

KAPPA GUIDE

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Introduction

Analysis of the non-Maxwellian effects in the observed optically thin line spectra presents a new research direction in the spectroscopy of the solar corona and transition region. Non-Maxwellian distributions in the solar corona and transition region can originate as a result of the strong gradient in density or temperature, due to plasma heating by reconnection during the solar flares or micro-flares, due to presence of some types of waves, or due to other physical processes such as turbulence.

The shape of a non-Maxwellian distribution function strongly influences the character of the emitted optically thin spectra. This occurs through the changes in rates, and in stationary conditions to ionization and excitation equilibria. The interpretation of spectra under the assumption of non-Maxwellian distribution usually leads to different diagnosed plasma parameters than those for Maxwellian one, especially for temperature. Therefore, the assumption of Maxwellian distribution of particles can lead to mis-interpretation of physical conditions in the observed plasma.

1. What is KAPPA package?

KAPPA package is a software and database allowing us to calculate line intensities and synthetic spectra for electron non-thermal distributions with high energy tail approximated by a κ -distribution. It is based on the CHIANTI software and database for spectral analysis under the assumption of Maxwellian distribution. KAPPA package uses and needs many CHIANTI routines and also its database. Therefore, it cannot be used as a stand-alone software.

2. Kappa-distributions

In-situ measurements of a distribution function in the solar wind plasma showed the presence of high-energy tail in the distribution. The origin of such distribution, in non-homogenous plasma, is related to the increase of the mean free path of particles with high energy. These particles are then able to penetrate without collisions to regions with different densities and temperatures and thus they produce high-energy tail.

The distributions with high-energy tail can be described by a κ -distribution:

$$f(E)dE = A_{\kappa} \frac{2}{\pi^{1/2}(k_B T)^{3/2}} \frac{E^{1/2}dE}{\left(1 + \frac{E}{(\kappa-1.5)k_B T}\right)^{\kappa+1}}, \quad (1)$$

where E is the particle energy, k_B Boltzmann constant, κ parameter of distribution, and A_{κ} is the normalization constant, $A_{\kappa} = \Gamma(\kappa + 1)/(\Gamma(\kappa - 1.5)(\kappa - 1.5)^{3/2})$. Temperature T in the κ -distribution has the same relation to the mean energy of particles as Maxwellian distribution:

$$\langle E \rangle = 3k_B T/2 \quad (2)$$

and parameter κ models the shape of the distribution. $\kappa \rightarrow 1.5$ is limit for strongly non-Maxwellian distribution, and for $\kappa \rightarrow \infty$ limit, the κ -distribution approaches Maxwellian. For the constant mean energy but different value of parameter κ , the number of high-energy particles increases when κ decreases, the number of the low energy particles increases too and maximum of distribution moves to lower energies ($E_{\max} = k_B T (\kappa - 1.5) / \kappa$), and (Figure 1). More details about kappa-distributions can be found e.g. in Livadiotis & McComas (2013).

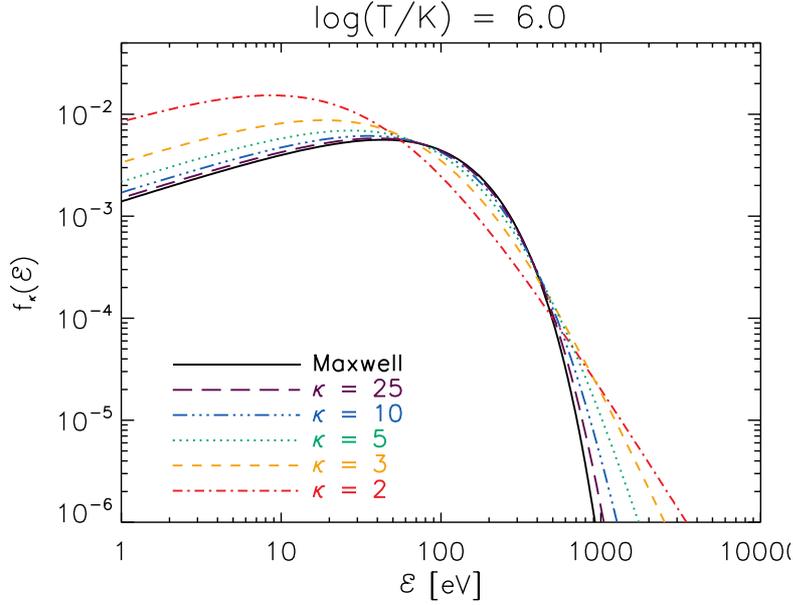


Figure 1. Comparison of the Maxwellian distribution with the κ -distributions for different $\kappa = 25, 10, 5, 3$ and 2 , and the same mean energy of particles corresponding to $T = 10^6$ K.

2.1. Ionization equilibrium

In the coronal conditions, the ionization equilibrium is given by equilibrium between total ionizing processes (direct ionization and autoionization) on one hand and, total recombination processes (radiative and dielectronic recombination) on the other hand:

$$n_k C_k^I = n_{k+1} C_{k+1}^R, \quad (3)$$

where n_k (n_{k+1}) is density of k -times ($k+1$ -times) ionized ions, C_k^I is the total ionization rate of k -times ionized ions and C_{k+1}^R is the total recombination rate of $k+1$ -times ionized atoms. The rates of the elementary processes are defined by:

$$C = \langle \sigma v \rangle = \int_0^\infty \sigma \frac{2E^{1/2}}{m} f(E) dE, \quad (4)$$

where σ is collisional cross section, v is the particle velocity, m particle mass, $f(E)$ is the particle distribution function.

The presence of the κ -distribution strongly affects the ionization rates. The effect depends on temperature, ion, and value of κ . Increase of the ionization rate by several orders of magnitude can occur at temperatures several times lower than temperature corresponding to the abundance maximum of given ion for the Maxwellian distribution. This results from the presence of the high-energy tail that increases the number of the high-energy electrons that are able to produce ionizing

transitions. The radiative recombination rates are less influenced. An increase of the recombination rate by a factor 2 for κ -distribution with $\kappa = 2$ compared to Maxwellian is typical. Collisional cross sections for this process decrease with electron energy, but the κ -distribution contains more low-energy electrons than the Maxwellian distribution with the same temperature (Figure 1). Therefore, the radiative recombination rates for the κ -distributions are higher. The changes in the dielectronic recombination rates are influenced by the shape of distribution, their peaks are wider and lower for κ -distributions (Dzifčáková and Dudík, 2013, for details).

