

SCIENTIFIC USE CASES FOR THE VIRTUAL ATOMIC AND MOLECULAR DATA CENTER

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Abstract. VAMDC Consortium is a worldwide consortium which federates interoperable Atomic and Molecular databases through an e-science infrastructure. The contained data are of the highest scientific quality and are crucial for many applications: astrophysics, atmospheric physics, fusion, plasma and lighting technologies, health, etc. In this paper we present astrophysical scientific use cases in relation to the use of the VAMDC e-infrastructure. Those will cover very different applications such as: (i) modeling the spectra of interstellar objects using the myXCLASS software tool implemented in the Common Astronomy Software Applications package (CASA) or using the CASSIS software tool, in its stand-alone version or implemented in the Herschel Interactive Processing Environment (HIPE); (ii) the use of Virtual Observatory tools accessing VAMDC databases; (iii) the access of VAMDC from the Paris solar BASS2000 portal; (iv) the combination of tools and database from the APIS service (Auroral Planetary Imaging and Spectroscopy); (v) combination of heterogeneous data for the application to the interstellar medium from the SPECTCOL tool.

Keywords: databases, software, atoms, molecules, solar physics, interstellar medium

1 Introduction

VAMDC(<http://www.vamdc.eu/>) (Dubernet et al. 2010) is a worldwide e-infrastructure which federates interoperable Atomic and Molecular databases. The contained data are of the highest scientific quality and are crucial for many applications: astrophysics, atmospheric physics, fusion, health, etc. In this paper we present astrophysical scientific use cases in relation to the use of the VAMDC e-infrastructure.

Those scientific science use cases reflect the strategy of the VAMDC Consortium towards users of atomic and molecular data. One objective consists in providing the scientific community with innovative tools for easily handling and processing results that are queried from the VAMDC interface portal (sect.2) or from standalone tools such as SPECTCOL(sect.3). Another strategy consists in porting the VAMDC capabilities and facilities into tools developed by institutes outside the consortium such as the SPECVIEW software (sect.4.1). This software is part of our main strategy of user software development as it can be used in many applications where visualisation of spectra is concerned, and for any type of users: researchers, education, business, outreach. In this paper we will present a science use case within the APIS service (sect. 4.2). A last objective consists in providing support so that external users can implement our VAMDC plugin in their software: this has been applied to the BASS2000 portal (sect.7), to the Cassis tool from IRAP (sect.~refcassis), and to the MyXCLASS interface for CASA (sect. 6).

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2 Link to Virtual Observatory Tools

A key element of the VAMDC infrastructure is the web portal (<http://portal.vamdc.eu>), that provides an unified way to query the VAMDC registered atomic and molecular databases. A request is built through a graphical user interface and sent to all the databases. They return data in a common XML format called XSAMS (<http://www.vamdc.eu/standards>).

The portal provides tools called “Processors” that can convert a XSAMS file into another format. The Processors called ‘Molecular Spectroscopy XSAMS to HTML’ and ‘Atomicxsams2HTML’ display for, respectively molecular and atomic spectroscopic data, an HTML page where columns and lines can be selected. The selected data can be exported into 2 formats: a CSV table where column are separated by “,” and a VOTable which is a Virtual Observatory (VO) standard used to exchange data among VO Tools.

The VOTable can be sent to any VO Tool launched on the users’ desktop using the “send via SAMP” functionality of the processor. SAMP is another VO Standard (<http://www.ivoa.net/documents/SAMP/>) that allows several applications to exchange data directly, without the need to save and load a file locally.

In the example below, the file is sent to an application called TOPCAT (<http://www.star.bris.ac.uk/~mbt/topcat/>) which is dedicated to the visualisation of tabular data. All functionalities of TOPCAT can be used on the selected VAMDC data.

