4th Spectral Line Shapes in Plasmas
Code Comparison Workshop

March 20–24, 2017

Baden, Austria

Call for Submissions (rev. March 8, 2017)

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 data files that we will be expecting.

The webpage of the meeting is at http://plasma-gate.weizmann.ac.il/slsp4/. 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 (2017):

January 22	—	web interface for file uploads opens
February 19	—	hotel booking deadline
March 5	—	submission deadline
March 20	—	workshop opens
March 24	—	workshop adjourns

Contents

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 ($T = T_\mathrm{e} = T_\mathrm{i}$). 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 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. If you feel that the best suggested model for a particular case is still too far from reality, you are encouraged to submit a separate result using an alternative model you see fit best, using "0" as the model index. Submissions of all such results should include an adequate description of the model used in the `<comments>` field of the file (see Sec. 4).

2 Justification of cases and details

The first [1], second ([2] and references therein), and third [**?**] SLSP workshops were a great success. We have covered a lot of interesting and physically sound spectral lines in a variety of plasma conditions.

The spread of results for some of the cases of SLSP1&2 demanded a deeper investigation, which was a focus at SLSP3. This detailed "debugging" will continue at SLSP4. There will also be new (for SLSP) topics, such as the quadrupole effects and influence of the magnetic field on the trajectories of plasma particles.

Following the SLSP2 & SLSP3 example, we also continue with the "experimental" cases, suggesting to interpret real-life spectroscopic data.

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. This time, like at SLSP2&3, the lines are hydrogen Lyman-α and Lyman-β. The "ideal" one-component plasma (OCP) model, extensively prescribed for many cases in the previous workshops, turned out [3] to be potentially problematic for computer simulations, as confirmed by specially crafted cases at SLSP3, due to a formally infinite Debye length. To avoid this issue, for this workhop an effective screening will be prescribed. This pseudo-ideal OCP (PIOCP) model assumes a set of *non-interacting* Debye pseudo particles with a fixed effective screening length $\bar{\lambda}$ to avoid the problem of very slow convergence of the impact width with the number of particles. Specifically, one should assume 100 particles in an effective Debye sphere, i.e.,

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

1. Hydrogen Lyman-α in an ideal plasma is a classical ion-dynamics test. This time, we hope to observe convergence between simulations and analytical models...

2. Hydrogen Lyman-β. Similarly to the previous case, but now a line with no central component.

2.2 Quadrupole corrections in H-like

Interest to quadrupole (in general, higher-than-dipole multipole) contributions to the Stark broadening has recently resurfaced [4], indicating an importance of these type of corrections. Since this is the first time the phenomenon is analyzed at SLSP, the atomic transitions are again selected to be the simplest ones—hydrogen Lyman-α and Lyman-β. Furthermore, the plasma model remains the same as in the "reference" cases, with the parameters as a strict subset:
$n_e = 10^{18}$ & $10^{19}\,\mathrm{cm}^{-3}$, $T = 1$ & $10\,\mathrm{eV}$.

3. Lyman-α with dipole and quadrupole effects ($\Delta n = 0$).

4. Lyman-β with dipole and quadrupole effects ($\Delta n = 0$).

Finally, the quadrupole and quadratic effects are believed to often be comparable. Thus, the following two cases, otherwise identical, respectively, to cases 3 and 4, add these corrections. For simplicity, we restrict the expansion of the basis sets to states with $n = 3$ and $n = 4$, respectively.

Table 1: Case definitions.

