The 7th Non-LTE Code Comparison Workshop

December 5-9, 2011

Vienna, Austria

Submission of Calculations

This document is intended to define the particulars of the workshop submissions. In the sections below we will define the case problems, the comparison quantities which we require and the detailed format of the data files that we will be expecting. The problems are completely defined by a specification of the ***electron temperature*** and ***electron density***. The goal is to compare the kinetic codes and therefore the problems are 'zero-dimensional', i.e., there are no consideration of plasma non-uniformity, boundary effects, or heavy-particle interactions.

The webpage of the meeting is at http://nlte.nist.gov/NLTE7. The submission files are to be uploaded to the same server nlte.nist.gov using a web interface with userid and password. Both will be provided to the participants upon request to yuri.ralchenko@nist.gov. To reduce the server load and accelerate the upload, it would be most convenient if the contributor(s) created an archive file containing all the individual result files. Submissions employing any modern data compression techniques (e.g., `zip/gzip/bzip2/arj/lha/rar`) along with the Unix `tar` archiving utility will be accepted. Also, please inform Yuri Ralchenko (email: *yuri.ralchenko@nist.gov*) when new files are uploaded.

Timeline:

1. **November 10 – submission deadline**
2. November 20 – online database available
3. December 5 – workshop opens
4. December 9 – workshop adjourns

I. STATEMENT OF CASES

We have selected a number of atoms to consider, and for each atom we are requesting results on a grid of electron temperatures and electron densities. In the following, temperatures are given in eV, particle densities in cm^{-3}, time in seconds.

The following problems have been established for the cases:

Element	Case ID	Total # of Cases	Parameter	Grid		
Neon	Ne	6×6	**T_e**	**10,30**		
			N_e	**10^{14},10^{18},10^{20}**		
			Spectra	**Range (eV)**	**Resolution (eV)**	**# of points**
				1-250	ΔE = 0.05	4981
			Extra info	Each case is to be calculated for six different values of n_{max}: only g.s. included, 3,4,8,12, ∞		
Argon	Ar	12	**T_e**	**10,20,40,60,80,100**		
			N_e	**10^{10},10^{20}**		
			Extra info	Include only Ar^{6+}, Ar^{7+}, Ar^{8+} and Ar^{9+} (Mg- through F-like ions)		
Argon	ArTD	3	**N_e**	**10^{14},10^{18},10^{20}**		
			T_e	**50**		
			Spectra	**Range (Å)**	**Resolution (Å)**	**# of points**
				4.17-4.2	Δλ = 0.0001	301
				40-50	Δλ = 0.01	1001
				400-800	Δλ = 0.1	4001
			Extra info	Time dependence: **t(0)**=0, **t(1)**=10^{-16} s, **t(i)**=**t(i-1)*dt** for **i**=2..200; **dt** = 1.15 for N_e=10^{14}, **dt** = 1.10 for N_e=10^{18}, **dt** = 1.08 for N_e=10^{20}. Initial condition: ALL population is in configuration $1s2s^2 2p^6 3p$.		
Krypton	Kr	3	**Pressure/Energy**	4 kBar/361 J (case **1**) 4 kBar/235 J (case **2**) 7 kBar/306 J (case **3**)		
			Spectra	**Range (Å)**	**Resolution (Å)**	**# of points**
			Case 1	5.8-7.8	Δλ = 0.001	2001
			Case 2	5.8-7.8	Δλ = 0.001	2001
			Case 3	5.8-7.8	Δλ = 0.001	2001

Tungsten	W	6	**T_e**	**2500, 3900, 5000, 7000, 9000, 12000**		
			N_e	**10^{14}**		
			Spectra	**Range (Å)**	**Resolution (Å)**	**# of points**
			For 3900 eV	3-9	$\Delta\lambda$=0.002	3001
			For 5000 eV	25-33	$\Delta\lambda$=0.004	2001

Table I. Case definitions.

The grid of plasma temperatures and densities is given in Table I. If your calculation requires an ion temperature, then you should assume it is identical to the electron temperature.

