ASTRONOMY & ASTROPHYSICS
SUPPLEMENT SERIES

Astron. Astrophys. Suppl. Ser. **112,** 525-535 (1995)

VALD: The Vienna Atomic Line Data Base

N.E. Piskunov[1,2], F. Kupka[1], T.A. Ryabchikova[3], W.W. Weiss[1] and C.S. Jeffery[4]

[1] Institut für Astronomie, Türkenschanzstr. 17, A-1180 Wien, Austria
email: LAST_NAME@GALILEO.AST.UNIVIE.AC.AT
[2] Joint Institute for Laboratory Astrophysics, Univ. Colorado, Boulder, CO 80309-0440, U.S.A.
[3] Institute for Astronomy, Russian Academy of Sciences, Pyatnitskaya 48, 109017 Moscow, Russia
[4] Department of Physics and Astronomy, Univ. St. Andrews, N. Haugh, St. Andrews, Fife KY16 9SS, UK

Received December 5, 1994; accepted March 4, 1995

Abstract. — The "Vienna Atomic Line Data Base" (VALD) consists of a set of critically evaluated lists of astrophysically important atomic transition parameters and supporting extraction software. VALD contains about 600 000 entries and is one of the largest collections of accurate and homogeneous data for atomic transitions presently available. It also includes specific tools for extracting data for spectrum synthesis and model atmosphere calculations. The different accuracies of data available in the literature made it necessary to introduce a ranking system and to provide a flexible method for extracting the best possible set of atomic line parameters for a given transition from all the available sources. The data base is presently restricted to spectral lines which are relevant for stars in which the LTE approximation is sufficient and molecular lines do not have to be taken into account. The provision was made that these requirements should not restrict the general design of VALD and the possibility of future expansion. In this paper we describe the structure of VALD, the available data sets and specific retrieval tools. The electronic-mail interface (VALD-EMS) created to allow remote access to VALD is also described. Both users and producers of atomic data are invited to explore the database, and to collaborate in improving and extending its contents.

Key words: atomic data — stars: abundances — astronomical data bases: miscellaneous

1. Introduction

The detailed analysis of stellar spectra provides a wealth of information, including the chemical composition of their atmospheres, the surface distribution of active regions (spots) and magnetic fields and the identification of pulsation modes. The extraction of such information always implies some kind of modelling of the stellar atmosphere and the calculation of a synthetic spectrum. Such modelling requires the solution of the radiative transfer equation in order to obtain the spectral distribution of the emerging flux and, hence, a detailed knowledge of the line opacities.

The ultimate goal of the Vienna research group was the computation of model atmospheres with individualized chemical compositions. Using one very large master list containing many million lines for each model would have been computationally very expensive. Instead, we developed a special tool which allows to extract only those transitions that contribute significantly to the total opacity. These tools, called PRESELECT and SELECT, are cornerstones of VALD (see Fig. 1 and Subsect. 5.2).

Send offprint requests to: W.W. Weiss

For the majority of spectral lines the absorption profile is sufficiently described by the product of central opacity and a broadening profile given by the Voigt function $H(\alpha,v)\cdot(\pi^{1/2}\Delta\nu_D)^{-1}$ – a convolution of Doppler and Lorentz profiles. The latter is characterised by the damping constants Γ_r (*radiative*), Γ_s (*Stark*) and Γ_w (*van der Waals*). In the approximation of local thermodynamic equilibrium (LTE), the central line opacity, neglecting stimulated emission, depends on

$$\kappa_{\lambda_c} \propto gf\lambda_0{}^2 e^{-E/kT}\cdot H(\alpha,0). \qquad (1)$$

where $\alpha = \Gamma/4\pi\Delta\nu_D$. Thus the atomic data required to characterise an atomic absorption line are $\lambda_0, gf, E, \Gamma_r, \Gamma_s, \Gamma_w$, and, in order to account for Zeeman splitting in the presence of a magnetic field, the effective Landé factor.

These data have been obtained by different authors in a number of different ways, both experimentally and theoretically. Consequently, the value of a datum for a given transition may vary from one line list to another (such lists will be called *source lists* in the following). This uncomfortable situation is a permanent source of confusion amongst researchers and often a reason for systematic

Table 1. The current VALD source lists

Source List	Elements / Ions	Number of Lines	References
Bell light:	Li to K	66794	Kurucz (1993)
Bell heavy:	Cu to U	38453	Kurucz (1993)
NLTE lines:	H, He, B, C, O, Na, Mg, Al, Si, K, Ca	39791	Kurucz (1993)
Kurucz-Peytreman:	He to U	265587	Kurucz & Peytremann (1975) (observed energy levels)
GFIRON ext.	Ca to Ni	406942	all lines between observed energy levels (Kurucz 1994)
NBS:	Sc to Ni	8124	Martin, Fuhr & Wiese (1988), A. Gulliver (included in Kurucz, 1993)
	Ti II	185	Bizzarri et al. (1993), Ryabchikova et al. (1994a)
	Cr II	57	Pinnington et al. (1993), Sigut & Landstreet (1990)
	Fe I	1814	O'Brian et al. (1991)
	Pr II, Nd II, Sm II, Eu II, Er II	332	Komarovskij (1991)
	Ce II	30	solar averaged gf-values
NBS Mono 145:	La II, Ce II, Pr II, Nd II, Sm II, Er II	4367	Meggers et al. (1975),
	Ga II, Xe II	49	Ryabchikova & Smirnov (1989, 1994), Wiese & Martin (1980)