ID	Transition(s)	# of subcases	n_e (cm^{-3})	T (eV)	Extra parameters
1	H Lyman-α	$3 \times 3 \times 3 \times 1 = 27$	10^{17}, 10^{18}, 10^{19}	1, 10, 100	—
			Model: $\Delta n \neq 0$ dipole interactions ignored (strictly linear Stark effect); no fine structure; straight path trajectories of Debye quasiparticles in **three** variants: only electrons, only protons, and electrons and protons together.		
2	H Lyman-β	$3 \times 3 \times 3 \times 1 = 27$	10^{17}, 10^{18}, 10^{19}	1, 10, 100	—
			Model: Same as above.		
3	H Lyman-α	$2 \times 2 \times 3 \times 1 = 12$	10^{18}, 10^{19}	1, 10	—
			Model: Same as above, but with quadrupole interactions included.		
4	H Lyman-β	$2 \times 2 \times 3 \times 1 = 12$	10^{18}, 10^{19}	1, 10	—
			Model: Same as above.		
5	H Lyman-α	$2 \times 2 \times 3 \times 1 = 12$	10^{18}, 10^{19}	1, 10	—
			Model: Same as above, but with $\Delta n = 1$ couplings included.		
6	H Lyman-β	$2 \times 2 \times 3 \times 1 = 12$	10^{18}, 10^{19}	1, 10	—
			Model: Same as above.		
7	Mg XI He-γ	$1 \times 1 \times 2 \times 1 = 2$	3×10^{22}	180	—
			Plasma model: Only electrons are accounted for. Two variants of the atomic model: without and with $\Delta n \neq 0$ interactions.		
8	Li I 2s–2p	$1 \times 6 \times 2 \times 1 = 12$	10^{17}	1, 2, 5, 10, 20, 50	—
			Model: 2s and 2p levels included, no fine structure. Only **fixed-energy** electron broadening is included. No Debye screening. Two variants of calculations: only dipole or dipole + quadrupole interactions.		
9	B III 2s–2p	$1 \times 6 \times 2 \times 1 = 12$	10^{18}	4, 7, 10, 20, 50, 100	—
			Model: Same as above.		
10	H Lyman-α	$1 \times 1 \times 3 \times 3 = 7$	10^{17}	5	$B = 0, 100, 200\,\mathrm{T}$
			Model: No fine structure. Electron OCP, no ions. For non-zero B, three variants of calculations (see the case description).		
11	H Ly-10	$1 \times 1 \times 3 \times 3 = 7$	10^{13}	1	$B = 0, 10, 20\,\mathrm{T}$
			Model: Same as above		
12	O VIII Lyman-α	$4 \times 2 \times 2 \times 3 = 48$	10^{20}, 2×10^{20}, 10^{21}, 2×10^{21} (see note)	100, 200	$\omega = 2.5 \times 10^{15}\,\mathrm{rad/s}$, $F = 0, 1, 2\,\mathrm{GV/cm}$
			Model: fine structure included, plasma ions: O nuclei, in **two** variants: either treating ions as static non-screened ones (Holtsmark) or realistic plasma (as realistically as your model can...).		
13	H $n = * \to 2$	$3 \times 1 \times 2 \times 1 = 6$	3×10^{17}, 10^{18}, 3×10^{18}	1	—
			Model: fully ionized H plasma, **two** variants: only bound–bound transitions included or both bound–bound and free–bound. Assume LTE populations.		
14	H Balmer-β	$2 \times 3 \times 1 \times 1 = 6$	10^{15}, 10^{16}	0.1, 0.2, 0.4	—
			Model: $n = 2$ and $n = 4$ states, no fine structure; helium plasma.		
14a	H Balmer-β	1	*	*	*
14b	H Balmer-β	1	*	*	*
14c	H Balmer-β	1	*	*	*
14d	H Balmer-β	1	*	*	*
14e	H Balmer-β	1	*	*	*
14f	H Balmer-β	1	*	*	*
			Model: Do your best (but in sync with 15a–f)!		
15	He I 492 nm	$2 \times 3 \times 1 \times 1 = 6$	10^{15}, 10^{16}	0.1, 0.2, 0.4	—
			Model: $2p$ and $4p$, d, f singlet levels included; helium plasma.		
15a	He I 492 nm	1	*	*	*
15b	He I 492 nm	1	*	*	*
15c	He I 492 nm	1	*	*	*
15d	He I 492 nm	1	*	*	*
15e	He I 492 nm	1	*	*	*
15f	He I 492 nm	1	*	*	*
			Model: Do your best (but in sync with 14a–f)!		
16	Cr XXIII He-β	$2 \times 1 \times 2 \times 1 = 4$	2×10^{24}, 4×10^{24}	2000	—
			Model: without and with Li-like satellites included; chromium plasma under LTE.		
16a	Cr XXIII He-β	1	*	*	*
			Model: Do your best!		

5. Lyman-α with dipole and quadrupole effects ($\Delta n \leq 1$).

6. Lyman-β with dipole and quadrupole effects ($\Delta n \leq 1$).

Please note that all cases below do NOT assume an ideal plasma, unless explicitly said so.

2.3 Electron impact broadening

Here it is proposed to compare electron broadening calculated with different models/approximations. The case of interest is Mg lines at $T = 180\,\mathrm{eV}$ and $n_e = 3 \times 10^{22}\,\mathrm{cm}^{-3}$ since these were used for the plasma diagnostics of the Fe opacity measurements [5]. Specifically, the line is Mg He-γ due to its potential model dependence [6, 7].

