7th Spectral Line Shapes in Plasmas
Code Comparison Workshop

September 30 – October 4, 2024

Gran Canaria, Spain

Call for Submissions (rev. September 9, 2024)

Introduction

This document defines the particulars of the workshop submissions. In the sections below we define the case problems, the comparison quantities which we require and the detailed format of the submission data files.

The webpage of the meeting is at `https://plasma-gate.weizmann.ac.il/slsp7/`. The submission files are to be uploaded to the same server using a web interface with userid and password. Details will be announced separately.

Timeline (2024):

~~July 07~~	—	~~hotel pre-booking deadline~~
August 18	—	web interface for file uploads opens
August 29	—	registration deadline
September 15	—	submission deadline
September 30	—	workshop opens
October 04	—	workshop adjourns

Contents

Table 1: Case definitions.

ID	Transition(s)	# of subcases	n_e (cm^{-3})	T (eV)	Extra parameters
1	Ar XVIII Lyman-α	$3 \times 3 \times 3 \times 2 = 54$	$10^{23}, 10^{24}, 10^{25}$	1000, 2000, 4000	LS off/on
	Model: $\Delta n \neq 0$ dipole interactions ignored (strictly linear Stark effect); straight path trajectories of Debye quasiparticles in **three** variants: only electrons, only protons, and electrons and protons together.				
2	Ar XVIII Lyman-β	$3 \times 3 \times 3 \times 2 = 54$	$10^{23}, 10^{24}, 10^{25}$	1000, 2000, 4000	LS off/on
	Model: Same as above.				
3	Ar XVIII Balmer-α	$3 \times 3 \times 2 \times 1 = 18$	$10^{23}, 10^{24}, 10^{25}$	1000, 2000, 4000	—
	Model: $\Delta n \neq 0$ dipole interactions ignored (strictly linear Stark effect); no fine structure; atomic model in **two** variants: without and with the interference term.				
4	He I 447nm	$2 \times 3 \times 3 \times 2 = 36$	$10^{16}, 10^{17}$	0.5, 1, 2	$\alpha = 1\%$ or 10%
	Model: plasma broadening in **three** variants: charged perturbers and neutrals separately, as well as the combined effect. The atomic model is limited to triplet states with $n = 2$ or $n = 4$ and $\ell \geq 1$ without fine structure.				
5	H Lyman-α	$1 \times 2 \times 3 \times 3 = 18$	10^{17}	1, 2	$B = 0, 1\,\mathrm{kT}, 10\,\mathrm{kT}$
	Model: broadening in **three** variants: plasma broadening and MSE separately, as well as the combined effect. The no-quenching approximation, no LS, no penetration effects, no spiral trajectories, but with the B^2 term (if your code can) included.				
6	H Balmer-β	$1 \times 2 \times 3 \times 3 = 18$	10^{17}	1, 2	$B = 0, 1\,\mathrm{kT}, 10\,\mathrm{kT}$
	Model: same as above.				
7	Li I 2s–2p	$1 \times 6 \times 3 \times 1 = 18$	10^{17}	1, 2, 5, 10, 20, 50	—
	Model: 2s and 2p levels included, no fine structure. Only electron broadening. **Three** variants: the "standard" dipole approximation, dipole and quadrupole, and full Coulomb with the penetrating collisions accounted.				
8	B III 2s–2p	$1 \times 6 \times 3 \times 1 = 18$	10^{18}	4, 7, 10, 20, 50, 100	—
	Model: Same as above.				
9	H Balmer-α	$1 \times 1 \times 2 \times 9 = 18$	10^{15}	1	$F = 0, 5F_0, 10F_0$ $B = 0, 3\,\mathrm{T}, 6\,\mathrm{T}$
	Model: the $\vec{F}$ and $\vec{B}$ fields (when both non-zero) are either parallel or perpendicular to each other. Assume the harmonic electric field to oscillate with the plasma or upper hybrid frequency, respectively. Linear Stark effect, no fine structure.				
10	H Balmer-β	$1 \times 1 \times 2 \times 9 = 18$	10^{15}	1	$F = 0, 5F_0, 10F_0$ $B = 0, 3\,\mathrm{T}, 6\,\mathrm{T}$
	Model: Same as above.				
11	Cu XIII Kα	$3 \times 1 \times 2 \times 3 = 18$	$10^{24}, 3 \times 10^{24}, 10^{25}$	100	—
	Hydrogen plasma (protons and electrons). **Two** variants of the Stark broadening: with the interference term off and on. **Three** variants of the atomic model: no $n \geq 3$ excited states, only 3d^1 excited states, and as complete one as possible.				
12	H Balmer series	6	*	*	*
	Model: Do your best!				