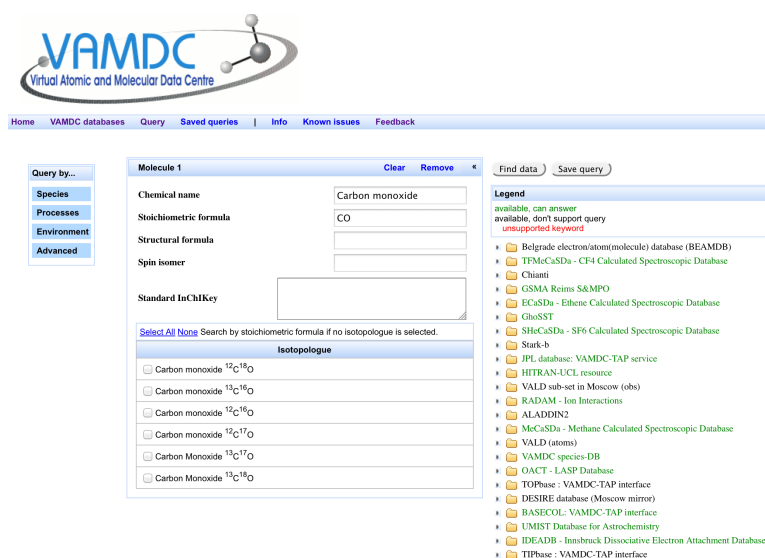


Fig. 1. VAMDC Portal:<http://portal.vamdc.eu>.

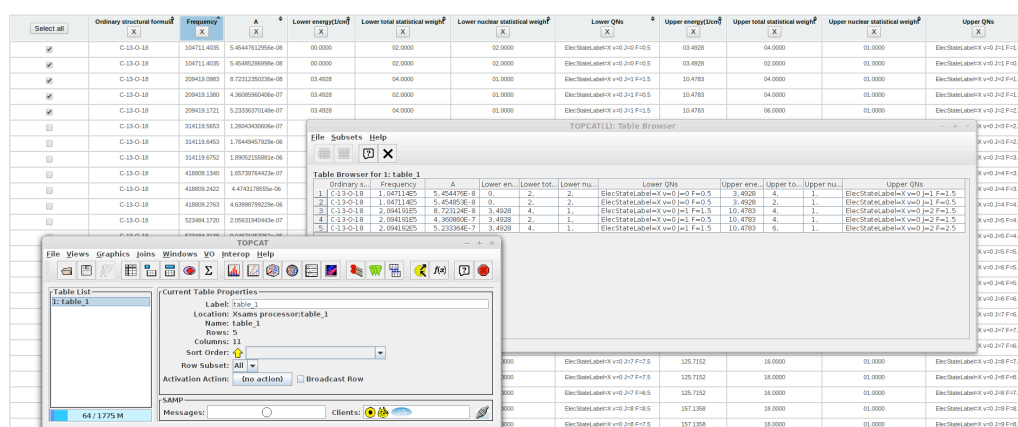


Fig. 2. Molecular data displayed by the processor and sent to TOPCAT VO Tool.

3 The Spectcol Tool

The aim of the client tool SPECTCOL (<http://www.vamdc.eu/software>) (Dubernet et al. 2012) is to associate spectroscopic data provided by spectroscopic databases with collisional data provided by collisional databases using the VAMDC technology.

The client tool interrogates the registries to find spectroscopic and collisional information about a molecule. It retrieves different possible sets of data from different databases. The user can associate sets of his own choice in order to create customized combination of spectroscopic and collisional data.

Indeed the usual difficulty met by astrophysical users is to combine collisional data from a database such as BASECOL Dubernet et al. (2013) (<http://basecol.obspm.fr>) with spectroscopic data coming from other native databases such as CDMS (<http://www.astro.uni-koeln.de/cdms>), JPL (<http://spec.jpl.nasa.gov/>) or any other spectroscopic databases. Combination of data implies the possibility to match molecular states that were very often described differently in JPL, CDMS and BASECOL, and this problem is now solved easily using VAMDC and SPECTCOL.

