

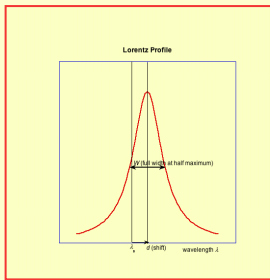
# The **STARK-B** database as a resource for “STARK” widths and shifts data: State of advancement and program of development *in the framework of the* European Consortium **VAMDC** *(Virtual Atomic and Molecular Data Center)*

S. Sahal-Bréchet<sup>(1)</sup>, M.S. Dimitrijević<sup>(2,1)</sup>, N. Moreau<sup>(1)</sup>,  
and N. Ben Nessib<sup>(3)</sup>

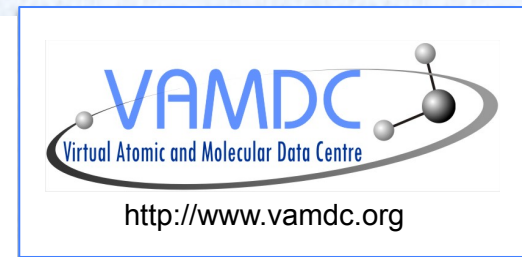
*(1) Observatoire de Paris, LERMA CNRS UMR 8112, France*

*(2) Astronomical Observatory, Volgina 7, 11060 Belgrade 38, Serbia*

*(3) Department of Physics and Astronomy, College of Science, King Saud University, Riyadh 11451, Saudi Arabia*



<http://stark-b.obspm.fr>



# STARK-B

broadening and shift of *isolated* spectral lines of atoms and ions, by *collisions* with electrons and ions in a plasma

*Overlapping lines and departures from impact approximation are outside the scope of STARK-B*

*Stark broadening of spectral lines can be applied to many subjects*

- Ionization degree  $\geq 1\%$
- Moderately hot to very hot plasmas ( $2.5 \cdot 10^3$  to  $\sim 6 \cdot 10^6$  K)
- Moderate electron density ( $10^{10}$  to  $10^{23} \text{ cm}^{-3}$ )
- Astrophysics
- Laboratory plasmas
- Technological plasmas

# Diagnosics and Modelling in Astrophysics: Understanding of the evolution of stars

- *Thanks to considerable developments of*
  - *Ground based and space-born missions*
  - *Increased sensitivity (S/N) and spectral resolution*
  - *Powerful computers*

## **Interpretation of the faint observed spectrum : faint objects, faint lines (trace elements)**

- Line intensities + line profiles
- Continuum
- Spectroscopic diagnostics:
  - Temperatures
  - pressure
  - Abundances
  - Chemical stratification of the atmosphere

## **Modelling of atmospheres**

- Synthetic spectra: a great number of lines of a same element are required
- Radiative transfer

## **Stellar interiors studies and Asterosimology**

- opacities: a great number of lines of highly ionized elements are required
- Nuclear processes: formation of elements, chemical enrichment

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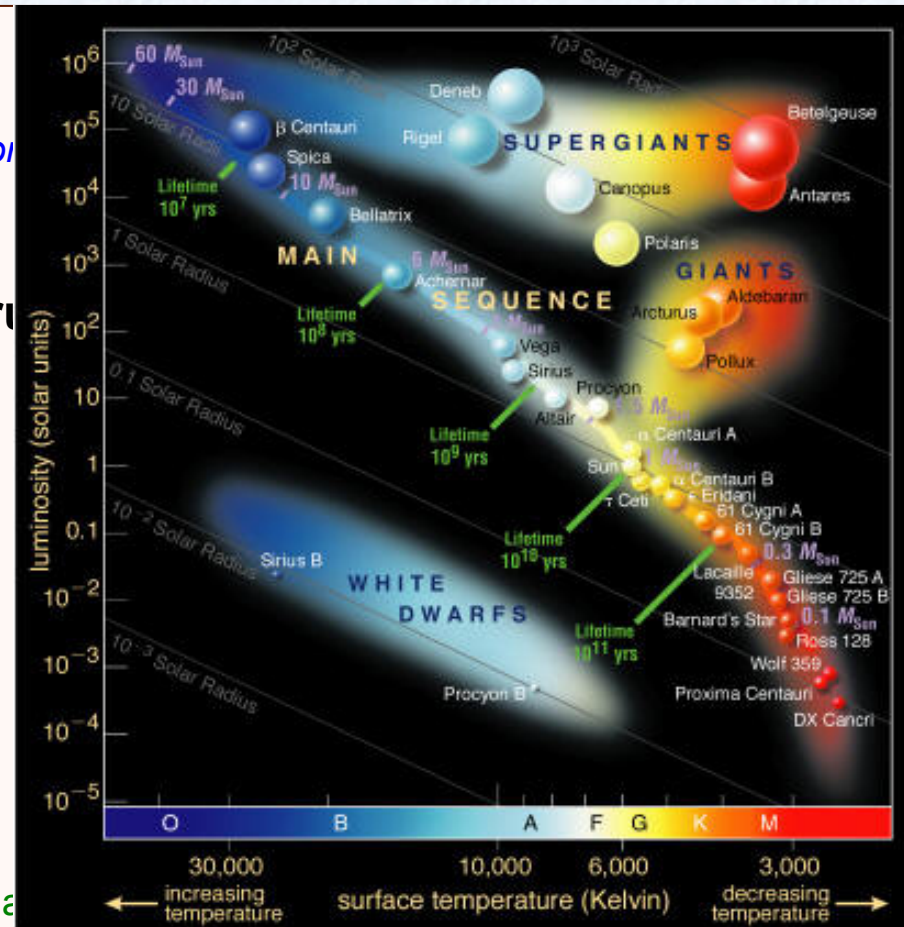
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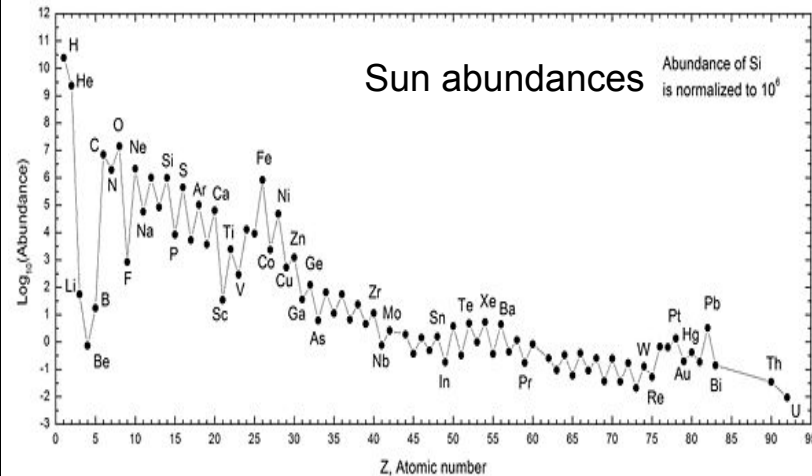
## Modelling of atmospheres

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## Stellar interiors studies and Asterosimology

- opacities: a great number of lines of highly ionized elements
- Nuclear processes: formation of elements, chemical

Group	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
Period 1	1 H																	2 He
Period 2	3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
Period 3	11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
Period 4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
Period 5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
Period 6	55 Cs	56 Ba		72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
Period 7	87 Fr	88 Ra		104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Uut	114 Uuq	115 Uup	116 Uuh	117 Uus	118 Uuo
Lanthanides	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu			
Actinides	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr			

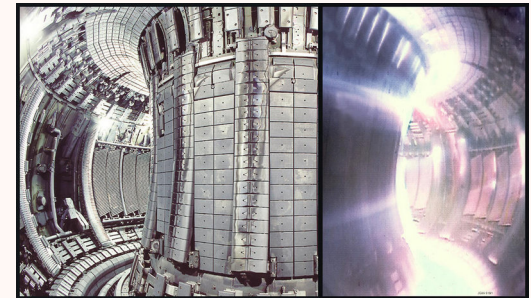


# Diagnostics and Modelling in Laboratory and Technological plasmas

- *Thanks to developments and needs (devices an research)*
  - *Magnetic confinement fusion: moderately dense and hot plasmas*
  - *Inertial confinement fusion (laser fusion, ion-beam fusion): dense and very hot plasmas*
  - *Low temperatures plasmas*
  - *Lighting discharges*

## Analysis and interpretation of the spectrum in fusion devices

- Light elements in the divertor and edge plasma regions
- Importance of Tin, Tungsten and impurities
  - Temperatures
  - Pressure



## Progress in low-energy light sources

- Discharge lamps and lighting :
  - optimisation of performances
  - cold light from hot atoms and molecules
    - . (white light 3000-5000K, discharge up to 45000K),
    - . high electron density (strong and broad emission in the visible spectrum)
  - Fluorescent lamps: improving efficacy (phosphors)
- Rare earth elements Dy, Ho, Ce: excellent radiation sources
- HID (*High Intensity Discharge*): MH (*Metal Halide*) lamps, e.g. Dy I<sub>3</sub>, In I, ZnI<sub>3</sub>
- (LED light-emitting diodes)



# STARK-B

Database for "Stark" broadening of isolated lines of atoms and ions in the impact approximation

<http://stark-b.obspm.fr>

- **Calculated widths and shifts:** more than 150 pubs (1984-2011)