1 Statement of cases

We have selected a number of transitions to consider, given in Table 1. For each transition we are requesting results on a grid of electron densities (n_e) and temperatures ($T = T_e = T_i$). For each case, the atomic and plasma models are specified, and for some cases, there are more than one atomic or plasma model suggested. Unless specified otherwise, plasma is assumed quasi-neutral, consisting of electrons and a single type of ions.

Each calculation will be referenced by its subcase name. The subcase name is of the form Case_ID.N.T.M.F, where Case_ID is from the first column of Table 1, and the N, T, M, and F correspond, respectively, to the n_e, T, model, and external-field (or another atomic feature) indices, each counting from 1.

The models suggested are limited – some by design, others by necessity, to make them manageable without too much computational resources and human time spent.

2 Justification of cases and details

The previous six SLSP workshops have been a great success. We have covered a lot of interesting and physically sound spectral lines in a variety of plasma conditions.

The new topics to be pursued at SLSP7 are van der Waals broadening, motional Stark effect (MSE), and periodic electric fields in the presence of a constant magnetic field.

2.1 Reference cases

The so called "reference" cases, involving simple atomic systems with many simplifying assumptions about the plasma environment, are the baseline of code comparisons. At the previous workshops, various H Lyman and Balmer lines were considered. However, some phenomena (including those considered in the cases below) are absent in neutral radiators. Therefore, singly-ionized hydrogenlike He II lines were added for SLSP6. This time, we deviate further from hydrogen, considering two first Lyman lines in H-like argon. Furthermore, for the first time the "reference" cases include the fine structure.

To avoid complications due to various approaches to plasma coupling in different codes, a pseudo-ideal one-component plasma (PIOCP) model should be used assuming a set of *non-interacting* Debye pseudo particles with a *prescribed* effective screening length $\bar{\lambda}$. Specifically, one should assume 100 particles of each type in an effective Debye sphere, i.e.,

$$\frac{4\pi}{3} n \bar{\lambda}^3 = 100. \tag{1}$$

1. H-like argon Lyman-α.

2. H-like argon Lyman-β.

2.2 The "interference" term

3. Ar XVIII Balmer-α. The simplest H-like transition for which the effect is non-zero. Calculations with and without the interference term should be submitted.

The plasma model remains the same as in the "reference" cases (but only the full, electrons+ions plasma model is used).

2.3 Neutral perturbers

Consider, for the first time in the SLSP workshops, the effect of neutral perturbers (specifically, the van der Waals broadening).

Assume two values of the ionization degree $\alpha = 1\%$ or 10%.

4. He I 447-nm line.

2.4 Motional Stark effect

This is another "for the first time in SLSP" case. The plasma conditions are typical for white dwarf atmospheres [1], for which the MSE due to the *thermal* motion of radiators is expected to be important [2, 3].

5. H Lyman-α

6. H Balmer-β

For each set of plasma parameters and magnetic field, the line shapes should be calculated in three variants: only the "usual" Stark broadening, the MSE, and both effects together.

