CHIANTI

An Astrophysical Database for Emission Line Spectroscopy

CHIANTI TECHNICAL REPORT No. 33

Data Files for the Advanced Models (ions, models, dilvl, ealvl, rrcoeffs, drcoeffs, ctilvl, ctrlvl)

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1 Description of the file types

The advanced models require global data files, which contain the parameters needed throughout the calculation, and ionisation and recombination data files for each ion. The former are stored in the <code>!xuvtop/advanced_models/ancillary_data</code> directory. Although the following description of the new files gives the length of each datum, in the current implementation of the CHIANTI routines only the radiative and dielectronic recombination fitting coefficient files are read as a fixed format.

1.1 Global data files

1.1.1 List of ions included in the advanced models

This file is called advmodel_list.ions and is similar to the masterlist.ions file. It is read by the routine 'ch_read_list_ions'.

Table 1: The format of the data in the energy files					
Col.	Format	ID	Comment		
1	a6	ION	Ion name		
2	i5	NLEV	Number of included levels		

Table 1: The format of the data in the energy files

Each column in the files has:

- 1. The name of the ion in CHIANTI format included in the advanced models, format=a6.
- 2. The number of levels to be included when calculating level populations for the overall ionisation and recombination rates, format=i5.

The file contains columns with a fixed number of characters, and the data entries are terminated by a line containing only a -1. All subsequent lines are considered to be comments.

1.1.2 Model atmosphere data for charge transfer rates

Model atmosphere parameters from various works which are required to calculate charge transfer rates are provided for the convenience of the user. They have filenames ending in .dat, e.g. fontenla_facula.dat and can be found in the !xuvtop/advanced_models/model_atmospheres subdirectory. The data come from the calculations of Avrett & Loeser (2008) and Fontenla et al. (2014). The latter has multiple files derived from their models of different regions, and their model numbers denoting the regions are found in the comments section of each file.

Each column in the file has:

1. The temperature in K, format=e9.3

Table 2: The format of the data in the model atmosphere DAT files

Col.	Format	ID	Comment
1	e9.3	TEMP	Temperature (in K)
2	e12.3	NELEC	Electron number density (in cm^{-3})
3	e12.3	HEIGHT	Height (in km)
4	e12.3	PRESS	Pressure (in K cm ⁻³)
5	e12.3	NHYD	Total hydrogen number density (in cm ⁻³)
6	e12.3	NH1	Ionisation fraction of neutral hydrogen
7	e12.3	NHE1	Ionisation fraction of neutral helium
8	e12.3	NHE2	Ionisation fraction of singly ionised helium

- 2. The electron number density in cm^{-3} , format=e12.3.
- 3. Height through the atmosphere in km as defined in the model atmosphere calculation, format=e12.3. The definition of zero height differs between works and the original works should be referred to for this value.
- 4. Pressure in K $\rm cm^{-3}$ derived from the product of temperature and electron density, format=e12.3.
- 5. Total hydrogen number density in cm⁻³, format=e12.3.
- 6. Population of neutral hydrogen as a fraction of the total hydrogen number density, format=e12.3.
- Optional column of population of neutral helium as a fraction of the total helium number density, format=e12.3.
- 8. Optional column of population of singly-ionised helium as a fraction of the total helium number density, format=e12.3.

The file contains columns with a fixed number of characters, and the data entries are terminated by a line containing only a -1. All subsequent lines are considered to be comments. The files are read directly with the routine 'ch_read_atmos', which is called by 'ch_adv_model_setup' when setting up the advanced models. The structure returned by 'ch_read_atmos' can also be input to 'ch_adv_model_setup' using the 'atmos_params' structure instead of giving the atmosphere file.

1.2 Ion-specific data files

Four new data files have been created for level-resolved ionisation and recombination rate coefficients. Two are for electron impact ionization and two are for charge transfer. The files are found in the usual ion-specific subdirectories, e.g. !xuvtop/c/c_2.

1.2.1 Level-resolved electron impact ionisation

There are two filetypes with different suffixes but which contain the same data layouts. The first type is c_2.dilvl, which is used for level-resolved direct electron impact ionisation. The second type is c_2.ealvl, which contains level-resolved indirect electron impact ionisation, also known as excitation—auto-ionisation. Both file types are read by 'ch_ioniz_rate_lr'. These files differ from the '.diparams' and '.easplups' used for ground level ionisation, in that the level-resolved files contain rate coefficients tabulated for a specific temperature range, while the ground level files tabulate parameters for a scaled, Burgess-Tully type domain (see Dere, 2007, for more details).

