
CHIANTI

An Astrophysical Database for Emission Line Spectroscopy

CHIANTI TECHNICAL REPORT No. 13

The CHIANTI epsilon files (ups and scups)

Ver. 1.1, Peter Young, 5 March 2018

Ver. 1.0, Peter Young, 4 February 2017

This document describes the format for the CHIANTI ups and scups files, which contain the electron effective collision strength for an ion. Note that the ups files are not distributed with CHIANTI, but are used by the CHIANTI team to generate the scups files.

1 General information

Effective collision strengths are often referred to as “upsilons”. They are the collision strengths integrated over a Maxwellian electron distribution and so are a function of temperature. The upsilons from a published calculation are re-formatted into an ups file, and then this file is processed to create a scaled-upson (scups) file. See CHIANTI Technical Report No. 4 for more information about this process.

2 The ups file

For each transition in this file, there will be three lines of data. The format for each line is described below. An example of the data format is given below for the case of a transition with upsilons only defined at three temperatures.

1	2	5.000e-01	0.000e+00	-1	3
1.000e+05	1.000e+06	1.000e+07			
1.152e+00	1.273e+00	1.405e+00			

2.1 Format – line 1

Column 1 – lower level index *i7*

The CHIANTI level index for the lower level of the transition.

Column 2 – upper level index *i7*

The CHIANTI level index for the lower level of the transition.

Column 3 – transition energy *e12.3*

The energy (E) of the transition in Rydberg units.

Column 4 – weighted oscillator strength *e12.3*

The weighted oscillator strength (gf) for the transition (dimensionless).

Column 5 – high temperature limit point *e12.3*

The high temperature limit point for the transition. For allowed transitions, this takes the value $4*gf/E$ (E in Rydbergs). If the high temperature limit is not defined, then this value should be set to -1.

Column 6 – number of temperatures *i5*

The number of temperatures at which the upsilons are defined.

2.2 Format – line 2

This line contains the temperatures (units: K) at which the upsilons are defined. The number of columns is specified in column 6 of line 1, and the format of each column is “e12.3”.

2.3 Format – line 3

This line contains the upsilons (no units) defined at the temperatures given in line 2. The number of columns is specified in column 6 of line 1, and the format of each column is “e12.3”.

2.4 Format – comments

At the end of the file, unformatted comments can be added by having a single line containing only ‘-1’, followed by the comments. An additional ‘-1’ at the end of the file is optional. An example:

```
-1
File: mg_5.ups
File prepared by Peter Young on 31-Jul-2010
```

2.5 Reading the ups file

The UPS file is read into an IDL structure as follows:

```
IDL> read_ups, upsfile, upsstr
```

where the structure, UPSSTR, has tags called INFO and DATA. These are both structures, and tags for INFO are described in Table 1, and the tags for DATA are described in Table 2.

Table 1. Tags for the upsstr.info structure.

Tag	Data	Type
ION_NAME	Ion name (CHIANTI format)	String*1
ION_Z	Atomic number	Integer*1
ION_N	Spectroscopic number	Integer*1
ION_ROMAN	Ion name (Roman numerals)	String*1
ION_LATEX	Ion name (latex format)	String*1
ION_LATEX_ALT	Ion name (alternative latex format)	String*1
COMMENTS	File comments	String array
CHIANTI_VER	Chianti version number	String*1
TIME_STAMP	Time file was made	String*1
FILENAME	Filename (including path)	String*1
MISSING	Value for missing data	Float*1
NTRANS	Number of transitions	Long*1

Table 2. Tags for the upsstr.data structure.

Tag	Data	Type
LVL1	Lower level index	Integer*1
LVL2	Upper level index	Integer*1
DE	Energy	Float*1
GF	Oscillator strength	Float*1
LIM	High temperature limit	Float*1
NT	Number of temperatures	Integer*1
TEMP	Temperatures	Float*NT_MAX
UPS	Effective collision strengths	Float*NT_MAX

The size of the TEMP and UPS arrays will be set to the maximum number of temperatures (NT_MAX) in the data-set. If NT_MAX=40 and a particular transition only has upsilons defined for 20 temperatures, say, then TEMP[0:19] and UPS[0:19] will contain these values, and TEMP[20:39] and UPS[20:39] will be set to the ‘missing value’, i.e., UPSSTR.INFO.MISSING. The number of temperature points for a transition is given by the NT tag.

3 The scups file

This file contains the effective collision strengths that have been scaled using the Burgess & Tully method. In addition, the collision strengths at scaled temperatures of 0 and 1 are given.

The file format is similar to that for the ups file, with each transition represented by three lines of data.

3.1 Format – line 1

Column 1 – lower level index *i7*

The CHIANTI level index for the lower level of the transition.

Column 2 – upper level index *i7*

The CHIANTI level index for the lower level of the transition.

Column 3 – transition energy *e12.3*

The energy (E) of the transition in Rydberg units.

Column 4 – weighted oscillator strength *e12.3*

The weighted oscillator strength (gf) for the transition (dimensionless).

