Virtual Laboratory Astrophysics: the STARK-B database for spectral line broadening by collisions with charged particles and its link to the European project VAMDC

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Abstract. Atomic physics in plasmas has been an essential tool for many years. Accurate spectroscopic diagnostics and modeling require the knowledge of numerous collisional line profiles. “Stark broadening” theories and calculations have been extensively developed for about 50 years. Nowadays, the access to such data via an on line database becomes essential. The aim of STARK-B is to reply to this need. It is a collaborative project between the Astronomical Observatory of Belgrade (AOB) and the “Laboratoire d’Etude du Rayonnement et de la Matière en Astrophysique” (LERMA) of the Paris Observatory and CNRS. It is a database of widths and shifts of isolated lines of atoms and ions due to electron and ion impacts that we have calculated and published in international refereed journals (more than 150 papers by Dimitrijević & Sahal-Bréchot, and colleagues). It is devoted to modeling and spectroscopic diagnostics of stellar atmospheres and envelopes, laboratory plasmas, magnetic fusion plasmas, laser equipments and technological plasmas. Hence, the domain of temperatures and densities covered by the tables is wide and depends on the ionization degree of the considered ion. The STARK-B database is in free access and is a part of VAMDC: the Virtual Atomic and Molecular Data Centre is an European Union funded collaboration between groups involved in the generation and use of atomic and molecular data. VAMDC aims to build a secure, documented, flexible and interoperable e-science environment-based interface to existing atomic and molecular data. STARK-B and its VAMDC context are presented in this paper.

1. Introduction
Pressure broadening of spectral lines arises when an atom or a molecule which emits or absorbs light in a gas or in a plasma, is perturbed by its interactions with the other particles of the medium. An atom or a molecule may be neutral as well as charged. The so-called Stark broadening is due to electron and ion colliders. The theory has been extensively developed for about 50 years and is currently used for many spectroscopic diagnostics and modeling. A number of its developments have been stimulated by the advances in Astrophysics, by the needs in laboratory and technological plasmas (tokamaks, laser produced plasmas, inertial fusion plasmas...), and also by the needs in industrial plasmas (discharge lighting). Due to the developments of the accuracy of observations in astrophysics and laboratory physics, many needs of atomic data appear at the end of the 20th century, and the needs are constantly...
increasing. Hence, calculations based on a simple but enough accurate and fast methods are necessary for obtaining numerous results. Furthermore, the development of powerful computers also stimulates the development of atomic data on a large scale. Besides, the access to these atomic data via on line databases becomes essential.

In section 2, we will recall the physical conditions where Stark broadening plays a role in different plasmas. Section 3 will be devoted to a brief review of the standard impact Stark broadening theory that is at the basis of the theory, calculations and the database presented in the present paper. In fact, Dimitrijević and Sahal-Bréchot have updated and operated at a large scale the numerical code (SCP) created by Sahal-Bréchot since about thirty years. This code is based on the impact semiclassical-perturbation theory for isolated spectral lines of neutral and ionized atoms broadened and shifted by collisions with electrons and ions, [1] [2] [3] [4]. More than 150 papers are issued from the first update [5]. Then, the new need of creation of an on-line database appeared in the beginning of the 21st century, particularly in correlation with the birth and the growth of virtual Observatories and to the increasing need of exchange of interoperable data. Thus, the database STARK-B (formerly called BELDATA) was initiated in the Astronomical Observatory of Belgrade (AOB), and then a collaborative project between AOB and LERMA was born and led to the present database. STARK B, which is in free access, is currently developed at Paris Observatory and has opened on line since the end of 2008 (http://stark-b.obspm.fr [6]), and now contains the published data of all our papers obtained through the SCP theory and code. It is a part of the atomic and molecular databases of the Paris Observatory, and there is a link to the Serbian Virtual Observatory (SerVO, http://servo.aob.rs/~darko). A mirror site is planned at AOB. More details are given in Section 4, as well as the scheduled developments. STARK-B has been a database of VAMDC (Virtual Atomic and Molecular Data Centre) since the end of 2009. This FP7 European project "Research Infrastructures" was created in summer 2009 for 3.5 years. It is an interoperable e-Infrastructure for exchange of atomic and molecular data. It is an international consortium that has built an e-science interoperable platform [7] [8] (http://www.vamdc.eu, and http://portal.vamdc.eu) permitting an automated exchange of atomic and molecular data. The software infrastructure is based on an ensemble of standards and softwares (http://www.vamdc.eu/software/). VAMDC addresses data producers and users, and gives a support for introducing new databases in the consortium, and for using standards and softwares. This will be presented in Section 5.