7. He-γ line of Mg XI, only electron broadening. Two variants of calculation, (i) only with $\Delta n = 0$ interactions and (ii) including effects of mixing with $n = 5$ levels.

2.4 Isolated lines

$\Delta n = 0$ transitions in Li-like species present a puzzle by disagreement between experimental and different theoretical calculations [8]. For the first SLSP meeting, the Li-like 3s–3p isoelectronic sequence was considered, while for the second one, the 2s–2p resonance lines of the same sequence were calculated. At SLSP3, the study was continued with a deeper analysis of the 2s–2p series, asking, for the first time, to provide 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 [9]. 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 [10]). 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 $T_e = E$.

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

9. B III – one that ignited a long discussion some time ago [11].

Each calculation will be done in two variants—only dipoles (as usual), or dipoles and quadrupoles together.

2.5 External fields

The external macro fields (both electric and magnetic) are always assumed to be parallel to the z axis.

2.5.1 B-induced trajectory effects

There are claims [12] about strong influence on Zeeman patterns through modifications of the electron trajectories ("spiraling") due to the magnetic field. We are going to test this phenomenon.

One-component electron plasma will be assumed for these cases. For non-zero magnetic field, three variants of its inclusion will be calculated: (i) the "standard" one, V_B is included in the radiator Hamiltonian, but no influence on the electron trajectories, (ii) only trajectories are affected, but no direct effect on the radiator, and (iii) "full" calculations.

10. Lyman-α. Typical "white dwarf" conditions: $n_e = 10^{17}\,\mathrm{cm}^{-3}$, $T = 5\,\mathrm{eV}$, $B = 0, 100, 200\,\mathrm{T}$.

11. Lyman-10. Typical "tokamak edge" conditions: $n_e = 10^{13}\,\mathrm{cm}^{-3}$, $T = 1\,\mathrm{eV}$, $B = 0, 10, 20\,\mathrm{T}$

2.5.2 Harmonic fields

12. O VIII Lyman-α under external harmonic perturbation. The functional dependence of the electric field is $F\cos(\omega t)$, with ω and F given in Table 1. The parameters chosen are similar to ones inferred in [13]. The atomic model includes fine structure. We will see whether a realistic treatment of plasma ions is important here. Please note that in the original revision of this document, the density values were mistakenly typed one order of magnitude smaller than intended ($\sim 10^{20}\,\mathrm{cm}^{-3}$ instead of $\sim 10^{21}\,\mathrm{cm}^{-3}$). To avoid the confusion with subcase numbering, the correct values are added to the list of densities, instead of replacing. Therefore, the real subcases of interest are 12.3.*.*.* and 12.4.*.*.* .

2.6 Ionization potential depression

Spectroscopy-wise, discrete transitions start to overlap between themselves and the free–bound continuum. A broad spectral region will be analyzed covering both discrete and continuum spectrum and a transition region in between.

13. H Balmer series at $T = 1\,\mathrm{eV}$ and three densities from 3×10^{17} to $3\times10^{18}\,\mathrm{cm}^{-3}$. Assume LTE level populations, but please do **not** include the trivial $\exp(-\hbar\omega/T)$ factor in the spectrum output (this corresponds to the equal bound-state populations). The suggested spectral range (see Table 6) for this case covers transitions from Balmer-α to continuum.

2.7 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. To have a better understanding of why different approaches might end up with different best-fit plasma parameters, we also ask to calculate the relevant line shapes on a small predefined grid of parameters.

For these calculations (on the predefined grid), please submit only the Stark-broadened profiles, i.e., no Doppler broadening etc, while in the "best-fit" subcases (14a–f, 15a–f, 16a), include any relevant effects. Please note that the experimental data are unpublished, and are provided solely for the purpose of this workshop. For any other use, please contact the authors (see below) directly.

14. Hydrogen Balmer-β and He I 492-nm line were simultaneously observed at a low-temperature corona discharges in helium. A poster paper with details of the experiment is attached. The challenge here is to find the plasma parameters satisfying profiles of the two lines *simultaneously*. Cases 14a–f correspond to cases 15a–f, respectively.