The ionization equilibria for κ -distributions show wider peaks of ion abundance. This means that the individual ions can exist in wider temperature ranges with relatively high abundances compared to the Maxwellian distribution. The maxima of these abundance peaks can also be shifted. The shift of peaks to the lower temperatures is very significant in the transition region, where it can be more than a half of order in temperature for $\kappa = 2$. To the contrary, in the solar corona at temperatures above 10^6 K, small shift to lower temperatures can be seen, typically for smaller deviation from the Maxwell distribution, or to higher temperatures, typically for higher deviation from the Maxwell distribution and high temperatures.

The latest version III of KAPPA contains density dependent ionization equilibria (density suppressed dielectronic recombination). Double ionization is also included. Note the density suppression of dielectronic recombination is only one of the effects changing intensities of transition-region lines, and its inclusion is not a substitute for generalized collisional-radiative modelling. User discretion is advised.

2.2. Excitation equilibrium

For temperatures and electron densities corresponding to the transition region, corona and solar flares, the excitation and de-excitation processes are dominated by electron collisional excitation and radiative de-excitation transitions. The statistical excitation equilibrium in this approximation is described by the equation:

$$n_i(\sum_j n_e C_{ij,j \neq i} + A_{ij,j > i}) = \sum_j n_j(n_e C_{ji,j \neq i} + A_{ji,j > i}), \quad (5)$$

where n_e is the electron density, n_i and n_j are the populations of levels i , and j , C_{ij} and C_{ji} are the electron excitation and de-excitation rates between the levels i and j , and A_{ij} , A_{ji} are Einstein coefficients for the spontaneous radiation. For transitions in optical or near UV region, it is necessarily to include photoexcitation. Its probability is proportional to $B_{ij} \bar{I}_{\nu_{ij}}$, where B_{ij} is Einstein absorption coefficient and $\bar{I}_{\nu_{ij}}$ is the mean intensity of radiation with frequency corresponding to the energy E_{ij} of the transition between the levels i and j .

The electron distribution influences the electron collisional excitation and de-excitation rates (Equation 3). In solar spectroscopy, collision strengths $\Omega_{ij}(E_i) = \Omega_{ji}(E_j)$ instead of the collisional cross sections are usually used:

$$\sigma_{ij} = \frac{\Omega_{ij}}{\omega_i E_i} \pi a_0^2, \quad (6)$$

where E_i (E_j) is the initial (final) electron energy before (after) the collision, ω_i is statistical weight of level i , and a_0 is the Bohr radius.

The electron excitation and de-excitation rates for κ -distributions can be written using distribution-averaged collisional strengths for excitation, $Y_{ij}(T, \kappa)$, and de-excitation, $Y_{ji}(T, \kappa)$ (e.g. Dzifčáková et al., 2015, Dudík et al., 2014):

$$C_{ij} = \frac{2\sqrt{2}a_0^2 I_H}{\sqrt{m_e \omega_i}} \left(\frac{\pi}{k_B T}\right)^{1/2} e^{-\frac{E_{ij}}{k_B T}} \Upsilon_{ij}(T, \kappa) \quad (7)$$

and

$$C_{ji} = \frac{2\sqrt{2}a_0^2 I_H}{\sqrt{m_e \omega_j}} \left(\frac{\pi}{k_B T}\right)^{1/2} \Upsilon_{ji}(T, \kappa) \quad (8)$$

where

$$\Upsilon_{ij} = A_\kappa \frac{E_{ij}}{k_B T} e^{\frac{E_{ij}}{k_B T}} \int_{E_{ij}}^{\infty} \frac{\Omega_{ij}(E_i)}{\left(1 + \frac{E_i}{(\kappa-1.5)k_B T}\right)^{\kappa+1}} \frac{dE_i}{E_{ij}} \quad (9)$$

and

$$\Upsilon_{ji} = A_\kappa \frac{E_{ij}}{k_B T} \int_0^{\infty} \frac{\Omega_{ji}(E_j)}{\left(1 + \frac{E_j}{(\kappa-1.5)k_B T}\right)^{\kappa+1}} \frac{dE_j}{E_{ij}}. \quad (10)$$

The calculations of excitation rates for the non-Maxwellian distribution is usually problematic (with several exceptions) due to unavailability of the cross sections or collision strengths data. Moreover, these data files are usually huge, having sizes of several tens of GiB. Therefore, only the integral products of the cross sections over the Maxwellian distribution, i.e. the electron excitation rates, are usually published. This is the case in CHIANTI (Dere et al. 1997, Landi et al. 2013, Del Zanna et al. 2015). Consequently, Dzifčáková (2006a), Dzifčáková (2008), and Dzifčáková et al. (2015) developed the unique inversion method which enables to approximate the collision strengths by an analytical function. The method employs the typical limit behaviour of the collision strengths for different types of atomic transitions.

A functional form for the approximation of Ω is assumed

$$\Omega = \sum_{n=0}^{n_{max}} C_n u^{-n} + D \ln(u) \quad (11)$$

where C_n and D are coefficients and $u = E_i/E_{ij}$. The Ω averaged over Maxwellian distribution, $\Upsilon_{ij}(T)$, is

$$\Upsilon_{ij} = \frac{E_{ij}}{k_B T} e^{\frac{E_{ij}}{k_B T}} \int_{E_{ij}}^{\infty} \Omega_{ij}(E_i) e^{-\frac{E_i}{k_B T}} \frac{dE_i}{E_{ij}}. \quad (12)$$

After the integration we have

$$\Upsilon_{ij} = C_0 + \left(\sum_{n=1}^{n_{max}} \frac{E_{ij}}{k_B T} C_n E_n \left(\frac{E_{ij}}{k_B T}\right) + D E_1 \left(\frac{E_{ij}}{k_B T}\right) \right) e^{\left(\frac{E_{ij}}{k_B T}\right)}. \quad (13)$$

where E_n is an n -the order exponential integral. The high-energy limit of Ω and corresponding behaviour of $\Upsilon_{ij}(T)$ provide conditions for the coefficients C_n and D . For electric dipole transitions we have

$$D = \frac{4\omega_{ifij}}{E_{ij}}, \quad \Upsilon_{ij}(\rightarrow \infty) = \sum_{n=0}^{n_{max}} C_n = \Omega(u = 1), \quad (14)$$

for non-electric dipole, non-exchange transitions

$$D = 0, \quad Y_{ij}(\rightarrow 0) = C_0, \quad Y_{ij}(\rightarrow \infty) = \sum_{n=0}^{n_{max}} C_n = \Omega(u = 1), \quad (15)$$

and for the exchange transitions

$$C_0 = C_1 = D = 0, \quad Y_{ij}(\rightarrow 0) = \frac{E_{ij}}{k_B T} \int_1^\infty \Omega du, \quad Y_{ij}(\rightarrow \infty) = \sum_{n=2}^{n_{max}} C_n = \Omega(u = 1). \quad (16)$$

The low-temperature and high-temperature limits of $Y_{ij}(T)$ can be found in the CHIANTI database. The coefficients C_n and D were evaluated from the Maxwellian collisional strengths in CHIANTI by the least square method. The approximations up to $n_{max} = 7$ were used to achieve the higher precision.