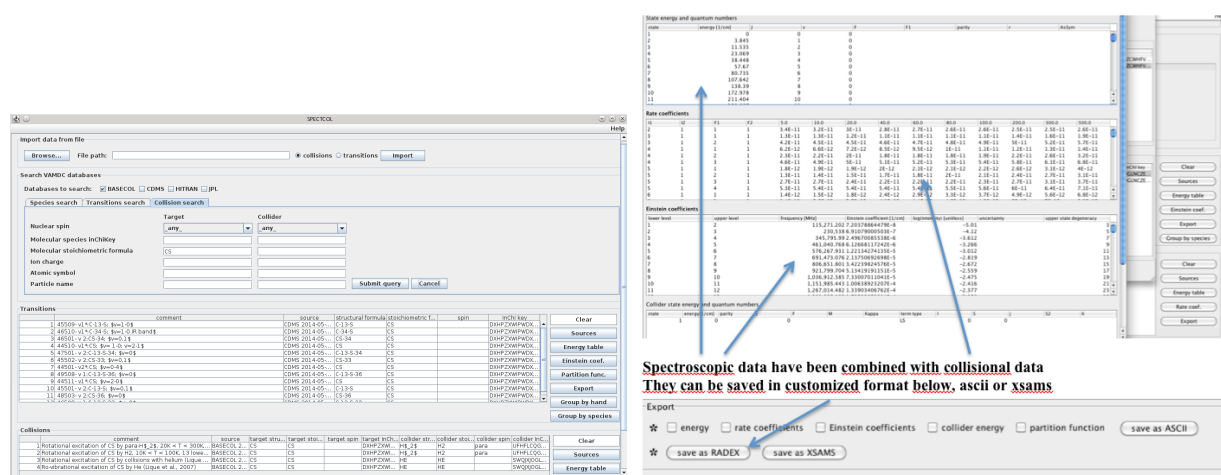


Fig. 3. Left: Spectcol Query Interface. **Right:** Spectcol output where matching has been done between spectroscopic data and collisional data.

4 Link within the APIS Service: Specview

4.1 SPECVIEW

Specview is a tool for 1-D spectral visualization and analysis of astronomical spectrograms from STScI (http://www.stsci.edu/institute/software_hardware/specview/). It is written in Java and thus can be run anywhere Java is supported. Specview is able to read all the Hubble Space Telescope spectral data formats, as well as data from several other instruments (such as IUE, FUSE, ISO, FORS and SDSS), preview spectra from MAST, and data from generic FITS and ASCII tables. It can also read data from Virtual Observatory servers, and read and write spectrogram data in Virtual Observatory SED format. It can also read files in the SPC Galactic format used in the chemistry field.

Specview can overplot spectral line identifications taken from a variety of line lists, including user-supplied lists. Its linelists' query form has been modified to include the VAMDC Query Module, called QueryBuilder (<http://www.vamdc.eu/developer>), thus providing the full capability of querying the VAMDC databases. In particular it allows to select finely the observed species and properties of linelists. Currently about 20 spectroscopic databases are inter-connected through VAMDC and accessible through VAMDC software and libraries.

4.2 APIS

The APIS service (Lamy et al. 2014) (for Auroral Planetary Imaging and Spectroscopy) is freely accessible at <http://apis.obspm.fr> since mid-2013. It consists of a high level database of auroral planetary observations

(images and spectra) of the outer planets and their satellites taken by the Hubble Space Telescope in the Far-UV window from 1997 up to now, including more than 5000 individual observations. The APIS database is archived at VO-PARIS Data Center. Associated metadata are built along the standard Europlanet-Table Access Protocol (EPN-TAP) (Erard et al. 2014a), so that the data can be queried externally to APIS by VO portals such as VESPA (<http://vespa.obspm.fr>) (Erard et al. 2014b), and be quickly and efficiently sorted out by a dedicated search interface (see left panel of Fig. 4). APIS finally proposes to interactively work with the data online, through VO tools, such as Aladin and Specview.

Both 1D and 2D spectra can be plotted online from APIS with Specview through a Simple Application Messaging Protocol (or SAMP) hub (see right panel of Fig. 4). As planetary aurorae result from the collisional excitation of the upper atmosphere by magnetospheric electrons, spectra of the outer planets provide a direct mean to probe the upper atmospheric composition, mainly populated by atomic and molecular hydrogen. Specview is able to retrieve transitions lines from VAMDC catalogues (H-Lya is provided by default with Specview, while H₂ lines can be retrieved from the SESAM database <http://sesam.obspm.fr>), and to superimpose them to the observations (see right panel of Fig. 4).

