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ARCHIVES OF ASTRONOMICAL SPECTRAL OBSERVATIONS AND ATOMIC/MOLECULAR DATABASES FOR THEIR ANALYSIS

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Abstract. We present a review of open-source data for stellar spectroscopy investigations. It includes lists of the main archives of medium-to-high resolution spectroscopic observations, with brief characteristics of the archive data (spectral range, resolving power, flux units). We also review atomic and molecular databases that contain parameters of spectral lines, cross-sections and reaction rates needed for a detailed analysis of high resolution, high signal-to-noise ratio stellar spectra.

Key words: atomic data – line: identification – molecular data – instrumentation: spectrographs – astronomical databases: miscellaneous – surveys – atlases

1. INTRODUCTION

Spectroscopy is the most powerful tool in astrophysics. A significant part of information about stellar temperature, gravity, chemical composition, dynamical structure of galaxies is extracted from the analysis of stellar spectra. Modern methods of determination of stellar atmospheric parameters and chemical abundances are based on fitting a synthetic spectrum to the observed one. Rapid development of techniques of astronomical observations and, in particular, unprecedented accuracy in spectroscopic observations require an adequate response from the laboratory and theoretical spectroscopy. The fitting quality depends on the accuracy of input atomic parameters: wavelengths (transition energy levels), transition probabilities, damping parameters, etc.

To analyze spectra of astronomical objects, one needs processed spectra, models of emitting matter, and a set of parameters for atomic and molecular lines that form the observed flux. In the era of photographic spectra, it was difficult to distribute observations, and each astronomer or group of astronomers had to carry out their own observations and perform the full reduction procedure. Today, practically all astronomical observations are carried out in digital format that allows us to collect data in archives and databases, providing access to these data for outer users.

At present, many ground-based and space telescopes produce a huge amount of observational data, including images in different filters, spectra in different spectral ranges (UV, optical, IR), polarization measurements. Each telescope has a schedule of observations based on approved proposals of scientific groups. Usually these observations become publicly available after one year since their official release. Many large observatories create special archives and provide an opportunity to download raw or reduced CCD observations from their websites. Thus, there is a chance that observations of your objects were already obtained by other astronomers, and you may extract the needed data from archives, with the acknowledgements specified by the archives.

Usually, processing of observations is carried out with the pipelines specific for individual spectrographs. A pipeline is a set of software tools that provides full automatic processing of raw 2-D spectra and produces an output in the form of 1-D spectra calibrated in absolute or relative units.

This article presents a review of open archives of spectral data, models of stellar atmospheres, and atomic and molecular data, necessary for spectroscopic analysis.

2. ARCHIVES OF SPECTRAL OBSERVATIONS

Usually, spectra are available at the website of the observatory. A menu on the main webpage provides links to the archive page or user portal. In some cases, registration is required. All data (raw or reduced) are presented in FITS (Flexible Image Transport System) format, which is the main format of astronomical data. One should remember that records in the FITS format may be different: data for a given wavelengths scale, ascii or binary tables.

The first online archive we would like to mention is the General Observation Archive of the Special Astrophysical Observatory of the Russian Academy of Sciences, North Caucasus, Russia:
http://www.sao.ru/oasis/cgi-bin/fetch
It starts with a list of instruments. This list includes one high-resolution spectrograph, NES (Nasmyth Echelle Spectrograph; resolving power R=35 000–60 000), used at the 6-m BTA telescope. An online form provides access to the spectra taken since 1994. The query form allows one to search by object name or coordinates, by date, by Principal Investigator (PI) of the proposal, by the type of data, and by observation mode. The available observations are in raw format. Access to the archive does not require registration.