2. Importance of Stark broadening in plasmas

On the one hand, in astrophysics, thanks to the considerable developments of the spectral resolution and sensitivity (high S/N) of the recent past years, and of large ground-based telescopes and space-born missions, it becomes possible to observe very faint objects and spectra in all ranges of wavelengths (from XUV to radio) with an unequalled accuracy. For interpreting the spectra, the atomic parameters responsible for their intensities and their profiles must be known. The development of realistic models of interiors and of atmospheres of stars including stratification, and the interpretation of their evolution and the creation of elements through nuclear reactions, requires the knowledge of numerous profiles, especially for trace elements. Abundances of elements are crucial parameters to be determined. This needs an accurate interpretation of the detailed line spectra of stellar objects and thus extensive sets of atomic data, including collisional broadening and especially Stark broadening. Neglecting Stark broadening can lead to 40% error in abundances. Nowadays collisional broadening data are needed, not only for strong lines of abundant elements (H, He, C, N, O, Ne) as in the past, but also for weak lines of abundant elements, for elements of lower abundance (the Iron-peak), and then, that is more recent, for heavy elements of very low abundance which are always very weak. Even some radioactive elements, such as thorium and uranium have been recently discovered in low-metallicity stars (stars of the first or second generation), and are used for chronometric age determination. An extreme domain of temperatures (about $10^6$ - $10^7$ K) and electron densities (about $10^{24}$ cm$^{-3}$) concern interiors of stars. They cannot be observed but are mirrored via asteroseismology, and Stark broadening of abundant ions plays an important role for modeling and for deriving radiative
opacities. In the very dense and hot atmospheres of neutron stars, the physical conditions are typical of those of stellar interiors, and highly-ionized atoms such as H and He-like Fe have been observed in X rays and the measured line strengths of lines indicate that the lines are significantly broadened by Stark effect [9], and this should provide an opportunity to determine both the mass and the radius of these exotic objects. On less extreme conditions of temperatures ($10^4$ to a few $10^5$ K) and densities ($10^{13}$ to $10^{15}$ cm$^{-3}$), Stark broadening is efficient for modeling and analyzing spectra of moderately hot (A), hot (B) and very hot (O) types of stars. It is dominant in comparison with thermal Doppler effect in deep layers of stellar atmospheres. In white dwarfs, collisional broadening and especially Stark broadening is dominant in all layers of the atmosphere (temperatures in the region of $10^8$ K, electronic densities of the order of $10^{18}$-$10^{19}$ cm$^{-3}$) In stars like sun, and especially in the chromosphere which lays above the photosphere, Stark broadening can be operative for lines arising from high excited levels.

On the other hand, in laboratory and technological plasmas, considerable developments are also in progress and require new and numerous atomic data for spectroscopic diagnostics and modeling. Magnetic confinement fusion plasmas (tokamaks, such as ITER) are moderately hot (electron and ion temperatures about 0.5 to 40 keV in the core and 0.05 to 10 keV at the edge) and dense ($10^{14}$ cm$^{-3}$), especially in the divertor and edge plasma regions. Expected impurities include a wide range of elements (such as tin), but some important elements are not the same as in astrophysics, with nuclear charge $Z$, ranging from above 70 (as tungsten) and down to 1. Light elements are also important, such as Helium-like krypton. Inertial confinement fusion plasmas (laser fusion, ion-beam fusion, such as JET, laser LMJ) are hot (several keV) and very dense (up to $10^{24}$ cm$^{-3}$ for the density) and their thermodynamical conditions look like those of stellar interiors.