Each calculation will be referenced by a case name, which is to be given in the submission data file (as described further below). The case name is constructed by appending a suffix to the Case_ID shown in the preceding table. The suffix consists of one or more digits. For most of the cases, the first digit corresponds to the electron temperature, and second to the electron density. Correspondingly, the Argon case with T_e = 40 eV and $N_e = 10^{20}$ cm^{-3} will be referred to as **Ar32** since 40 eV is the third value in the list of T_e and 10^{20} cm^{-3} is the second density. The neon cases will have a third digit indicating the highest principal quantum number in the model (1 for ground-state-only case etc.), e.g., **Ne213** corresponds to 30 eV, 10^{14} cm^{-3} and n_{max}=4.The tungsten case of 12 keV/10^{14} cm^{-3} will be referred to as **W31** and so on. The krypton cases will be identified by one digit only, that is, the 4 kBar/361 J case will be **Kr1** and so on.

The quantities to be computed for each case are described below. Most of the cases will also require *calculation of emission spectra*. All cases but the ArTD should be calculated in a steady-state condition.

The submissions file should be named as **<case>.<contributor_name>.<code_name>**, so that Dr. A. Einstein's calculations with his code GToE for one of the Argon cases would be in the file `ar31.einstein.gtoe` (case insensitive).

II. JUSTIFICATION OF CASES AND DETAILS

1. Ne

The Ne case is designed to explore convergence of CR models with the highest principal quantum number n_{max} included in a model. Accordingly, we ask the participants to perform calculations for six different cases per T_e/N_e combination: first with only ground states included, and then for five different values of n_{max} = 3, 4, 8, 12 and *infinity* (e.g., the highest n_{max} your particular model can handle). Please include continuum (ionization potential) lowering using the ion density $\mathbf{N_i=N_e/Z}$. Again, the last digit in the case names will be referred to the n_{max} value, e.g., **Ne235** for 30 eV, 10^{20} cm^{-3} and n_{max}=12 and **Ne231** for the ground-state-only calculation.

2. Ar

The steady-state case for Ar aims at the in-depth analysis of dielectronic recombination (DR) and excitation-autoionization (EA). As we found at NLTE-6, all participating codes virtually agree when EA/DR are excluded, and therefore a better understanding of how EA/DR are treated in different models becomes a timely undertaking. The Ar calculation should include only *four ionization stages* which are simple yet representative of contributions of Δn=0 and $\Delta n \neq 0$ channels. The table below specifies the autoionizing states which are to be included for DR from F-, Na- and Na-like ions:

Ion	**Initial states**	**Intermediate states (Δn=0 channels)**	**Intermediate states (Δn>0 channels)**
F-like Ar^{9+}	$(2)^7$	$(2)^7 nl$	$(2)^6 3ln'l'$ $(n'\geq 3)$ $(2)^6 4ln'l'$ $(n'\geq 4)$
Ne-like Ar^{8+}	$(2)^8$		$(2)^7 3ln'l'$ $(n'\geq 3)$ $(2)^7 4ln'l'$ $(n'\geq 4)$
Na-like Ar^{7+}	$(2)^8 3l$	$(2)^8 3l'$ nl	$(2)^8 4ln'l'$ $(n'\geq 4)$ $(2)^7 3l3l'n''l''$ $(n''\geq 3)$

Table II. Autoionizing states for the steady-state case of Ar.

The allowed $n'l'$ values of the captured electron may be different in different codes. Notation $(2)^6$ denotes all possible combinations of 6 electrons in n=2 shell, i.e., $2s^2 2p^4$, $2s2p^5$ and $2p^6$.

3. Ar-TD

The time-dependent case for Ar was inspired by the selective K-shell photoexcitation that can be accomplished on the existing XFELs, such as LCLS. The goal here is to study the density-sensitive collisional-radiative cascades and population redistribution in Ne-like Ar, and especially the ensuing emission in x-ray, soft x-ray and EUV parts of spectra. It is assumed that at time t=0 **all** population is in the $1s2s^22p^63p$ configuration. Since this configuration has two terms and four levels, the term- or level-based codes should assume statistical distribution of population with $1s2s^22p^63p$.