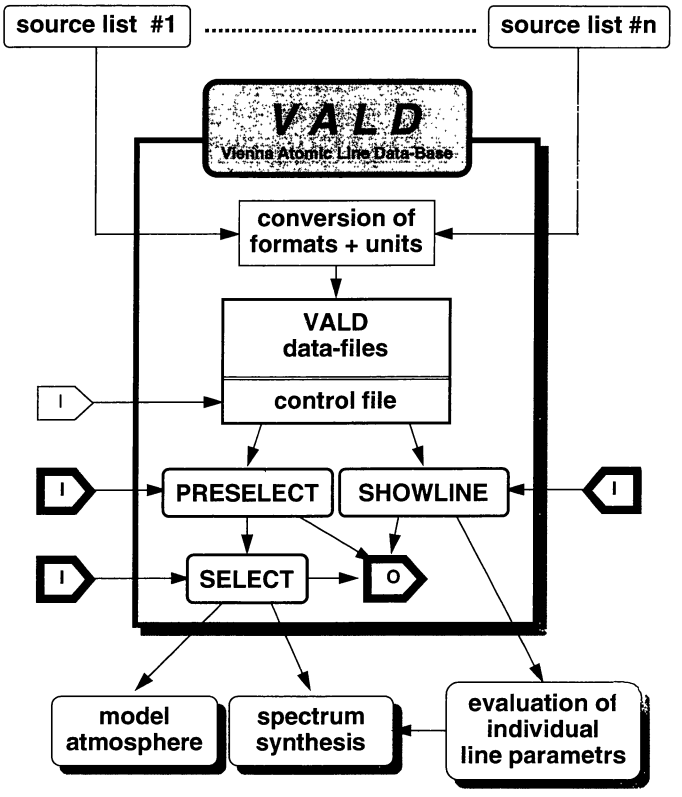

Fig. 1. Block diagram showing the logical structure of VALD. Individual components are described in the text. I – input of extraction parameters by a user in the interactive mode, **I** – input **also** via electronic mail (VALD-EMS) possible, **O** – output to the user via e-mail or in the interactive mode as a file

differences between published analyses, even when based on the same observations.

1.1. *Main goals of VALD*

The main goals of the VALD project are therefore:
- to compile the most accurate and complete lists of spectral lines relevant to stellar atmospheres (presently we focus on atomic lines observed in stars of spectral types late B, A, F and G. These restrictions, however, are not fundamental to the design of VALD),
- to evaluate the source lists in terms of reliability of different parameters and to rank the lists accordingly, and
- to provide a data base which can
  - be easily expanded by adding new data files and/or new line parameters,
  - provide simple access for computer software written in a high-level language,
  - ensure quick access to individual entries (interactive queries),
  - provide a quick and simple overview of parameters available from different lists,
  - compile all the references for transitions,
  - provide quality criteria,
  - generate output files for spectrum synthesis or model atmosphere calculations.

1.2. *Main features of VALD*

At present, the source lists of spectral lines given in Table 1 have been converted to the VALD standard binary format and included in the data base. Where necessary, line parameters have been converted to the physical units

used in VALD. The lists have been critically evaluated and ranked (see Sects. 2 to 3).

Control files let users restrict the search to particular subsets and to create output files with a flexible format. These files are needed for computing opacity distribution function tables compatible with Kurucz' (1993) model atmosphere code ATLAS9, for the spectrum synthesis program SYNTH-II, (Piskunov 1992; Ryabchikova et al. 1994a), and the interactive program ROTATE (Piskunov 1992; Ryabchikova et al. 1994a) which fits synthetic spectra to observations.

2. Structure of VALD

VALD consists of files with entries for transitions which are characterized by a set of parameters:

1. Central wavelength in Å
2. Ion identifier $kk.jj$ - kk = atomic number, jj = ionisation
3. $\log gf$ - logarithm of the oscillator strength f times the statistical weight g of the parent level
4. E_i - excitation energy of the lower level (in eV)
5. J_i - principal quantum number of the lower energy level
6. E_k - excitation energy of the upper level (in eV)
7. J_k - principal quantum number of the upper energy level
8. g_i - Landé factor of the lower energy level
9. g_k - Landé factor of the upper energy level
10. $\log \Gamma_r$ - logarithm of the radiation damping constant in $(4\pi s)^{-1}$
11. $\log \Gamma_s$ - logarithm of the Stark damping constant in $(4\pi s N_e)^{-1}$ at 10 000 K
12. $\log \Gamma_w$ - logarithm of the Van der Waals damping constant in $(4\pi s N_H)^{-1}$ at 10 000 K
13. Spectroscopic terms of lower and upper energy levels (ASCII text)
14. Index of accuracy for $\log gf$ - where available
15. Comments, e.g. multiplet number (Martin et al. 1988), relative accuracy for $\log gf$

In general, a source list is considered for VALD if at least the first seven parameters are given. If any of the next five quantities are missing from the source list, *default values* of '0' for the damping constants and '99' for Landé factors (to avoid confusion with real zero Landé factors) are inserted. The remaining parameters are text strings and are filled with blanks if no information is provided by the source list.

Most of the spectral lines in VALD are extracted from four large line lists: BELLLIGHT, BELLHEAVY, GFIRON and NLTElines (Kurucz 1992). These lists are used as the primary source for wavelengths, energy levels, J-values, damping constants and Landé factors. Presently, damping constants are available for iron group elements (from GFIRON) and for some light elements.

Although much effort has been put into checking and cross-checking the input data for VALD, the user must still be careful. Not all gf-values are accurate enough for an abundance analysis. Some observed lines are missing, and some nonexistent lines show up in synthetic spectra (see Sect. 4.3). Lists with more accurate gf-values are continually being added to VALD.

3. The VALD extraction software

The software written for VALD consists of several programs written in standard Fortran to ensure portability. The required flexibility of the system is achieved by using control files describing the layout of VALD data files, ranking etc. Interactive users can create their own control files. The e-mail service provided by VALD always uses a default control file. Program control and data exchange is based on standard input and output to allow several programs to be combined into a pipeline.

3.1. *The VALD standard format*

The number of different formats used for published line lists comes close to the number of authors. Furthermore, different units were used in the literature for the physical quantities. To eliminate the conversion problem, to save storage space and data retrieval time, we have chosen common units and a common file format for VALD.

A line list in VALD can be split into several files. Every file in VALD format consists of an arbitrary number of records with a fixed size and format. Each record holds the complete data for one atomic transition (hereafter simply called "line"). These quantities are stored sequentially in binary format. Different files can contain the same line, but each line inside a given file has to be unique.

Currently, to add a new source to VALD, a specific conversion program has to be written in order to transform the data values to the physical units used in VALD, to fill in the default values (if needed), and to produce a VALD binary data file.

3.2. *Control files*

An example of a typical control file for VALD is given in Table 2.