Col.	Format	ID	Comment
	1 0111100		
	e11.3	TEMP	Temperatures (in K) (1st line)
1	i5	L1	Initial level of transition
2	i5	L2	Final level of transition
3	e11.3	IP	Energy of transition (in eV)
4	e11.3	RATE	Rate coefficient for each temperature given in the first line (in $\text{cm}^3 \text{ s}^{-1}$)

Table 3: The format of the data in the DILVL and EALVL files

Each file contains in the first line a list of temperatures in K at which the rate coefficients are tabulated. Each column of the remaining lines in the file has:

- 1. The initial level of the ion before ionisation takes place, format=i5. The index corresponds to the level in the c_2.elvlc file.
- 2. The final level of the ion after ionisation takes place, format=i5. The index corresponds to the level in the c_3.elvlc file.
- 3. The energy input in eV required for the transition to take place, format=e11.3.
- 4. The rate coefficients for the transition in cm³ s⁻¹, format=e11.3. They are given for each of the temperatures listed in the first line of the file.
- 5. The remainder of the line may have further comments giving details of the initial and final levels, but they are not read by the software.

The file contains columns with a fixed number of characters, and the data entries are terminated by a line containing only a -1. All subsequent lines are considered to be comments.

1.2.2 Level-resolved recombination fitting coefficients

These files are used to reconstruct the total recombination rate coefficients for ground and metastable levels using the formulæ provided by N.R. Badnell. These data are provided as part of the Atomic Processes for Astrophysical Plasma (APAP) Network, at http://apap-network.org/DATA_AS/DR/ and http://apap-network.org/DATA_AS/RR/. The same coefficients for the ground level, used for the coronal approximation modelling, are found in the ion-specific .rrparams and .drparams files.

For an electron temperature T (in K) the radiative recombination (RR) rate coefficients are reconstructed using the formula

$$\alpha_{RR}(T) = A \left\{ \left(\frac{T}{T_0} \right)^{\frac{1}{2}} \left[1 + \left(\frac{T}{T_0} \right)^{\frac{1}{2}} \right]^{1-B} \left[1 + \left(\frac{T}{T_1} \right)^{\frac{1}{2}} \right]^{1+B} \right\}^{-1} . \tag{1}$$

In some cases, such as for low charge ions, B is replaced by $B+C\exp\left(\frac{-T_2}{T}\right)$. The former type, which just uses coefficient B, is designated a Type 1 formula, while the latter case is designated a Type 2 case. The various coefficients in the formulæ above are provided in the fitting coefficients files in the ion-specific sub-directories and use the suffix .rrcoeffs. The files are read by the existing 'ch_rad_recomb' routine, but the keyword 'level_resolved' should be used to read them. A Type 3 case is used for some other sources of data, although they are not used for the APAP data. Details of this last case can be found in the technical report for the .rrparams files.

Table 4: The format of the data in the RRCOEFF	Table	4. The	format	of the	data i	in the	RRCOEFFS	file
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Type	Col.	Format	ID	Comment
				(First line)
All	1	i5	Z	Atomic number
	2	i5	ION	Spectroscopic number
	3	i5	NMETA	Number of levels in ion for which there is data
				(Remaining lines)
All	1	i5	LVL	Level index
	2	i5	2J+1	Statistical weight of level
	3	i5	TYPE	Data type used for fitting formula
Type 1	4	e11.3	A	Fitting coefficient A
	5	f10.5	В	Fitting coefficient B
	6	e12.4	T0	Fitting coefficient T_0
	7	e12.4	T1	Fitting coefficient T_1
Type 2	4	e12.4	A	Fitting coefficient A
	5	f10.5	В	Fitting coefficient B
	6	e11.4	T0	Fitting coefficient T_0
	7	e11.4	T1	Fitting coefficient T_1
	8	f10.5	\mathbf{C}	Fitting coefficient C
	9	e12.4	T2	Fitting coefficient T_2

The first line in the file has:

- 1. The atomic number of the element, format=i5.
- 2. The spectroscopic number of the ion before recombination, format=i5.
- 3. The number of energy levels for which fitting coefficients are provided, format=i5.

 The remaining lines in the file give recombination data for individual energy levels and contain:

- 4. The index of the initial level in the ion before recombination, format=i5. The indices correspond to the initial levels in the CHIANTI energy level files. In a few cases, these differ from the level indexing in the original level-resolved recombination data file provided by the APAP Network website given above.
- 5. Statistical weight of the initial level, format=i5.
- 6. The type of fitting formula used, format=i5.
- 7. The remaining columns give the fitting coefficients in the order they appear in the formula for RR. The formats for each of these coefficients varies; see the above table for exact details.

The dielectronic recombination (DR) fitting coefficients are reconstructed using the formula

$$\alpha_{DR}(T) = T^{-\frac{3}{2}} \sum_{i} C_i \exp\left(-\frac{E_i}{T}\right) . \tag{2}$$

The various coefficients in the formulæ above are provided in the fitting coefficients files in the ion-specific sub-directories and use the suffix .drcoeffs. The files are read by the existing 'ch_diel_recomb' routine, but the keyword 'level_resolved' should be used to read them. The APAP Network data in these files are represented by one type to date, that designated Type 1 data.