Next, there are two online archives of the Haute-Provence Observatory, France. The first one is the archive of observations obtained with the fibre-fed echelle spectrograph, ELODIE, at the 1.93-m telescope:
http://atlas.obs-hp.fr/elodie/
The resolving power is R=42 000. The archive contains 35 535 spectra in the 4000–7000 Å spectral range. The spectra are available as raw and reduced data. The reduced 1-D spectra are in relative flux units. Low resolution spectra with R=10 000 are calibrated in absolute flux units (reduced above the Earth's atmosphere), with a broad-band photometric precision of 2.5% and narrow-band precision of 0.5%. The web interface allows the user to preview the selected data. The search is performed by object name or coordinates. Some additional search possibilities are available. Access to the archive does not require registration. ELODIE was decommissioned in mid-August 2006, after more than 12 years of observations, so the archive is completed.

ELODIE was replaced by the new echelle spectrograph SOPHIE:
http://atlas.obs-hp.fr/sophie/

The resolving power of the SOPHIE spectrograph is R=40 000, 75 000. Observations cover the spectral range 4000–7000 Å. The web query form is exactly the same as in the ELODIE archive. The current version of the archive (June 3, 2015) contains 81 483 spectra of 6144 objects. 55 980 spectra are open to download. The archive does not require registration.

The largest amount of spectral data is collected in the archive of the European Southern Observatory (ESO):
http://archive.eso.org/eso/eso_archive_main.html
The ESO archive has separate query forms for raw and reduced data. The second one is operated only for the HARPS and UVES high-resolution stellar spectrographs. The search is performed by object name or coordinates, by spectrograph name, by date, by program ID, by PI of the proposal, by type of data, and by additional parameters. Several high-resolution spectrographs are included in the archive: the CRIRES installed at the 8-m VLT telescope ($R \lesssim$100 000), the EMMI installed at the 4-m NTT telescope (R=77 000), the FEROS installed at the MPG/ESO 2.20-m telescope and the full VLT array (R=48 000), the HARPS installed at the 3.6-m telescope (R=115 000), and the UVES installed at the 8-m VLT telescope (R=80 000–110 000). The user should register at the ESO User Portal.

Recently, a new archive of stellar spectra was opened. It is the archive of the ESPaDOnS spectrograph (Echelle SpectroPolarimetric Device for the Observation of Stars) installed at the Canada-France-Hawaii telescope:
http://www.cfht.hawaii.edu/Instruments/Spectroscopy/Espadons/
The resolving power of this instrument is R=68 000, 80 000. Spectroscopic observations cover the 3700–10 500 Å wavelength range. The query form provides a search by object name or coordinates, by observation ID, by PI name, by proposal ID or title, by keywords, by date, by the type of data, and by additional parameters. Spectral data are presented in relative units separately for individual echelle orders. The web interface allows one to preview the selected data. Access to the archive requires preliminary registration.

Additionally, we mention two open archives of spectra calibrated in absolute flux units. The first one is the archive of the Space Telescope Imaging Spectrograph (STIS) of the Hubble Space Telescope. Now it is a part of the Mikulski Archive for Space Telescopes (MAST):
http://archive.stsci.edu/
STIS has many different spectral modes with R=500–114 000 and covers different spectral bands in the overall range 1140–10270 Å. For the initial query, the user needs only the target name or coordinates. Observational data from different space missions are also available in MAST. It is not necessary to register for an account to search the archive catalogs or retrieve public data. However, to retrieve proprietary data, such as recently archived HST data, a registration in the STScI's Institute-wide Single Sign On (SSO) system is required.

The next archive is the science archive of the Sloan Digital Sky Survey (SDSS):
http://dr12.sdss3.org/
The basic search requires Plate ID, modified Julian date (MJD), and Fiber. The advanced search includes selection of objects by the range of magnitudes, coordinates, object type, instruments, redshift, and specific flags. The archive does not require registration.

Finally, we mention the Asiago Database of Spectroscopic Databases, which is

a compilation of published data:
http://web.pd.astro.it/adsd
Query interface has two forms: looking for a star, and looking for a catalog. In the first form, you indicate only the object name; in the second one, the user indicates spectral range, spectral type, luminosity class, data type, and resolution. The archive does not require registration.