In addition, industrial plasmas also require atomic data for optimizing the performances of discharge lamps and lighting sources [10]. The temperatures are various: the discharge can attain 45000K, whereas the emitted white light corresponds to 3000-5000K. The electron density is rather high, so Stark broadening can play an important role in the modeling. The interesting elements are rare earth phosphors (Dy, Ho, Ce) because they are excellent radiation sources in fluorescent lamps. Temperatures of HID (High Intensity Discharge) lamps, such as metal halides, are about 1000K on the wall and 7000K on axis. The buffer gas is usually mercury vapor at high pressure. Ga and Al atomic data are needed.

### 3. Basis of STARK-B data: the standard theory of Stark impact broadening of isolated lines

The theory and calculation of collisional line broadening in the impact approximation follows the founding work by Baranger [11] [12] [13].

#### 3.1. The impact approximation

First, the impact approximation is the fundamental one: the interactions are separated in time. Consequently the duration of an interaction $\tau = \rho_{np} / v_{np}$, where $\rho_{np}$ is a typical impact parameter and $v_{np}$ a typical relative velocity, must be much smaller than the mean time interval between two collisions $\Delta t$, which is of the order of the inverse of the collisional line width $N v_{np} \pi \rho_{np}^2$, where $N$ is the density of the perturbers. The condition of validity of the impact approximation can be written as $\rho_{np} / v_{np} \ll \Delta t$, or, which is equivalent, $N v_{np} \ll 1$, $v_{np}$ being the collision volume [11] [12], i.e., $\rho_{np} \ll N^{-1/3}$.

In other words, the studied radiating atom interacts with one perturber only at a time, and the perturbers are independent and their effects are additive.

#### 3.2. The complete collision approximation

Second, the collision is assumed to be complete. This means that the atom has no time to emit or absorb a photon during the collision process. This is valid if the duration of an interaction is much smaller than the interval between two successive emissions (or absorptions) of photons, which is of the
order of the inverse of the detuning, when larger than the line width. So, if the impact approximation is valid, the complete collision approximation is valid in the line center but can be invalid in the wings. In the very far wings the interactions can become “quasistatic”, which means that a photon can be emitted or absorbed before the perturbers had time to move. The data of STARK-B do not apply in this case. Consequently, within the complete collision approximation, radiative and collision processes are decoupled and the impact broadening theory becomes an application of the theory of collisions between an emitting (or absorbing) neutral (or ionized) atom and interacting particles. These two approximations are at the basis of the STARK-B data.

3.3. The case of “isolated lines”

Third, STARK-B data apply to “isolated lines” only and do not apply to “overlapping lines” [12]. This means that the levels next to the upper or lower level of the studied transition and likely to modify the broadening by introducing optical coherences do not overlap with them. So, hydrogen and hydrogenic ionic lines are excluded from the database, as well as some specific helium lines and some lines arising from Rydberg levels.

3.4. Lorentz profile

Therefore the profile of the i-f line emitted or absorbed between the i and f levels studied is Lorentzian, with a full width at half maximum $W$ (in angular frequency units) and a shift $d$ [13]. $W$ can be expressed in terms of inelastic cross-sections and elastic processes as (cf. [13]):

$$W = N \int v f(v) \left( \sum_{i \neq f} \sigma_{fi}(v) + \sum_{f \neq i} \sigma_{fi}(v) + \sigma_{el}(v) \right),$$

where $N$ is the density of the colliding perturbers, $f(v)$ the Maxwell distribution of the relative atom-perturber velocity $v$, $\sigma_{fi}$ and $\sigma_{fi'}$ the inelastic cross-sections between the initial level $i$ (resp. $f$ final level) and the perturbing levels $i'$ (resp. $f'$) of the i-f transition. $\sigma_{el}(v)$ represents the contribution of elastic collisions and includes Feshbach resonances when ion-electron collisions are studied.

The shift is not given in the present paper, and we refer to [13] for its quantum expression.

We notice that the widths and shifts are proportional to the density $N$ in the above expression, and depend on the temperature of the plasma through the distribution of velocities. In fact, since interactions with charged particles are concerned, at high densities, the Debye screening has to be taken into account and reduces the cross-sections. So, the widths and shifts become reduced. Consequently, for a series of lines of a given neutral or ionized atom, STARK-B displays widths $W$ and shifts $d$ for a set of temperatures and densities and for various perturbers (electrons and ions). For low densities, which are not on the tables, the data, which are provided at medium densities, can be deduced through a linear extrapolation. At high densities some data are not given because the impact approximation is not valid; an asterisk, which replaces the data, indicates this. Data which are given but preceded by an asterisk mean that the impact approximation reaches its limit of validity, i.e. when $0.2 < N V_{typ} \leq 0.5$.