The first line determines the extraction parameters. Presently, they are:

- the *wavelength window*, defining the wavelength range in Å for which lines in different files are assumed to be the same, provided they refer to the same ion, J-values and, to within 0.1%, upper energy level. This quantity is necessary, because different VALD source lists may give slightly different wavelengths for the same transition.
- the *maximum spectrum number* (ionization stage + 1),

Table 2. An example of a VALD control file

```
0.01,5,50.
; wavelength window in A, maximum spectrum number
; (ionization stage + 1), and maximum excitation
; potential of lower level in eV
;
'ree.exp',  5,57,71,2,5,3,3,0,0,0,0,'REE lines, experimental'
'ree.main', 6,57,71,3,3,3,3,0,0,0,0,'REE lines, main list'
'C.nlt',    9, 6, 6,3,3,3,3,0,1,1,1,'NLTE lines: C'
'O.nlt',   10, 8, 8,3,3,3,3,0,1,1,1,'NLTE lines: O'
;'Li20.kp',17, 3, 8,1,1,1,1,0,0,0,0,'KP 1975: Li to O'
'kur4000', 30,20,28,2,2,2,2,2,2,2,2,'GFIRON ext. 4000-5000'
'iron.nbs',41,26,26,0,5,0,0,0,0,0,0,'NBS: Iron'
```

and

• the *maximum excitation potential* of the lower energy level in eV for lines to be extracted.

All the other lines in the control file are either comments (beginning with a semi-colon) or a reference to a VALD data file. The reference has the following format: filename, reference index (unique number assigned to each data file which can be chosen by the user), followed by the range of elements covered (in line 7 of Table 2 the string '57,71' indicates that lines of La to Lu are listed in 'ree.main'). The next eight numbers describe the quality (ranking parameters) of the values given for a line (see Subsect. 3.3) and are followed by a short text describing the source list. This text will also appear in the output files.

3.3. *Ranking parameters*

An important aspect of VALD, which allows the line data to be tested and the most reliable values to be used, is the ranking of quantities in each file of the data base. This is achieved by choosing *ranking parameters* in the control file (Subsect. 3.2).

The ranking of a quantity is defined by a non-negative integer number. Eight ranking parameters are given in the data base control file and provide, in sequence, quality assessments for each of λ, gf, E_i, E_k, $\overline{g}_{\rm eff}$, $\Gamma_{\rm r}$, $\Gamma_{\rm s}$, and $\Gamma_{\rm w}$. If entries to the same line in different files are found, the parameters with the highest respective ranking are extracted. The example control file in Table 2 addresses files 'ree.exp' and 'ree.main' which partially contain the same lines from RE elements. Wavelength and all '0'-ranked parameters would always be taken from file 'ree.main' due to its higher wavelength ranking (which is '3'). The same would happen for the energy levels. On the other hand, the gf-value would be taken from 'ree.exp' (the ranking is '5' against '3' in the other list).

Except for '0' and '1' the numerical value of a ranking parameter has no immediate significance. It is the whole *set* of ranking parameters assigned to a given *set* of lists which matters. Any integer value could be used for a given parameter and a particular list as long as the preferred list has the highest value for that parameter.

Two ranking values have a special meaning: '0' indicates that for all lines in the list only the default value (see Sect. 2) is given for that parameter. Both lists in our example have a 0-ranking for $\overline{g}_{\rm eff}$, hence all lines have the same default value of '99' for both Landé factors g_i and g_k. If a line, however, is included in one of the other files with a non-zero ranking, the value encountered at the first occurrence (if ranking is equal) or with the highest ranking will be returned to the query,

A '0' ranking for the wavelength indicates that the whole list is considered to be a *replacement* list. This means that a quantity will be extracted from such a list only in the case where a line is present in another list with a non-zero wavelength ranking. Consider the example of 'iron.nbs' in Table 2. The gf-values of 'iron.nbs' have the ranking of '5' compared to '2' in 'kur4000'. Hence, gf-values of lines included in both files, 'kur4000' and 'iron.nbs', will be taken from the latter file. However, if a line in 'iron.nbs' is not found in one of the other lists, it will not be extracted. The purpose of *replacement* lists is to supply VALD with the most accurate values for one or several particular quantities. Such files are usually generated from experimental data with many other VALD quantities missing and/or of poor accuracy, especially the wavelength. We have chosen this policy to ensure that a particular line is not extracted twice due to a wavelength error in the *replacement* list being larger than the wavelength window defined in Subsect. 3.2. The only but time consuming remedy is a careful wavelength calibration, as is currently done for all Fe I *replacement* lists.

The second ranking value with a special meaning is '1'. It is used to flag very unreliable data. All programs accessing VALD have an option to ignore lists, which have '1' as the wavelength's ranking. This low quality ranking is chosen for all files containing data from the old Kurucz-Peytremann list (1975).

A comment sign (before 'Li2O.kp' in our example) causes no lines to be extracted from that file, no matter which queries are asked.

Various rankings can be applied to the same list for testing. In general, there is one primary data base control file, which has ranking for all lists in VALD, and which is based on discussions similar to those presented for several examples in the following section. The most recent control file can be obtained on request via email to the VALD manager (see Appendix). The advantage of this flexible ranking system is the possibility of a continuous readjustment according to current experience of the user community.

Usually, experimental data are preferred over theoretical calculations. If a list has only a few but highly accurate VALD-relevant quantities, it is considered as a replacement list. If a list fails in applications several times it is reranked.

Some VALD source lists already represent extensive compilations, for which individual data items cannot always be identified with their original sources. Since each source list can only be associated with a single quality ranking, VALD cannot make any allowance for internal inhomogeneity within a given source. Where specific improvements to the ranking within a source are identified, these can, however, be provided by the addition of supplementary source lists (e.g. Sect. 4.2).

4. Source list improvements and homogeneity of VALD

VALD uses source lists of very different origin. Therefore, the problem of homogeneity becomes important. Driven by our present scientific needs, we have investigated this question first for lines of iron peak and Rare-Earth elements, which are the most prominent features in the spectra of chemically peculiar (CP) stars. Due to the available observations, we have focussed this study on the visual spectral region.

As an important tool for checking the accuracy of gf-values from various sources and for supplementing missing data, we derived so-called *astrophysical gf-values* from high quality observations. The procedure is described in Ryabchikova et al. (1994a) and basically relies on an a priori accepted abundance value and the optimum fit of spectral lines to observations, where the gf-value is a free parameter.