2.5 Isolated lines

This set of cases is similar to the respective one at SLSP4. That time, no reliable fully QM results were submitted, hence the idea is to repeat the comparison. However, in addition to the SLSP4 variants, calculations with the penetrating collisions are included.

A fairly extensive amount of calculated data is requested, including partial inelastic cross-sections.

For semiclassical models and simulations, these are to be calculated in the following way: The Lth partial wave contribution to the inelastic cross-section of transition from level i to level f ($i \neq f$) is, for a given energy E,

$$\sigma_{if}^{(L)}(E) = \frac{2\pi}{g_i} \int_{R_{min}^{(L)}}^{R_{max}^{(L)}} \rho d\rho \sum_{m_i, m_f} |\langle J_i m_i | T(\rho, E) | J_f m_f \rangle|^2, \tag{2}$$

where g_i is the initial level degeneracy. T may be the S-matrix since the states are different and a square is taken. Different choices of R_{max} and R_{min} are discussed in [4]. A simple one that we adopt here is

$$R_{min}^{(L)} = L \frac{\hbar}{mv}, \tag{3}$$

$$R_{max}^{(L)} = (L+1)\frac{\hbar}{mv}, \tag{4}$$

where $v = \sqrt{2E/m}$. Now, we add calculation of the elastic contribution in the form of pseudo "cross-section" $\tilde{\sigma}$, defined as

$$\tilde{\sigma}_{if}^{(L)}(E) = \frac{2\pi}{g_i g_f} \int_{R_{min}^{(L)}}^{R_{max}^{(L)}} \rho d\rho \sum_{m_i, m_f} |\langle J_i m_i|T(\rho, E)|J_i m_i\rangle - \langle J_f m_f|T(\rho, E)|J_f m_f\rangle|^2. \tag{5}$$

Furthermore, we are looking separately for contributions of so called "weak" and "strong" collisions. The relative "strongness" of a collision is defined based on breaking the perturbative unitarity,

$$\delta_{if}(\rho, E) = \frac{1}{g_i g_f} \left| \sum_{m_i, m_f} [\langle J_i m_i|S(\rho, E)|J_i m_i\rangle \langle J_f m_f|S(\rho, E)|J_f m_f\rangle^* - 1] \right| \tag{6}$$

(e.g., see the unnumbered expression above Eq. (4-46) and arguments in [5]). To make correspondence to $\sigma_{if}^{(L)}(E)$, one should average Eq. (6) over the partial wave "rings", i.e.,

$$\delta_{if}^{(L)}(E) = \frac{2}{\left[R_{max}^{(L)}\right]^2 - \left[R_{min}^{(L)}\right]^2} \int_{R_{min}^{(L)}}^{R_{max}^{(L)}} \rho d\rho\, \delta_{if}(\rho, E). \tag{7}$$

These $\sigma_{if}^{(L)}(E)$, $\tilde{\sigma}_{if}^{(L)}(E)$, and $\delta_{if}^{(L)}(E)$ should be provided at least for L's from 0 through 10 (please go up to 100, if possible). Each of the two species (below) is asked to be calculated for a single representative density. The plasma model for these cases consists only of electrons. Contrary to all other cases, here the electrons should be assumed to have a fixed energy (i.e., **not** a Maxwellian distribution). The width and shift (which are required, too) should also be calculated for the same fixed energy of the electrons. The energy values are listed in the "T" column of Table 1. Please also ignore the Debye screening, but if this is problematic for your calculations, assume screening corresponding to $T_e = E$.