In addition, when the density increases, the lines, which are isolated at low densities, can overlap; the impact width becomes comparable to the separation $\Delta E(nl, nl')$ between the perturbing energy levels and the initial or final level. The isolated line approximation becomes invalid. This is indicated in the database by a parameter $C$ defined in [5] and in following papers. $C$ is provided in the tables and can be used as follows: for a perturber density $N$ lower than the limiting value $N_{lim}$ (cm$^{-3}$) = $C/W$, the line can be treated as isolated even if a weak forbidden component due to the failure of this approximation remains in the wing.

3.5. Effect of fine structure and hyperfine structure on the widths and shifts

The following remark holds in LS coupling. The atomic electronic spin $S$ and the orbital kinetic momentum $L$ are decoupled. For electronic collisions and most often by collisions with ions, the
collision time (of the order of $\rho_{typ}/v_{typ}$) is very much smaller than the fine structure splitting. So the electronic spin has no time to rotate during the collision and can be ignored. Thus all the fine structure components have the same widths and shifts, which are equal to those of the multiplet. This is a fortiori the same for the hyperfine components. So our calculations have most often been performed for multiplets only, and STARK-B data are most often given for multiplets. This remark does not apply for heavy atoms where departures from LS coupling can be important.

3.6. Compared orders of magnitude of electron and ion Stark widths and shifts
For isolated lines, the widths and shifts due to electron collisions are generally ten times higher than the widths and shifts due to ion collisions. This is due to the fact that inelastic collisions with positive ions are generally negligible, owing to the mass effect that decreases the relative velocity, and, in addition, if the radiator is an ion, the Coulomb repulsion acts. This can be not the case when the perturbing levels are very close to the levels of the studied transition. This can also be not the case at very high temperatures, and especially for ion radiators when the Coulomb repulsion becomes weak.

3.7. Calculation of the cross-sections, and then widths and shifts
3.7.1. The Semi-Classical Perturbation (SCP) approach. For the purposes of STARK-B, the semi-classical-perturbation treatment is adapted and gives results with a sufficient accuracy (about 20%). This is especially the case if the perturbing levels are not too far from the levels of the studied line. The basic formalism has been developed and discussed in detail in [1] [2]. Classical straight rectilinear paths for neutral radiators, and hyperbolic paths have been introduced for ion-electron and ion-ions collisions. Then the $S$-matrix has been obtained within the second order perturbation theory. The needed cross-sections are obtained through integration over the impact parameter of the transition probabilities. The needed cut-offs are determined in order to maintain the unitarity of the scattering $S$-matrix, and Debye screening is taken into account. A very fast computer code has been created. This formalism, and the computer code, have been updated and optimized several times: [3] for complex atoms, [4] for the inclusion of Feshbach resonances in the elastic ion-electron cross-sections, [5] and further papers, and [14] for transitions arising from very complex configurations.

3.7.2. The atomic structure. In the semiclassical picture, oscillator strengths and needed energy levels enter the expressions of the inelastic cross-sections. They are input data of the numerical code. The STARK-B data issued from our oldest papers (eighties and nineties), the Coulomb approximation with quantum defect (Bates & Damgaard approximation, [15]) was used, together with measured or calculated energy levels.
In the more recent papers modern ab initio methods are used (cf. [14]). The different atomic structure computer codes or the data can be downloaded on line. Thus the calculations of widths and shifts can be made from the beginning to the end without any additional external input or experimental adjustment. The chosen atomic structure package enters our computer semi-classical code and that allows, when these methods are applicable, to obtain widths and shifts for one-two hundred of lines:
- TOPbase, the Opacity Project atomic database, contains accurate calculated oscillator strengths and energy levels for abundant neutral atoms and ions of astrophysics. They have been obtained within the close-coupling scattering theory by means of the R-matrix method with innovative asymptotic techniques [17] [18]. L-S coupling is assumed. So, TOPbase data have been especially used to light and low and moderately ionized atoms and ions.
- The Cowan code [19] is an online atomic structure package consisting of a set of computer programs for calculation of energy levels, radiative transition wavelengths and probabilities, electron impact excitation and photoionization cross sections, etc. The Hartree-Fock-Slater multi-configuration expansion method with statistical exchange is the normal option since it is most computationally efficient. The relativistic corrections are treated by perturbations. So this method is especially suited to moderately heavy atoms which are little and moderately ionized.
- SUPERSTRUCTURE (SST) [20] is well suited for computation of large quantities of atomic data for highly charged ions. The wave functions are determined by diagonalization of the nonrelativistic
Hamiltonian using orbitals calculated in a scaled Thomas-Fermi-Dirac-Amaldi potential. Relativistic corrections are introduced according to the Breit-Pauli approach. Atomic data are obtained in intermediate coupling.