The first time step is 10^{-16} s for all three densities. The following 199 logarithmic steps depend on the electron density as given in Table I. The population output is requested at every 10^{th} step (total of 20 points) while the spectra output should be integrated over the whole time of calculation.

4. **Kr**

The objective of the Kr case is to discuss in detail how different researchers approach analysis of experimental spectra. The Kr gas jet measurements were performed on LULI2000 facility and provided well-resolved time-integrated spectra between 5.5 and 8 Å as well as four time-resolved frames (0-4 ns) between 20 and 220 Å. The Thomson scattering measurements were used to determine plasma density and temperature, however initial theoretical analysis showed rather different values of T_e. We ask the participants to do their best (e.g., no restrictions and/or recommendation on the CR model to be used) and try to explain the three experimental spectra of Fig. 4(b). The case names will be **Kr1** for **4 bar/361 J**, and **Kr2** for **4 bar/235 J** and **Kr3** for **7 bar/306 J**. Note that this analysis may require account of opacity effects.

The experimental spectra of intensities vs. wavelength are available at http://nlte.nist.gov. Also the 20-220 Å spectra for the 4 bar/230 J shot at three times (Fig. 7 of the original paper) are available. We do not plan to compare the time-resolved spectra but they can be used to deduce plasma parameters needed for time-integrated simulations.

5. **W**

This is a continuation of the effort started at NLTE-5 with calculation of ionization balance and radiative power losses for W in magnetic fusion plasmas (see AIP Conference Proceedings **1161**, p. 242 [2009]). Here we, on the one hand, add a new spectral range in soft x-ray to compare against available experimental data, and on the other, suggest comparisons with our previous calculations. Moreover, the low-T_e case was found to show the largest disagreement as compared with experiment.

III. SUBMISSION FILE DESCRIPTION

We are asking for a fairly large amount of information. To simplify the specification for the contributors we have adopted a keyword approach within the submissions file. In this approach, all quantities are space delimited. In Section V, we give a schematic of the file format. For clarity we will use the `courier` font to indicate the keywords (the actual submissions should be unformatted plain ASCII text). The user-supplied data that are problem-dependent are indicated by a **bold-face** parameter name in brackets (e.g., **<pop_frac>**). We anticipate that not all information will be provided by every user. However, since the information is space delimited, and not fixed in a particular column, then *some* value must be given for each field. The best default value is to put a zero. The longer records, such as the `ion` and `elev` lines, may continue over several lines at the contributor's discretion. Do not break a line in the middle of a keyword or a number. Blank lines may be used anywhere within the file to make the text more readable. While some of the names we use suggest integer quantities, please use decimal values if appropriate to your calculation. For floating point numbers, an **`e11.4`** format is generally adequate although for level energies a high accuracy may be necessary. The exact definitions of the quantities requested, including units, are given in Section V.

The submissions file is structured in 5 sections. These sections are identified by keywords. In some cases, an integer follows the section keyword to indicate the number of records which follow for that section. Some codes will not be able to provide information for every section. Thus, an entire section may be omitted. If all information is provided, then there will be a certain amount of redundancy. This redundancy is intentional and has at least two uses. First, it can be used to detect errors in the file formatting. Second, it is often possible to compute overall quantities more accurately internal to the kinetics code than by post-processing the results.

The *initial section* provides general problem identification information. This section begins with the keyword `data`.

The *second section* gives overall quantities describing the plasma population and energy distribution. This section is signaled by the keyword `summary_quantities`. Note there are no spaces in the keywords.

The *third section* gives information by ionization stage. This section is signaled by the keyword `ion_stages`. Within this section, information for each ionization stage begins with the keyword `ion`. As mentioned above, multiple lines may be used if desired (we intentionally used multiple lines in the schematic file listing below to improve its readability). Important note: we use <**Nbound**>, the number of bound electrons, *not* the ion stage charge, to label the ion stages.

The *fourth section* gives information by energy level (keyword `energy_levels`). Since many codes employ some form of continuum lowering and/or moving calculational windows, we require that energy level definitions be provided for every case. The shell occupation numbers (**<occK>**, **<occL>** etc.) as defined for each `elev` record will be used to compare codes for the cross-over from a ladder-like de-excitation regime to one which is in Saha-Boltzmann equilibrium with the continuum.