7. Li I – the first, neutral, species in the sequence;

8. B III – one that ignited a long discussion some time ago [6].

2.6 Periodic electric fields

We investigate a simultaneous effect of the plasma microfields, an external harmonic field, and a static magnetic field. The harmonic field is of the form of $\vec{F}\cos(\omega t + \phi)$, where the phase ϕ is assumed random for different radiators (but not changing within the light train formation time for a given radiator) (e.g., see [7]). $\vec{F}$ should be assumed to lie in the z direction, while F, in units of the Holtsmark field F_0, is given in Table 1. The magnetic field $\vec{B}$ is either parallel or perpendicular to $\vec{F}$ (in the later case, assume $\vec{B}$ along the x axis). Assume the harmonic electric field to oscillate with the plasma or upper hybrid frequency, respectively:

$$\omega = \begin{cases} \omega_{pe} & , \vec{F} \parallel \vec{B} \\ \omega_h = \sqrt{\omega_{pe}^2 + \omega_{ce}^2} & , \vec{F} \perp \vec{B} \end{cases}, \tag{8}$$

with

$$\omega_{pe} = \sqrt{4\pi n_e e^2/m_e} \tag{9}$$

and

$$\omega_{ce} = \frac{eB}{m_e c}. \tag{10}$$

9. Balmer-α

10. Balmer-β

2.7 Copper Kα in WDM

In a recent study [8], Cu 1s-2p line spectra from several charge states with open M-shells, emitted from a WDM plasma, were measured. The modeled lineshapes, however, appeared to be significantly narrower. Hence, the challenge is to check whether we can do it better (or agree upon the same result).

11. Cu Kα

2.8 Modeling experimental data

A "real life" type of calculations. The objective of these cases is to discuss in detail how different researchers approach analysis of experimental spectra.

12. The hydrogen Balmer series.

The data are kindly provided by Motoshi Goto and colleagues. The experimental setup is described in Ref. [9]. The instrumental resolution is 1 nm.

Six different spectra are provided. The data can be downloaded as a single archive. It containing both the original spectra (abscissas in the units of nm, ordinates in the units of W/nm, i.e., the volume-integrated radiation power per unit wavelength) and the spectra converted to the wavenumber units. The latter were also area-normalized to unity (fitting intensities in the absolute numbers is beyond the scope of this exercise).

Please note that the experimental data are provided solely for the purpose of this workshop. For any other use, please contact the leading author directly.

3 Atomic data

In all cases, we assume the dipole approximation both for the radiation ($E1$) and the perturbation due to the plasma micro-fields. The relevant matrix elements are

$$\langle \alpha j m | r_q | \alpha' j' m' \rangle = (-1)^{j-m} \begin{pmatrix} j & 1 & j' \\ -m & q & m' \end{pmatrix} (\alpha j \| r \| \alpha' j'), q = 0, \pm 1. \tag{11}$$

The reduced radius-vector matrix elements $(\alpha j \| r \| \alpha' j')$, relevant for the cases considered, are given below. For some cases, quadrupole interaction is also considered. Then similarly, the quadrupole matrix elements are

$$\langle \alpha j m | Q_q | \alpha' j' m' \rangle = (-1)^{j-m} \begin{pmatrix} j & 2 & j' \\ -m & q & m' \end{pmatrix} (\alpha j \| Q \| \alpha' j'), q = 0, \pm 1, \pm 2. \tag{12}$$

3.1 Hydrogen-like

For hydrogen ($Z = 1$) and hydrogen-like cases, the data are to be calculated analytically. For cases where the fine structure is neglected, the binding energies to be assumed are (in atomic units, $1 \, \text{hartree} \approx 27.211 \, \text{eV}$, corresponding to $\approx 2.1947 \times 10^5 \, \text{cm}^{-1}$)

$$E_n^0 = -\frac{Z^2}{2n^2}. \tag{13}$$

When the fine structure is asked to be accounted for, the energies are

$$E_{nj} = E_n^0 - \frac{\alpha^2 Z^4}{2n^3} \left(\frac{1}{j+1/2} - \frac{3}{4n} \right), \tag{14}$$

where $\alpha \approx 7.2974 \times 10^{-3}$ is the fine-structure constant.