- **SCP theory updated and operated** by M.S. Dimitrijević and S. Sahal-Bréchet and colleagues

- STARK B is currently developed at Paris Observatory

  - *the database has been opened since September 2008:*

- It is a part of the atomic and molecular databases of the Paris Observatory

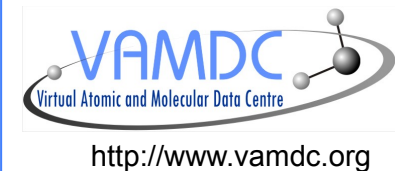
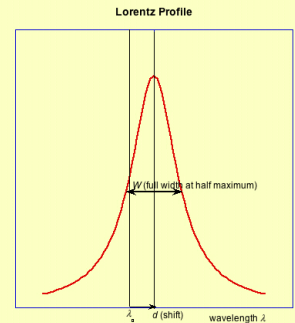
- Link to SerVO - Serbian Virtual Observatory

<http://servo.aob.rs/~darko/>

- It is node of VAMDC- Virtual Atomic and Molecular Data Centre

- it follows the standards of VAMDC and Virtual Observatories

(Europe: IVOA *International Virtual Observatory Alliance*)



# STARK-B data: Basic approximations (theory and calculations)

## • Impact approximation

- Collisions between radiators and perturbers act independently and are additive

## • Complete collision approximation

- → line broadening theory becomes an application of the theory of collisions

## • Isolated lines

- Neighbouring levels do not overlap

→ Lorentz profile; S-matrix, cross-sections

• LS coupling: fine (hyperfine) structure can be neglected during the collision (S or I : no time to rotate)

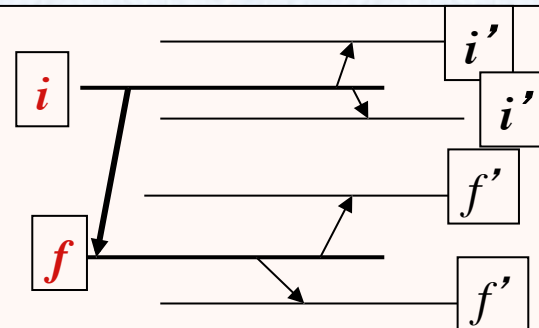
- → The fine structure (hyperfine) components have the same width and the same shift, that of the multiplet

## • High densities:

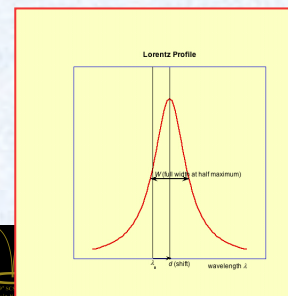
- → Debye screening effect

$$\tau \approx \rho_{\text{typ}} / \nu \ll \Delta T \text{ i.e. } \rho_{\text{typ}} \ll N^{-1/3}$$

The atom has no time to emit or absorb a photon during the collision process, the collision is not broken off.

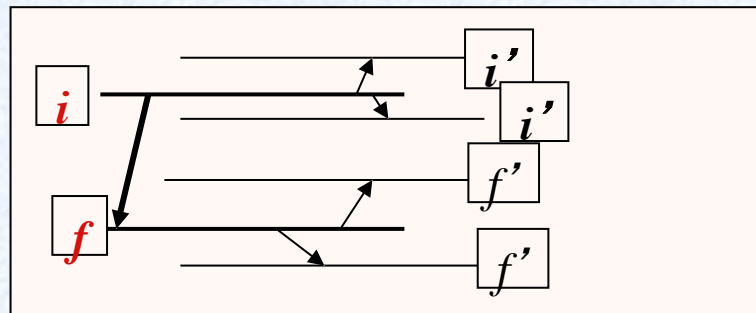


$$W = N \int \nu f(\nu) \left( \sum_{i' \neq i} \sigma_{ii'}(\nu) + \sum_{f' \neq f} \sigma_{ff'}(\nu) + \sigma_{el}(\nu) \right)$$





# STARK-B data: need to calculate S-matrix and cross-sections



$$w + id = N_P \int_0^\infty v f(v) dv \int_0^\infty 2\pi \rho d\rho \langle 1 - S_{ii} S_{ff}^* \rangle_{\text{angular average}}$$

$$= N_P \int_0^\infty v f(v) dv \int_0^\infty 2\pi \rho d\rho \times$$

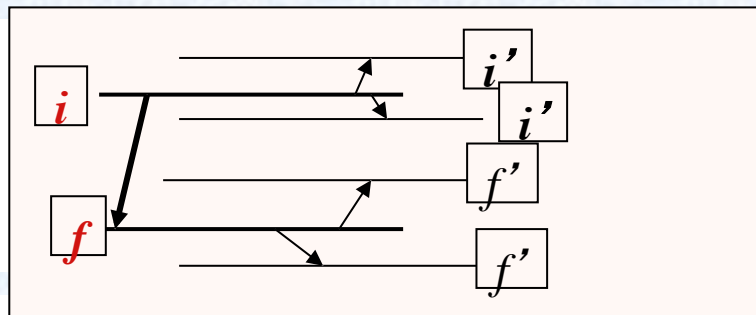
$$\left[ 1 - \sum_{\substack{M_i M'_i \\ M_f M'_f \\ \mu}} (-1)^{2J_f + M_f + M'_f} \begin{pmatrix} J_i & 1 & J_f \\ -M_i & \mu & M_f \end{pmatrix} \begin{pmatrix} J_i & 1 & J_f \\ -M'_i & \mu & M'_f \end{pmatrix} \times \right. \\ \left. \langle \alpha_f J_f M_f | S^* | \alpha_f J_f M'_f \rangle \langle \alpha_i J_i M_i | S | \alpha_i J_i M'_i \rangle \right]$$

# STARK-B data:

need to calculate and cross-sections for the width

With the  $T$  matrix:  $T=1-S$ , and using  $T^*T=2 \operatorname{Re} (T)$   
 $(2 l+1) \pi / k^2=2 \pi \rho d \rho$

$$k = \frac{mv}{\hbar}$$



$$W = 2w = N_p \int v f(v) dv \left[ \left( \sum_{\alpha J} \sigma(\alpha_i J_i \rightarrow \alpha_i' J_i') + \sum_{\alpha' J'} \sigma(\alpha_f J_f \rightarrow \alpha_f' J_f') \right) - 2 \operatorname{Re} \int_0^\infty 2\pi \rho d\rho \times \right. \\ \left. \left[ 1 - \sum_{\substack{M_i M_i' \\ M_f M_f' \\ \mu}} (-1)^{2J_f + M_f + M_f'} \begin{pmatrix} J_i & 1 & J_f \\ -M_i & \mu & M_f \end{pmatrix} \begin{pmatrix} J_i & 1 & J_f \\ -M_i' & \mu & M_f' \end{pmatrix} \right] \times \right. \\ \left. \left[ \langle \alpha_f J_f M_f | T^* | \alpha_f J_f M_f' \rangle \langle \alpha_i J_i M_i | T | \alpha_i J_i M_i' \rangle \right] \right]$$

$\sigma$  is the cross-section for a given velocity:

$$\sigma(\alpha_i J_i \rightarrow \alpha J) = \int_0^\infty 2\pi \rho d\rho \sum_{M_i M} \left| \langle \alpha_i J_i M_i | T | \alpha J M \rangle \right|^2$$

$P$  is the transition probability for a given impact parameter  $\rho$  (or a given orbital angular momentum  $l$ )

$$P(\alpha_i J_i \rightarrow \alpha J) = \sum_{M_i M} \left| \langle \alpha_i J_i M_i | T | \alpha J M \rangle \right|^2$$

# STARK-B

## Methods of calculations of the data 1 - The atomic structure (wave functions, levels and line strengths)

- Coulomb approximation with quantum defect (*Bates & Damgaard 1949*) with levels taken from tables
- NIST atomic data: levels and line strengths
- VALD (Vienna Atomic Line Database of levels and line strengths)
- TOPbase (R-matrix in LS coupling)
- Cowan code (HFS multi-conf with exchange and relativistic effects by perturbations)
- SUPERSTRUCTURE (scaled Thomas-Fermi-Dirac-Amaldi potential + relativistic effects by perturbations(Breit-Pauli))

# STARK-B

## Methods of calculations of the data

### 2. The scattering S-matrix and the cross-sections

- **SCP: Semi-Classical** : atom = quantum description (atomic structure),  
perturber= particle moving on a classical path  
+ **Perturbation theory (2<sup>nd</sup> order)**
  - (Sahal-Bréchet (SSB), A&A1970 and further papers, 6-8 basic papers)
    - unitarity and symmetrization of the S-matrix, adequate cut-offs
    - hyperbolae for ion-electron and ion-ion (SSB 1970),
    - complex atoms (SSB 1974), very complex (Mahmoudi, Ben Nessib & SSB 2008)
    - Feshbach resonances for ion-electron collisions (Fleurier, SSB 1977)
    - Updated and operated with MS. Dimitrijević (1984 and after)
    - accuracy: 20%, sometimes better, sometimes worse
- **MSE: Modified Semi-Empirical** : atom = simplified quantum description  
Dimitrijević and colleagues, JQSRT1980 and further A&A papers)