Si V and Ne V line widths and shifts data have been calculated with both Bates & Damgaard and SST atomic data [21] [22]. The difference does not exceed 30%. C II widths and shifts data have been calculated with both TOPBase and Bates & Damgaard atomic data [23], and the difference does not exceed a few percent, except when configuration interaction plays an important role by making permitted a forbidden transition. This gives an idea and an order of magnitude of the importance of the chosen atomic structure on the Stark broadening data.

3.7.3. The Modified Semi-Empirical Method (MSE). A number of applications were also achieved with the Modified Semi-Empirical (MSE) method [24] [25] [26] and other papers cited in [27]. It is less accurate, though simpler to use due to the considerably smaller set of atomic data needed in comparison with the SCP theory. It can effectively replace the SCP method when this one cannot be used due to a lack of atomic data. The MSE data have not still been introduced in STARK-B.

4. Organization of the database

Since STARK-B is devoted to modeling and spectroscopic diagnostics in various plasmas, the domain of temperatures and densities covered by the tables is wide and depends on the ionization degree of the considered ion. The temperatures can vary from several thousands for neutral atoms to several millions of Kelvin for highly charged ions. The electron or ion densities can vary from $10^{12}$ (case of stellar atmospheres) to several $10^{22}$ cm$^{-3}$ (some white dwarfs, subphotospheric layers and some laboratory and fusion plasmas). The datamodel, especially the definition of configurations, terms and levels follow the VAMDC standards, in order to allow interoperability with other atomic databases.

It is important to notice that the provided wavelengths (Å units) are most often calculated from the energy levels that are used in the calculations. Consequently, these wavelengths can be different from the measured ones, especially if energy levels originate from TOPBase, SST or Cowan code. The lines can be identified through the configurations, terms and levels. In addition, the widths and shifts data are provided in units of wavelengths (Å) and not in angular frequency units. So, if widths and shifts data are needed for measured wavelengths ($\lambda_{\text{measured}}$), or for fine structure data whereas the data are only provided for multiplets (cf. section 3.5), one has to multiply the STARK-B data by $(\lambda_{\text{measured}}/\lambda_{\text{STARK-B}})^2$.

We refer to section 3.4 for the cases of departures from the impact approximation and from the isolated line approximation at high densities.

Currently, STARK-B contains Stark widths and shifts for spectral lines of the following elements and ionization degrees:

Ag I, Al I, Al III, Al XI, Ar I, Ar II, Ar VIII, Au I, B II, B III, Ba I, Ba II, Be I, Be II, Be III, Br I, C II, C III, C IV, C V, Ca I, Ca II, Ca V, Ca IX, Ca X, Cd I, Cd II, Cl I, Cl VII, Cr I, Cr II, Cu I, F I, F II, F III, F IV, F V, F VI, F VII, Fe II, Ga I, Ge I, He I, Hg II, I I, In II, In III, K I, K VIII, K IX, Kr I, Kr II, Kr VIII, Li I, Li II, Mg I, Mg II, Mg XI, Mn II, Mn II, N I, N II, N III, N IV, N V, Na I, Na X, Ne I, Ne II, Ne III, Ne IV, Ne V, Ne VIII, Ni II, O I, O II, O III (in progress), O IV, O V, O VI, O VII, P IV, P V, Pb I, Pd I, Pb II, S III, S IV, S V, S VI, Sc III, Sc III, Sc X, Se XI, Se II, Si I, Si II, Si IV, Si V, Si VI, Si XI, Si XII, Si XIII, Sr I, Te I, Ti IV, Ti XII, Ti XIII, Ti III, V V, V XIII, Y III, Zn I.