3. GRIDS OF STELLAR ATMOSPHERE MODELS

It was mentioned in Sec. 1 that one needs a model of the emitting matter for a detailed spectral analysis. In stellar spectroscopy, it is the model of stellar atmosphere. There are two commonly used grids of stellar-atmosphere models with open access. The first of them contains models calculated with the famous Kurucz's codes, ATLAS9 and ATLAS12. These 1-D plane-parallel LTE (local thermodynamic equilibrium) models are collected in the Castelli & Kurucz database:
http://www.oact.inaf.it/castelli/
Model atmospheres are calculated in the effective temperature range $T_{\rm eff}$=3 500–50 000 K, surface gravity range $\log g = 0.0$–5.0 dex, metallicity range [Fe/H]=–5.5 to +0.5 dex with mixing length parameters l/H=0.5, 1.25. The grid also includes models with enhanced abundances of helium and alpha-elements. Besides models, the Castelli & Kurucz database contains fluxes calculated for each model. Fluxes are calculated for 1221 spectral points distributed over the 90–1 600 000 Å interval. A useful part of the database is the grid of theoretical color indices calculated for a number of photometric systems, including *Johnson*, *Cousins*, *Strömgren*, *Geneva*, *Walraven*, *Sloan*, *HST* systems, and others. No registration is required to download data from the Castelli & Kurucz database.

The second popular grid of model atmospheres is Models of Atmospheres in Radiative and Convective Scheme (MARCS):
http://marcs.astro.uu.se/
These are 1-D, hydrostatic, plane-parallel and spherical LTE models of cool stellar atmospheres (Gustafsson et al. 2008). The MARCS collection contains about 52 000 stellar-atmosphere models of F-, G-, K-, and M-type stars in three different formats. The user has to register, then choose the necessary models and retrieve them via ftp as tar archives.

Next is the multipurpose stellar atmosphere code PHOENIX (Hauschildt et al. 1996). Two grids of models were produced with this code. For dwarfs, the NextGen model grid was calculated from 3000 K to 10 000 K (in steps of 200 K), for surface gravity $\log g$ between 3.5 and 5.5 dex in steps of 0.5, and metallicities [M/H] between –4.0 and 0.0 dex in steps of 0.5 (Hauschildt et al. 1999a). For giants, the NextGen model grid with effective temperature between 3000 and 6800 K, surface gravity between 0.0 and 3.5 dex, and metallicity between –0.7 and 0.0 dex was calculated by Hauschildt et al. (1999b). We did not find these model grids in open access; however, low-resolution synthetic spectra grids based on these models are available at
http://www.am.ub.edu/∼carrasco/models/synthetic.html

The last stellar-atmosphere code we mention is LLmodels (line-by-line) code, where each line contributing to opacity is taken into account for modeling the atmosphere, similar to synthetic spectrum calculations (Shulyak et al. 2004). A model grid calculated with this code for the microturbulent velocity 2.0 $\mathrm{km\,s^{-1}}$ contains models ranged from 4500 to 22 000 K in effective temperature, from 2.5 to 5.0 dex in surface gravity, and from –0.8 to +0.8 dex in metallicity (see Table 5 in Tkachenko et al. 2012). The corresponding steps are 0.1 dex in $\log g$, 0.1 dex in metallicity, 100 K in the 4500–10 000 K effective temperature range and 250 K for higher T_{eff} values. This grid is currently available at *https://fys.kuleuven.be/ster/meetings/binary-2015/gssp-software-package*

4. DATABASES OF ATOMIC AND MOLECULAR DATA, CROSS SECTIONS AND REACTION RATES

The third ingredient in spectral analysis is the input parameters of spectral lines: wavelengths (transition energy levels), transition probabilities, damping parameters, etc. Below we briefly describe several main databases of atomic and molecular data, cross sections, and reaction rates.