Reduced matrix elements of radius-vector are

$$(n\ell \| r \| n'\ell') = (-1)^{\ell+\ell_>} \sqrt{\ell_>} R_{n\ell}^{n'\ell'}, \tag{15}$$

where $\ell_> = \max(\ell, \ell')$ and

$$R_{n\ell}^{n\ell-1} = -\frac{3}{2Z} n \sqrt{n^2 - \ell^2} \tag{16}$$

for diagonal terms (e.g., Eq. (63.5) in [10], but notice the wrong sign there!) and

$$R_{n\ell}^{n'\ell-1} = Z^{-1} \frac{(-1)^{n'-\ell}}{4(2\ell-1)!} \sqrt{\frac{(n+\ell)!(n'+\ell-1)!}{(n-\ell-1)!(n'-\ell)!}} \frac{(4nn')^{\ell+1}(n-n')^{n+n'-2\ell-2}}{(n+n')^{n+n'}} \times$$
$$\left\{ F_{21}\left(-n_r, -n_r', 2\ell, -\frac{4nn'}{(n-n')^2}\right) - \left(\frac{n-n'}{n+n'}\right)^2 F_{21}\left(-n_r-2, -n_r', 2\ell, -\frac{4nn'}{(n-n')^2}\right) \right\} \tag{17}$$

for off-diagonal ones (Eq. (63.2) in [10]). Here, F_{21} is the Gauss hypergeometric function and $n_r = n - \ell - 1$, $n_r' = n' - \ell$ are the radial quantum numbers of the two states. For convenience, the reduced matrix elements up to $n = 5$ are given in Table 2.

Table 2: Hydrogen reduced matrix elements up to $n = 5$. Note that in the SLSP4 version, the $\Delta n \neq 0$ signs were flipped!

	1s	2s	2p	3s	3p	3d	4s	4p	4d	4f	5s	5p	5d	5f
2p	1.29	-5.20												
3s			-0.938											
3p	0.517	3.06		-12.7										
3d			6.71		-14.2									
4s			-0.382		-2.44									
4p	0.305	1.28		5.47		-1.84	-23.2							
4d			2.418		10.7			-29.4						
4f						17.7			-27.5					
5s			-0.228		-0.970			-4.60						
5p	0.209	0.774		2.26		-0.683	8.52		-4.31		-36.7			
5d			1.38		4.20			15.6		-2.88		-48.6		
5f						5.75			24.4				-52.0	
5g										35.4				-45.0

The reduced matrix elements of the quadrupole operator are

$$(n\ell|Q|n'\ell') = (-1)^\ell \sqrt{(2\ell + 1)(2\ell' + 1)} \begin{pmatrix} \ell & 2 & \ell' \\ 0 & 0 & 0 \end{pmatrix} {}^{(2)}R_{n\ell}^{n'\ell'} . \tag{18}$$

For $n = n'$, ${}^{(2)}R_{n\ell}^{n\ell'}$ can be derived using recurrent relations [11]:

$$^{(2)}R_{n\ell}^{n\ell} = \frac{n^2}{2Z^2} \left[5n^2 + 1 - 3\ell(\ell + 1) \right] \tag{19}$$

and

$$^{(2)}R_{n,\ell\pm2}^{n\ell} = \frac{5n^2}{2Z^2} \sqrt{(n^2 - \ell_>^2) \left[n^2 - (\ell_> - 1)^2 \right]} . \tag{20}$$

3.2 Isolated lines

The data are taken from the NIST on-line compilation [12]. The level energies, averaged over the fine-structure components for $\ell > 0$, are given in Table 3. The absolute values of the matrix elements are obtained from the respective multiplet-averaged absorption oscillator strengths f according to

$$|(n\ell|r|n'\ell')| = \sqrt{\frac{3f(2\ell' + 1)}{2(E_{n\ell} - E_{n'\ell'})}} , \tag{21}$$

and sign as in respective H-like from Eqs. (15) – (17). The data are summarized in Table 4.

Table 3: Atomic level energies for non-hydrogenic lines.