The method was tested for the first time by Dzifčáková and Mason (2008) and subsequently more extensively by Dzifčáková et al. (2015). The comparison of the excitation rates calculated using the approximations with direct calculations of collision strengths showed that in most cases the precision is better than a few percents. Bigger differences appear with decreasing κ , and for $\kappa = 2$, the extreme differences do not exceed 10% which is comparable with typical precision of atomic data themselves.

The presence of the κ -distributions in plasma changes the excitation rates. The character of changes depends on the type of the atomic transition, its excitation energy, temperature and parameter κ (Dzifčáková and Kulinová, 2003, Dzifčáková, 2006, Dzifčáková et al., 2015). Typically, the excitation rate increases for low temperatures. This increase can be several orders of magnitude for $\kappa = 2$ in comparison with the Maxwellian case. However, for temperatures $k_B T \geq E_{ij}$ (Dzifčáková, 2006a), the excitation rates for the κ -distributions are lower than for Maxwellian distribution. The differences increase with decreasing κ .

For known excitation rates, the equations of the statistical equilibrium (Equation 5) can be solved for non-Maxwellian distributions and the intensity of the spectral lines can be calculated in the usual way as an integral along line of sight l :

$$I_{ij} = \frac{hc}{4\pi\lambda_{ij}} A_{j \rightarrow i} \int n_{j,X}^k dl = \frac{hc}{4\pi\lambda_{ij}} A_{j \rightarrow i} \int \frac{n_{j,X}^k n_X^k n_X n_H}{n_X^k n_X n_H n_e} n_e dl, \quad (17)$$

where $n_{j,X}^k$ is density of k -times ionized ions of element X in level j , n_X^k is the density of all k -times ionized ions of element X , n_X is the density of all ions of element X , and n_H is the Hydrogen density. The distribution function affects the line intensity through the ratio of the relative population of level j given by the excitation equilibrium as well as the ratio n_X^k/n_X (abundance of k -times ionized ions of element X) given by the ionization equilibrium for the equilibrium plasma.

2.3. Satellite lines

The rate of dielectronic excitation from level i to level j for a distribution function $f(E)$ can be written (Seely et al., 1987)

$$C^{diel} = \left(\frac{2}{m_e \Delta E_{ji}} \right)^{1/2} \frac{h^3 \omega_j}{16\pi m_e \omega_i} f(\Delta E_{ji}) A_a, \quad (18)$$

where ω_j and ω_i are statistical weights of double excited state and lower level and A_a is the autoionization (Auger) rate. The transition occurs at discrete energy ΔE_{ji} which corresponds to the energy difference between states. For the Maxwellian distribution, this equation leads to the well-known expression (Phillips et al., 2008)

$$C^{diel} = \frac{h^3}{2(2\pi m_e k_B T)^{3/2}} \frac{\omega_j}{\omega_i} e^{-\frac{\Delta E_{ji}}{k_B T}} A_a . \quad (19)$$

Similarly, for κ -distributions we can write

$$C_{\kappa}^{diel} = \frac{A_{\kappa} h^3}{2(2\pi m_e k_B T)^{3/2}} \frac{\omega_j}{\omega_i} \frac{A_a}{\left(1 + \frac{\Delta E_{ji}}{(\kappa-1.5)k_B T}\right)^{\kappa+1}} , \quad (20)$$

leading to the expression used in KAPPA package (Dzifčáková et al., 2015):

$$C_{\kappa}^{diel} = C_{Maxw}^{diel} \frac{A_{\kappa} e^{\frac{\Delta E_{ji}}{k_B T}}}{\left(1 + \frac{\Delta E_{ji}}{(\kappa-1.5)k_B T}\right)^{\kappa+1}} . \quad (21)$$

2.4. Recombination and ionization from excited levels

Power-law dependence on energy for the cross-section of the radiative recombination σ_{RR} from the excited levels is assumed (Osterbrock, 1974)

$$\sigma_{RR} = \frac{C_{RR}}{E^{\eta+0.5}} , \quad (22)$$

where C_{RR} is a constant and $\eta + 0.5$ is a power law index. Subsequently, for the radiative recombination rate of κ -distributions R_{RR}^{κ} it is possible to write (Dzifčáková et al., 2013)

$$R_{RR}^{\kappa} = R_{RR}^{Maxw} \frac{\Gamma(\kappa+\eta-0.5)(1.5-\eta)^{\eta}}{\Gamma(\kappa-0.5)} , \quad (23)$$

where R_{RR}^{Maxw} is Maxwellian radiative recombination rate.

The ionization rates from the excited levels are also included in CHIANTI 9. The approximations of κ -distributions by a sum of Maxwellians by Hahn and Savin (2012) were used

$$f_{\kappa}(E, T) = \sum_0^n a_n \times f_{Maxw}(E, c_n \times T), \quad (24)$$

where a_n and c_n are constants tabulated by Hahn and Savin (2012). The direct ionization rate of κ -distributed electrons from excited levels, $R_{DI}^{\kappa}(T)$, is

$$R_{DI}^{\kappa}(T) = \sum_0^{n_{max}} a_n \times R_{DI}^{Maxw}(c_n \times T), \quad (25)$$

where $R_{DI}^{Maxw}(T)$ is Maxwellian averaged direct ionization rate.

These rates are included in the calculation of the excitation equilibrium by the same way as in CHIANTI 9.

CHIANTI 9 contains also joint ionization and recombination rates with included cascade effects for some ions. These rates cannot be separated from cascade effects and recalculated for κ -distributions, therefore, only Maxwellian rates are available for these ions.

2.5. Continuum

Besides of the calculations of the spectral line intensities, the KAPPA package also allows for calculation of non-Maxwellian continua (Dzifčáková et al., 2015). Dudík et al (2012) calculated continuum for the κ -distributions. They considered contributions from free-free and free-bound continuum only. The contribution from two-photon continuum can be neglected (Phillips et al. 2008).