    ICSLS-2016 poster paper describing the experiment: exp_H_He.pdf

Experimental spectrum of Balmer-β, pressure 1 bar (case 14a): exp_H_Hea.dat

Experimental spectrum of Balmer-β, pressure 1.5 bar (case 14b): exp_H_Heb.dat

Experimental spectrum of Balmer-β, pressure 2 bar (case 14c): exp_H_Hec.dat

Experimental spectrum of Balmer-β, pressure 3 bar (case 14d): exp_H_Hed.dat

Experimental spectrum of Balmer-β, pressure 4 bar (case 14e): exp_H_Hee.dat

Experimental spectrum of Balmer-β, pressure 5 bar (case 14f): exp_H_Hef.dat

The data were kindly provided by Nelly Bonifaci and her colleagues. Units: nm.

15. The He I 492-nm counterpart to case 14.

16. Spectrum of the $n = 3 \to n = 1$ emission of He-like chromium, together with its Li-like satellites. The experiment was performed at the Orion laser facility, where a chromium foil was hit by a 1-ps, 82-J laser pulse yielding a $2.45 \times 10^{19}\,\mathrm{W/cm^2}$ irradiation intensity [14].

Exp. spectrum of Cr XXIII He-β with Li-like satellites (case 16a): exp_CrXXIIIa.dat

The data were kindly provided by Peter Beiersdorfer and his colleagues. Units: eV.

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

$$\langle \alpha j m | r_q | \alpha' j' m' \rangle = (-1)^{j-m} \begin{pmatrix} j & 1 & j' \\ -m & q & m' \end{pmatrix} (\alpha j | r | \alpha' j') \,, q = 0, \pm 1 \,. \tag{8}$$

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

$$\langle \alpha j m | Q_q | \alpha' j' m' \rangle = (-1)^{j-m} \begin{pmatrix} j & 2 & j' \\ -m & q & m' \end{pmatrix} (\alpha j | Q | \alpha' j') \,, q = 0, \pm 1, \pm 2 \,. \tag{9}$$

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, $1\,\mathrm{hartree} \approx 27.211\,\mathrm{eV}$, corresponding to $\approx 2.1947 \times 10^5\,\mathrm{cm^{-1}}$)

$$E_n^0 = -\frac{Z^2}{2n^2} \,. \tag{10}$$

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

$$E_{nj} = E_n^0 - \frac{\alpha^2 Z^4}{2n^3} \left(\frac{1}{j + 1/2} - \frac{3}{4n} \right) \,, \tag{11}$$

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

Reduced matrix elements of radius-vector are

$$(n\ell | r | n'\ell') = (-1)^{\ell + \ell_>} \sqrt{\ell_>} R_{n\ell}^{n'\ell'} \,, \tag{12}$$

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

$$R_{n\ell}^{n\ell-1} = -\frac{3}{2Z} n \sqrt{n^2 - \ell^2} \tag{13}$$

for diagonal terms (e.g., Eq. (63.5) in [15], but notice the wrong sign there!) and

$$R_{n\ell}^{n'\ell-1} = Z^{-1} \frac{(-1)^{n'-\ell}}{4(2\ell-1)!} \sqrt{\frac{(n+\ell)!(n'+\ell-1)!}{(n-\ell-1)!(n'-\ell)!}} \frac{(4nn')^{\ell+1}(n-n')^{n+n'-2\ell-2}}{(n+n')^{n+n'}} \times$$
$$\left\{ F_{21}\left(-n_r, -n'_r, 2\ell, -\frac{4nn'}{(n-n')^2}\right) - \left(\frac{n-n'}{n+n'}\right)^2 F_{21}\left(-n_r - 2, -n'_r, 2\ell, -\frac{4nn'}{(n-n')^2}\right) \right\} \tag{14}$$

Table 2: Hydrogen reduced matrix elements up to $n = 5$.

	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

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

Species	Level	Energy (cm^{-1})
Li I	2s	0.00
	2p	14903.89
B III	2s	0.00
	2p	48381.07
He I	2p (^{1}P)	171134.897
	4d (^{1}D)	191446.456
	4f (^{1}F)	191451.897
	4p (^{1}P)	191492.712

for off-diagonal ones (Eq. (63.2) in [15]). 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.