Species	Level	Energy (cm^{-1})
He I	2p (^{3}P^0)	169086.91
	4p (^{3}P^0)	191217.06
	4d (^{3}D^0)	191444.48
	4f (^{3}F^0)	191451.88
Li I	2s	0.00
	2p	14903.89
B III	2s	0.00
	2p	48381.07

Table 4: Oscillator strengths for non-hydrogenic lines.

Species	Transition	f
He I	2p (^{3}P^0) — 4d (^{3}D^0)	1.23e-1
	4p (^{3}P^0) — 4d (^{3}D^0)	2.01e-1
	4d (^{3}D^0) — 4f (^{3}F^0)	2.99e-3
Li I	2s — 2p	7.47e-1
B III	2s — 2p	3.63e-1

The quadrupole reduced matrix elements, needed for cases 7.*.*.2.1 and 8.*.*.2.1 are given in Table 5. These data were calculated with the R. D. Cowan's code [13].

Table 5: Quadrupole reduced radial matrix elements for non-hydrogenic species.

Species	Transition	$(|Q|)$
Li I	2p — 2p	−30.48
B III	2p — 2p	−3.328

3.3 Van der Waals broadening

For the vdW broadening (case 4), assume all He neutrals have a *randomly* oriented dipole moment with the absolute value of $d = 4\,\mathrm{a.u.}$

4 Submission format

We use an XML-based format for submissions, with an example shown schematically in Listing 1.

Listing 1: An example of submission.

```xml
<?xml version="1.0"?>
<slsp>
  <case>1.1.1.3.1</case>
  <contributor>E. Stambulchik</contributor>
  <affiliation>WIS</affiliation>
  <code>simu</code>
  <version>1.9.0/1.4.0</version>
  <date>2011-12-13 18:34:39</date>

  <comments>
      These are my comments on this calculation.
  </comments>

  <time1>6.826e-11</time1>
  <nruns>400</nruns>

  <accuracy>-10 +5</accuracy>

  <field_distribution unit="128196">
     0.000000 0.000000
     0.025000 0.000421
     0.075000 0.002919
      ...
      ...
     29.875000 0.000333
     29.925000 0.000324
     29.975000 0.000316
  </field_distribution>

  <spectrum unit="1">
     -200.0 0.000741852
     -199.8 0.000751194
     -199.6 0.000747932
      ...
      ...
     199.6 0.000738701
     199.8 0.000752916
     200.0 0.000735306
  </spectrum>
</slsp>
```

Everything is included between the `<slsp>` and `</slsp>` tags. The meaning of other tags is described below:

`<case>` The subcase identification in the Case_ID.N.T.M.F format, see Sec. 1.

`<contributor>` The person who submits these results.

`<affiliation>` His/her affiliation.

`<code>` Name of the code/approach.

`<version>` Version of the code (optional).

`<date>` Date/time when the calculations were made.

`<comments>` Any comments you may like to make. The comments are optional, **except for fitting experimental data)**. In these cases, please describe the model employed with sufficient details. If the comments must contain "<" or "&" characters, enclose the entire text with "<![CDATA[" and "]]>":

```
<comments><![CDATA[
   Some  bizarre  & < >  comments .
]]></comments>
```

`<time1>` Physical time (not CPU!), in seconds, the evolution of the atomic system is calculated for in a single run. (This and the following entry are specific for MD simulations. When irrelevant, skip or set to zero.)

`<nruns>` Number of runs used for averaging.

`<accuracy>` The estimated accuracy (in %) of the calculations, say of the FWHM. Only uncertainties introduced by the calculations should be included (in particular, not those due to an idealized/simplified plasma or atomic models suggested for this specific case). If the error bars are asymmetric, list two numbers with proper signs.