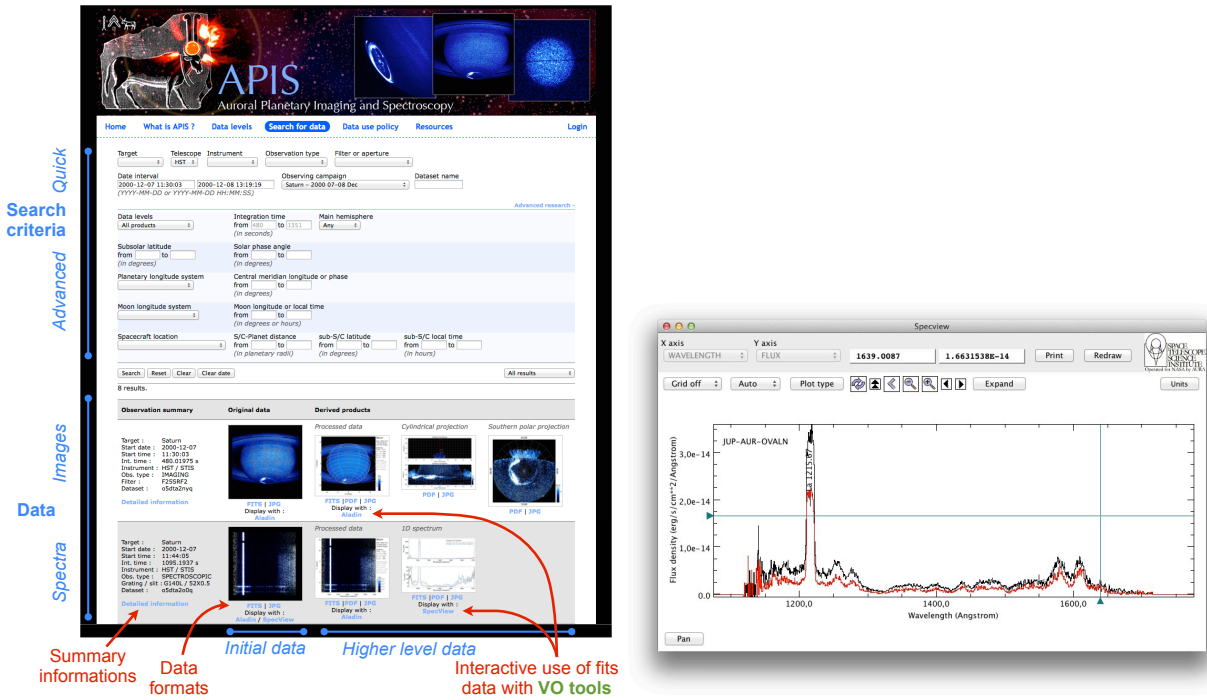


Fig. 4. Left: Example of data query with the APIS search interface. **Right:** Far-UV spectrum of Jupiter plotted with Specview. The H-Lya transition is marked by a vertical line.

5 Link from CASSIS Application

The CASSIS (Centre d'Analyse Scientifique de Spectres Instrumentaux et Synthétiques) software has been developed by CESR/IRAP since 2005 (<http://cassis.irap.omp.eu>). It allows to generate synthetic spectra to prepare astronomical observations or to compare with actual observations, provides the means to perform a quick line identification (necessary for large spectral surveys), and helps to determine the sources parameters (line width, column density, temperature, density, beam dilution) with LTE or non-LTE minimisation scripts or rotational diagram analysis when many transitions are available. CASSIS is available as a stand-alone application or as a plug-in of the Herschel Interactive Processing Environment (HIPE).