Finally, the *fifth section* contains calculated spectral characteristics.

A relational database tool will be used to manage the data during the course of the workshop.

If necessary, additional clarification regarding the submission format will be provided at the Workshop's web site.

IV. SUBMISSION FILE FORMAT

The text that follows is a schematic of a submissions file:

```
data                    <user comment... >
case                    <case_id>
code                    <name>
atom                    <name>  <Znuc>
calctime                <CPU>  <human>


summary quantities
plasma                  <Te>  <Ne>
time                    <time>
zbar                    <zbar>
m2                      <2nd central moment>
m3                      <3rd central moment>
eint                    <internal_energy>
deintdt                 <dE_int/dT_e>
pfn                     <partition_fn>
nmax eff                <n_value>
ploss                   <P_bb>  <P_bf>  <P_ff>  <P_total>



ion stages              <count>
ion                                 <Nbound> <pop_frac> <nouter>
                                    <S_tot> <f_S_coll> <f_S_photo> <f_S_auto>
                                    <α_tot>  <f_α_coll> <f_α_photo> <f_α_auto>
...

ion                                 <N_bound> <pop_frac> <nouter>
                                    <S_tot> <f_S_coll> <f_S_photo> <f_S_auto>
                                    <α_tot> <f_α_coll> <f_α_photo> <f_α_auto>


energy levels           <count>
elev                                <N_bound> <level> <stwt> <energy> <population>
                                    <Γ_tot> <f_Γ_collbb> <f_Γ_photobb> <f_Γ_collbf> <f_Γ_photobf> <f_Γ_auto>
                                    <Θ_tot> <f_Θ_collbb> <f_Θ_photobb> <f_Θ_collbf> <f_Θ_photobf> <f_Θ_auto>
                                    <occK> <occL> <occM>    ...         <nouter>
...
elev                                <N_bound> <level> <stwt> <energy> <population>
                                    <Γ_tot> <f_Γ_collbb> <f_Γ_photobb> <f_Γ_collbf> <f_Γ_photobf> <f_Γ_auto>
                                    <Θ_tot> <f_Θ_collbb> <f_Θ_photobb> <f_Θ_collbf> <f_Θ_photobf> <f_Θ_auto>
                                    <occK> <occL> <occM>    ...         <nouter>
…
…
```

The energy levels are to be provided for all steady state cases.

Spectrum Output

For the cases where we request spectra, the spectral information will be given in this same text file, following the information above. The spectrum will be in the format:

spectrum1	**<case>**		**<count$_1$>**		
<wavelength1>	**<ε_{bb}1>**		**<ε_{bf}1>**	**<ε_{ff}1>**	**<ε_{tot}1>**
<wavelength2>	**<ε_{bb}2>**		**<ε_{bf}2>**	**<ε_{ff}2>**	**<ε_{tot}2>**
.....					
<wavelengthN>	**<ε_{bb}N>**		**<ε_{bf}N>**	**<ε_{ff}N>**	**< ε_{tot}N>**
spectrum2	**<case>**		**<count$_2$>**		
<wavelength1>	**<ε_{bb}1>**		**<ε_{bf}1>**	**<ε_{ff}1>**	**<ε_{tot}1>**
<wavelength2>	**<ε_{bb}2>**		**<ε_{bf}2>**	**<ε_{ff}2>**	**<ε_{tot}2>**
.....					
<wavelengthN>	**<ε_{bb}N>**		**<ε_{bf}N>**	**<ε_{ff}N>**	**< ε_{tot}N>**
spectrumW	Z1	Z2	…		
<wavelength1>	**<ε_{bb}1_Z1>**	**<ε_{bb}1_Z2>**	…		

where wavelengths are in Å, and spectra **ε** for bound-bound (bb), bound-free (bf), and free-free (ff) transitions are explained later.