# STARK-B

## Methods of calculations of the data

### 3. Calculations leading to a great number of data

Atomic structure coupled to the S-matrix calculation:

*Many widths and shifts for a set of several temperatures and densities in a same run*

Ab initio calculations: no external data insertion

– Coupling to atomic structure codes and databases:

data for 100-150 lines and more in a same run

– TopBase + SCP

– SST + SCP

– Cowan code + SCP

– Coupling to VALD: data for more than 1000 lines in a same run

# 2012: **SCP** data inserted for 114 neutral and ionized atoms (*more than 150 publications*)

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,+ *Cr II (MNRAS,2013 , new results to be inserted)*  
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  
N I, N II, N III, N IV, N V  
Na I, Na X  
Ne I, Ne II, Ne II, Ne III, Ne IV, Ne V, Ne VIII  
Ni II  
O I, O II, O III , O IV, O V, O VI; O VII  
P IV, P V  
Pb IV,+ *Pb IV (MNRAS, 2013, new results to be inserted)*  
Pd I  
Rb I  
S III, S IV, S V, S VI  
Sc III, Sc X, Sc XI  
Se I  
Si I, Si II, Si IV, Si IV, Si V, Si VI, Si XI, Si XII, Si XIII  
Sr I  
Te I  
Ti IV, Ti XII, Ti XIII  
Tl III  
V V, V XIII  
Y III  
Zn I

# 2013: New step for insertion of widths and shifts data: the **MSE** (Modified Semi Empirical) method

**Convenient** when the **knowledge of the atomic structure is incomplete**  
(lack of levels and/or line strengths: case of complex neutral and ionized atoms)  
Dimitrijević and colleagues, JQSRT1980 and further papers  
→ atom: **simplified quantum description**

1- Cf. Griem (*Phys. Rev.*1968): SE (Semi-Empirical) method

$$W = 2w = N_p \int v f(v) dv \left[ \left( \sum_{\alpha J} \sigma(\alpha_i J_i \rightarrow \alpha J) + \sum_{\alpha' J'} \sigma(\alpha_f J_f \rightarrow \alpha' J') \right) + \sigma_{\text{elastic}} \right]$$

- Elastic contribution taken into account by extending the inelastic cross-sections under the threshold
- Cross-sections calculated with an effective Gaunt factor  $g$  (Van Regemorter ApJ 1962)

2- **MSE**: Separation between  $\Delta n=0$  and  $\Delta n \neq 0$

- Perturbing levels lumped together for  $\Delta n \neq 0$ , → use of oscillator strengths sum rules
- $g$  revisited, and convenient for ions with  $Z > 1$
- accuracy of the method: 30-50%

# 2013: **MSE data to be inserted:** 90 neutral and ionized atoms *(about 50 publications)*

Ag II  
Al III, Al V  
Ar II, Ar III, Ar IV  
As II, As III  
Au II  
B III, B IV  
Ba II  
Be III  
Bi II, Bi III  
Br II  
C III, C IV, C V  
Ca II  
Cd II  
Cl III, Cl IV, Cl VI  
Co II  
Cu III, Cu IV

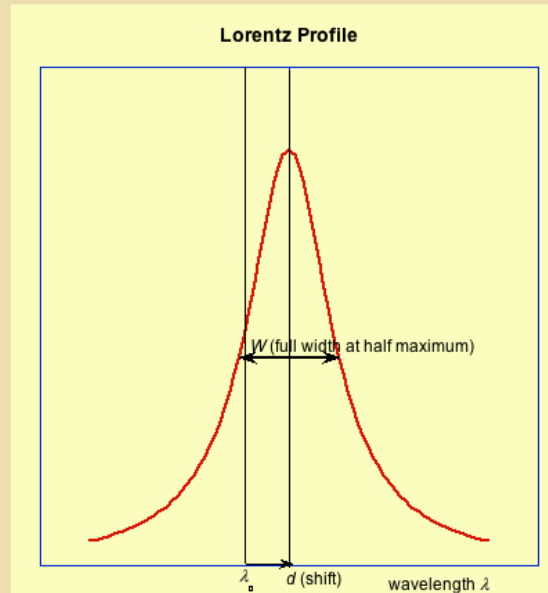
Eu II, Eu III  
F III, F V, F VI  
Fe II  
Ga II, Ga III  
Ge III, Ge IV  
I II  
Kr II, Kr III  
La II, La III  
Mg II, Mg III, Mg IV  
Mn II  
N II, N III, N IV, N VI  
Na III, Na VI  
Nd II  
Ne III, Ne IV, Ne V, Ne VI  
O II, O III, O IV, O V  
P III, P IV, P VI

Pt II  
Ra II  
S II, S III, S IV  
Sb II  
Sc II  
Se III  
Si II, Si III, Si IV, Si V, Si VI  
Sn III  
Sr II, Sr III  
Ti II, Ti III  
V II, V III, V IV  
Xe II  
Y II  
Zn II, Zn III,  
Zr II



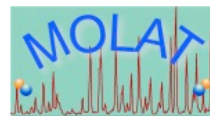
## STARK-B

Database for "Stark" broadening of isolated lines of atoms and ions in the impact approximation



The STARK-B database is now fully opened though not yet complete.

Last data update : 2012-03-30



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## Introduction

This is a database of calculated widths and shifts of isolated lines of atoms and ions due to electron and ion collisions.

This database is devoted to modelling and spectroscopic diagnostics of stellar atmospheres and envelopes. In addition, it is also devoted to laboratory plasmas, laser equipments and technological plasmas. So, the domain of temperatures and densities covered by the tables is wide and depends on the ionization degree of the considered ion. The temperature can vary from several thousands for neutral atoms to several hundred thousands of Kelvin for highly charged ions. The electron or ion density can vary from  $10^{12}$  (case of stellar atmospheres) to several  $10^{19} \text{ cm}^{-3}$  (some white dwarfs and some laboratory plasmas).

The impact approximation and the isolated line approximation are applied, so that the line profile is Lorentzian. The basis for calculations is the computer code which evaluates electron and ion impact broadening of isolated spectral lines of neutral atoms and ions, using the semiclassical-perturbation approach developed by Sahal-Br  chot (1969ab, 1974), and supplemented in Fleurier et al. (1977), see below. This computer code has been updated by Dimitrijevic and Sahal-Br  chot in their series of papers, Dimitrijevic and Sahal-Br  chot (1984) and following papers. The data are derived from this series of papers and are cited in the tables.

The accuracy of the data varies from about 15-20 percent to 35 percent, depending on the degree of excitation of the upper level, and on the quality of the used atomic structure entering the calculation of scattering S-matrix leading to the widths and shifts. The more the upper level is excited, the more the accuracy is good. In the earlier papers, the used atomic structure was the so-called "Bates and Damgaard" one (Coulomb wavefunctions + quantum defect). More recent atomic structure data are introduced in the latest papers. The reader is invited to refer to the papers cited in the tables for the used atomic data and atomic levels, and for more details.

### The impact approximation

The impact approximation is valid when the mean duration  $\tau$  of a collision is much smaller than the mean interval  $\Delta T$  between two collisions (Baranger 1958 abc).  $\Delta T$  is of the order of the inverse of the collisional line width  $\gamma$  expressed in angular frequency units.

$\tau$  can be written as :

$$\tau = \langle \rho \rangle / \langle v \rangle ,$$

where  $\langle \rho \rangle$  is a typical impact parameter and  $\langle v \rangle$  the mean velocity of the collider :

$$\langle v \rangle = (8kT / \pi\mu)^{1/2} ,$$

$\mu$  being the reduced mass, T the temperature, and k the Boltzmann constant.

An order of magnitude of  $\langle \rho \rangle$  can be derived from the line width  $\gamma$  and is obtained by writing (N being the density of the perturbers)

$$\gamma = N \langle v \rangle \pi \langle \rho \rangle^2 .$$

The validity condition of the impact approximation can be written as

$$N V \ll 1 ,$$

$V = \pi \langle \rho \rangle^3$  is the collision volume (Baranger 1958abc).

The impact values of the widths and shifts are given in the tables, except when  $N V > 0.5$ . Then the cells are empty and marked by an asterisk preceding the cell. Widths values for  $0.1 < N V \leq 0.5$  are marked by an asterisk in the cell preceding the value. See the Section "Data description" for more details.

In the far wings,  $\Delta\omega$  being the detuning in angular frequency units, the validity condition for the generalized impact approximation becomes

$$\tau \Delta\omega \ll 1 .$$

When the impact approximation is not valid (especially for ion colliders), the quasistatic approximation can be used. As shown by Baranger (1962) for ion emitters and polarization interaction potential, and by Sahal-Br  chot (1991) for the quadrupolar interaction which is in fact dominant due to the Coulomb repulsion, the quasistatic broadening is completely negligible in the wings. For neutrals emitters, the polarization part of the interaction is most often dominant and can be obtained by the A parameter of Griem (1974). This A parameter is provided in a few tables, where it is calculated with the method described by Ben Nessib et al. (1996).

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## The isolated line approximation

At high densities or for lines arising from high levels, the electron impact width becomes comparable to the separation  $\Delta E(nl, n\pm 1)$  between the perturbing energy levels and the initial or final level : the corresponding levels become degenerate and the isolated line approximation is invalid (Griem 1974). In order to check the validity of this approximation, we have defined a parameter C in Dimitrijevic and Sahal-Bréchet (1984) which is given in the tables. See "Data description" for more details.