CASSIS uses the Single Spectral Access (SSA) Protocol to access the IVOA services in order to retrieve any spectra (Hubble, Corot, ISO, Pollux, etc) via our SSA module. Also CASSIS uses the SAMP messaging protocol that enables astronomy software tools to interoperate and communicate. CASSIS is able to retrieve informations on the spectroscopic data necessary for the modeling (LTE or non-LTE: see <http://cassis.irap.omp.eu/docs/RadiativeTransfer.pdf> for details) or identification from databases (CDMS, JPL) through the VAMDC

TAP protocol based on IVOA format. TAP provides virtual data and allows to plug in the query language VSS2 and the data model VAMDC-XSAMS (the latter being an output format)(<http://www.vamdc.eu/standards>).

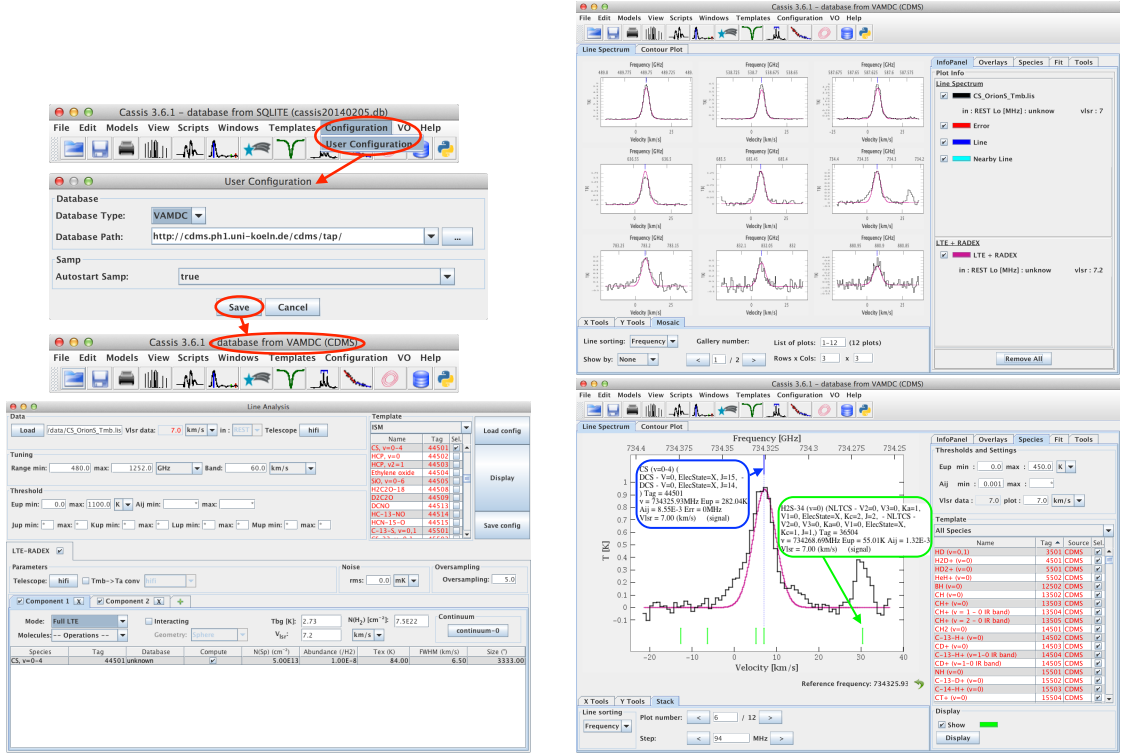


Fig. 5. Left: The top panels show how to change the user configuration in order to swap from a local SQLite database to the VAMDC database. The bottom panel is a snapshot of the Line Analysis module with parameters such that CASSIS will search all the CS transitions having an $E_{up} < 1100$ K, potentially present in the selected data file and will overlay an LTE model. The result is displayed in the figure to the right. **Right:** The top panel shows the result corresponding to the Line Analysis window (left panel). All the transitions found are displayed as a mosaic and clicking on one of the lines allows the user to zoom on it. The bottom panel shows a zoom of the 6th transition over which transitions (with $E_{up} < 450$ K and $A_{ij} > 10^{-3}$) from other species have been overlaid, allowing the identification of an H_2^{34}S line next to the CS line (Herschel/HIFI data).