CHIANTI: *http://www.chiantidatabase.org* is an Atomic Database for Spectroscopic Diagnostics of Astrophysical Plasmas. This database consists of a critically evaluated set of up-to-date atomic data for different isoelectronic sequences, together with user-friendly programs written in Interactive Data Language (IDL) and Python to calculate radiation from astrophysical plasmas (Dere et al. 1997; Landi et al. 2013). The database includes atomic energy levels, wavelengths, radiative transition probabilities, collision excitation rate coefficients, ionization and recombination rate coefficients, as well as data to calculate free-free, free-bound, and two-photon continuum emission mainly for highly ionized atoms. The access to CHIANTI package is free.

NIST Atomic Spectra Database: *http://www.nist.gov/pml/data/asd.cfm* This database provides access and search capability for NIST critically evaluated data on atomic energy levels, wavelengths, and transition probabilities that are reasonably up-to-date (Ralchenko et al. 2013). The NIST database is subdivided in two parts: Lines and Levels. Critical compilations are carried out by the Atomic Spectroscopy Data Center, located in the Physical Measurement Laboratory at the National Institute of Standards and Technology (NIST), USA.

KURUCZ's data collection: *http://kurucz.harvard.edu* is an online collection of a huge amount of laboratory and theoretical data for atomic and molecular lines. It includes energy levels, transition probabilities, calculated damping parameters and Landé factors, hyperfine splitting and isotopic components when available (Kurucz 2011). All transitions in Kurucz's data are divided into the observable part (transitions between experimentally measured energy levels) and the predicted part. The second, largest part of data is used for opacity calculations, while the first part is used for fine spectral analysis. A description of file formats and Fortran codes to read the data are available.

The Vienna Atomic Line Database (VALD) is a collection of atomic and molecular transition parameters of astronomical interest (Kupka et al. 1999, 2000; Ryabchikova et al. 2015). VALD offers tools for selecting subsets of lines for typical astrophysical applications: line identification, abundance analysis and radial velocity measurements, model atmosphere calculations etc. The VALD Electronic Mail Service (VALD-EMS) is the main data transfer protocol for small data set extraction. For extraction of a large amount of data, VALD users are recommended to use the 'via ftp' option. The VALD web portal is the main user interface to VALD. It offers the full functionality of the extraction tools and the flexibility of data access. VALD has three mirror sites:

- Uppsala *http://vald.astro.uu.se/∼vald3*

- Moscow *http://vald.inasan.ru/∼vald3*

- Vienna *http://vald.astro.univie.ac.at/∼vald3/php/vald.php*

We list below the main ideas behind the VALD concept that may help using it in the most efficient way:

- VALD extraction tools are constructed for intelligent selection of data relevant for a specific astronomical problem.
- VALD is regularly updated with critically evaluated data sets. The VALD project experts investigate statistical properties of the data, extensively compare the results obtained from different data sources, and establish a quality rating for each new source, which is a basis for data selection. This portal offers the user a possibility of creating and saving an alternative ranking table that would also ensure reproducibility of the extraction.
- VALD data access is free but requires registration. Registration helps in rejecting spam, collecting statistics, and informing the users about updates.

TOPBASE: *http://cdsweb.u-strasbg.fr/topbase/topbase.html*
This database contains the most complete dataset of LS-coupling term energies, f-values, and photoionization cross sections for astrophysically abundant ions ($Z = 1 - 26$) that is currently available (Cunto & Mendoza 1992). They have been computed in the close-coupling approximation by means of the R-matrix method with innovative asymptotic techniques. In most cases, the accuracy of the data is comparable with that obtained by other state-of-the-art atomic physics numerical approaches. The user can either ftp the original raw files or make use of the interactive searching facilities to display custom views of: Table of content, Energy levels, f-values, Photoionization cross sections.