## The semiclassical perturbation approximation (SCP)

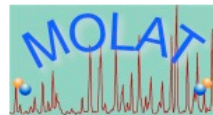
When the impact approximation is valid, the collisional broadening becomes an application of the theory of collisions (Baranger 1958abc). In the semiclassical approximation, rectilinear trajectories are used for neutral emitters (or absorbers), and hyperbolic trajectories for ionic emitters (or absorbers) colliding with charged particles. Within the second order perturbation approximation, dipolar, polarization and quadrupolar interactions are taken into account (Sahal-Bréchet 1969ab and earlier papers), updated for complex atoms and ions (Sahal-Bréchet 1974). The details of calculations of the widths and shifts can be found on these papers. For ionic emitters, the original computer code has been updated by including Feshbach resonances in elastic and fine structure transitions by using the semiclassical limit of the Gailitis formula (Fleurier et al. 1977). Debye shielding effect is also taken into account. It is negligible at low densities or for lines arising from low levels. Then widths and shifts are proportional to the density.

## Other data

When SCP calculations cannot be performed, this database will include data obtained using the MSE (Modified Semi-Empirical) method (Dimitrijevic & Konjevic 1980, Dimitrijevic 1982, Dimitrijevic & Krsljanin 1986), supplemented by Popovic & Dimitrijevic (1996) for complex atoms. These data will be included in a future version.

selected experimental data will also be included in another future version.

- [Baranger, M. 1958a](#), Phys. Rev. A, 111, 481
- [Baranger, M. 1958b](#), Phys. Rev. A, 111, 494
- [Baranger, M. 1958c](#), Phys. Rev. A, 112, 855
- [Baranger M., 1962](#) "Spectral line broadening by plasmas", edited by D. R. Bates. Library of Congress Catalog Card Number 62-13122. in "Atomic and Molecular Processes", pp. 493-548, Acad. Press Inc., New-York
- [Ben Nessib, N., Ben Lakhdar, Z. et Sahal-Bréchet, S., 1996](#), Phys. Scr., 54, 608-613.
- [Dimitrijevic, M.S., and Sahal-Bréchet, S.:](#) 1984, [JQSRT](#) 31, 301-313
- [Dimitrijevic M.S., & Konjevic J.](#), 1980, [JQSRT](#), 24, 451
- [Dimitrijevic M.S.](#), 1982, [A&A](#), 112, 251
- [Dimitrijevic M.S. & Krsljanin, V.](#) 1986, [A&A](#), 165, 269
- [Fleurier C., Sahal-Bréchet, S., and Chapelle, J.:](#) 1977, [JQSRT](#), 17, 595-604
- [Griem, H. R. 1974](#), "Spectral line broadening by plasmas", Pure and Applied Physics, New York: Academic Press, USA
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- [Sahal-Bréchet, S.:](#) [1969b](#), [A&A](#) 2, 322-354
- [Sahal-Bréchet, S.:](#) [1974](#), [A&A](#) 35, 319-321
- [Sahal-Bréchet, S.:](#) [1991](#), [Astron.Astrophys.](#) 245, 322-330



## Data description

### Periodic table of elements

Click on a yellow case corresponding to the chosen element and then on an ionization degree. There are no data on the non-coloured cases. Then a new page appears, requiring your detailed choice.

### Tables description

#### Column 1

Perturber density  $N$  in  $\text{cm}^{-3}$

#### Column 2

Lower level or lower term

#### Column 3

Upper level or upper term

#### Comments to columns 2 and 3

When the fine structure splitting is small, namely if the difference between energy levels of a same multiplet is small compared to the distance to the next level linked by an allowed transition, all the fine structure lines of a same multiplet have the same width and shift. In that case the data are given for the multiplet only and for an average wavelength for the whole multiplet. If needed, the width value for a particular line within a multiplet can be obtained from :

$$W_{\text{line}} = W_{\text{mult}} I_{2\text{line}} / \lambda_{\text{mult}}^2$$

Idem for the shift

#### Column 4

Multiplet when it is available

#### NB

It is the multiplet number generated on line from the NIST Atomic Spectra Database \*. Therefore we have chosen not to select any wavelength range, because the multiplets numbers vary if the the selected wavelength range varies. In addition, the data for multiplets as a whole are only generated on the NIST Atomic Spectra Database if all fine structure components are known and if it is in LS coupling. \* NIST Atomic Spectra Database (version 3.1.5), [Online].

Available: <http://physics.nist.gov/asd3> Ralchenko, Yu., Kramida, A.E., Reader, J., and NIST ASD Team (2008), National Institute of Standards and Technology, Gaithersburg, MD.

#### Column 5

Wavelength in Å

#### Comment to column 5 :

These wavelengths are calculated wavelengths with the computer code. In particular, they are averaged over the multiplet when multiplet data are given.

#### Column 6

Parameter  $C$  for the validity condition of the isolated line approximation

#### Comment to column 6

The isolated line approximation is valid for a kind of perturbers  $a$  ( $a$  = electrons, protons, He II, ...) if  $C/W_a$  is higher than the corresponding perturber density. For a perturber density  $N$  lower than  $N_i$  ( $\text{cm}^{-3}$ )= $C/W_a$ , the line can be treated as isolated even if a weak forbidden component due to the failure of this approximation remains in the wing.  $W_a$  is the full width at half-intensity given in the

## Column 6

Parameter C for the validity condition of the isolated line approximation

### Comment to column 6

The isolated line approximation is valid for a kind of perturbers  $a$  ( $a$  = electrons, protons, He II, ...) if  $C/W_a$  is higher than the corresponding perturber density. For a perturber density  $N$  lower than  $N_i$  ( $\text{cm}^{-3}$ )= $C/W_a$ , the line can be treated as isolated even if a weak forbidden component due to the failure of this approximation remains in the wing.  $W_a$  is the full width at half-intensity given in the corresponding following columns (9, 11, 13...). See the "Introduction" for definition of the validity condition of the isolated line approximation.

## Column 7

Temperature T in Kelvin

## Column 8

A (quasistatic parameter for neutral atoms, cf. Introduction for details) if available

## Column 9

Full width at half intensity  $W_e$  in Å (electron colliders)

## Column 10

Shift  $\delta_e$  in Å (electron colliders). A positive shift is towards the red, a negative one is towards the blue

- Empty cells which are not preceded by an asterisk mean that the data are not available
- Empty cells which are preceded by an asterisk mean that the impact approximation is not valid, because  $NV > 0.5$  (cf. Introduction for details), and thus the corresponding data are not provided
- Non-empty cells preceded by an asterisk mean that the impact approximation reaches its limit of validity,  $0.1 < NV \leq 0.5$  (cf. Introduction for details) (cf. Introduction for details)

### NB

When the shift is negative, due to the additional minus sign, only the width value is marked with the asterisk.

## Columns 11 and 12

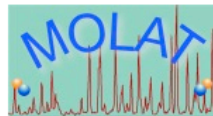
same as columns 9 and 10, but for protons colliders (subscript p)

## Columns 13 and following columns :

same as columns 9 and 10, but for other ion colliders (other corresponding subscripts)

### NB

Some widths and shifts appear at medium and not at low densities. This means that they are proportional with the density. Thus data at low densities can be deduced from those at medium densities by linear interpolation with the perturber density.

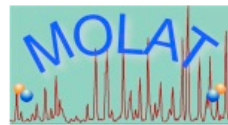


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Choose an element and an ionization degree

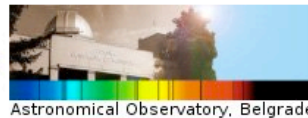
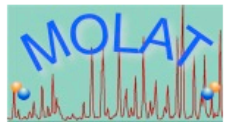
H																	He	
Li	Be											B	C	N	O	F	Ne	
Na	Mg											Al	Si	P	S	Cl	Ar	
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr	
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe	
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn	
Fr	Ra	Ac																
			Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu		
			Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr		



Choose an element and a ionization degree

- [Si I](#)
- [Si IV](#)
- [Si V](#)
- [Si VI](#)
- [Si XI](#)
- [Si XII](#)
- [Si XIII](#)

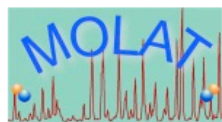
H																	He	
Li	Be											B	C	N	O	F	Ne	
Na	Mg											Al	Si	P	S	Cl	Ar	
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr	
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe	
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn	
Fr	Ra	Ac																
			Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu		
			Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr		



Select your dataset

Select your dataset

Si IV, electron Hydrogen II Helium II



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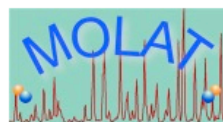
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Si IV, electron Hydrogen II Helium II

Select your Perturber density ( cm<sup>-3</sup> )

or enter a value:

OK



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Si IV, electron Hydrogen II Helium II

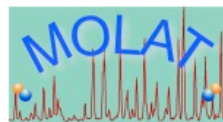
1.00e+17

or enter a value:

Select your transition

or a wavelength interval

min (Å):  max (Å):



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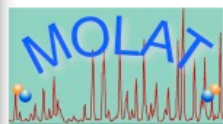
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Si IV, electron Hydrogen II Helium II