6 Link from myXCLASS Interface for CASA

Spectroscopic data as it is accessible via VAMDC is essential to model and analyze astronomical spectra. VAMDC has supported the development of a toolbox (<http://www.astro.uni-koeln.de/projects/schilke/myXCLASSInterface>) for the Common Astronomy Software Applications package (CASA) in order to include access to its databases. The toolbox contains the myXCLASS program, which is used to model astronomical spectra by solving the radiative transfer equation for an isothermal object in one dimension, whereas the finite source size and dust attenuation are considered as well.

The spectroscopic data, such as transition frequencies, state energies, Einstein A coefficients, degeneracies and partition functions, required for the modeling, is retrieved via the VAMDC infrastructure from the CDMS and the JPL catalogs, and then stored in a local database. Besides the access to the databases, the toolbox also includes the model optimizer package MAGIX Möller et al. (2013) (Modeling and Analysis Generic Interface for eXternal numeric codes). This optimizer helps to find the best description of the data using a given model, i.e., helps to find the parameter set that most closely reproduces the data.

A recent example, where the toolbox has been successfully used, is the analysis of spectra recorded towards the Sgr B2(M) cloud core which exhibits strong absorption features of gas located in the spiral arms of our galaxy. One of these spectra is shown in left panel of Fig. 6. It shows a spectrum of $^{36}\text{ArH}^+$ (1-0) (blue) recorded towards the star forming region SgrB2(M). The optimizer has been used to fit the spectrum (red)

and to derive column densities and excitation temperatures as a function of relative velocity of the molecular gas. The derived column density per velocity as shown in the right hand side figure for the above example including other species provides important insights into the physical, chemical and structural composition of these objects Schilke et al. (2014).

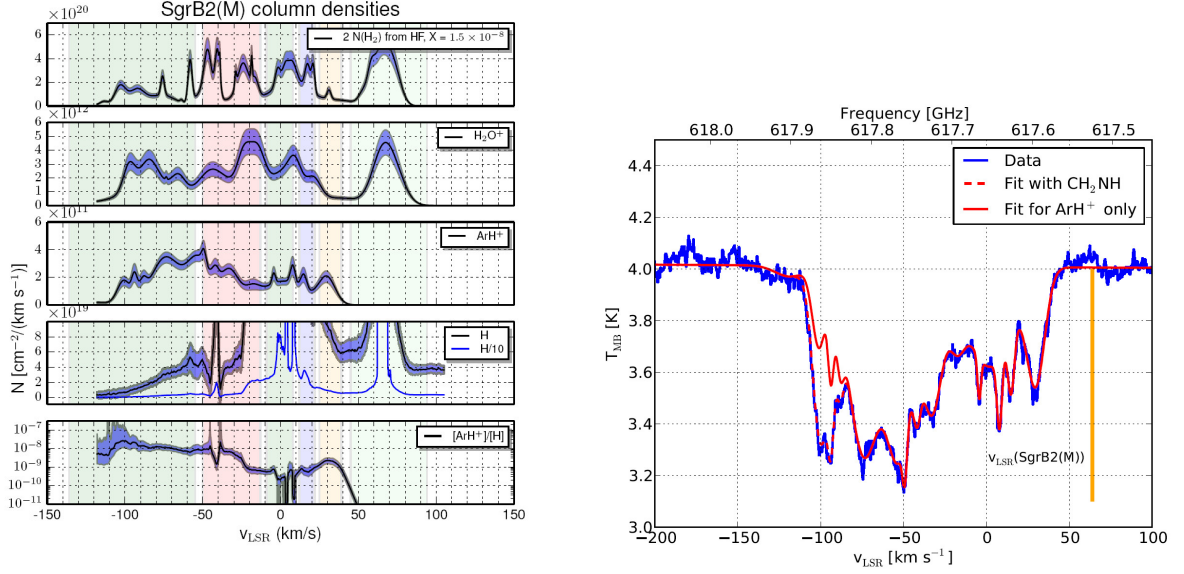
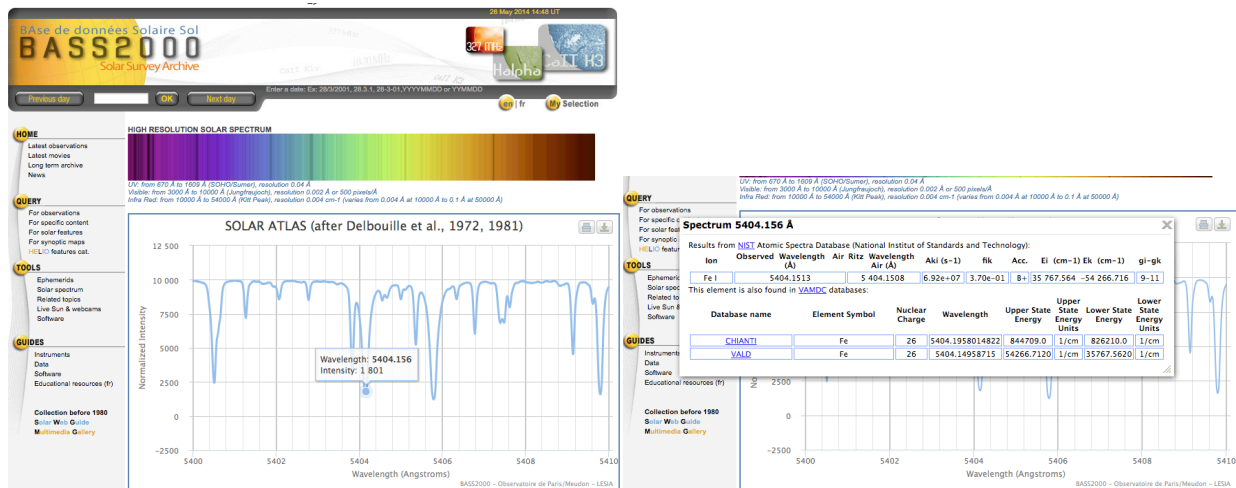