HITRAN: *http://hitran.org*
is an acronym for high-resolution transmission molecular absorption database. HITRAN is a compilation of spectroscopic parameters that a variety of computer codes use to predict and simulate the transmission and emission of light in the Earth's atmosphere (McClatchey et al. 1973; Gordon et al. 2013). The HITRAN compilation, and the analogous HITEMP (high-temperature spectroscopic absorption parameters) database, are developed at the Atomic and Molecular Physics Division, Harvard-Smithsonian Center for Astrophysics. The current edition of HITRAN is now available to users on an interactive internet application called HITRANonline. HITRANonline and the HITRAN Application Programming Interface, HAPI, provide the user with many new features. The features include the convenient ability to filter, plot, download data in user-defined outputs, calculate absorption and transmission, apply advanced line-shape functions, and many

new capabilities. Users can log in to the database portal, but for data extraction registration is required.

CDMS: *http://cdms.ph1.uni-koeln.de/cdms/portal*

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 occur in the interstellar or circumstellar medium or in planetary atmospheres (Müller et al. 2001). A catalog section contains mostly rotational transition frequencies, uncertainties, intensities, and a wealth of other information on atomic and molecular species that may occur in the ISM or CSM or in planetary atmospheres. Supported by the University of Cologne. Registration is not required.

KIDA: *http://kida.obs.u-bordeaux1.fr*

is a database of KInetic Data of interest for Astrochemical (interstellar medium and planetary atmospheres) studies (Wakelam et al. 2012). In addition to available referenced data, KIDA provides recommendations over a number of important reactions. The database is supported by the Astrophysical laboratory of Bordeaux, Bordeaux University, CNRS. Chemists and physicists can add their data to the database through several paths listed at the website. Astrophysicists can download the database through the download form. You need to log in to add or download data. Online forms allow the users to consult and download the data.

Different databases have different error evaluation procedures. The NIST team carefully studies the quality of experiments and/or theoretical calculations and then supplies the data with a corresponding quality parameter. The VALD team checks each new set of data by calculating synthetic spectra and comparing them with the observed spectra of benchmark stars, Sun, Procyon, etc. Fig. 1 shows a comparison between the observed and calculated spectrum in the region of the Fe I λ4235.386 Å line. This line is in the list of experimental data reported by O'Brian et al. (1991) and has a quality parameter D+ ($\sim$20%) in the NIST compilation, while the line does not appear in stellar spectra. Synthetic spectra fit observations if the transition probability for Fe I λ4235.386 Å line is taken from theoretical Kurucz's calculations. Note that a difference between the cited experimental and theoretical transition probabilities exceeds 2 dex. Therefore, this Fe I line, as well as several other lines recommended by NIST, were removed from experimental data of the VALD collection.

All above-mentioned atomic and molecular (A&M) databases have different formats of data presentation that is a certain difficulty for the users. Moreover, each of these databases was created for a specific class of scientific tasks; therefore, they are not complete from the point of view of A&M spectroscopy. To make the access to A&M data easier for the user, it was decided to create a well documented interoperable interface to the differently organized existing A&M databases.

VAMDC (Virtual Atomic and Molecular Data Centre): *http://vamdc.eu*

is a consortium of institutes and research institutions that share a common technical and political framework for the distribution and curation of atomic and molecular data (Dubernet et al. 2010; Rixon et al. 2011). The VAMDC Consortium technical framework relies on the use of the e-science VAMDC infrastructure that provides the international research community with access to a broad range of A&M data compiled within a set of A&M databases accessible through the provision of a single portal. VAMDC uses XML-based well documented format XSAMS to exchange data between hosts and users. There exist tools to convert XSAMS