V. DEFINITIONS OF REQUESTED QUANTITIES

Before proceeding to a detailed description of the requested quantities, we would like to comment on the ion density. In absence of heavy-particle interactions, the influence of ion density would mostly be exposed through the ionization potential lowering. To provide a description of N_i, for all cases the electron and ion densities are to be related via the plasma neutrality condition, i.e., $N_i = N_e/Z$.

In *section 1*, the identification section, the following quantities are requested:

`data` Calculation identifier and user comment line. Comment should be limited to this one line only and should include the contributor's name, institution, the version of the code, and the date at which calculation was run. This can be invaluable in maintaining order in large number of submissions.

`case` All calculations will have a case identification of the form `Ar12` or the like (see Section I). These identifiers are assigned in the section below where the specific calculations are called out.

`code` An identifier for each contributor's code which may be chosen by the contributors. For convenience in post-processing and tabulation the names should not be excessively long. The names will be used in all tables and graphs of comparisons, and must be the same from case to case.

`atom` Identifies the atom under study. The field **<name>** is a convenience for the contributor. In many cases, calculations are driven by atomic data found in a file. The file **<name>** may be used to specify that name. The field **<Znuc>** is the nuclear charge of the atom.

`calctime` Provides information on the CPU time (computer) and total time (human) spent on calculation of this particular case.

In *section 2*, the `summary_quantities` section, the following items are requested:

`plasma` This record specifies the plasma conditions used in this calculation. The electron temperature is in units of eV. The electron density is in units of cm-3.

`time` A value (e.g., zero) for steady-state cases.

`zbar` Average charge of the plasma.

`m2` Second central moment of the charge state distribution.

`m3` Third central moment of the charge state distribution.

`eint` Specific internal energy of the atom.

`pfn` Partition function of the atom.

`nmax_eff` For this calculation, the principal quantum number of the outermost electron in any bound state. We will be interested in sensitivity of comparison quantities to the highest bound states accounted for by the model. This quantity will also be used as a measure of continuum lowering.

`ploss` The radiative power losses: bound-bound, bound-free, free-free, and total. Units: erg/sec/cm^3.

The **central moments** are defined as:

$$m_N = \sum_j y_j \left(q_j - \bar{Z} \right)^N ,$$

where y_j is the fractional population of ion stage j, q_j is the ion charge, and $\bar{Z}$ is the average charge.

The **specific internal energy** is the sum of level populations, n_j, multiplied by their energy value, E_j, divided by the total ion density N_i:

$$E_{\text{int}} = \sum_j \frac{E_j n_j}{N_i} \quad .$$

The energy reference is the ground state of the neutral atom. We recognize that a kinetics model may not include all ionization stages of the atom – the ground state of the most neutral ion is the most reasonable substitute. For intercomparisons, this quantity will likely need zero point shifts. Units are eV/atom.

The **specific heat** is the derivative with respect to electron temperature of the specific internal energy of the atom. Units are eV/atom/eV. If computed by finite difference, the step size is to be chosen by the contributor.

The **partition function** is defined as the classical partition function:

$$Q = \sum_j g_j \exp\left(-E_j / T_e \right) ,$$

where g_j is the statistical weight of level j and E_j is the energy of the level, with respect to the ground state of the most neutral ion.

The total **power loss** is the most important quantity, so that if one has difficulties separating different contributions, then it would suffice to have zeros in fields other than <**P$_{\text{total}}$**>.

Note that many of the "thermodynamic" quantities are intentionally sensitive to continuum lowering models. Quantities possibly affected are <**eint**> and <**pfn**>. If your continuum lowering model alters the energy levels or statistical weights, please include these effects in the appropriate "thermodynamic" quantities.

High-lying bound states can be included in the population kinetics in a variety of ways. The field `nmax_eff` is intended to give information on the highest-lying bound state, which is affecting the calculation of the populations. It is thus an "effective" principal quantum number. If a code includes a level, which accounts for more than one *n* value, then for this field we recommend giving the *largest* value that is being modeled.

In *section 3*, the `ion_stages` section, the following quantities are requested:

<Nbound> The number of bound electrons in this ionization stage.

<pop_frac> The fraction of atoms in this ionization stage. Sum over all ions should be normalized to unity.