Column 5 – high temperature limit point *e12.3*

The high temperature limit point for the transition. For allowed transitions, this takes the value $4*gf/E$. If the high temperature limit is not defined, then this value should be set to -1. For the latter, it is recommended to use the format i12.

Column 6 – number of temperatures *i5*

The number of scaled temperatures at which the scaled upsilons are defined.

Column 7 – transition type *i5*

Each transition is categorized into one of several types. These types originate from the original Burgess & Tully (1992) paper but have been expanded since then (see Table 3). The type determines how the upsilons are scaled within the CHIANTI software.

Table 3. Transition types used in CHIANTI.

Type	Description
1	Allowed transitions (i.e., non-zero gf value)
2	Forbidden transition
3	Intercombination transition
4	Allowed transitions with a small gf value.
5	Dielectronic capture transitions (CHIANTI 3; Dere et al. 2001)
6	Log-scaling intended for proton transitions (CHIANTI 4; Young et al. 2003)

Column 8 – scaling parameter *e12.4* or *f12.5*

A single parameter determines how the scaled upsilons are distributed over the scaled temperature range. For allowed transitions, the scaling parameter has to be greater than 1, and for some transitions the value is so close to 1 that the 4th or 5th decimal places can be significant. For

this reason, it is better to use the f12.5 format. This is automatically handled by the WRITE_SCUPS routines (Technical Report No. 4).

3.2 Format – line 2

This line contains the scaled temperatures at which the scaled upsilons are defined. They take values between 0 and 1. The number of columns is specified in column 6 of line 1, and the format of each column is “e12.3”.

3.3 Format – line 3

This line contains the scaled upsilons defined at the temperatures given in line 2. The number of columns is specified in column 6 of line 1, and the format of each column is “e12.3”.

3.4 Format – comments

At the end of the file, unformatted comments can be added by having a single line containing only ‘-1’, followed by the comments, and then a final line containing ‘-1’. For example,

```
-1
File: mg_5.scups
File prepared by Peter Young on 31-Jul-2010
-1
```

3.5 Reading the SCUPS file

The SCUPS file is read into an IDL structure as follows:

```
IDL> read_scups, splfile, scupstr
```

where SCUPSTR has two tags called INFO and DATA that are both structures. The tags for SCUPSTR.INFO are described in Table 4, and the tags for SCUPSTR.DATA are described in Table 5.

Table 4. The tags for scupstr.info.

Tag	Data	Type
ION_NAME	Ion name (CHIANTI format)	String*1
ION_Z	Atomic number	Integer*1
ION_N	Spectroscopic number	Integer*1
ION_ROMAN	Ion name (Roman numerals)	String*1
ION_LATEX	Ion name (latex format)	String*1
ION_LATEX_ALT	Ion name (alternative latex format)	String*1
COMMENTS	File comments	String array
CHIANTI_VER	Chianti version number	String*1
TIME_STAMP	Time structure was created	String*1
FILENAME	Filename (including path)	String*1
MISSING	Value for missing data	Float*1
NTRANS	The number of transitions	Long64*1

Table 5. The tags for scupstr.data.

Tag	Data	Type
LVL1	Lower level index	Integer*1

LVL2	Upper level index	Integer*1
DE	Energy	Float*1
GF	Oscillator strength	Float*1
LIM	High temperature limit	Float*1
T TYPE	Transition type	Integer*1
C UPS	Scaling parameter	Float*1
NSPL	Number of temperatures	Integer*1
STEMP	Scaled temperature values	Float*NT_MAX
SPL	Spline node values	Float*NT_MAX

The size of the SCUPSTR.DATA.STEMP and SCUPSTR.DATA.SPL arrays is determined by the transition with the most number of data-points. For example, suppose one transition has 10 data points, and all other transitions have 8 data-points. NT_MAX will be 10 and so all transitions will have STEMP and SPL arrays of size 10. However, for the 8 data-point transitions, entries STEMP[8:9] and SPL[8:9] will be set to the missing value (SCUPSTR.INFO.MISSING). Note that for the latter transitions, SCUPSTR.DATA.NSPL will be set to 8

4 De-scaling upsilons

For most users, the best way to de-scale the data in the scups file is to use the routine SPL2UPS.PRO. For example:

```
IDL> ups=sp12ups('fe_13',[1,20],temp)
```

where TEMP is an array of temperatures at which the upilon values are required, and the atomic transition is given by [1,20] for the excitation from the level 1 to level 20.

A low-level routine for de-scaling upsilons used within the CHIANTI software is DESCALE_SCUPS.PRO, which is called as:

```
IDL> descale_scups, temp, scupstr, index, ups
```

where SCUPSTR is the scups structure, INDEX is a transition index with SCUPSTR, and UPS contains the upsilons at the temperatures TEMP.

Appendix

A. Document history

Version 1.1, 5-Mar-2018. Added Appendix; updated information on formats in Sect. 3.

B. Converting a SPLUPS file to a SCUPS file

Prior to CHIANTI 8 the electron excitation upsilons were stored in a SPLUPS file. To convert one of these files to a SCUPS file, the IDL call is:

```
IDL> convert_splups_to_scups, 'ionname.splups', 'ionname.scups'
```