`<spectrum>` For all cases **except those concerned with isolated lines (7 – 8)**, we ask to provide entire line shapes on a reasonably dense grid, typically ~ 1000 points (see Table 6). When the spectral range is symmetric ($\pm$ something), it means relative to the unperturbed position ω_0, calculated as a difference between the weighted-average energies of the initial and final levels:

$$\hbar\omega_0 = \frac{\sum_i g_i E_i}{\sum_i g_i} - \frac{\sum_f g_f E_f}{\sum_f g_f} \,. \tag{22}$$

The spectral windows and distances between the consecutive abscissas defined are recommended values. The relatively wide spectral windows are defined on purpose, to investigate far wings of the spectral lines. You can use denser and/or wider grids as you see fit. It is suggested to use equidistant grids. The units are cm^{-1}. The optional `unit` attribute allows for scaling the abscissas, e.g., by using `unit="8065.5"` one can output spectra in eV's. Where the spectra are requested and external fields specified the π ($\Delta M = 0$) and σ ($\Delta M = \pm 1$) polarizations will be needed separately (to be provided as the second and third columns, respectively):

```
  ...
  ...
  <spectrum>
    w_1  I_pi(w_1)  I_sigma(w_1)
    w_2  I_pi(w_2)  I_sigma(w_2)
    ...
    ...
    w_N  I_pi(w_N)  I_sigma(w_N)
  </spectrum>
  ...
  ...
```

It is assumed that

$$I_{\mathrm{tot}}(\omega) = I_\pi(\omega) + 2I_\sigma(\omega) \,. \tag{23}$$

In all cases, no normalization condition is imposed, but do preserve correct ratio between I_π and I_σ.

`<field_distribution>` Quasi-static field distribution (normalized) used for the calculation (due to all plasma particles, but excluding external fields, if any). The fields are in V/cm. The optional `unit` attribute allows for scaling the field strength values conveniently, e.g., by setting it to the Holtsmark normal field strength F_0 one obtains the distribution of the reduced field strengths. The distributions should be calculated on an equidistant grid covering at least $0 - 10$ with a step not exceeding 0.1 (in units of F_0).

`<width>` FWHM, **for isolated lines only (cases 7 and 8)**. In units of cm^{-1}.

`<shift>` Shift, for the same cases. In units of cm^{-1}.

`<fit_n_e>` Best-fit n_e used for the calculations, **only for the "experimental" cases**.

`<fit_T>` Best-fit T used for the calculations, **only for the 'experimental" cases**.

`<partial_xs>` Partial cross-sections; these are also specific to the 7 and 8 cases. The format is

Table 6: Recommended spectral grids.

Subcase	Spectral range (cm^{-1})	Step (cm^{-1})
1.1.*.*.*	$\pm 1e5$	100
1.2.*.*.*	$\pm 4e5$	400
1.3.*.*.*	$\pm 2e6$	2000
2.1.*.*.*	$\pm 5e5$	500
2.2.*.*.*	$\pm 2e6$	2000
2.3.*.*.*	$\pm 1e7$	1e4
3.1.*.*.*	$\pm 2e5$	200
3.2.*.*.*	$\pm 1e6$	1000
3.3.*.*.*	$\pm 4e6$	4000
4.1.*.*.*	± 1500	1.5
4.2.*.*.*	± 5000	5
5.1.*.*.1	± 100	0.1
5.1.*.*.2	± 600	0.1
5.1.*.*.3	± 6000	0.1
6.1.*.*.1	± 1000	1
6.1.*.*.2	± 2000	1
6.1.*.*.3	± 20000	1
9.1.*.*.*	± 30	0.03
10.1.*.*.*	± 100	0.1
11.1.*.*.*	$\pm 2e5$	500
11.2.*.*.*	$\pm 5e5$	1000
11.3.*.*.*	$\pm 2e6$	2000
12.1.1.1.1	14,000–27,000	10

```
   ...
   ...
 <partial_xs>
   L_1  sigma_e(L_1)  sigma_d(L_1)  sigma_el(L_1)  delta(L_1)
   L_2  sigma_e(L_2)  sigma_d(L_2)  sigma_el(L_2)  delta(L_2)
   ...
   ...
   L_N  sigma_e(L_N)  sigma_d(L_N)  sigma_el(L_N)  delta(L_N)
 </partial_xs>
   ...
   ...
```