4.1. *Iron-peak elements*

We have supplemented the NBS compilation for iron lines with data based on new experimental measurements of oscillator strengths for Fe I by O'Brian et al. (1991) to provide a homogeneous set of gf-values. For high excitation Fe II lines ($E_{\rm lower} \geq 10$ eV), the NBS gf-values are comparable to those derived from semiempirical gf-calculations (Ryabchikova et al. 1994a).

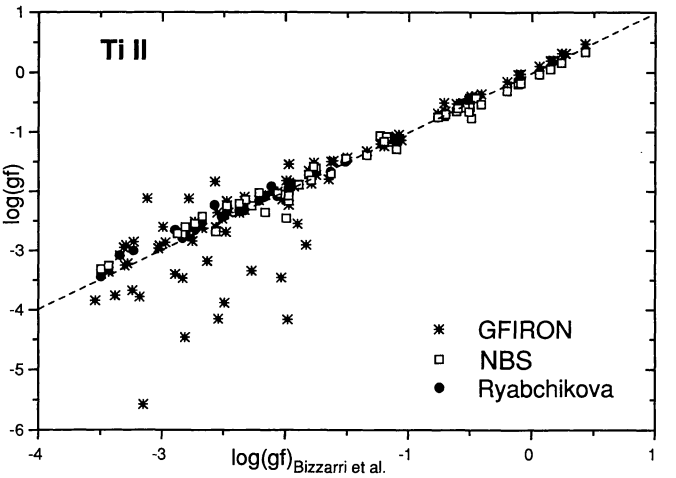

Fig. 2. Oscillator strengths for Ti II lines from GFIRON, NBS-Martin et al. (1988), and Ryabchikova et al. (1994a: *astrophysically* derived values, see second paragraph of Sect. 4) are compared with values from Bizzarri et al. (1993). The dotted line is not a fit, but represents an ideal correlation

The accuracy of NBS data for the other iron peak elements, in particular for Ti II, Cr II, and Mn II, is lower.

Bizzarri et al. (1993) measured transition probabilities for 100 Ti II lines in the λ 3050−10000 Å spectral region with a mean accuracy of 0.04 dex. These data are compared with NBS, GFIRON, and Ryabchikova et al. data in Fig. 2. A comparison of these measurements with the astrophysical gf-values extracted from Ryabchikova et al. (1994a) shows a good correlation between both data sets, with a correlation coefficient of 0.995 and a dispersion of 0.08 dex. A small zero-point shift of 0.05 dex is related to the difference for the solar titanium abundance which was used for calibrating the astrophysical oscillator strengths.

A linear least-squares fit for NBS data (Fig. 2) results in a correlation coefficient of 0.991 and a dispersion of 0.13 dex. For the semi-empirically calculated GFIRON values we find a large scatter with a dispersion of 0.52 dex, but with a slope of the linear fit which is nearly the same as for the two other data sets.

In conclusion, we combined the data from Bizzarri et al. (1993) and Ryabchikova et al. (1994a) to create one replacement list for Ti II oscillator strengths. Furthermore, precise measurements from the Oxford group (Blackwell et al. 1982), corrected by +0.09 dex, as proposed in Bizzarri et al. (1993), were added to this replacement list, which finally contains 185 Ti II lines.

For the Cr II lines two new sets of measurements were available which form the basis for our VALD Cr II replacement list: experimental transition probabilities by Pinnington et al. (1993), and astrophysical gf-values extracted from Sigut & Landstreet (1990). A comparison of

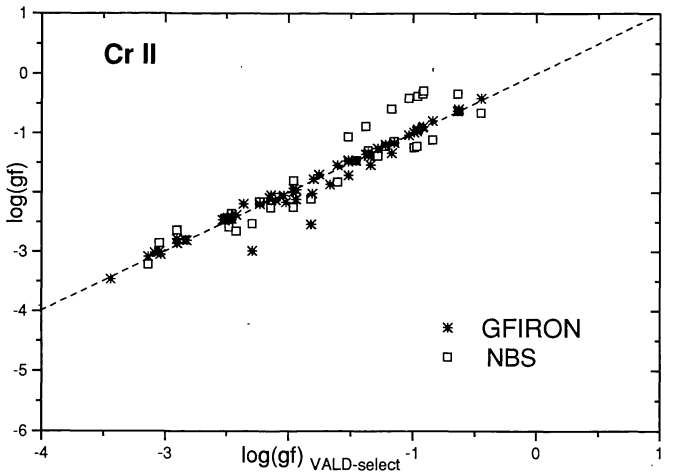

Fig. 3. Oscillator strengths for Cr II lines from GFIRON, and NBS-Martin et al. (1988) are compared with values from our Cr II replacement list. The dotted line is not a fit, but represents an ideal correlation

these sets shows a close correlation between both sources, which is again better than for the NBS data. The final replacement list for Cr II lines contains 57 entries.

Figure 3 shows a comparison of the oscillator strengths from our replacement list (VALD-select) with NBS and Kurucz's GFIRON data. The correlation between VALD-select and GFIRON data is evident, except for two lines of Multiplet No. 39 at λ4539.62 and 4565.78 Å for which the deviation is 0.70 dex.

Pinnington et al. (1993) measured radiative lifetimes of 14 low energy levels in Cr II and found good agreement with calculated lifetimes, which lends further credit to the absolute scale of Kurucz's Cr II oscillator strengths. The same authors also used Kurucz's gf-values as branching ratios to transform lifetimes to oscillator strengths, a procedure which causes the previously mentioned good correlation between semi-empirical calculations and experimental measurements. In other words, the intrinsic accuracy of Pinnington et al. data depends on the *relative* accuracy of Kurucz's calculations. However, a chromium abundance analysis for the solar atmosphere (Pinnington et al. 1993) corroborates an accuracy of their gf-values of better than 10–15%, which still is higher than the accuracy of current NBS Cr II data in the optical spectral region.

4.2. *Rare-Earth (RE) elements*

Atomic data for neutral ions of RE elements were taken entirely from BELLHEAVY. They have an estimated accuracy for most of the gf-values of at least 0.3 dex. On the other hand, data for singly ionized RE elements were supplemented by two additional sources to provide better gf-values than given by BELLHEAVY.