1.00e+17

or enter a value:

- Select your transition
- Select your transition
- All
- 2p6.3d 2D -> 2p6.4f 2Fo
  - 2p6.3d 2D -> 2p6.4p 2Po
  - 2p6.3d 2D -> 2p6.5f 2Fo
  - 2p6.3d 2D -> 2p6.5p 2Po
  - 2p6.3d 2D -> 2p6.6f 2Fo
  - 2p6.3d 2D -> 2p6.6p 2Po
  - 2p6.3p 2Po -> 2p6.3d 2D
  - 2p6.3p 2Po -> 2p6.4d 2D
  - 2p6.3p 2Po -> 2p6.4s 2S
  - 2p6.3p 2Po -> 2p6.5d 2D
  - 2p6.3p 2Po -> 2p6.5s 2S
  - 2p6.3p 2Po -> 2p6.6d 2D
  - 2p6.3p 2Po -> 2p6.6s 2S
  - 2p6.3s 2S -> 2p6.3p 2Po
  - 2p6.3s 2S -> 2p6.4p 2Po
  - 2p6.3s 2S -> 2p6.5p 2Po
  - 2p6.3s 2S -> 2p6.6p 2Po
  - 2p6.4d 2D -> 2p6.4f 2Fo



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Si IV, electron Hydrogen II Helium II

1.00e+17

or enter a value:

OK

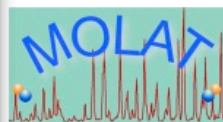
Select your transition

Select your transition

All

2p6.3d 2D -> 2p6.4f 2Fo  
2p6.3d 2D -> 2p6.4p 2Po  
2p6.3d 2D -> 2p6.5f 2Fo  
2p6.3d 2D -> 2p6.5p 2Po  
2p6.3d 2D -> 2p6.6f 2Fo  
2p6.3d 2D -> 2p6.6p 2Po  
2p6.3p 2Po -> 2p6.3d 2D  
2p6.3p 2Po -> 2p6.4d 2D  
2p6.3p 2Po -> 2p6.4s 2S  
2p6.3p 2Po -> 2p6.5d 2D  
2p6.3p 2Po -> 2p6.5s 2S  
2p6.3p 2Po -> 2p6.6d 2D  
2p6.3p 2Po -> 2p6.6s 2S  
**2p6.3s 2S -> 2p6.3p 2Po**  
2p6.3s 2S -> 2p6.4p 2Po  
2p6.3s 2S -> 2p6.5p 2Po  
2p6.3s 2S -> 2p6.6p 2Po  
2p6.4d 2D -> 2p6.4f 2Fo

OK



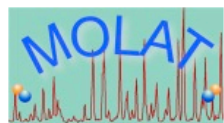
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or enter a value:

or a wavelength interval

min (Å):  max (Å):



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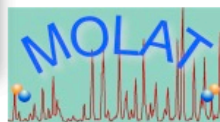
or enter a value:

or a wavelength interval

min (Å):  max (Å):

Select your temperature

All  
20000  
50000  
80000  
100000  
150000  
200000



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or enter a value:  


or a wavelength interval

 min (Å):  max (Å):  


When using these data, please refer to the original papers and to this database as :

Sahal-Bréchet, S., Dimitrijević, M.S., Moreau N., 2013. Stark-B database, [online]. Available: <http://stark-b.obspm.fr> [Apr 19, 2013]. Observatory of Paris, LERMA and Astronomical Observatory of Belgrade

## References

REFERENCES							
ARTICLE	AUTHORS	SOURCE	YEAR	METHOD	ADS REFERENCE	DOI REFERENCE	OTHER REFERENCE
Stark broadening of spectral lines of multicharged ions of astrophysical interest. II: Si IV lines.	Dimitrijević M.S., Sahal-Bréchet S., Bommier V.	A&AS, Vol.89, p.591-598	1991	SCP	<a href="http://cdsads.u-strasbg.fr/abs/1991A%26AS...89..591D">http://cdsads.u-strasbg.fr/abs/1991A%26AS...89..591D</a>	Not available	Not available
Stark broadening parameters tables for spectral lines of multicharged ions of astrophysical interest. II: Si IV lines	Dimitrijević M.S., Sahal-Bréchet S., Bommier V.	Bull. Obs. Astron. Belgrade, Vol.144, p.81-99	1991	SCP	<a href="http://cdsads.u-strasbg.fr/abs/1991BOBeo.144...81D">http://cdsads.u-strasbg.fr/abs/1991BOBeo.144...81D</a>	Not available	Not available

## Line shiftings and broadenings




N (CM-3)	LOWER LEVEL	UPPER LEVEL	MULTIPLT	WAVELENGTH (Å)	C (Å/CM-3)	T (K)	A	ELECTRON			HYDROGEN II			HELIUM II		
								*W	W (Å)	*D	D (Å)	*W	W (Å)	*D	D (Å)	*W
1.000e+17	2p6.3s 2S	2p6.3p 2Po	1	1396.7	1.400e+20	20000		1.760e-2		5.190e-5	9.070e-5	-3.040e-5	1.590e-4		-3.040e-5	
1.000e+17	2p6.3s 2S	2p6.3p 2Po	1	1396.7	1.400e+20	50000		1.120e-2		-1.740e-4	2.720e-4	-7.840e-5	3.890e-4		-7.610e-5	
1.000e+17	2p6.3s 2S	2p6.3p 2Po	1	1396.7	1.400e+20	80000		8.990e-3		-1.660e-4	4.040e-4	-1.180e-4	5.070e-4		-1.100e-4	
1.000e+17	2p6.3s 2S	2p6.3p 2Po	1	1396.7	1.400e+20	100000		8.120e-3		-1.190e-4	4.620e-4	-1.390e-4	5.710e-4		-1.290e-4	
1.000e+17	2p6.3s 2S	2p6.3p 2Po	1	1396.7	1.400e+20	150000		6.840e-3		-1.620e-4	5.710e-4	-1.810e-4	6.700e-4		-1.570e-4	
1.000e+17	2p6.3s 2S	2p6.3p 2Po	1	1396.7	1.400e+20	200000		6.120e-3		-1.870e-4	6.490e-4	-2.050e-4	7.070e-4		-1.810e-4	

## Fitting coefficients




Below are the equations used to get the fitted data :

- $\log(w) = a_0 + a_1 \log(T) + a_2 (\log(T))^2$
- $d/w = b_0 + b_1 \log(T) + b_2 (\log(T))^2$

S. Sahal-Bréchet, M. S. Dimitrijević, N. Ben Nessib, "Comparisons and comments on electron and ion impact profiles of spectral lines", 2011, Baltic Astronomy, Vol. 20, pp. 523-530

N (CM-3)	LOWER LEVEL	UPPER LEVEL	MULTIPLT	WAVELENGTH (Å)	C (Å/CM-3)	ELECTRON						HYDROGEN II						HELIUM II					
						A0	A1	A2	B0	B1	B2	A0	A1	A2	B0	B1	B2	A0	A1	A2	B0	B1	B2
1.000e+17	2p6.3s 2S	2p6.3p 2Po	1	1396.7	1.400e+20	1.6628	-1.06541	0.06301	0.24246	-0.0772	0.00494	-20.4375	6.21713	-0.55915	-3.60832	1.37118	-0.14175	-18.04533	5.47708	-0.50319	-1.38595	0.55571	-0.06457

## Updates

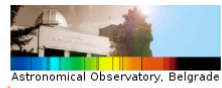
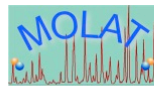
RECENTLY ADDED DATA		
ION	PERTURBERS	DATE OF IMPORTATION
O III	e, H II, He II	2012-07-24
C IV	e, H II, He II	2012-07-10
Si IV	e, H II, He II	2012-03-22
Pb IV	e, H II, He II	2012-03-14
Si XIII	e, H II, He III	2012-02-15
Ca V	e, H II, He II	2011-11-16
F I	e	2011-11-16
Ne IV	e	2011-11-10
O IV	e, H II, He III, C III, C IV, C V, O III, O IV, O V, O VI	2011-11-10
Br I	e	2011-11-09

UPDATED DATA			
ION	PERTURBERS	DATE OF IMPORTATION	REPLACED BY
C II	electron proton He II	2010-01-27	2013-02-10
Ti XII	electron proton He III	2008-08-27	2012-08-05
In III	electron proton He II	2012-03-04	2012-08-05
Ti XI	electron proton He III	2008-06-18	2012-08-05
Mg I	electron proton Ar II	2009-05-15	2012-08-05
In III	electron proton He II	2008-08-29	2012-08-05
Mg I	electron proton Si II Fe II Mg II	2009-05-15	2012-08-05
Ba II	electron proton He II	2009-09-17	2012-08-04
Pb IV	electron proton He III	2008-08-09	2012-08-04
In II	electron proton He II	2012-07-25	2012-08-04
Zn I	electron proton He II	2010-07-20	2012-08-04
F VII	electron proton He III	2008-08-30	2012-08-04
In II	electron proton He II	2008-06-18	2012-08-04
S VI	electron proton He III	2009-09-09	2012-08-04
Be III	electron proton He II	2010-07-19	2012-07-24
Mg XI	electron proton He III	2010-07-20	2012-06-30
Ca I	electron proton He II	2010-07-20	2012-06-30
Ca I	electron proton He II Mg II Si II Fe II	2008-06-18	2012-06-30
Ag I	electron proton He II	2010-07-08	2012-05-30
Al I	electron proton He II	2010-07-19	2012-05-30
Cu I	electron proton Cu II	2011-11-15	2012-03-24
Ne II	electron proton He II	2011-01-29	2012-03-14
Ne III	electron proton He II	2010-05-28	2012-03-13
Ar I	electron proton Ar II	2009-08-10	2012-02-03
Ar I	electron proton He II	2011-02-17	2012-02-03
He I	electron proton He II	2009-03-26	2011-12-19
Na I	electron proton He II	2008-09-02	2011-12-14
Ar II	electron proton Ar II	2010-02-08	2011-11-22
K I	electron proton He II	2010-07-20	2011-11-22
Cr I	electron proton He II	2010-02-14	2011-11-20
N II	electron proton He II	2010-02-11	2011-11-20