<nouter> The principal quantum number of the outermost electron for any state in this ion stage.

<S_{tot}> The total (effective) ionization rate out of this ion stage, averaged over all initial states in this ion stage (weighted by the fractional populations of the initial states), and summed over all final states. This quantity is further summed over all ionization processes.

<f_S_{coll}> The fractional contribution of electron collisional ionization processes to <S_{tot}>.

<f_S_{photo}> The fractional contribution of photo-ionization processes to S_{tot}>.

<f_S_{auto}> The fractional contribution of auto-ionization processes to <S_{tot}>.

<α_{tot}> The total (effective) recombination rate out of this ion stage, averaged over all initial states in this ion stage (weighted by the fractional populations of the initial states), and summed over all final states. This quantity is further summed over all recombination processes.

<f_α_{coll}> The fractional contribution of three-body recombination to the total <α_{tot}>.

<f_α_{photo}> The fractional contribution of radiative-recombination to the total <α_{tot}>.

<f_α_{auto}> The fractional contribution of dielectronic capture processes to the total <α_{tot}>.

We note that the total effective ionization and recombination rates are rates, and not rate coefficients. It is also important to be precise about the direction of these total rates. <S_{tot}> is the total effective rate out of the indicated ion into the more ionized ion. Similarly, <α_{tot}> is the total effective rate out of the indicated ion into the less ionized ion.

The definitions of S_{tot} and α_{tot} are best clarified through an example. Consider a three-ion stage problem consisting of levels in Li-like, He-like, and H-like ions. For the He-like ion, S_{tot} is the sum of all ionization rates *out* of He-like, weighted by the appropriate He-like initial state populations, and summed over all final states in the H-like ion. The averaging over initial states is completed by dividing the above sum by the total population of the He-like ion. α_{tot} for the He-like ion is the sum of all recombination rates out of He-like, weighted by the appropriate He-like initial state populations, and summed over all final states in the Li-like ion. The averaging over initial states is completed by dividing the above sum by the total population of the He-like

ion. With these definitions, we can define a set of ionization rate equations. In the case of the He-like ion, we write:

$$\frac{dn(He)}{dt} = \alpha_{tot}(H)n(H) - \left[\alpha_{tot}(He) + S_{tot}(He)\right]n(He) + S_{tot}(Li)n(Li).$$

Units of <$\mathbf{S_{tot}}$> and <$\boldsymbol{\alpha_{tot}}$> are 1/sec.

In *section 4*, the `energy_levels` section, the following quantities are requested:

<Nbound> Identifies the ionization stage to which this energy level belongs. As always, this quantity is the number of bound electrons in the level.

<level> A sequential level number within this ionization stage. This index begins at 1 within each ionization stage for use as a label in model comparisons. The ground state of each ion stage will be identified by locating the state of lowest energy within the ion stage.

<stwt> The statistical weight of this energy level.

<energy> The energy of the level relative to the overall model. Ionization potentials will be obtained by subtraction of successive ground state energies. Units are in eV. The overall energy reference is the ground state of the most neutral ion in the problem.

<population> The **normalized** ion density of this level. *Sum of all level populations over all ions is unity*.

<$\boldsymbol{\Gamma_{tot}}$> The **total population flux out** of this level. This definition is different from the previous workshops. Units are 1/sec.

<**f_**$\boldsymbol{\Gamma_{collBB}}$> The *fractional* contribution of electron collision excitation/de-excitation processes to <$\boldsymbol{\Gamma_{tot}}$>.

<**f_**$\boldsymbol{\Gamma_{photoBB}}$> The *fractional* contribution of bound-bound radiation processes to <$\boldsymbol{\Gamma_{tot}}$>.

<**f_**$\boldsymbol{\Gamma_{collBF}}$> The *fractional* contribution of electron collision ionization-recombination processes to <$\boldsymbol{\Gamma_{tot}}$>.

<**f_**$\boldsymbol{\Gamma_{photoBF}}$> The *fractional* contribution of photo-ionization-recombination to <$\boldsymbol{\Gamma_{tot}}$>.