Total emissivity of free-free continuum due to electron-ion bremsstrahlung for κ -distributions can be expressed (Dudík et al., 2012)

$$\epsilon_{ff}(\lambda, \kappa, T) = \frac{A_\kappa T^{1/2}}{\lambda^2} n_e n_H \sum_Z K_Z(\kappa, T) A_Z \int_0^\infty \frac{g_{ff}(y, w)}{\left(1 + \frac{y+w}{\kappa-1.5}\right)^{\kappa+1}} dy, \quad [\text{ergs cm}^{-3} \text{ s}^{-1} \text{ sr}^{-1} \text{ \AA}^{-1}] \quad (26)$$

where A_Z is the element abundance relative to hydrogen, $w = hc/\lambda k_B T$ is scaled photon energy, g_{ff} is free-free Gaunt factor, and

$$K_Z(\kappa, T) = \frac{1}{4\pi} \frac{32\pi}{3} \frac{e^6}{m_e c^2} \sqrt{\frac{2\pi k_B}{3m_e}} \sum_k k^2 \frac{n_k}{n_Z} \quad (27)$$

where k is the ionization degree. The bremsstrahlung spectrum is strongly enhanced for low values of kappa mainly at short wavelengths (Dudík et al., 2012, Figs. 2 and 3) in the comparison with the Maxwellian distributions.

The emissivity of free-bound continuum originated by recombination of κ -distributed electrons which forms k -times ionized ions of element X with excited electron on the level j can be expressed (Dudík et al., 2012)

$$\epsilon_{fb}(\lambda, \kappa, T) = \frac{1}{4\pi} \sqrt{\frac{2}{\pi}} \frac{\epsilon}{(m_e k_B T)^{3/2}} n_e n_H \sum_{k,X} \frac{n_{k+1}}{n_k} A_X \frac{\omega_j}{\omega_0} \sigma_j^{bf} A_\kappa \frac{1}{\left(1 + \frac{\epsilon - I_j}{(\kappa-1.5)k_B T}\right)^{\kappa+1}}, \quad (28)$$

where $\epsilon = hc/\lambda = E + I_j$ is the photon energy, I_j is the ionization potential from the level j with statistical weight ω_j , and σ_j^{bf} is the ionization cross section from level j .

Free-bound spectra for the κ -distributions showed greatly enhanced ionization edges (Dudík et al., 2012, Fig. 5). This is mainly the result of the increase of low energy electrons for the κ -distributions comparing with the Maxwellian ones with the same temperature.

2.6. Effects and diagnostics

To demonstrate the effect of κ -distribution to a synthetic spectrum, in Figure 2 we depict synthetic spectrum calculated for the extreme non-thermal distribution, $\kappa = 2$ (red), and for the

Maxwell distribution (black). For both spectra the constant electron density $N_e = 10^9 \text{ cm}^{-3}$ was adopted, and the line ratio of Fe XI 180.40 Å / Fe XII 195.12 Å was chosen to be equal. Thus it can be seen that κ -distribution enhances line intensities of some allowed lines and the diagnosed T is higher than for the Maxwell distribution.

The sets of synthetic spectra calculated under the assumption of κ -distribution allow for construction of diagnostic models. Picking up specific line ratios one can diagnose plasma parameters as κ , T, electron density and DEM under the assumption on non-thermal κ -distribution. The κ -distribution has significant influence on the diagnosed T. The diagnosed electron densities are typically lower than Maxwellian ones, for $\kappa = 2$ by about 0.1 dex in the log.

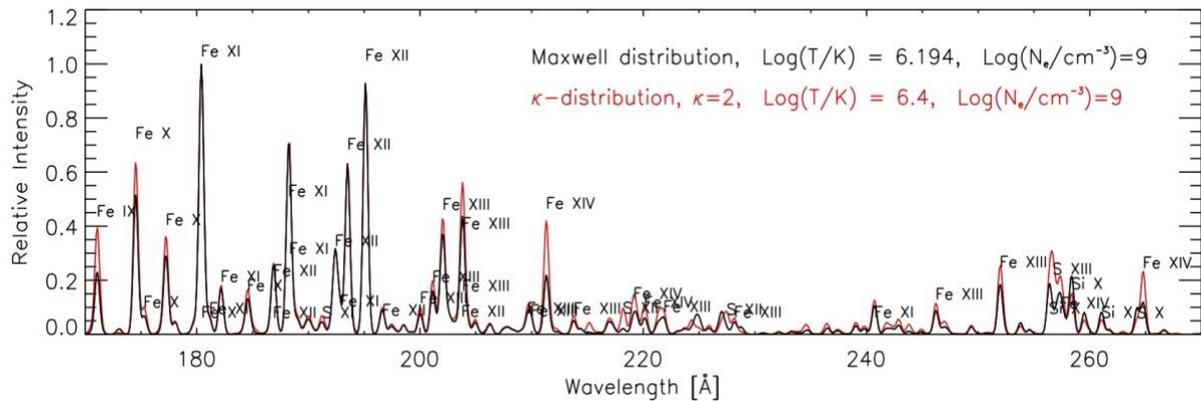


Figure 2. Example of the synthetic spectrum calculated by KAPPA for the Maxwellian distribution (black line) and kappa-distribution with $\kappa = 2$ (red line). The line ratio of Fe XI 180.40 Å / Fe XII 195.12 Å is chosen to be the same in both spectra.

Generally, successful diagnostics of κ -distribution requires high precision of the observed line intensities. This requires good photon statistics as well as high precision of spectrometer calibration.

3. KAPPA Package

The KAPPA database and software is based on CHIANTI, the freely available atomic database and software (Dere et al. 1997; Landi et al. 2013, Dere et al., 2019,). Similarly as CHIANTI, it works under Interactive Data Language (IDL). KAPPA software uses many modified CHIANTI routines and CHIANTI two ions model to calculate an excitation equilibrium.

The software and database of KAPPA package allows to calculate the synthetic spectra for integer values of $\kappa = 1.7, 1.8, 1.9, 2, 2.5, 3, 4, 5, 7, 10, 15, 25,$ and 33. These values of kappa allow for sufficient approximation to cover the observed cases. Ionization equilibria for these values of kappa are tabulated and included in database of the package.

The KAPPA package has its own, separate folders, where all routines and the database are located. It cannot be installed within the directory of CHIANTI itself in order to prevent its automatic removal by CHIANTI updates. The path to the folder can be set by an IDL system variable in the IDL startup.pro file:

```
defsysv, '!data_pth', 'path to package' .
```

The KAPPA folder contains original and the modified CHIANTI routines to calculate spectra for the κ -distributions, with the 'data9_k' subfolder having the same structure as the CHIANTI's 'dbase' subfolder.

In the past, the first versions of KAPPA package corresponding to CHIANTI 5.2 (Dzifčáková 2006b) contained directly the coefficients for the approximation of Ω . In this case, the calculation of the spectrum for the κ -distributions was approximately ten times longer compared with that of CHIANTI using the Maxwellian distribution. Therefore, following the second version (corresponding to CHIANTI 7, Dzifčáková et al., 2015), $Y_{ij}(T, \kappa)$'s were pre-calculated for a grid temperatures and κ and included into its database.