The first contains experimental oscillator strengths from Komarovskij (1991) for Pr II, Nd II, Sm II, Eu II, and Er II, and solar averaged gf-values for 30 Ce II lines extracted from the papers by Grevesse & Blanquet (1969), Andersen et al. (1975), Gurtovenko & Kostyk (1989), Thevenin (1989), and by Meylan et al. (1993). All solar data were scaled to [Ce]=1.55 (Anders & Grevesse 1989) in the hydrogen abundance scale of [H]=12.0.

The second source is based upon intensities from NBS Mon. 145 (Meggers et al. 1975). For La II and Ce II lines interpolated gf-values were derived according to Magazzu & Cowley (1986). Using experimental gf-values from Komarovskij (1991) we calibrated the NBS intensities for Pr II, Nd II, Sm II, and Er II lines following the procedure described by Cowley & Corliss (1983) and by Ward (1985) to obtain interpolated gf-values for lines of these ions. The coefficients for the new calibration were kindly provided by C.R. Cowley (private communication).

We subsequently investigated the accuracy of these three sources in order to decide their rankings. All experimental data from the first additional source (Komarovskij 1991, and solar data for Ce II) have been given the highest ranking. The most extensive list of gf-values has been given the next lower ranking, and consists of lines for La II (Magazzu & Cowley 1986), lines for Pr II, Sm II, Nd II, and Er II (new calibration, see previous paragraph), and lines for all the other singly ionized RE elements (BELLHEAVY). The lowest ranking was given to a third list, which supplies additional data for Ce II (Magazzu & Cowley 1986), and for Pr II, Sm II, Nd II, and Er II (BELLHEAVY). The few lines of ionized RE elements for which oscillator strengths were derived from solar spectra (see above) helped to cross-check our calibration procedure.

4.3. *Other elements*

A separate list of gf-values is provided for Ga II and Xe II lines. The data were extracted from Ryabchikova & Smirnov (1994) for the Ga II lines, from Wiese & Martin (1980) and from Ryabchikova & Smirnov (1989) for Xe II lines.

The first extensive use of VALD (at that time called VLDB) is described by Kupka (1994). Several obviously incorrect entries in source lists were identified by him. In particular the NLTE source list (Kurucz 1993) contains quite a number of false lines of Si I, Si II, Ca I, Ca II and possibly also of S II, S III, and Al III. The Si II line at λ6029.869 Å, for example, gives a distinct feature in the spectrum of a solar abundant star with $T_{\rm eff}$= 8000 K and log g= 4.0, but contrary to the other synthesized Si lines this feature cannot be found in α Cir (CP2, SrEuCr) spectra (Fig. 4).

Other examples for controversial Si II lines have wavelengths of 4002.585, 4028.459 and 4035.272 Å. They are very strong in the synthetic spectrum of the extremely Si–rich star ET And (HD 219749), but cannot be detected in the stellar spectrum (Ryabchikova et al. 1994b).

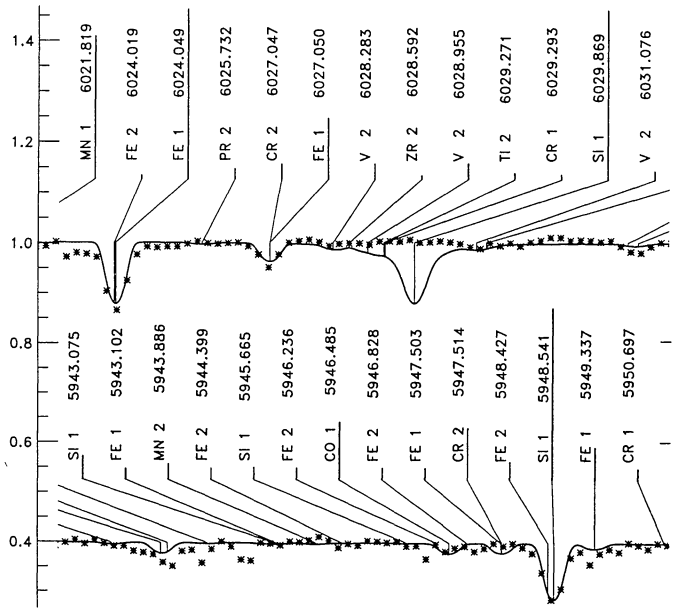

Fig. 4. Two sections of a synthesized and observed spectrum of α Cir, with the same relative scale. Note the discrepancy for the Si I line at λ 6029.869 Å, whereas the Si I line at λ 5948.541 Å is well synthesized, which confirms - among other Si lines - the correct Si abundance. The length of the vertical bar next to the element designation and wavelength is proportional to the computed core-depth. This feature helps to estimate the importance of blends

5. Data retrieval from VALD and examples

Information about a specific line including all parameter values from different source lists with their corresponding bibliography and ranking can be requested from VALD. One can also request an extraction of all lines in a given wavelength range and with certain parameters.

5.1. *Selecting individual line information (SHOWLINE)*

The purpose of the program SHOWLINE is to gather all information on an individual line. In general, only the approximate wavelength, element and spectrum number of a line are known and some or all data from various sources should be displayed.

SHOWLINE extracts from VALD all the lines satisfying the specified criteria and puts the data including the ranking parameters to the standard output device. Table 3 shows the result of a data base query on Mn I at λ 4436.35 Å (wavelength window 0.01 Å).

The parameters for automatic ranking are taken into account for all lines found. Those lines, which turn out to be identical within the given wavelength window (by their J-values and upper energy levels, see Sect. 3.2) are merged to give a single entry containing the best parameters for that line. The result is printed on the same output device (see Table 3, bottom). Only two of three lines remained in our example. One line (λ 4436.360 Å, source = NBS) was used to replace the gf-value of a line from Kurucz' GFIRON list (λ 4436.357 Å).

5.2. *Automatic line selection (PRESELECT and SELECT)*

VALD has two tools for the automatic selection of relevant lines for spectrum synthesis and for model atmosphere calculations (see Fig. 1).

A pre-selection is performed to find data on all lines in a given wavelength range. The search can be limited by specifying a certain element or even a particular ion. The program PRESELECT ignores all lines of higher spectrum number and higher excitation potential for the lower energy level according to the control file. For the lines found in the data base an automatic ranking is used to replace line data in the given wavelength window. In addition, all line data with low accuracy (wavelength ranking '1') can be ignored.