<**f_**$\boldsymbol{\Gamma_{auto}}$> The *fractional* contribution of auto-ionization/dielectronic recombination processes to <$\boldsymbol{\Gamma_{tot}}$>.

<$\boldsymbol{\Theta_{tot}}$> The **total population flux into** this level. For steady-state condition <$\boldsymbol{\Theta_{tot}}$> = -<$\boldsymbol{\Gamma_{tot}}$>. Units are 1/sec.

<**f_**$\boldsymbol{\Theta_{collBB}}$> The *fractional* contribution of electron collision excitation/de-excitation processes to <$\boldsymbol{\Theta_{tot}}$>.

<**f_**$\boldsymbol{\Theta_{photoBB}}$> The *fractional* contribution of bound-bound radiation processes to <$\boldsymbol{\Theta_{tot}}$>.

<**f_**$\boldsymbol{\Theta_{collBF}}$> The *fractional* contribution of electron collision ionization-recombination processes to <$\boldsymbol{\Theta_{tot}}$>.

<f_Θ$_{photoBF}$>	The *fractional* contribution of photo-ionization-recombination to **<Θ$_{tot}$>**.
<f_Θ$_{auto}$>	The *fractional* contribution of auto-ionization/dielectronic recombination processes to **<Θ$_{tot}$>**.
<occK>	Occupation number: for this energy level, the number of electrons in the K shell. Users of configuration interaction codes might wish to use the dominant configuration to assign this value.
<occL>	The number of electrons in the L shell.
...	
<nouter>	The principal quantum number of the outermost electron in that energy level.

Parameter **Γ** describes all processes originating from a particular level while **Θ** describes all processes ending on this level. The population flux is defined as a product of the population by the corresponding rate, so that, for instance, the total **Θ** for a level *i* is:

$$\Theta_i = \sum_j POP_j \times R_{ij} ,$$

where POP_j is the population of level *j* and R_{ij} is the rate of a physical process originating in level *j* and ending in level *i* (e.g., probability for a radiative transition from the upper level *j* into the lower level *i*). Note that at the previous workshops, we were asking for rates rather than population fluxes.

The shell occupation numbers (**<occK>**, **<occL>**, etc.) could be variable in number for each code, plasma condition, and energy level. Contributors are not constrained on this point: they may specify as many shells as necessary, and as relevant to their calculational approach. The final entry for this energy level record should be the principal quantum number of the outermost electron in that level. In the case of highly-excited levels, the shell occupation numbers may be simplified by only specifying the core, <**Nbound**>-1, electrons. In this case the field <**nouter**> will be used to set the location of the remaining electron. We will be using the values given in this section to compute some of the quantities given in section 2 for consistency checks.

In *section 5*, the `spectrum` section, the data requested are summarized below:

Ne

x-axis:	energy (in eV),
spectrum units:	erg/s/cm^3/eV;

Ar,W

x-axis:	wavelength (in Å),
spectrum units:	erg/s/cm^3/Å;

Ar-TD

x-axis:	wavelength (in Å),
spectrum units:	erg/cm^3/Å;

The spectrum for the present optically thin cases is requested per unit volume. The required data are bound-bound <ε_{bb}>, free-bound <ε_{fb}>, free-free <ε_{ff}> and total <ε_{tot}> spectra (except for Ar-TD case where only bound-bound spectrum is required). The field <**count**> specifies the number of *(wavelength, spectra)* rows which follow. For the W cases, a section in the spectrum file that describes total spectra should be followed by a section containing bound-bound spectra for the most populated ion stages (with relative ion populations $POP(W_Z)/POP(W) \geq 10^{-5}$).

Finally, the line broadening should be natural+Doppler for all cases.

Example of a spectrum file for W:

```
…
spectrum2     W21           2501
1.000e1       1.000e-15     1.000e-16     2.500e-15     3.600e-15
1.002e1       2.000e-15     2.000e-16     5.000e-15     7.200e-15
…             …             …             …             …
6.000e1       1.000e-15     1.000e-16     2.500e-15     3.600e-15

spectrumW     45            46            47            48            49
1.000e1       1.300e-16     1.700e-16     2.000e-16     5.000e-16     0.000e-16
…
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