VALD – an atomic and molecular database for astrophysics

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Abstract. The VALD database of atomic and molecular data aims to ensure a robust and consistent analysis of astrophysical spectra. We offer a convenient e-mail and web-based user interface to a vast collection of spectral line parameters for all chemical elements and in the future also for molecules. An international team is working on the following tasks: collecting line parameters from relevant theoretical and experimental publications, computing line parameters, evaluating the data quality by comparison of similar data from different sources and by comparison with astrophysical observations, and incorporating the data into VALD. A unique feature of VALD is its capability to provide the most comprehensive spectral line lists for specific astrophysical plasma conditions defined by the user.

1. Introduction

The VALD database was created in 1995 as the “Vienna Atomic Line Database” [1] and aimed at providing the relevant information for atomic transitions significantly contributing to absorption in stellar spectra.

The goals of VALD are to
- compile accurate and complete lists of spectral lines relevant to stellar atmospheres and spectroscopy
- evaluate line lists and suggest rankings according to the quality of line data
- provide a database allowing
  - easy expansion with respect to data type and size
  - simple and fast access to individual entries
  - extraction of references and quality criteria
  - extraction of best data sets according to default or user ranking.

For each transition, the database contains at least the central wavelength, a species identifier, the energies and total angular momentum quantum numbers of the two levels and the oscillator strength. For many lines, Landé factors, damping constants, term designations, oscillator
strength accuracy and an identifier for the source of the data are also included. Data originating
from different sources are converted to common units. The data are stored in binary format in
fixed length records. The data files are further processed by a compression algorithm specifically
written for VALD. The compression reduces the size of the database by a factor of five, while
allowing independent access to each record.

2. VALD today – VALD-2

2.1. VALD data

VALD-2 contains the line lists from Kurucz CD-ROMs 18 and 20–22 [2–6], as well as line
lists compiled by the VALD team from numerous sources (about 34 000 lines for about 60
ions), and van der Waals constants calculated by [7]. The data quality is determined by error
estimates given in the original sources, by intercomparison of data from different sources, and
by astrophysical verification (comparison of synthetic spectra to observations). Extraction of
data from VALD is based on a default ranking of line lists according to data quality, which is
determined by VALD team members. However, users have the option to provide their own
rankings for the source lists (via the so-called “personal configuration” on the VALD web
interface, see Section 2.2). For a detailed description of the use of ranking parameters see [1]
and [8]. These two publications, together with [9], constitute the main published documentation
of VALD-2. An up-to-date version of the documentation is made available on-line on the VALD
web page (see Section 2.2). The database content is being updated from time to time, and
detailed information about each update is given in the “News” section on the VALD web page.

The last major update of VALD-2, at the end of 2007, resulted in more than 100 000 additional
lines for about 30 ions. For example, data for lanthanides from the DREAM database [10] are
now included in the extraction by default on all mirror sites, and a new classification of the Nd III
spectrum [11] is provided. The update further consisted of corrections and additions to data for
existing lines, such as new van der Waals constants [12] and new experimental Landé factors.
A detailed description of the latest additions to the data content will be given in forthcoming
publications (see also the contribution by Ryabchikova et al. to this volume).

For the selection of new oscillator strength data to be included in VALD, the preferred sources
are experimental determinations of \( f \)-values (i.e. laboratory measurements of branching fractions
and level lifetimes), followed in preference by theoretical calculations of \( f \)-values. Occasionally,
these data are supplemented by “astrophysical” \( f \)-values, i.e. determination of the oscillator
strengths from fits of synthetic spectra to high-quality observed spectra of well-known stars or
other astrophysical objects. This method has to be regarded with caution, since it depends
on a number of assumptions for modelling the stellar spectrum. The two most important
assumptions are a fixed, known abundance of the concerned species in the star and the physics
of the atmospheric model, which can introduce systematic errors in the derived \( f \)-values [see
also 13]. Nevertheless, large compilations of astrophysical \( f \)-values, such as [14] and [15] might
be included as optional source lists in VALD, accessible for users by editing their personal
configuration.

2.2. Accessing VALD

The VALD web interface and documentation can be accessed on three mirror sites, in
Vienna (http://ams.astro.univie.ac.at/vald/), Uppsala (http://www.astro.uu.se/~vald/) and
Moscow (http://vald.inasan.ru/~vald/). New VALD clients register via e-mail to the VALD
administrator or on the web interface. VALD requests are sent to the E-Mail Service (VALD-
EMS) via e-mail, which can be composed by using the web interface (see Fig. 1). VALD serves
about 1000 users from 70 countries and processes over 200 requests per day.

Four different request types are available: Show Line – extract all information about a few
spectral lines within a small wavelength interval from all sources, Extract Element – extract
transition data with highest ranking for all lines of a species within a certain wavelength interval, Extract All – same as Extract Element, but for all species contained in VALD, Extract Stellar – effective temperature, surface gravity, microturbulence and chemical composition are provided by the user; extract all spectral lines with highest ranked data producing significant absorption within a certain wavelength interval. A request of the latter type uses atmospheric models from R.L. Kurucz’s website (ATLAS9 ODFNEW grids with microturbulence parameter 2 km s$^{-1}$, [16]). The radiative transfer equation is solved at the central wavelength of each line ignoring blending. Lines with a central depth larger than a given threshold are extracted. This type is the most requested by users (see Fig. 1).

3. VALD tomorrow – VALD-3 developments
The next major release of the database – VALD-3 – will contain a significant amount of new data, including recently published lists of atomic data, data for diatomic molecules (e.g. TiO, see Fig. 2), and information on autoionization, isotopic shifts, extended van der Waals broadening and Zeeman pattern calculation. The extraction tools will be upgraded with additional capabilities, such as new partition functions for a large number of molecules (for Extract Stellar requests), an update of the web interface and the extraction tools with new options, and references to original sources in BibTeX format in the output. VALD-3 data-providing teams include R. Kurucz (CfA Cambridge), S. Johansson, H. Nilsson et al. (Fe peak elements, Th, U, Lund University), J.E. Lawler, E.A. Den Hartog, et al. (lanthanides, Univ. of Wisconsin), E. Biémont, et al. (lanthanides, Univ. Liège), J.S. Sobeck et al. (Cr, Univ. of Texas at Austin) and J.C. Pickering, R.J. Blackwell-Whitehead et al. (e.g. Ti, Imperial College, London), as well as some of the authors of this paper (PB, RK, BP).

We hope that the database will continue to be a valuable tool for astrophysical applications. In the longer term, we envisage an extension of the database to further data needed for calculations of astrophysical spectra (hyperfine structure constants, photo-ionization and collision cross-sections), or at least efficient links from the VALD database to other databases providing such data. Furthermore, a standardized format of atomic data would be of great advantage. We are addressing this issue by considering the possibility of providing VALD output in Virtual Observatory format (VOTable) and creating an interface to the Virtual Observatory.

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Figure 2. Astrophysical verification of TiO line lists – ESO/VLT/UVES spectrum of M dwarf GJ 628 (green dots) and model spectrum for $T_{\text{eff}} = 3400$ K and solar metallicity with TiO data from [17] (red line).

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