The output of PRESELECT is sent to the standard output as plain ASCII text and has two different output modes: The more important one is for further processing by the VALD tools and does not include information on J-values, transition designations, accuracy and multiplet numbers. Instead of separate Landé factors for each level one effective Landé factor is calculated according to Beckers (1969):

$$\overline{g}_{\rm eff} = \frac{g_i + g_k}{2} + \frac{g_i - g_k}{4}\Big[j_i\,(j_i+1) - j_k\,(j_k+1)\Big] \quad (2)$$

and included in the output. An example for a pre-selection is shown in Table 4.

In a less frequently used retrieval mode *all* the data on a line are displayed, including a computed $\overline{g}_{\rm eff}$. This mode is important when term designation and Landé factors are required (Zeeman splitting, etc.).

A final selection program, called SELECT, is designed to meet the needs of stellar spectroscopists. SELECT has two modes of operation: SYNTH for spectrum synthesis and MODEL for model atmospheres. In both modes a model atmosphere is used. The abundances are solar by default, can alternatively be taken from the model atmosphere, or may be specified by the user. The value for microturbulence must always be supplied by the user.

In SYNTH mode, SELECT solves the radiative transfer equation for the central wavelength of each line ignoring blending. Next, it checks the central depth and compares it to a given threshold. Lines deeper than the threshold will be extracted. In this way SELECT can help to find spectral regions suitable for observations and to analyze complex blends. The output of SELECT in SYNTH mode (see Table 5) contains one extra column – the relative line depth. The abundances of the first 99 elements follow the file name of the model atmosphere used. SELECT does

Table 3. A query on data about Mn I at 4436.35 Å with SHOWLINE (line data only)

```
Lines found:

Wavelength in A  Element/Ion  log gf      E(low) in eV      E(high) in eV
Lande: eff.      low   high   gamma.Rad   gamma.Stark       gamma.VdW
                 terms (low -> high)  accuracy  (multiplet or comments)
                                      database reference for all values
-------------------------------------------------------------------------------
 4436.343 ( 2)   Mn 1        -0.087 ( 2)    4.827 ( 2)   2.5   7.621 ( 2)   2.5
    0.86 ( 2)    0.86  0.86  7.916 ( 2)   -6.169 ( 2)         -7.796 ( 2)
                3F2)4   2F    3F)4  2F
                                      GFIRON ext. (Ca-Ni) 4000-5000
 4436.357 ( 2)   Mn 1        -0.465 ( 2)    2.920 ( 2)   2.5   5.714 ( 2)   1.5
    1.50 ( 2)    1.37  1.20  7.848 ( 2)   -5.507 ( 2)         -7.784 ( 2)
                (5D)4   4D   (5D)4   4D
                                      GFIRON ext. (Ca-Ni) 4000-5000
 4436.360 ( 0)   Mn 1        -0.288 ( 5)    2.920 ( 0)   2.5   5.714 ( 0)   1.5
   99.00 ( 0)   99.00 99.00  0.000 ( 0)    0.000 ( 0)         0.000 ( 0)
                a 4D          z 4D*        B    (22)
                                      NBS: Manganese
-------------------------------------------------------------------------------

These data should be combined to the following lines:

WL in A  El/Ion log(gf)  Ei[eV]   Ji  Ek[eV]   Jk   gl   gam.r   gam.s   gam.w
-------------------------------------------------------------------------------
 4436.343  Mn 1  -0.087   4.827  2.5   7.621  2.5  0.86  7.916  -6.169  -7.796
                                          GFIRON ext. (Ca-Ni) 4000-5000
 4436.357  Mn 1  -0.288   2.920  2.5   5.714  1.5  1.50  7.848  -5.507  -7.784
                                          NBS: Manganese
-------------------------------------------------------------------------------
```

Table 4. A sample output of a VALD-EMS request to PRESELECT. The columns are: element, ion, wavelength (Å), E_i, $\log(gf)$, Γ_r, Γ_s, Γ_w, $\overline{g}_{eff}$, and the reference

```
    Damping parameters  Lande
Elm Ion  WL(A)     Excit(eV) log(gf) Rad.   Stark  Waals factor Reference
'AR 2', 5700.0010, 23.6740, -2.570, 0.000, 0.000, 0.000,99.000,'Bell light: Si to K          '
'FE 1', 5700.1280,  3.3010, -4.948, 7.623,-6.223,-7.870, 0.000,'GFIRON ext. (Ca-Ni) 5000-6000'
'F  1', 5700.1380, 14.6830, -2.550, 0.000, 0.000, 0.000,99.000,'Bell light: F  to Al         '
'SC 1', 5700.1640,  1.4330,  0.290, 7.765,-6.129,-7.854, 0.920,'GFIRON ext. (Ca-Ni) 5000-6000'
'MN 2', 5700.2190, 11.0880, -3.078, 8.938,-5.730,-7.737, 1.830,'GFIRON ext. (Ca-Ni) 5000-6000'
```

not take into account stellar rotation. The threshold must be adjusted correspondingly for fast rotating objects.

In MODEL mode, a threshold is set for the ratio of line opacity to continuous opacity. Only lines contributing significantly to the total opacity are extracted. Typically, SELECT would process much larger spectral intervals in MODEL mode than in SYNTH mode. For that reason the output file is in binary format. The MODEL mode of SELECT is therefore not available via VALD-EMS (see Appendix).

6. Conclusions

We have compiled an archive of data for atomic lines (VALD) observed in the atmospheres of late B to G type stars. We have developed a set of tools for the extraction of data selected according to flexible ranking criteria and appropriate to the atmosphere of a star with specific dimensions. We have evaluated the atomic data adopted into the archive in terms of reliability and have proposed a ranking for them. VALD can be easily expanded by the addition of new data files and/or new line parameters, access to the entries is quick and simple, and a user friendly