Table 5: The format of the data in the DRCOEFFS file					
Type	Col.	Format	ID	Comment	
				(First line)	
All	1	i5	Z	Atomic number	
	2	i5	ION	Spectroscopic number	
	3	i5	NMETA	Number of levels in ion for which there is data	
				(Remaining pairs of lines)	
All	1	i5	LVL	Level index	
	2	i5	2J+1	Statistical weight of level	
	3	i5	TYPE	Data type used for fitting formula	
Type 1	4-12	e12.4	Ei	Fitting coefficients E_i	
All	1	i5	LVL	Level index	
	2	i5	2J+1	Statistical weight of level	
	3	i5	TYPE	Data type used for fitting formula	
Type 1	4-12	e12.4	Ci	Fitting coefficients C_i	

Each column in the DRCOEFFS files has:

- 1. The atomic number of the element, format=i5.
- 2. The spectroscopic number of the ion before recombination, format=i5.

- 3. The number of energy levels for which fitting coefficients are provided, format=i5.

 For the remainder of the file, there is a pair of lines for each energy level and these contain:
- 4. The level index of the initial level in the ion before recombination, format=i5. The indices correspond to the initial levels in the CHIANTI energy level files. In a few cases, these differ from the level indexing in the original level-resolved recombination data file provided by the APAP Network website given above.
- 5. Statistical weight of the initial level, format=i5.
- 6. The type of fitting formula used, format=i5.
- 7. The remaining columns give in the first line of the pair the fitting coefficients E_i , while the second line of the pair gives the fitting coefficients C_i , format=e12.4.

1.2.3 Level-resolved charge transfer

There are two filetypes with different suffixes but which contain the same data layouts. The first type is c_1.ctilvl, which is used for level-resolved charge transfer ionisation. The second type is c_2.ctrlvl, which contains level-resolved charge transfer recombination. Both file types are read by 'ch_ioniz_rate_lr'.

Col.	Format	ID	Comment
	e11.3	TEMP	Temperatures (in K) (1st line)
1	i5	L1	Initial level of transition
2	i5	L2	Final level of transition
3	i5	PZ	Atomic number of perturber
4	i5	PELEC	Number of electrons in perturber
5	e11.3	IP	Energy of transition (in eV)
6	e11.3	RATE	Rate coefficient for each temperature given in the first line (in cm ³ s ⁻¹)

Table 6: The format of the data in the CTILVL files

Each file contains in the first line a list of temperatures in K at which the rate coefficients are tabulated. Each column of the remaining lines in the file has:

- 1. The initial level of the ion before ionisation takes place, format=i5. The index corresponds to the level in the c_1.elvlc file.
- 2. The final level of the ion after ionisation takes place, format=i5. The index corresponds to the level in the c_2.elvlc file.
- 3. The atomic number of the perturber involved in the transition, format=i5.
- 4. The number of electrons in the perturber before the transition takes place, format=i5.

- 5. The energy input in eV required for the transition to take place, format=e11.3. A negative energy means that there is an energy release during the transition.
- 6. The rate coefficients for the transition in cm³ s⁻¹, format=e11.3. They are given for each of the temperatures listed in the first line of the file.
- 7. The remainder of the line may have further comments giving details of the initial and final levels, but they are not read by the software.

The file contains columns with a fixed number of characters, and the data entries are terminated by a line containing only a -1. All subsequent lines are considered to be comments.

Col. Format ID Comment e11.3**TEMP** Temperatures (in K) (1st line) L1Initial level of transition 1 i52 i5L2Final level of transition 3 PZAtomic number of perturber i5 4 i5PELEC Number of electrons in perturber

Rate coefficient for each temperature given in the first line (in cm³ s⁻¹)

Table 7: The format of the data in the CTRLVL files

Each file contains in the first line a list of temperatures in K at which the rate coefficients are tabulated. Each column of the remaining lines in the file has:

- 1. The initial level of the ion before recombination takes place, format=i5. The index corresponds to the level in the c_2.elvlc file.
- 2. The final level of the ion after recombination takes place, format=i5. The index corresponds to the level in the c_1.elvlc file.
- 3. The atomic number of the perturber involved in the transition, format=i5.

Energy of transition (in eV)

5

6

e11.3

e11.3

IP

RATE

- 4. The number of electrons in the perturber before the transition takes place, format=i5.
- 5. The energy release in eV that occurs during the transition, format=e11.3. A negative energy means that an input of energy is required for the transition to take place.
- 6. The rate coefficients for the transition in cm³ s⁻¹, format=e11.3. They are given for each of the temperatures listed in the first line of the file.
- 7. The remainder of the line may have further comments giving details of the initial and final levels, but they are not read by the software.

The file contains columns with a fixed number of characters, and the data entries are terminated by a line containing only a -1. All subsequent lines are considered to be comments.

References

Avrett, E. H., & Loeser, R. 2008, ApJS, 175, 229

Dere, K. P. 2007, A&A, 466, 771

Fontenla, J. M., Landi, E., Snow, M., & Woods, T. 2014, Sol. Phys., 289, 515

A Document history

Ver.~1.1,~11-Aug-2025. Updates were made to Sect. 1.1.2 in order to mention the 'ch_read_atmos' routine.

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