The reduced matrix elements of the quadrupole operator are

$$(n\ell|Q|n'\ell') = (-1)^{\ell}\sqrt{(2\ell+1)(2\ell'+1)}\begin{pmatrix} \ell & 2 & \ell' \\ 0 & 0 & 0 \end{pmatrix} {}^{(2)}R^{n'\ell'}_{n\ell}\,. \tag{15}$$

For $n = n'$, ${}^{(2)}R^{n\ell'}_{n\ell}$ can be derived using recurrent relations [16]:

$${}^{(2)}R^{n\ell}_{n\ell} = \frac{n^2}{2Z^2}\left[5n^2 + 1 - 3\ell(\ell+1)\right] \tag{16}$$

and

$${}^{(2)}R^{n\ell}_{n,\ell\pm2} = \frac{5n^2}{2Z^2}\sqrt{(n^2-\ell_>^2)\left[n^2-(\ell_>-1)^2\right]}\,. \tag{17}$$

3.2 Non-hydrogen

The data are taken from the NIST on-line compilation [17]. 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

$$|(n\ell|r|n'\ell')| = \sqrt{\frac{3f(2\ell'+1)}{2(E_{n\ell}-E_{n'\ell'})}}\,, \tag{18}$$

and sign as in respective H-like from Eqs. (12 – 14). The data are summarized in Table 4.

The quadrupole reduced matrix elements, needed for cases 8.*.*.2.1 and 9.*.*.2.1 are given in Table 5. These data were calculated with the R. D. Cowan's code [18].

3.3 Data for case 7

Attached is the Cowan's [18] atomic data for Mg XI.

Table 4: Oscillator strengths for non-hydrogenic lines.

Species	Transition	f
Li I	2s — 2p	7.472e-1
B III	2s — 2p	3.629e-1
He I	2p (^{1}P) — 4d (^{1}D)	1.203e-1
	4d (^{1}D) — 4p (^{1}P)	2.390e-2
	4d (^{1}D) — 4f (^{1}F)	1.596e-3

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

Data for case 7 : Mg_XI.dat

The file has two blocks: i) energy levels and ii) transitions. In the energy level block, the first column is the level index, and the last column is the state energy in kilo kayser (10^3 cm^{-1}). In the transition block,

1st—transition index
2nd—upper state index
3rd—lower state index
4th—electric dipole moment
5th—transition energy (k kayser)
6th—transition energy (eV)
7th—transition wavelength (angstrom)

4 Submission format

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

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 advanced models (M=0 in the subcase id) and fitting experimental data (cases 16* and 14*)**. In the later 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.

Listing 1: An example of submission.

```
<?xml version="1.0"?>
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  <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>

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  <nruns>400</nruns>

  <accuracy>-10 +5</accuracy>

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    0.025000 0.000421
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      ...
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    29.975000 0.000316
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  <spectrum unit="1">
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    -199.8 0.000751194
    -199.6 0.000747932
      ...
      ...
    199.6 0.000738701
    199.8 0.000752916
    200.0 0.000735306
  </spectrum>
</slsp>
```

`<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 (8 – 9)**, 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:

$$\hbar\omega_0 = \frac{\sum_i g_i E_i}{\sum_i g_i} - \frac{\sum_f g_f E_f}{\sum_f g_f} \,. \tag{19}$$

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

$$I_{\mathrm{tot}}(\omega) = I_\pi(\omega) + 2I_\sigma(\omega) \,. \tag{20}$$

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 8 and 9)**. In units of cm^{-1}.

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

`<partial_xs>` Partial cross-sections; these are also specific to the 8 and 9 cases. The format is

```
...
...
<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).

Table 6: Recommended spectral grids.

Subcase	Spectral range (cm^{-1})	Step (cm^{-1})
1.1.*.*.*	$\pm$ 200	0.2
1.2.*.*.*	$\pm$ 1,000	1
1.3.*.*.*	$\pm$ 5,000	5
2.1.*.*.*	$\pm$ 1,000	2
2.2.*.*.*	$\pm$ 5,000	20
2.3.*.*.*	$\pm$ 25,000	100
3.1.*.*.*	$\pm$ 1,000	1
3.2.*.*.*	$\pm$ 5,000	5
4.1.*.*.*	$\pm$ 5,000	20
4.2.*.*.*	$\pm$ 25,000	100
5.1.*.*.*	$\pm$ 1,000	1
5.2.*.*.*	$\pm$ 5,000	5
6.1.*.*.*	$\pm$ 5,000	20
6.2.*.*.*	$\pm$ 25,000	100
7.*.*.*.*	$\pm$ 500,000	2,000
10.*.*.*.*	$\pm$ 200	0.2
11.*.*.*.*	$\pm$ 30	0.1
12.*.*.*.*	$\pm$ 30,000	150
13.*.*.*.*	$(1.3 - 3.0) \times 10^4$	5
14.1.*.*.*	$\pm$ 100	0.25
14.2.*.*.*	$\pm$ 400	1
15.1.*.*.*	$\pm$ 100	0.25
15.2.*.*.*	$\pm$ 400	1
16.*.*.*.*	$\pm$ 10^6	1000

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