Table 5. An example of SELECT output in SYNTH mode

```
 5700.0000, 5705.0000,   10,   123,  Wavelength region, lines selected, lines processed
                                     Damping parameters  Lande  Central
Elm Ion  WL(A)    Excit(eV) Vmct log(gf) Rad.   Stark  Waals factor  depth  Reference
'CR 1', 5700.5180,  3.5510, 2.0, -1.440, 7.538,-5.991,-7.845, 1.330, 0.572, 'GFIRON ext. (Ca-Ni) 5000-6000'
'CR 1', 5700.5500,  3.4490, 2.0, -2.574, 7.812,-6.185,-7.822, 1.120, 0.227, 'GFIRON ext. (Ca-Ni) 5000-6000'
'S  1', 5700.5800,  7.8680, 2.0, -1.040, 0.000, 0.000, 0.000, 0.000, 0.120, 'Bell light: Si to K          '
'SI 1', 5701.1040,  4.9300, 2.0, -2.050, 8.310,-4.410, 0.000, 0.000, 0.110, 'NLTE lines: Si              '
'CR 2', 5701.4640,  3.8270, 2.0, -3.845, 8.677,-6.611,-7.929, 0.960, 0.649, 'GFIRON ext. (Ca-Ni) 5000-6000'
'FE 1', 5701.5450,  2.5590, 2.0, -2.216, 8.167,-6.052,-7.840, 1.120, 0.266, 'GFIRON ext. (Ca-Ni) 5000-6000'
'CR 2', 5701.9090,  6.5780, 2.0, -4.251, 8.431,-6.647,-7.900, 1.200, 0.063, 'GFIRON ext. (Ca-Ni) 5000-6000'
'CR 1', 5702.3230,  3.4490, 2.0, -0.970, 7.797,-6.171,-7.822, 1.090, 0.638, 'GFIRON ext. (Ca-Ni) 5000-6000'
'CR 1', 5702.7060,  4.6130, 2.0, -2.089, 8.114,-6.171,-7.840, 1.030, 0.135, 'GFIRON ext. (Ca-Ni) 5000-6000'
'CR 1', 5704.1480,  3.1040, 2.0, -3.378, 7.182,-6.205,-7.865, 1.320, 0.095, 'GFIRON ext. (Ca-Ni) 5000-6000'
'08000G45.KRZ',
'H : -0.04','HE: -1.05','LI:-10.88','BE:-10.89','B : -9.44','C : -3.48',
'N : -3.99','O : -3.11','F : -7.48','NE: -3.95','NA: -5.71','MG: -4.46',
'AL: -5.57','SI: -4.49','P : -6.59','S : -4.83','CL: -6.54','AR: -5.48',
.....this list is complete in the original output table.....
'PA:-20.00','U :-12.51','NP:-20.00','PU:-20.00','AM:-20.00','CM:-20.00',
'BK:-20.00','CF:-20.00','ES:-20.00','END'
```

overview of parameters from different source lists, with ranking criteria, is provided.

VALD has enabled us to economically compute opacity distribution function tables, to investigate the quality of data on atomic transitions given in various references, and to have quick access to relevant lines for abundance analyses, Doppler mapping, etc. (Piskunov et al. 1993; Hiesberger et al. 1994; Kupka 1994; Kupka et al. 1994; Kuschnig et al. 1994; Piskunov et al. 1994a-c; Ryabchikova et al. 1994b).

Some activities planned for the future include:
- adding missing parameters for existing lines, completion of the line lists, in particular in the UV and IR, and the inclusion of molecular lines,
- careful ranking of all parameters and improvement of the ranking system,
- including information on isotopic effects, hyperfine structure and Zeeman patterns,
- compiling a list for telluric lines,
- comparing synthetic spectra based on VALD lists to high quality observations of solar and stellar spectra,
- including references to original sources.

Our goal is to develop and improve VALD to become an internationally recognised resource for the retrieval of astrophysically important atomic data. This can only be achieved by the close collaboration of both the users and producers of such data working in diverse areas of astronomy.

Remote access to the database is provided (at no cost) by the VALD electronic mail service (VALD-EMS: see appendix).

Several important and valuable collections of data on transitions have been omitted from the current installation of VALD. We are currently considering how best to assimilate f-values and lifetimes from the Opacity Project database (Cunto et al. 1993) into VALD. We also invite other producers and assessors of atomic data to contribute their results, with the assurance that contributions will be properly attributed.

Acknowledgements. Computing resources and financial support for this international collaboration were provided by the Fonds zur Förderung der wissenschaftlichen Forschung (project *P 8776-PHY*), Österreichische Akademie der Wissenschaften (project *Asteroseismologie*), and Bundesministerium für Wissenschaft und Forschung (project *Numerical modelling of radial and non-radial pulsation*). Collaborative Computational Project No. 7 (CCP7) for the Analysis of Astronomical Spectra is funded by the UK Particle Physics and Astronomy Research Council. The contribution of many linelists, latterly on CD-ROM, by Dr. Robert Kurucz is gratefully acknowledged.

A. Appendix

VALD Electronic Mail Service (**VALD-EMS**) is the main interface for accessing VALD by external users and contains the following features:

- Subsets of spectral line lists can be extracted with tools adapted for stellar spectroscopy. VALD-EMS strongly discourages bulk data transfer and is designed for intelligent search and extraction.
- The VALD data base is regularly updated in a transparent way with critically evaluated data-sets by

the VALD project team. Feedback from the user-community is very much welcomed and encouraged.
- VALD-EMS has control over the mail request queue and the processing of the requests on VALD computers. These machines are not solely dedicated to the VALD project.

A.1. *How to register for VALD*

The first step is to register in the list of VALD clients, which contains INTERNET e-mail addresses from where VALD-EMS requests will be accepted. To do so, send an e-mail message to the VALD manager at the address:

VALDADM@GALILEO.AST.UNIVIE.AC.AT

with your full name and your e-mail address.

If you intend to access VALD-EMS from more than one computer, you must send your e-mail address on each.

A.2. *VALD-EMS requests*

VALD-EMS requests are ordinary electronic mail messages sent via INTERNET to:

VALD@GALILEO.AST.UNIVIE.AC.AT.

Each mail can include *only one* request which consists of several lines. *Only the first 80 characters of each line are interpreted by VALD-EMS.* The request starts with a line containing a string:

BEGIN REQUEST

and ends with a line:

END REQUEST

VALD is case **in**sensitive and blanks are ignored. Every line or part of a line starting with the symbol # is ignored by VALD and can be used for comments.

All mail is processed at certain times of the day and valid requests are interpreted and submitted for execution in the order of arrival. The output file is mailed back to the client. This file contains the VALD-EMS request number, all diagnostic information (syntactic errors, wrong parameter values, etc.) and the data extracted from VALD.