The KAPPA database contains ionization, recombination, excitation, deexcitation rates, and ionization equilibria for κ -distributions.

3.1. Database

Database of KAPPA package is located in 'data10' subfolder. It has the same structure as "dbase" subfolder in CHIANTI, e.g. for C we have directory 'c/'. Each element has its own directory.

A series of ancillary data are contained in additional directories of 'data9_k' subfolder:

```
'masterlist/' - the list of the ions currently present in the database (a copy from the CHIANTI
                database 9.0),
'abundance/'  - elemental abundance files (a copy from the CHIANTI database 9.0),
'continuum/'  - contains files for the continuum calculations (a copy from the CHIANTI
                database 9.0),
'dem/'        - DEM files (a copy from the CHIANTI database 9.0),
'ioneq/'      - ionization fraction files for kappa-distributions,
'ip/'         - ionization potentials (a copy from the CHIANTI database 9.0).
```

The 'ioneq/' directory contains ionization equilibria with names such as 'Dz23_logn10_kappa_2.ioneq' where the number following 'logn' is logarithm of the electron density (in this case 10). Zero density ionization equilibria are named 'logn0'. The 'kappa_2' in the name means the ionization equilibrium for kappa=2. Values of kappa=1.7, 1.8, 1.9, and 2.5 are denoted 'kappa_1p7', 'kappa_1p8', 'kappa_1p9', and 'kappa_2p5'.

Element directories contain subdirectory for each ion. For example, in 'c/' directory we have subdirectories e.g. for C I - C VII we have subdirectories 'c_1/' - 'c_7/'. The filename for each ion follows spectroscopic notation.

The subdirectories for ions within the database contain data for the ionization and recombination rates for the κ -distributions together with tabulated $Y_{ij}(T, \kappa)$ and $Y_{ji}(T, \kappa)$ files in the ASCII format and as well as IDL save files with the extension '.sav'. Files have their names according to the ion and the κ with extension '.ups' for $Y_{ij}(T, \kappa)$ and '.dwns' for $Y_{ji}(T, \kappa)$, e.g., 'fe_10_k2.ups' for $Y_{ij}(T, \kappa)$ of Fe X and $\kappa=2$. Current version of KAPPA package fully corresponds to the atomic data contained in the CHIANTI database version 9.0.

The ion atomic data taken from CHIANTI database 9.0 have a name corresponding to ion's name (e.g. 'c_4') and filename extension:

- ' .elvlc' - Level labelling, energy (a copy from the CHIANTI database 9.0),
- ' .wgfa' - wave lengths, Einstein probabilities for spontaneous emission, oscillator strengths (a copy from the CHIANTI database 9.0),
- ' .fb1vl1' - Data for the free-bound calculations (a copy from the CHIANTI database 9.0),
- ' .auto' - autoionization rates (a copy from the CHIANTI database 9.0)

Those depending on kappa have suffix '_k' plus value of kappa (e.g. 'c_6_k2' means C VI data for the kappa-distribution with kappa=2). They have filename extensions

- ' .ups' - scaled upsilons
- ' .dwns' - downsilons
- ' .sav' - upsilons + downsilons in IDL save file
- ' .tionr' - total ionization rates
- ' .trechr' - total recombination rates
- ' .rr1vl1' - level resolved radiative recombination rates
- ' .cilvl1' - level resolved ionization rates

3.2. Software

KAPPA can be run mainly on Macs and on PCs with Linux. KAPPA is not standalone and needs CHIANTI software and database. KAPPA directory contains all KAPPA routines. To preclude incompatibility problems with CHIANTI software due to its upgrade CHIANTI, the most important CHIANTI 9.3.1 routines are also located in the KAPPA directory and their names have suffix '_m' before the extension (e.g. 'ch_synthetic_m'). Some of them have been also slightly modified.

All the IDL routines have documentation in their extensive headers giving detailed descriptions and examples.

The main widget-type routine 'kappa' is based on the CHIANTI routine 'ch_ss' and has the same widgets. It allows to select the type of calculation by the selection of the ionization equilibrium file. The ion-equilibrium file name (extension '.ioneq') with 'kappa_' plus the κ value (e.g. 'kappa_02.ioneq') selects calculation for the κ -distribution with $\kappa=2$. The selection of the ion equilibrium file without this syntax runs Maxwellian calculations. Outputs from 'kappa' can be in form of ASCII arrays or structures compatible with CHIANTI.

Some of main routines like 'ch_synthetic_k', 'izothermal_k', are modified CHIANTI routines having the same names but with an extra '_k' in their name. They can be called also directly from the command line. These routines follow the original CHIANTI routines as closely as

possible. The calling parameters of these routines are kept the same, except that the first parameter is always the value of kappa. Their outputs are also arrays or structures compatible with CHIANTI. Corresponding main Maxwellian routines from CHIANTI are also located in KAPPA folder and their names have an extra suffix '_m' in their names. The routines usually have a list of options. We recommend to read them.

The other routines are typically original routines (e.g. for the free-free continuum). They can be called by the main routines or directly from the command line. As an input, they can require a structure produced as an output from other routines.

The output structures usually have the same tags as CHIANTI output but they have one extra tag with value of kappa. Therefore, they can be used as input to the original CHIANTI routines.

Please report to us any problems you might find using the software.

Table 1: List of main-level routines

<i>Synthetic spectra</i>	
kappa	Multi-purpose widget to calculate line intensities, synthetic spectra with the continuum, and various outputs.
ch_synthetic_k	Multi-purpose routine that calculates line intensities (without any abundance factor), output is an IDL structure.
isothermal_k	Computes spectra from isothermal plasmas, output is an IDL structure
make_kappa_spec_k	Creates a synthetic spectrum. Works with structures.
<i>Line emissivities</i>	
emiss_calc_k	Calculation of the emissivities of all lines of a specified ion over given ranges of temperature and density.
gofnt_k	calculation of the line contribution function $G(n,T)$ (line intensity per unit emission measure) for kappa distributions
<i>Continuum</i>	
freefree_k	Calculation of the free-free (bremsstrahlung) continuum.
freebound_k	Calculation of the free-bound continuum.
<i>Ionization and recombination</i>	
read_rrlvl_k	Reads level resolved radiative recombination rates.
read_tion_k	Reads total ionisation rates.
read_trec_k	Reads total recombination rates.
<i>Excitation rates</i>	
excit_rate_kappa	Calculates excitation and de-excitation rates for the specified ion and transition over given range of temperature.
ups_kappa_interp	Converts KAPPA fits to upsilons (thermally-averaged collision strengths) for a specified κ -distribution, ion, transition and temperature

