute the wavelengths directly from the energy levels in the .elvlc file.

Column 4 – weighted oscillator strength *e15*

The weighted oscillator strength (often referred to as a *gf* value) is a dimensionless parameter. It is non-zero only for allowed transitions. The statistical weight is that of the lower level involved in the transition. The *gf*-values are typically given to three decimal places.

Column 5 – radiative decay rate *e15*

Generally this will be the radiative decay rate (or *A*-value) in units of s^{-1}. It can also be the autoionization rate or the two-photon decay rate, both in units of s^{-1}. The latter are identified by zero values for the wavelength. The *A*-values are typically given to three decimal places.

Column 6 – free format

After the data columns, there can be a free-format string giving the transition information for the transition. This is used to aid reading the file by eye, and the transition information is not read by the software.

Comments section

The comments section will be free format. It is recommended that, in addition to specifying the citation to a data source, the data assessor should also specify a DOI, or a URL to the ADS page for the paper. For example:

%collision strengths:
Mason, H.E., 1975, MNRAS, 170, 651

DOI: 10.1093/mnras/170.3.651
http://adsabs.harvard.edu/abs/1975MNRAS.170..651M

4 Reading the wgfa file

The main routine for reading the wgfa file is read_wgfa2.pro, which is called as:

IDL> read_wgfa2, filename, lvl1, lvl2, wvl, gf, a_value, wgfaref

where the outputs lvl1, lvl2, wvl, gf and a_value are each 1D arrays containing the five data columns from the file. Note that for those transitions that have both a radiative decay rate and an autoionization rate, then the transition will be represented twice in the output arrays. In preparation for input to the level population solving routine, the rates are summed within the routine setup_ion.pro. The output wgfaref is a string array containing the comment string at the bottom of the data-file.

There is also a routine that reads the wgfa file into a structure:

IDL> read_wgfa_str, filename, wgfastr, wgfaref

where the tags of the output are:

lvl1: column 1
lvl2: column 2
wvl: column 3
gf: column 4
aval: the radiative decay rates
auto: the autoionization rates and two-photon rates

Thus the radiative decay rates are separated from the autoionization and two-photon rates.

There is also a routine read_wgfa.pro, but this is now obsolete.

Appendix

1 Update history

Ver. 1.2, 22-Feb-2019: added Section 2 ("Computing the wavelengths"); added comment to Section 1 about CHIANTI 9; adjusted document format.

Ver. 1.1, 11-Dec-2017: now mentions significance of -1 in the file (Sect. 2); updated document header.