A.3. *Types of request*

VALD-EMS currently supports 4 types of requests with compulsory and optional parameters:

SHOW LINE	extracts all information available in VALD for a specific spectral line
EXTRACT ALL	extracts the best parameters for lines in a given spectral window
EXTRACT ELEMENT	extracts the best parameters for spectral lines of a particular element or ion in a given spectral window
EXTRACT STELLAR	extracts all spectral lines (with their best parameters) which produce significant absorption in an atmosphere with given $T_{\rm eff}$ and log g.

The request is defined by one of the keywords listed above, placed in the second line of the request in the e-mail. A detailed description is sent to each VALD client after registering. This description is also available from CCP7, the WWW, or the Strasbourg Data Center.

For VALD-EMS, only model atmospheres (Kurucz 1993) with solar abundance are accessible. If a user specifies values for $T_{\rm eff}$ and log g for which no model is published by Kurucz, the model with parameters nearest to those given is used.

A.4. *Errors in VALD*

The VALD project team does not take any responsibility for errors in the data base, but we are very interested in improvements. VALD users are therefore encouraged to send us any information about problems and better and/or additional sources for transitions. Please send all your comments to the VALD managers (VALDADM@GALILEO.AST.UNIVIE.AC.AT), who currently are F. Kupka (Vienna) and N. Piskunov (Vienna, presently at JILA).

References

Anders E., Grevesse N. 1989, Geochim. Cosmochim. Acta 53, 197

Andersen T., Poulsen O., Ramanujan P.S., Petrakiev Petkov A., 1975, Sol. Phys. 44, 257

Beckers J.M. 1969, AFCRL-69-0115, Phys. Sc. Res. Papers No. 371, Air Force Cambridge Res. Lab., Office of Aerospace Res.

Bizzarri A., Huber M.C.E., Noels A. et al. 1993, A&A 273, 707

Blackwell D.E., Menon S.L.R., Petford A.D. 1982, MNRAS 201, 603

Blaise J., Wyart J.-F., Tahar Djerad M., Zeineb Ben Ahmed. 1984, Phys. Scripta 29, 119

Cowley C.R., Corliss C.H. 1983, MNRAS 203, 651

Cunto W., Mendoza C., Ochsenbein F., Zeippen, C.J. 1993, A&A 275, L5

Fuhr J.R., Martin G.A., Wiese W.L. 1988, J. Phys. Chem. Ref. Data 17, Suppl. 4

Grevesse N., Blanquet G. 1969, Sol. Phys. 8, 5

Gurtovenko E.A., Kostyk R.I. 1989, "Fraunhofer Spectrum and the Solar Oscillator Strength System", Naukova Dumka, Kiev

Hiesberger F., Piskunov N., Bonsack W.K. et al. 1994, A&A, in press

Komarovskij V.A. 1991, Optika Spectroscopia 71, 559

Kurucz R.L., Peytremann E. 1975, SAO Special Report No. 362

Kurucz R.L. 1979, ApJS 40, 1

Kurucz R.L. 1992, Rev. Mex. Astron. Astrof. 23, 45

Kurucz R.L. 1993, SAO KURUCZ CD-ROM NO. 13 and 18

Kurucz R.L., 1994, SAO KURUCZ CD-ROM NO. 20 to 22

Kupka F. 1994, "Modellatmosphären und Synthetische Spektren am Beispiel von α Circini", master thesis, Univ. of Vienna

Kupka F., Ryabchikova T., Bologova G. et al. 1994, in proc. Chemically Peculiar and Magnetic Stars, eds. J. Zverko and J. Ziznovsky, Astron. Inst. Slovak Acad. Sc., pg. 130
Kuschnig R., Weiss W.W., Piskunov N., Ryabchikova T., Kreidl T.J. et al. 1994, in proc. IAU Symp. 162, Pulsation, Rotation and Mass Loss in Early-Type Stars, eds. L.A. Balona et al. (Kluwer Acad. Publ.) 43
Lanz T., Dimitrijevic M.S., Artru M.-C. 1988, A&A 192, 249
Magazzu A., Cowley C.R. 1986, ApJ 308, 254
Martin G.A., Fuhr J.R., Wiese W.L. 1988, J. Phys. Chem. Ref. Data 17, Suppl. 3
Meggers W.F., Corliss C.H., Scribner B.F. 1975, NBS Monograph No. 145, US Government printing Office, Washington, DC
Meylan T., Furenlid I., Wiggs M.S., Kurucz R.L. 1993, ApJS 85, 163
O'Brian T.R., Wickliffe M.E., Lawer J.E., Whaling W., Brault J.W. 1991, J. Opt. Soc. Am. B 8, 1185
Pinnington E.H., Ji Q., Guo B., Berends R.W., van Hunen J. 1993, Can. J. Phys. 71, 470
Piskunov N.E. 1992, in Stellar Magnetism, eds. Yu.V. Glagolevskij & I.I. Romanuk, Nauka, St. Petersburg, p. 92
Piskunov N.E, Huenemoerder D.P., Saar S.H. 1993, in 8th Cambridge Workshop on Cool Stars, Stellar Systems, and the Sun J.-P. Caillault ed., ASP Conf. Ser. Astron. Soc. of Pacific, San Francisco, in press
Piskunov N.E., Wehlau W.H. 1994a, A&A., in press
Piskunov N.E., Ryabchikova T.A., Kuschnig R., Weiss W.W. 1994b, A&A, in press
Piskunov N.E., Mathys G., Wehlau W.H. 1994c, A&A, submitted
Ryabchikova T.A., Smirnov Yu. M. 1989, Astron. Tsirk. No. 1534, 21
Ryabchikova T.A., Smirnov Yu. M. 1994, Russian Astron. J. 71, 83
Ryabchikova T.A., Hill G.M., Landstreet J.D., Piskunov N., Sigut T.A.A. 1994a, MNRAS 267, 697
Ryabchikova T.A., Kuschnig R., Piskunov N.E., Weiss W.W. 1994b A&A, in press
Sigut T.A.A., Landstreet J.D. 1990, MNRAS 247, 611
Thevenin F. 1989, A&AS 77, 137
Ward L. 1985, MNRAS 213, 71
Wiese W.L., Martin G.A. 1980, NSRDS-NBS 68, Wavelengths and Transition Probabilities for Atoms and Atomic Ions, Part 2. US Government Printing Office, Washington, DC