For each L, partial excitation and de-excitation (for the same *incident* energy) cross-sections should be listed in the second and third columns, respectively [see Eq. (2) for semiclassical calculations and simulations]. The fourth column is the elastic "cross-section", Eq. (5). The units are cm^2. Finally, the last column is the measure indicating how "strong" collisions of the given partial wave are, Eq. (7).

References

[1] D. Saumon, S. Blouin, and P.-E. Tremblay. Current challenges in the physics of white dwarf stars. *Physics Reports*, 988:1–63, November 2022. `doi:10.1016/j.physrep.2022.09.001`.

[2] J. Rosato. Effect of collisions on motional Stark broadening of spectral lines. *J. Quant. Spectrosc. Radiat. Transfer*, 306:108628, September 2023. `doi:10.1016/j.jqsrt.2023.108628`.

[3] T. A. Gomez, M. C. Zammit, C. J. Fontes, and J. R. White. A quantum-mechanical treatment of electron broadening in strong magnetic fields. *Astrophys. J.*, 951(2):143, July 2023. `doi:10.3847/1538-4357/acda28`.

[4] S. Alexiou, R. W. Lee, S. H. Glenzer, and J. I. Castor. Analysis of discrepancies between quantal and semiclassical calculations of electron impact broadening in plasmas. *J. Quant. Spectrosc. Radiat. Transfer*, 65(1–3):15–22, 2000. `doi:10.1016/S0022-4073(99)00051-5`.

[5] H. R. Griem. *Plasma spectroscopy*. McGraw-Hill Book Company, New York, 1964.

[6] H. R. Griem, Yu. V. Ralchenko, and I. Bray. Stark broadening of the B III $2s - 2p$ lines. *Phys. Rev. E*, 56(6):7186–7192, 1997. `doi:10.1103/PhysRevE.56.7186`.

[7] I. Hannachi, R. Stamm, J. Rosato, and Y. Marandet. Calculating the simultaneous effect of ion dynamics and oscillating electric fields on Stark profiles. *Advances in Space Research*, December 2021. `doi:10.1016/j.asr.2021.12.009`.

[8] S. X. Hu, D. T. Bishel, D. A. Chin, P. M. Nilson, V. V. Karasiev, I. E. Golovkin, M. Gu, S. B. Hansen, D. I. Mihaylov, N. R. Shaffer, S. Zhang, and T. Walton. Probing atomic physics at ultrahigh pressure using laser-driven implosions. *Nat. Commun.*, 13(1):6780, November 2022. `doi:10.1038/s41467-022-34618-6`.

[9] M. Goto, G. Motojima, R. Sakamoto, B. Pégourié, A. Matsuyama, T. Oishi, T. Kawate, and Y. Kawamoto. Better understanding of hydrogen pellet ablation cloud spectra through the occupation probability formalism in LHD. *Atoms*, 12(1):1, January 2024. `doi:10.3390/atoms12010001`.

[10] H. A. Bethe and E. E. Salpeter. *Quantum Mechanics of One- and Two-Electron Atoms*. Plenum, New York, 1977.

[11] J. D. Hey. On the determination of radial matrix elements for high-n transitions in hydrogenic atoms and ions. *J. Phys. B: At. Mol. Opt. Phys.*, 39(12):2641, 2006. `doi:10.1088/0953-4075/39/12/003`.

[12] NIST Atomic Spectra Database. URL: `http://physics.nist.gov/asd/`, `doi:10.18434/T4W30F`.

[13] R. D. Cowan. *The Theory of Atomic Structure and Spectra*. University of California Press, Berkeley – Los Angeles – London, 1981.