Apart O III data, all the data corresponding to our already published papers have now been implemented.

The homepage (Fig.1) proposes several menus, among which “Introduction”, “Data Description” and “Access to the Data”. “Introduction” briefly recalls the approximations and methods of calculation. “Data Description” describes the data that are in the files. A graphical interface is provided in “Access to the Data” (Fig.2): first, the consumer clicks on the wished element in the Mendeleev periodic table and then on the ionization degree of interest. Yellow cells contain data, while white cells are empty. Next, with a few clicks, the user chooses the colliding perturber(s), the perturber density, the
transition(s) by quantum numbers and the plasma temperature(s). The consumer can also make a query by domain of wavelengths instead by transitions. Then a table displaying the widths and shifts is generated. Bibliographic references are given and linked to the publications via the SAO/NASA ADS Physics Abstract Service [55] and/or within DOI. They can be freely downloaded if the access is not restricted. The widths and shifts data can be downloaded in ASCII and in VOTable format (XML format), adapted to Virtual Observatories.

Figure 1. The STARK-B home page: http://stark-b.obspm.fr

Figure 2. "Access to the data": the graphical interface

The database will be completed when new data will be calculated and published (e.g. C II results of [23]). The implementation of MSE data is planned for a next future. The implementation of our quantum data will be another future step. The further developments also concern insertion of little apps (fitting along temperatures, along principal quantum number for a given multiplet, charge of the ion collider along isoelectronic sequences, of the radiating ion, homologous ions…) by using fittings or systematic trends in order to obtain data that are missing on the database.

5. The STARK-B database and VAMDC (Virtual Atomic and Molecular Data Centre)

Many fields in astronomy, physics, energy production and industry depend on databases for atomic, molecular and particle-surface interaction processes. A reliable exchange of such data has become crucial for decades. Nowadays, many databases do exist, but they are organized and presented in different manners, with heterogeneous standards, rules and selection criteria. This is a barrier for an efficient search for data and their use. The free exchange of atomic and molecular data requires the definition both of standards which model the data structure and of tools that implement these standards and that help to carry out science using these data. Developments in computer technologies offer opportunities for new distributed tools and applications in various fields of physics. The convenient and reliable exchange of data is clearly an important component of such applications. So VAMDC [7] [8] was created in summer 2009 for 3.5 years in the framework of the FP7 "Research Infrastructures - INFRA-2008-1.2.2 - Scientific Data Infrastructures" initiative. It is an European collaboration between groups involved in the generation and use of atomic and molecular data. VAMDC involves 15 administrative partners representing 24 teams from 6 European Union member states, partners in non-EU countries (Serbia, the Russian Federation and Venezuela), and external partners in the US. It includes scientists in atomic and molecular physics with a strong coupling to the users of their data (astrochemistry, atmospheric physics, plasmas) and scientists and engineers from the Information and Communication Technologies community used to deal with interoperable e-infrastructure. The core of the VAMDC-infrastructure is founded on the databases detailed in [7]. VAMDC aims to build a secure, documented, flexible and interoperable e-science environment-based interface to existing atomic and molecular data. The VAMDC portal (http://portal.vamdc.eu/) has been released in the mid-April 2012 for the external users. It can be tested and is frequently updated from the development version that is still in progress. The results of the queries can be downloaded in XSAMS format (XML Schema for Atoms, Molecules and Solids). The XSAMS schema provides a framework for a structured presentation of atomic, molecular, and particle-solid-interaction data in an XML file. XML
(Extensible Markup Language) is the current standard for exchange of such data. It enables an automated exchange of complex contents between heterogeneous information systems through interoperability. STARK-B is one of the databases of VAMDC and participates to this undertaking.

6. Conclusion
Nowadays, numerical databases in Atomic and Molecular Physics are essential for both the modeling and the interpretation of spectra provided by observations and laboratory measurements of various plasmas. The free exchange of atomic and molecular data requires the definition both of standards which model the data structure and of tools that implement these standards and that help to carry out science using these data. The continuation of such developments and services of powerful and constantly updated online databases, like STARK-B, is crucial.

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