3.3. Routines

3.3.1. Line intensities calculation:

'ch_synthetic_k.pro' calculates line intensities assuming constant pressure or density (or a model T, N), without the abundance factor. The calling sequence is:

```
IDL> ch_synthetic_k, kappa, wmin, wmax, output=output, $
      err_msg=err_msg, msg=msg, $
      pressure=pressure, density=density, $
      model_file=model_file, all=all,snl_ion=snl_ion, $
      photons=photons, masterlist=masterlist, $
      save_file=save_file, verbose=verbose, $
      logt_isothermal=logt_isothermal, $
      logem_isothermal=logem_isothermal, $
      goft=goft, ioneq_name=ioneq_name, dem_name=dem_name, $
      noprot=noprot, rphot=rphot, radtemp=radtemp, progress=progress
```

where the most important inputs are

kappa	- κ value,
wmin, wmax	- minimum and maximum of wavelength range,
density	- the electron density,
ioneq_file	- the name of the ion-equilibrium file with full path. They must contain the same value of κ as has kappa in calling sequence, in other case software uses the default ion equilibrium file for the κ -distribution (e.g. 'kappa_02.ioneq' for $\kappa=2$),
logt_isothermal	- array of logarithmic temperatures

Detailed description of inputs, outputs and key words is in the header of the routine.

Example:

Calling sequence:

```
IDL> ch_synthetic_k, 2, 10., 20., output=str2, density=1.e+9,$
      ioneq_name=!data_path+'ioneq/kappa_02.ioneq',$
      logt_isothermal=6.8, /photons, /noprot, /all, $
      snl_ion=['fe_17', 'fe_18']
```

calculates the line intensities in the spectral range 10 - 20 Å for $\kappa = 2$, $\log(T/K) = 6.8$, density 10^9 cm^{-3} , without included proton rates, for two ions Fe XVII and Fe XVIII, and intensities are in photon $\text{cm}^{-2} \text{ s}^{-1} \text{ sr}^{-1}$. The output is a structure 'str2'. The structure is nearly the same as the output from CHIANTI 'ch_synthetic.pro', but it has a one more tag '.kappa' with the value of κ (see Appendix 2).

3.3.2. Continuum calculation

The routines 'freebound_k' and 'freefree_k' calculate intensities of the free-bound and free continuum for κ -distributions. The calling sequences are:

```
freebound_k, kappa, temp, wvl, int, sumt=sumt, photons=photons, $  
    noverner=noverner, iz=iz, ion=ion, no_setup=no_setup, $  
    min_abund=min_abund, dem_int=dem_int, verbose=verbose, $  
    kev=kev, em_int=em_int
```

```
freefree_k, kappa, temp, wvl, int, min_abund=min_abund, $  
    iabund=iabund, no_setup=no_setup, photons=photons, $  
    ff=ff,int_precalc=int_precalc, $  
    kev=kev, dem_int=dem_int, em_int=em_int, sumt=sumt
```

where the most important inputs are:

kappa value of κ
temp Temperature in K (can be an array).
wvl Wavelength in angstroms (can be an array). If /keV is set, then WVL
 is assumed to contain energies in keV units.

Output is

int free-bound continuum intensity, array [10^{-40} erg cm³ s⁻¹ sr⁻¹ Å⁻¹].

Detailed description of inputs, outputs and key words is in the header of the routine.

Example:

Calling sequences:

```
IDL> freefree_k, 3, 5.e+6, findgen(50)+1.,ff  
IDL> freebound_k, 3, 5.e+6, findgen(50)+1.,fb
```

calculate free-free and free-bound continuum for $\kappa=3$, $T = 5 \times 10^6$ K and for wavelengths at 1 Å intervals between 1 and 50 Å.

3.3.3. Calculation of synthetic spectra

Isothermal synthetic spectra for the κ -distributions can be calculated using routine 'isothermal_k'. The calling sequence is:

```
isothermal_k, kappa, wmin, wmax, wavestep, temp, lambda, spectrum, $
    list_wvl, list_ident, pressure=pressure, edensity=edensity, $
    photons=photons, ergs=ergs, sngl_ion=sngl_ion, $
    abund_name=abund_name, ioneq_name=ioneq_name, $
    verbose=verbose, min_abund=min_abund, cont=cont, $
    masterlist=masterlist, noprot=noprot, radtemp=radtemp, $
    rphot=rphot, em=em, all=all
```

where the most important inputs are:

kappa	value of κ
wmin	Minimum of the wavelength range in Å.
wmax	Maximum of the wavelength range in Å.
wavestep	Bin size of spectrum (in Å).
temp	Electron temperature (or array) in K.
edensity	Electron density in cm^{-3} .

Outputs are:

lambda	Wavelength array of calculated synthetic spectrum
spectrum	Intensity array
list_wvl	A list of wavelengths for use with synthetic_plot.pro
list_ident	A list of line identifications for use with synthetic_plot.pro

Detailed description of inputs, outputs and key words is in the header of the routine.

'kappa' is user-friendly, widget-based approach to calculate synthetic spectra. It is a modification of CHIANTI routine 'ch_ss'.

IDL > kappa

This widget allows the user to calculate synthetic spectra in two basic steps. Basically, you follow the various widgets from top left to lower right to set the desired parameters. First calculate the line intensities. These values can be saved for later use. Next, specify further parameters such as the elemental abundances and instrumental spectral resolution and then calculate and plot the spectrum. These values can also be saved for later use. The HELP buttons in the widget provide short descriptions of the required information. More details are given below.

Example:

Calling sequence:

```
IDL> isothermal_k, 5, 10., 20., 0.02, 8.e+6, lambda, spectrum, $
    list_w, list_i, edensity=3.e+9, sngl_ion=[fe_17, fe_18], /cont
```

calculates the isothermal spectrum of Fe XVII and Fe XVIII with continuum for the κ -distribution with $\kappa = 5$ in the spectral range 10 - 20 Å, bin size 0.02 Å, $T = 8 \times 10^6$ K, and the electron density $= 10^9 \text{ cm}^{-3}$.

The routine 'make_kappa_spec_k' creates synthetic spectra for the κ -distributions using an output from 'ch_synthetic_k':

```
make_kappa_spec_k, kappa, transitions, lambda, output, bin_size=bin_size, $
    instr_fwhm= instr_fwhm, wrange=wrange, all=all, $
    continuum=continuum, abund_name=abund_name, min_abund=min_abund, $
    photons=photons, file_effarea=file_effarea, $
    err_msg=err_msg, verbose=verbose, kev=kev, $
    no_thermal_width=no_thermal_width
```

where the most important inputs are:

kappa	value of κ
transitions	the structure created by ch_synthetic_k.pro.
lambda	array of wavelengths. If not defined as input, it is calculated on the basis of BIN_SIZE, and returned as an output.
bin_size	bin size in Angstroms of the spectrum.
wrange	allows a subset of the wavelength range to be turned into a spectrum.
instr_fwhm	instrumental FWHM (Angstroms).