## Contact

For further enquiries or user support, contact:

- [Sylvie Sahal-Bréchet, Observatoire de Paris, LERMA, Meudon, France](#)
- [Milan S. Dimitrijevic, Astronomical observatory, Beograd, Serbia](#)
- [Nabil Ben Nessib, King Saud University, Riyadh, Saudi Arabia,](#)
- [Nicolas Moreau, Observatoire de Paris, LERMA, Meudon, France](#)



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# STARK-B: Next steps

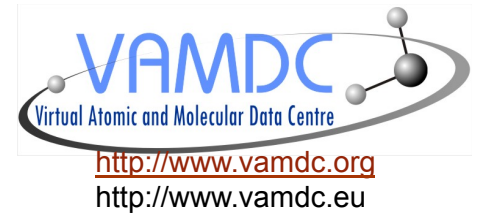
- Insertion of MSE data(in progress)
- Insertion of little “applets” on line for users:
  - ✓ extrapolation or interpolation
    - along principal quantum numbers,
    - charge of the radiating ions (isoelectronic sequences),
    - homologous ions,
    - charge of the ion collider
- Future:
  - ✓ SCP code on line: STARK-C project
  - ✓ Insertion of quantum data in intermediate coupling: SST + DW, AS
    - especially adapted to highly charged ions and resonance lines (*Sahal-Bréchet with Elabidi & Ben Nessib (2004 and after, an also with Dubau and Cornille 2007 and after)*)

# VAMDC Consortium

## *Virtual Atomic and Molecular Data Center*

- European project FP7 "Research Infrastructures summer 2009 - end of 2012
- Interoperable e-Infrastructure for exchange of atomic and molecular data
- 15 administrative partners: 24 teams
  - from 6 European Union member states,
  - Serbia, Russian Federation and Venezuela
- strong coupling
  - to the users (astrochemistry, atmospheric physics, plasmas)
  - scientists and engineers from the ICT community (*Information and Communication Technologies*) used to deal with deploying interoperable e-infrastructure

e.g. Europlanet IDIS  
IVOA (*International Virtual Observatory Alliance*)  
Members: Euro-VO , AstroGrid...



VAMDC Consortium

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This meeting will be held at the Meudon Campus of the Observatory of Paris, France, from First issue of the VAMDC newsletter is available for download. 14-16 Novem...

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**VAMDC Portal**

The VAMDC Portal is a search engine for the VAMDC databases. It works very much in the same way as an internet search engine such as Google or Bing, in that you use the portal to find out whether the database nodes may contain the information that you want, and then if a particular node does, you are presented with a link to the data directly from the node. The portal enables you to construct complex queries and the resulting data returned from the database nodes will be in the **XSAMS** common data format. If you are not yet familiar with the XSAMS data format or if you just want a quick view of your data, then the portal can send the XSAMS data from a node to an XSAMS processor, which can present the data to you in a more convenient format.

There are three links to access the portal. In the next section, you will find links marked in blue followed by a short text by way of explanation. **You can also visit our portal user guide here where you can find accompanying tutorials and how to use the interface.**

**List of VAMDC Portal**

- 1. The **portal for the external users** is at [vamdc\\_portal](#). This is a released version of portal, using 11.12 version of standards. New nodes and new xsams processors might appear after the release. Source code is considered stable and will not change for now.
- 2. The **portal for VAMDC testing** is at [vamdc\\_portal\\_test](#). If you are a VAMDC person testing nodes, please use this portal. This one sees all the latest changes and is frequently updated from the dev version. Eventually this version will be updated to use 12.07 standards.
- 3. The **development VAMDC portal** is at [vamdc\\_portal\\_dev](#). This is a pure development version that is not guaranteed to work at any given time. It is automatically updated from the latest sources overnight.

**News From AstroAtom**

- [Expanded Iron UTA spectra — probing the thermal stability limits in AGN clouds](#)
- [Suppression of Dielectronic Recombination Due to Finite Density Effects](#)
- [Photoionization modeling of oxygen K absorption in the interstellar medium: the Chandra grating spectra of...](#)
- [The 2013 Release of Cloudy Influence of Departures from LTE on Oxygen Abundance Determination](#)

# VAMDC: portal user

VAMDC Portal

portal.vamdc.org/vamdc\_portal/home.seam

Actualiser Arrêter Google

SLSP utility À la une Débuter avec Fir... Page de démarr... Les plus visités WIS Plasma Labo... VAMDC Project Observatoire de ... Webmail de l'Ob... STARK-B Marque-pages


**VAMDC**  
Virtual Atomic and Molecular Data Centre

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**Welcome to the VAMDC portal!**

Currently we have 22 databases running and ready to serve you with the data.

e-infrastructure SEVENTH FRAMEWORK PROGRAMME UCL UNIVERSITY OF CAMBRIDGE UPPSALA UNIVERSITET INSTITUTE OF ATMOSPHERIC OPTICS INSTITUTE OF ASTRONOMY RUSSIAN ACADEMY OF SCIENCES HARVARD UNIVERSITY universität wien