Fig. 6. Left: Spectrum of $^{36}\text{ArH}^+$ (1-0) toward SgrB2(M) with fit including the H_2CNH line blending at -110 km s^{-1} as dashed red line, and fit $^{36}\text{ArH}^+$ only in red. **Right:** Column density per km s^{-1} of HF, H_2O^+ , $^{36}\text{ArH}^+$, and H. The error estimate for $^{36}\text{ArH}^+$ was done using the MAGIX Interval Nested Sampling algorithm. The uncertainty is marked by the blue shading around the curves.

7 Link from BASS2000 Portal

BASS2000 (<http://bass2000.obspm.fr>) provides access to a wide range of the Solar spectrum, from 67 nm to 5 400 nm. This spectrum is obtained from Curdt et al. (2001) for the UV part using SOHO/SUMER data; from Delbouille et al. (1972) for the visible part, using Kitt Peak National Observatory observations; from Delbouille et al. (1981) for the infrared part, also based on Kitt Peak observations. The visible part of the spectrum is very much used both for preparing and processing observations. Spectro-polarimeters take full advantage of the detailed knowledge of atomic data concerning the observed lines in order to be able to calculate local magnetic field. Therefore, Solar spectrum has been connected to VAMDC in order to provide directly useful information to the user. This helps for data processing, but also in order to prepare observations, for instance tagging atmospheric molecular lines, such as water, that may serve for wavelength calibration.



8 Conclusions

The VAMDC Consortium provides support for all those strategies: you can implement protocols that VAMDC has designed: see <http://www.vamdc.eu/standards>. You might want to save time and to use our libraries in Java or other languages: <http://www.vamdc.eu/developers>. You may need some tutorials: see <http://tutorial.vamdc.org>. You may need some help: send a mail to support@vamdc.eu. You may want to exchange: <http://forum.vamdc.org> and to create your own sub-topics. You may want that our services are improved, then contact the relevant people: <http://www.vamdc.eu/contact>.

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