Detailed description of inputs, outputs and key words can be found in the header of the routine.

Example:

Calling sequence:

```
IDL> make_kappa_spec_k, 2, str2, lambda, output, binsize=0.02, instr_fwhm=0.25,
/all, /continuum
```

calculates synthetic spectrum with continuum ('output', array) in the spectral range of input 'str2', with bin size 0.02 Å and instrumental FWHM 0.25 Å ('lambda', array).

3.3.4. Emissivity calculation

Function 'emiss_calc_k' calculates emissivities of all lines of a specified ion over given ranges of temperature and density for the κ -distributions with specified κ . The calling sequence is:

```
emiss_calc_k, kappa, iz, ion, temp=temp, dens=dens, radtemp=radtemp, $
    rphot=rphot, path=path, no_de=no_de, noprot=noprot $
    quiet=quiet, pressure=pressure, diel=diel, $
    ioneq_file=ioneq_file, abund_file=abund_file, $
    no_setup=no_setup, sum_mwl_coeffs=sum_mwl_coeffs, $
    radfunc=radfunc, no_calc=no_calc, noionrec=noionrec, $
    no_rrec=no_rrec
```

where the most important inputs are:

kappa	value of κ
iz	Either the atomic number of the ion, or the name of the ion in CHIANTI format (e.g., 'fe_17').
ion	The spectroscopic number of the ion (e.g., 12 = XII).
temp	Direct specification of the temperature range (log T). Default temperature corresponds to the maximum of the specific ion abundance
dens	Direct specification of the density range (log Ne). Default density range is 8 to 12 in .5 intervals

Detailed description of inputs, outputs and key words can be found in the header of the routine.

Example:

Calling sequences:

```
IDL> output=emiss_calc_k(2,26, 12)
IDL> output=emiss_calc_k(2, 'fe_12')
IDL> output=emiss_calc_k(2,26, 12, temp=[6.2], dens=findgen(5)+8.)
IDL> output=emiss_calc_k(2, 'fe_12', temp=findgen(11)/100.+5.5, pressure=10.e+15)
```

calculate emissivity of Fe XII lines for κ -distribution with $\kappa = 2$. The first and the second output corresponds to default temperature and electron density, the third one corresponds to $\log(T/K) = 6.2$ and default electron densities, and the fourth one to the temperature array from $\log(T/K)=5.5$ to $\log(T/K) = 6.5$ and pressure 10^{15} cm^{-3} . The output is a structure which is nearly the same as output from CHIANTI 'emiss_calc', but it has a one more tag '.kappa' with the κ value (see Appendix 2).

The routine 'gofnt_k.' calculates the line contribution function $G(n,T)$ (line intensity per unit emission measure) of a given ion over given ranges of temperature and density for the κ -distributions with specified κ . The calling sequence is:

```
gofnt_k, kappa, ion, wmin, wmax, temperature, gof, description,$
      pressure=pressure, density=density, $
      psfile=psfile, outfile=outfile, photons=photons, $
      noabund=noabund, noprot=noprot, rphot=rphot, radtemp=radtemp, $
      abund_name=abund_name, ioneq_name=ioneq_name, all=all, $
      lower_levels=lower_levels, upper_levels=upper_levels, $
      arcsecs=arcsecs, VERBOSE=VERBOSE, logt0=logt0, value=value
```

where the most important inputs are:

kappa	value of κ
ion	Ion name in the CHIANTI format (e.g., 'fe_17').
logt0	Direct specification of the temperature array (log T).
density	Direct specification of the density, e.g. density=1.e+12.

Detailed description of inputs, outputs and key words can be found in the header of the routine.

Example:

Calling sequence:

```
IDL> gofnt_k, 2, 'o_5', 1000., 1500., temp, goft, desc, density=1.e+12
```

calculates $G(n,T)$ for O V lines for κ -distribution with $\kappa=2$, electron density 1.e+12, and temperature stored in 'temp'.

3.3.5. Calculation of electron excitation rates

The routine 'excit_rate_kappa' calculates the excitation and de-excitation rates for κ -distributions for the specified ion and transition over given range of temperature.

```
excit_rate_kappa, kappa, ion, trans, temp, e_rate, d_rate
```

where

kappa	The value of κ .
ion	The name of the ion in CHIANTI format (e.g., 'fe_17').
trans	The index of transition, can be an array
temp	The temperature (in Kelvins), can be an array.
e_rate	The excitation rate associated with temperature.
d_rate	The de-excitation rate associated with temperature.

The routine calls 'ups_kappa_interp' and 'read_kappa_ups'

Example:

Calling sequence:

```
IDL> excit_rate_kappa, 2, 'fe_17', indgen(3), [8.e+6,9.e+6],e_rate,d_rate
```

calculates the excitation and de-excitation rates for the κ -distribution with $\kappa=2$, for transitions with index 0-2 (between levels 1 and 2, 3, 4) of Fe XVII for temperatures 8×10^6 K and 9×10^6 K. Resulting rates are in arrays with [3x2] elements.

Appendix 1 - Data

Upsilon and downsilicon data files with the extensions **' .ups '** or **' .dwns '**

1-th line

Column	Format	ID	Comment
1	i7	n	number of transitions
2	i4	nt	number of temperatures

2-nd line

nt columns f5.2

3-rd - n+2 lines

Column	Format	ID	Comment
1	i3	ZET	element (ZET=26 - 'Fe')
2	i3	ION	ionization degree (ion=21 - XXI)
3	i4	L1	index of the lower energetic level
4	i4	L2	index of the lower energetic level
5	10.e3	DE	energy difference between levels L1 and L2 in Ry
6 - 6+nt-1	e12.5	UPS	Scaled upsilons

Comments are located at the end of data file between two '-1'.