Home VAMDC databases Query Saved queries Info Known Issues Login Register

Name	Description	Maintainer	Status
<a href="#">Cologne Database for Molecular Spectroscopy VAMDC-TAP service</a>	The Cologne Database for Molecular Spectroscopy (CDMS) contains a catalog of radio frequency and microwave to far-infrared spectral lines of atomic and molecular species that (may) occur in the interstellar or circumstellar medium or in planetary atmospheres. The catalog is continuously updated.	endes@gh1.uni-koeln.de	OK
<a href="#">MeCaSDa - Methane Calculated Spectroscopic Database</a>	Calculated line lists for methane (12CH4, 13CH4 and 12CD3D). The data on methane contain the vibration-rotation energy levels, line positions and line intensities in the range from 0 to 6200 cm <sup>-1</sup> .	Christian.Wenger@u-bourgogne.fr	OK
<a href="#">VALD (atoms)</a>	The Vienna Atomic Line Database (VALD) is a collection of atomic line parameters (wavelengths, transition energies and quantum numbers, oscillator strengths, Lande factors, radiative and collisional broadening). This resource is the VAMDC-TAP representation of the atomic data in VALD3.	thomas.marquart@yysast.uu.se	OK
<a href="#">OACT - LASP Database</a>	Laboratorio di Astrofisica Sperimentale (Catania-LASP for short) has been active in Catania starting from the eighties. The eldest of the group, after some training at the Physics department of the Catania University, started the activity at the Catania Astrophysical Observatory. Since then and thanks to several funding agencies (Consiglio Nazionale delle Ricerche, Italian CNR; Ministero dell'Istruzione, dell'Università e della Ricerca, MIUR; Agenzia Spaziale Italiana, ASI; etc.) and to the help of many colleagues (and directors) of the Observatory the LASP has grown. Today Catania-LASP means a group of 6 people with permanent position plus some students and guests, a laboratory building equipped with high vacuum chambers, facilities for the deposition of ice films, ion and Lyman-alpha irradiation experiments, many spectrometers in the range from 190 nm up to 200 micron, and also raman spectrographs.	gle@oact.inaf.it	OK
<a href="#">BASECOL VAMDC-TAP interface</a>	This database, called BASECOL is devoted to collisional non-vibrational excitation of molecules by colliders such as atom, ion, molecule or electron. It is supervised by an international working group of molecular physicists and astrophysicists involved in the calculations and use of vibrational cross-sections, in order to ensure the continuity and the quality of the database.	misha@doronic.org	OK
<a href="#">TOPbase VAMDC-TAP interface</a>	TOPbase lists LS-coupling energy levels, g-f values and photoionization cross sections for astrophysically abundant ions (Z=1,14; Z=16; Z=18; Z=20; Z=26) computed in the Opacity Project.	nicolas.moreau@obspm.fr-franck.delahaye@obspm.fr	OK
<a href="#">Theoretical spectral database of polycyclic aromatic hydrocarbons</a>	The Cagliari/Toulouse PAH database is a collection of theoretical spectroscopic data about Polycyclic Aromatic Hydrocarbons and carbon clusters. It provides basic geometric characteristics, energetics, harmonic analyses and electronic photoabsorption data. It is maintained by the Astrochemistry group at INAF-Observatory of Cagliari and the Institut de Recherche en Astrophysique et Planétologie in Toulouse.	gmulas@ca-cagliari.inaf.it	OK
<a href="#">IEADB - Innsbruck Dissociative Electron Attachment Database</a>	This database contains informations about dissociative electron attachment upon interaction of low energy electrons with molecules.	johannes.postler@uibk.ac.at	OK
<a href="#">Chianti</a>	Chianti consists of a critically evaluated set of up-to-date atomic data, together with user-friendly programs written in Interactive Data Language (IDL), to analyse the spectra from astrophysical plasmas. The VAMDC interface presents just the data from the Chianti-v7 release.	gr@ast.cam.ac.uk	OK
<a href="#">TIPbase VAMDC-TAP interface</a>	TIPbase lists fine-structure levels, A-values, collision strengths and effective collision strengths for astrophysically abundant ions, mainly from the Fe ionuclear sequence computed in the Iron Project.	nicolas.moreau@obspm.fr-franck.delahaye@obspm.fr	OK
<a href="#">OSMA Deima S&amp;MPO</a>	Calculated line lists for ozone (16O3, 16O18O16O and 18O3). The data on methane contain the vibration-rotation energy levels, line positions and line strengths in the range from 0 to 8000 cm <sup>-1</sup> . UV ozone absorption cross sections in wavelength range 195-830 nm at various temperatures.	yl@iao.ru-vladimir.yulterev@univ-reims.fr	OK
<a href="#">ECASDa - Ethene Calculated Spectroscopic Database</a>	Calculated data of ethylene (12C2H4). The data on ethylene contain the vibration-rotation energy levels, line positions and line intensities in the range from 500 to 7500 cm <sup>-1</sup>	ludovic.daumont@univ-reims.fr-mauri.rotger@univ-reims.fr	OK
<a href="#">Carbon Dioxide Spectroscopic Databank - 296K</a>	Carbon Dioxide spectroscopic Data Base for atmospheric applications (CDSD-296) contains spectral line parameters of 7 most abundant in the Earth's atmosphere isotopologues of the carbon dioxide molecule: <sup>12</sup> C <sup>16</sup> O <sup>16</sup> O, <sup>13</sup> C <sup>16</sup> O <sup>16</sup> O, <sup>12</sup> C <sup>16</sup> O <sup>18</sup> O, <sup>13</sup> C <sup>16</sup> O <sup>18</sup> O, <sup>12</sup> C <sup>18</sup> O <sup>16</sup> O, <sup>13</sup> C <sup>18</sup> O <sup>16</sup> O, <sup>12</sup> C <sup>18</sup> O <sup>18</sup> O, <sup>13</sup> C <sup>18</sup> O <sup>18</sup> O. It covers 5.9 - 12784.1 cm <sup>-1</sup> spectral range and contains more than 419600 lines. The line parameters (line position, line intensity, energy of lower state, air-broadening coefficient, self pressure induced broadening coefficient and exponent of temperature dependence of air broadening coefficients) have the calculated values. The line list has been generated using intensity cutoff 10 <sup>-sup&gt;27</sup> -sup>28 cm/molecule at reference temperature 296 K.	vip@its.lao.ru	OK
<a href="#">GhoSST</a>	The GhoSST database ( Grenoble Astrophysics and Planetary Solid Spectroscopy and Thermodynamics" database service) provides laboratory data on spectra (from UV to FIR) of natural and synthetic solids (ices, molecular solids, minerals, salts, inorganic materials, organic materials, meteorites, adsorbed molecules, hydrated solids, ?) of space sciences, Earth sciences and astrophysical interest. It is completed with band list data (NIR to FIR) on molecular solids and adsorbed/hydration molecules. The GhoSST data come from laboratory experiments performed since 1989 at IRIG (and formerly at LGGE and LPG) with different spectroscopy techniques (transmission, bidirectional reflection, micro-spectroscopy, ATR, Raman, Fluorescence, ...)	bernard.schmitt@obs-ufgrenoble.fr	OK
<a href="#">Carbon Dioxide Spectroscopic Databank - 1000K</a>	Carbon Dioxide spectroscopic Data Base for atmospheric applications (CDSD-296) contains spectral line parameters of 7 most abundant in the Earth's atmosphere isotopologues of the carbon dioxide molecule: <sup>12</sup> C <sup>16</sup> O <sup>16</sup> O, <sup>13</sup> C <sup>16</sup> O <sup>16</sup> O, <sup>12</sup> C <sup>16</sup> O <sup>18</sup> O, <sup>13</sup> C <sup>16</sup> O <sup>18</sup> O, <sup>12</sup> C <sup>18</sup> O <sup>16</sup> O, <sup>13</sup> C <sup>18</sup> O <sup>16</sup> O, <sup>12</sup> C <sup>18</sup> O <sup>18</sup> O, <sup>13</sup> C <sup>18</sup> O <sup>18</sup> O. It covers 257 - 9548 cm <sup>-1</sup> spectral range and contains more than 395000 lines. The line parameters (line position, line intensity, energy of lower state, air-broadening coefficient, self pressure induced broadening coefficient and exponent of temperature dependence of air broadening coefficients) have the calculated values. The line list has been generated using intensity cutoff 10 <sup>-sup&gt;27</sup> -sup>27 cm/molecule at reference temperature 1000 K.	vip@its.lao.ru	OK
<a href="#">Lund laboratory spectroscopy database</a>	Experimental data for transitions and lifetimes	hampus@astro.lu.se	OK
<a href="#">Stark-b</a>	Database for "Stark" broadening of isolated lines of atoms and ions in the impact approximation	sylvie.sahai-brechot@obspm.fr	OK
<a href="#">Spectr-V3</a>	The information accumulated in the SPECTR-V3 ADB contains over 450,000 records and includes factual experimental and theoretical data on ionization potentials, energy levels, wavelengths, radiation transition probabilities, oscillator strengths, and (optionally) the parameters of analytical approximations of electron-collisional cross-sections and rates for atoms and ions. Those data were extracted from publications in physical journals, proceedings of the related conferences, special-purpose publications on atomic data, and provided directly by authors. The information is supplied with references to the original sources and comments, elucidating the details of experimental measurements or calculations, where necessary and available. To date, the SPECTR-V3 ADB is the largest factual database in the world containing the information on spectral properties of multicharged ions.	p_a_luboda@mail.ru	OK
<a href="#">Water internet Accessible Distributed Information System</a>	Database containing information on water spectra, notably data on H216O, HDO, D2O, H217O and H218O.	faz@iao.ru	OK
<a href="#">HITRAN-LICJ resource</a>	The HITRAN database - truncated version for beta testing, from http://www.cfa.harvard.edu/HITRAN/	christian.hill@ucl.ac.uk	OK
<a href="#">VALD sub-set in Moscow (obs)</a>	The part of Vienna Atomic Line Database (VALD) with accurate wavelength and energy levels. It also provides laboratory and calculated transition probabilities, Lande factors and broadening parameters. It is used for line identification and spectral synthesis.	pakhomov@inasan.ru	OK
<a href="#">KIDA VAMDC-TAP interface</a>	KIDA is a database of kinetic data interesting for astrophysical (interstellar medium and planetary atmospheres) studies. In addition to the available referenced data, KIDA provides recommendations over a number of important reactions. Chemists and physicists can add their data to the database.	Valentine.Wakeham@obs-ubordeaux.fr	OK



# Query



- Query by...
- Species
  - Processes
  - Environment
  - Advanced

Find data Save query

### Legend

available, can answer  
available, don't support query  
unsupported keyword

- » Cologne Database for Molecular Spectroscopy: VAMDC-TAP service
- » ICB Dijon Methane
- » VALD (atoms)
- » Carbon Dioxide Spectroscopic Databank (VAMDC-TAP)
- » BASECOL: VAMDC-TAP interface
- » TOPbase : VAMDC-TAP interface
- » Theoretical spectral database of polycyclic aromatic hydrocarbons
- » Chianti
- » TIPbase : VAMDC-TAP interface
- » GSMA Reims S&MPO
- » GSMA Reims Ethylene
- » TAP-XSAMS for GhoSST database
- » Lund laboratory spectroscopy database
- » Stark-b
- » Spectr-W3
- » Water internet Accessible Distributed Information System
- » HITRAN-UCL resource
- » VALD sub-set in Moscow (obs)



# Query by species



Query by...

**Species**

Atom

Processes

Molecule

Environment

Particle

Advanced

Find data Save query

## Legend

available, can answer

available, don't support query

unsupported keyword

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# Query by species: atom



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Query by...

- Species
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  - Molecule
  - Particle
- Processes
- Environment
- Advanced

Find data Save query

### Legend

available, can answer  
available, don't support query  
unsupported keyword

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# Query by species: atom (following)



Query by...

Species

Processes

Environment

Advanced

Atoms Clear Remove

Atom symbol

Mass number  to

Nuclear charge  to

Ion charge  to

InChIKey

State energy  to  1/cm to 1/cm

Equivalent to

Find data Save query

### Legend

available, can answer  
available, don't support query  
unsupported keyword

- Cologne Database for Molecular Spectroscopy: VAMDC-TAP service
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e-infrastructure



SEVENTH FRAMEWORK PROGRAMME



# Query by species: atom, processes



Query by...