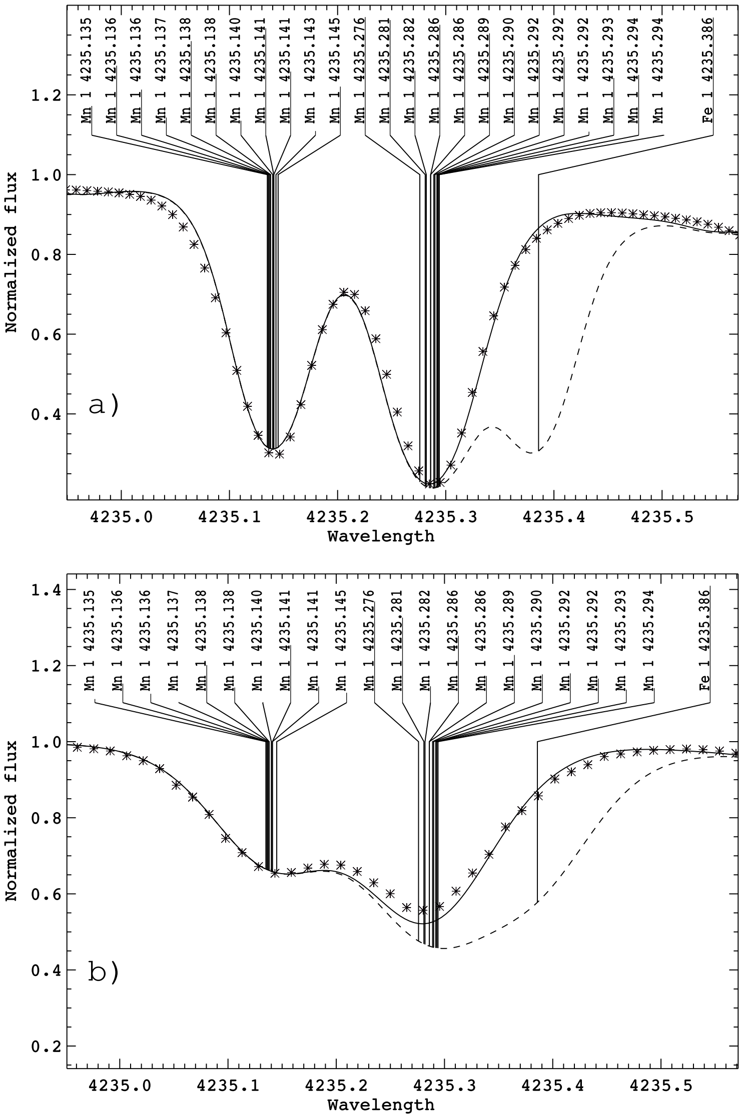

Fig. 1. Example of spectral fitting in the region of Fe I 4235.386 Å line for the Sun (a) and Procyon (b). Observations are plotted as asterisks; the synthetic spectrum calculated with the experimental transition probability for this line is represented by the dashed curve; the solid curve is the synthetic spectrum calculated with the theoretical transition probability.

into human readable formats. For simple queries, registration is not needed. To get access to wide data collections and to internal VAMDC tools, the user has to register at the VAMDC User Portal. Currently, VAMDC includes about 30 databases.

Finally, we would like to show an example of a spectral analysis package that

uses data from most of the above-mentioned databases. This is the SME (Spectroscopy Made Easy) package: *http://www.stsci.edu/∼valenti/sme.html*
SME was designed as a tool that performs analysis of stellar spectra using spectral fitting techniques in a consistent and reproducible way (Valenti & Piskunov 1996). SME uses spectral observations, grids of model atmospheres, and lists of spectral lines with their parameters as input data and returns the stellar-atmosphere parameters (effective temperature, surface gravity, metallicity, rotational velocity, etc.) that fit the observed stellar spectrum.

5. SUMMARY

Using these online references, it is possible to carry out an analysis of stellar atmospheres without leaving a computer. Nevertheless, we note that the user should have basic knowledge in theoretical astrophysics and some experience in spectral analysis to get reliable results.

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