The routine **' read_kappa_ups '** reads upsilons and downsilons for selected kappa-distribution:

```
IDL> read_kappa_ups, name, data_e, data_d, tmp, energy
```

Input:

name - name of the **' .ups '** or **' .dwns '** file with its full path and without its extension
e.g. name=!data_path+'fe/fe_15/fe_15_k2'

Output:

data_e - double array(nt0,n) - scaled upsilons
data_d - double array(nt0,n) - downsilons
tmp - array(nt0) - temperatures (in Kelvin)
energy - array(n) - excitation energy

where

nt0 - number of temperatures, n - number of transitions

It is possible to restore data_e, data_d, tmp, and energy in the same format from IDL save file:

```
IDL> restore, name+'.sav'
```

The routine **' ups_kappa_interp '** reads and descales upsilons and downsilons for selected κ -distribution and required temperatures:

```
ups_kappa_interp, kappa, ion, te, ups_e, ups_d, energy
```

The routine calls: read_kappa_ups

Input:

kappa - κ value

ion - ion in CHIANTI format (e.g. 'fe_17')

te - temperature in K (can be an array) for which upsilons and downsilons are required

Output:

data_e - double array(nt,n) - upsilons

data_d - double array(nt,n) - downsilons

energy - array(n) - excitation energy

where

nt - number of te, n - number of transitions

Data for total ionization or recombination rate '.tionr', '.trechr'

1-th line

Column	Format	ID	Comment
1	i7	NT	number of temperatures

2-nd - NT+1 lines

Column	Format	ID	Comment
1	e12.4	TMP	temperatures (in Kelvin)
2	e12.4	TIONRATE	total ionization rates
or	e12.4	TRECRATE	total recombination rates

NT+2 line 1-st column '-1' i2 format data end

Comments are located at the end of data file between two '-1'.

Routine '**read_kappa_tionr**' reads total ionization rates for selected κ -distribution:

```
IDL> read_kappa_tion, name, tmp, tionrate
```

Input:

name - name of the '.tionr' file with its full path and without its extension

e.g. name=!data_path+'fe/fe_15/fe_15_k2'

Output:

tmp - array(nt) - temperatures

tionrate - array(nt) - total ionization rates

where

nt - number of temperatures

The routine '**read_kappa_trechr**' reads total recombination rates for selected κ -distribution:

```
IDL> read_kappa_trechr, name, tmp, trecreate
```

Input:

name - name of the '.trechr' file with its full path and without its extension

e.g. name=!data_path+'fe/fe_15/fe_15_k2'

Output:

tmp - array(nt) - temperatures

trecreate - array(nt) - total ionization rates

where

nt - number of temperatures

The routine `'tionrec_rate_kappa'` calculates total ionization and rates for selected κ -distribution and temperature:

```
IDL> tionrec_rate_kappa, kappa, ion, te, tionr, trecr
```

The routine calls: `read_kappa_tionr`, `read_kappa_trecr`

Input:

kappa - κ value

ion - ion in CHIANTI format (e.g. 'fe_17')

te - temperature in K (can be an array) for which total ionization and recombination are required

Output:

tionr - array(n) - total ionization rates

trecr - array(n) - total recombination rates

where

n - number of te

Data for level resolved radiative recombination rate `' .rrlv1 '`

1-th line

Column	Format	ID	Comment
1	i7	N	number of transitions
2	i7	NT	number of temperatures

2-nd line

1 - NT column	e10.2	Temp	temperatures
---------------	-------	------	--------------

3-rd - 2+N line

Column	Format	ID	Comment
1	i5	Z	atomic number
2	i5	ION	ion
3	i7	initial_level	initial level
4	i7	final_level	final level
5 - 4+N	e10.2	rate	rate

Comments are located at the end of data file between two `'-1'`.

The function `'read_rrlv1_k'` reads level resolved radiative recombination rates for the κ -distributions

```
IDL> str = read_rrlv1_k (kappa, fname, status)
```

Input:

kappa - κ value

fname - The name for an ion in CHIANTI format (e.g. 'fe_17')

Output:

Structure `'str'` with several tags: kappa, rates, temperatures, levels and references. The output structure is nearly the same as in CHIANTI but it has one more tag `' .kappa '` (see Appendix 2).

Appendix 2 - Output structures

ch_synthetic_k - output structure contains the line intensities and details of transitions in tags:

.kappa	float, κ value
.lines	a structure containing information about the lines with tags: <ul style="list-style-type: none"> .iz integer, the atomic number of the elements (e.g., 26=Fe) .ion integer, the ionisation stage (e.g., 17=XVIII) .snote string, the identification of the ion (e.g., 'Fe XXIV d') .ident string, the identification of the transition, configuration and terms in text form. .ident_latex string, the identification of the transition, configuration and terms in latex form. .lvl1 integer, the lower level of the transition .lvl2 integer, the upper level for transition. .tmax float, the temperature of maximum emission of the line. .wvl float, wavelength of the transition, in Angstroms. .flag a flag -1 if the line has only theoretical energy levels or not. Otherwise 0. .int float, the intensity of line (erg/cm²/s/sr or phot/cm²/s/sr) .goft float, the G(T) of the line (optional /exclusive with .int).
.ioneq_name	string, the ion balance file used (full path).
.ioneq_logt	float array, the he Log10 T values associated.
.ioneq_ref	string, the references.
.dem_name	string, the differential emission measure file eventually used (full path).
.dem	float array, the Log10 DEM values
.dem_logt	float array, the Log10 T values associated.
.dem_ref	string, the DEM references.
.model_name	string indicating the model used.
.model_file	string, full path of the (Te,Ne) file if defined. Null string otherwise.
.model_ne	float (array), the Ne value(s).
.model_pe	float, the Pe value.
.model_te	float, the Te values if 'Function' is selected. Otherwise 0.
.wvl_units	string, the wavelength units.
.wvl_limits	float, the wavelength limits specified by the user.
.int_units	string, the intensity units.
.logt_isothermal	float (array), the Log10(T) values used.
.logem_isothermal	float, the Log10(EM) values used.
.date	string, the date and time when the structure was created.
.version	string, the version number of the CHIANTI database used.
.add_protons	a flag (0/1) to indicate whether proton data were used
.photoexcitation	aA flag (0/1) to indicate if photoexcitation was included
.radtemp	float, the blackbody radiation temperature (if photoexcitation was included).
.rphot	float, distance from the centre of the star in stellar radius units (if photoexcitation was included).

emiss_calc_k - output structure contains the line emissivities and details of transitions in tags:

.kappa	integer, value of κ
.ion_name	string; contains ion name, e.g., 'Fe XII'
.lambda	float; contains wavelength
.level1	integer; contains lower level of transition
.lv1_desc	string; gives configuration and term of lower level
.level2	integer; contains upper level of transition
.lv2_desc	string; gives configuration and term of upper level
.flag	integer; a flag to mark particular transitions
.em	fltarr(nt,nd); contains emissivities at particular temperatures and densities.

read_rrlvl_k - output structure contains the level resolved radiative recombination rates and details of transitions in tags:

.kappa	integer, value of κ
.rate	float array, contains level resolved radiative recombination rates
.temp	float array; contains associated temperatures
.final_level	integer array; contains final levels of transition
.initial_level	integer array; contains initial levels of transition
.ref	string; references

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