Species

Processes

Environment

Advanced

Atoms Clear Remove

Radiative

Collision  to

Nuclear charge  to

Ion charge  to

InChIKey

State energy  to  1/cm

Equivalent to  to  1/cm

Find data Save query

### Legend

available, can answer  
available, don't support query  
unsupported keyword

- » Cologne Database for Molecular Spectroscopy: VAMDC-TAP service
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- » VALD sub-set in Moscow (obs)



- Query by...
- Species
  - Processes
  - Environment
  - Advanced

**Atoms** Clear Remove

Atom symbol

Mass number  to

Nuclear charge  to

Ion charge  to

InChIKey

State energy  to  1/cm

Equivalent to  to  1/cm

**Environment** Clear Remove

Temperature  to  K

Equivalent to  to  10000.0 to 50000.0 K

Pressure  to  Pa

Equivalent to  to  Pa

Number Density  to  1/cm3

**Radiative** Clear Remove

Wavelength  to  A

Equivalent Wavelength  to  2000.0 to 3000.0A

Upper state energy  to  1/cm

Equivalent to  to  1/cm

Lower state energy  to  1/cm

Equivalent to  to  1/cm

Probability, A  to  1/s

Find data Save query

**Legend**

available, can answer  
 available, don't support query  
 unsupported keyword

- » Cologne Database for Molecular Spectroscopy: VAMDC-TAP service
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# Query : result, click on download



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Done

Modify query Stop waiting Save query

select \* where (EnvironmentTemperature >= 10000.0 AND EnvironmentTemperature <= 50000.0 AND EnvironmentTotalNumberDensity = 1E17) AND (RadTransWavelength >= 2000.0 AND RadTransWavelength <= 3000.0) AND ((AtomSymbol = 'Si' AND IonCharge = 3))

Comments

XSAMS processors

- BibTeX from XSAMS
- Table views of XSAMS
- Xsams2SME

Process

Name	Response	Download	Species	States	Processes	Radiative	Collisions	Non Radiative
<input type="checkbox"/> Stark-b	OK	<a href="#">XSAMS</a>	3	9	5	5	0	0



**Xsams:** XML Schema for Atoms, Molecules and Solids  
**XML:** Extensible Markup Language  
**Xsams2SME:** converts XML document into the CSV-format wanted by Spectroscopy Made Easy (SME)

# XSAMS

XML Schema for Atoms, Molecules, and Solids



**IAEA**  
International Atomic Energy Agency  
Atoms for Peace



Done

Modify query Stop waiting Save query

select \* where (EnvironmentTemperature >= 10000.0 AND EnvironmentTemperature <= 50000.0 AND EnvironmentTotalNumberDensity = 1E17) AND (RadTransWavelength >= 2000.0 AND RadTransWavelength <= 3000.0) AND ((AtomSymbol = 'Si' AND IonCharge = 3))

Comments

**XSAMS processors**

BibTeX from XSAMS  
 Table views of XSAMS  
 Xsams2SME

Process

General views of data in XSAMS format. The display is tabular and textual. Initial display is a list of states, with links to details of each state. An alternate display of radiative transitions is available.

Name	Response	Download	Species	States	Processes	Radiative	Collisions	Non Radiative
<input checked="" type="checkbox"/> Stark-b	OK	<a href="#">XSAMS</a>	3	9	5	5	0	0



# Result of the download: code in XML language for users



Home VAMDC databases Query Saved queries Help

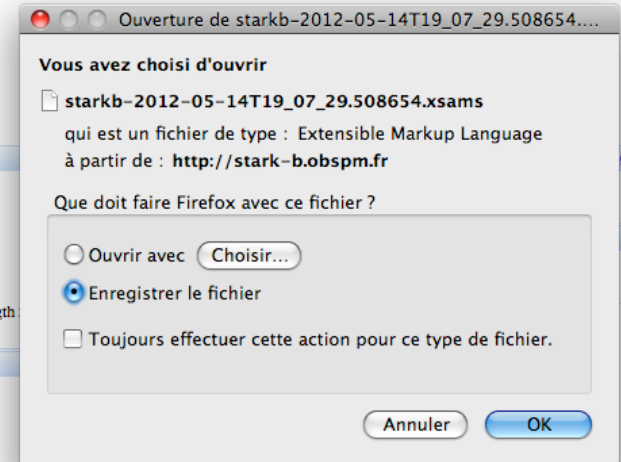
Done

Modify query Stop waiting Save query

select \* where (EnvironmentTemperature >= 10000.0 AND EnvironmentTemperature <= 50000.0 AND EnvironmentTotalNumberDensity = 1E17) AND (RadTransWavelength RadTransWavelength <= 3000.0) AND ((AtomSymbol = 'Si' AND IonCharge = 3))

Comments

Name	Response	Download	Species	States	Processes	Radiative	Collisions	Non Radiative
<input type="checkbox"/> Stark-b	OK	<a href="#">XSAMS</a>	3	9	5	5	0	0



Xsams  
XML Schema for Atoms, Molecules and Solids

Done

Modify query Stop waiting Save query

select \* where (EnvironmentTemperature >= 10000.0 AND EnvironmentTemperature <= 50000.0 AND EnvironmentTotalNumberDensity = 1E17) AND (RadTransWavelength >= 2000.0 AND RadTransWavelength <= 3000.0) AND ((AtomSymbol = 'Si' AND IonCharge = 3))

Comments

**XSAMS processors**

BibTeX from XSAMS  
 Table views of XSAMS  
 Xsams2SME

**Process**

General views of data in XSAMS format. The display is tabular and textual. Initial display is a list of states, with links to details of each state. An alternate display of radiative transitions is available.

Name	Response	Download	Species	States	Processes	Radiative	Collisions	Non Radiative
<input checked="" type="checkbox"/> Stark-b	OK	<a href="#">XSAMS</a>	3	9	5	5	0	0



**XSAMS processors**

BibTeX from XSAMS  
 Table views of XSAMS  
 Xsams2SME

**Process** [Result](#)

General views of data in XSAMS format. The display is tabular and textual. Initial display is a list of states, with links to details of each state. An alternate display of radiative transitions is available.



(Switch to view of radiative transitions)

Bstarkb-2012-06-04-19-34-56

Species	State	Energy
Si <sup>3+</sup>	— 2p6.4p <sup>2</sup> P <a href="#">— detail</a>	
Si <sup>3+</sup>	— 2p6.5p <sup>2</sup> P <a href="#">— detail</a>	
Si <sup>3+</sup>	— 2p6.6p <sup>2</sup> P <a href="#">— detail</a>	
Si <sup>3+</sup>	— 2p6.5s <sup>2</sup> S <a href="#">— detail</a>	
Si <sup>3+</sup>	— 2p6.4d <sup>2</sup> D <a href="#">— detail</a>	
Si <sup>3+</sup>	— 2p6.5d <sup>2</sup> D <a href="#">— detail</a>	
Si <sup>3+</sup>	— 2p6.6d <sup>2</sup> D <a href="#">— detail</a>	
Si <sup>3+</sup>	— 2p6.4f <sup>2</sup> F <a href="#">— detail</a>	
Si <sup>3+</sup>	— 2p6.5f <sup>2</sup> F <a href="#">— detail</a>	

# Line-list view of XSAMS

(Switch to view of states)

Bstarkb-2012-06-04-19-34-56

Species	$\lambda/v/n/E$	Probability	Upper state	Lower state	Broadening
Si <sup>3+</sup>	$\lambda=2125.0$ A		— 2p6.5s <sup>2</sup> S	— 2p6.4p <sup>2</sup> P	Detail
Si <sup>3+</sup>	$\lambda=2675.2$ A		— 2p6.5d <sup>2</sup> D	— 2p6.4f <sup>2</sup> F	Detail
Si <sup>3+</sup>	$\lambda=2676.6$ A		— 2p6.6d <sup>2</sup> D	— 2p6.5p <sup>2</sup> P	Detail
Si <sup>3+</sup>	$\lambda=2483.7$ A		— 2p6.6p <sup>2</sup> P	— 2p6.5s <sup>2</sup> S	Detail
Si <sup>3+</sup>	$\lambda=2287.0$ A		— 2p6.5f <sup>2</sup> F	— 2p6.4d <sup>2</sup> D	Detail

# Broadening of a single radiative-transition in XSAMS

Bstarkb-2012-06-04-19-19-48

Transition ID: Pstarkb-R3057

Wavelength = 2125.0 Å

Type	Temperature	Pressure	Density	Composition	Profile	Parameters	Comments
pressure	20000 K		1e+17 1/cm3	• electron	Lorentzian	gammaL = 0.205	
pressure	20000 K		1e+17 1/cm3	• Hydrogen (H <sup>+</sup> )	Lorentzian	gammaL = 0.00567	
pressure	20000 K		1e+17 1/cm3	• Helium (He <sup>+</sup> )	Lorentzian	gammaL = 0.00628	
pressure	50000 K		1e+17 1/cm3	• electron	Lorentzian	gammaL = 0.15	
pressure	50000 K		1e+17 1/cm3	• Hydrogen (H <sup>+</sup> )	Lorentzian	gammaL = 0.0116	
pressure	50000 K		1e+17 1/cm3	• Helium (He <sup>+</sup> )	Lorentzian	gammaL = 0.011	

# Thank you for your attention