

VALD–2: Progress of the Vienna Atomic Line Data Base[★]

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Abstract. We describe the updated version of the “Vienna Atomic Line Data Base” (VALD, Piskunov et al. 1995) which represents a considerable improvement over the first installation from 1994. The original line lists have been complemented with critically evaluated data obtained from experimental measurements and theoretical calculations which are necessary for computing state-of-the-art line opacities in stellar atmospheres, as well as for synthesizing spectra for high precision analyses. In this paper, we present new and improved data sets for neutral species and ions of Si, P, Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Y, Zr, Ru, Xe, La, Ce, Pr, Nd, Sm, Eu, Gd, Dy, Ho, Er, Tm, Yb, Lu, Re, Pt, Au, Hg, and Pb. For some species data are available in VALD for the first time. We explain our choice of quality rankings by reviewing the literature for the new data and by comparison with source lists included into VALD. For some cases, we produced new line data by weighted averaging of data from different sources with individual error estimates in order to increase the reliability of VALD line lists.

Software modifications allow remote users of VALD to specify individual extraction parameters as an alternative to the default settings of the VALD team and to have direct control over the quality ranking of line data. A World-Wide-Web interface is described which provides easy access to all new features.

To simplify proper crediting of all authors of atomic data, VALD now includes a compilation of all publications used in each type of reply.

Finally, we briefly discuss the future roadmap of VALD developments, including the incorporation of molecular transitions and integration with external data bases.

Key words: atomic data — techniques: spectroscopic — sun: abundances — stars: abundances — stars: atmospheres — stars: chemically peculiar

1. Introduction

A more complete knowledge of atomic transition parameters has always been crucial for progress in astronomical spectroscopy and for the modelling of stellar atmospheres. Although stellar structure models have benefited from the development of the OP and OPAL projects (see e.g. Hummer & Mihalas 1988; Iglesias & Rogers 1996), more reliable line opacities and thus more accurate and more complete atomic data are still a key requirement for the study of the surface layers of stars (cf. Baschek 1995). Hence, stellar spectroscopists had to create the line lists for their work from inhomogeneous and constantly changing data sets making the quality ranking of these data an important issue.

The “Vienna Atomic Line Data Base” (VALD, Piskunov et al. 1995, Paper I) has originally been created in order to merge such data sets for the computation of opacity distribution functions (cf. Piskunov & Kupka 1999). The computation of line blanketing effects involves the handling of bulk data with emphasis on completeness rather than on accuracy. On the other hand, stellar spectroscopy usually requires the compilation of a relatively small amount of highly accurate atomic data. Driven by the research interests of our group, VALD was designed to satisfy both requirements. Public access to the data base through an automatic e-mail interface (VALD-EMS, see Paper I) has attracted a continuously growing community of users working in astrophysics, plasma physics, and laboratory spectroscopy. Today VALD-EMS is the main user interface to our data base: at the time of writing

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[★] <http://www.astro.univie.ac.at/~vald>
<http://www.astro.uu.se/~vald>

of this paper more than 240 clients from all around the world are using it. The feedback from users and our own experience has provided an important input for the improvement of the software and line data.

VALD-2 represents the extended and improved version of VALD. We added new line lists for 34 atoms (Resp. 51 ions, see Fig. 1) with the best available measured or computed line parameters, in many cases verified by using astrophysical abundance analyses. The new referencing system helps to achieve adequate acknowledgements for researchers who are providing atomic data and to stimulate their collaboration. Major changes to the VALD software include new extraction options, while the extraction became more efficient. Compressed format of data storage allows to more than double the amount of information stored on the same disk. The data base is portable and two mirror sites are now processing VALD requests.

In this paper, we describe improvements to the software, the user interface and extraction capabilities, as well as extensions and corrections to the data archive. These changes are significant enough to call the current implementation VALD-2. The version described in Paper I will be referred to as VALD-1.

In Sect. 2 we provide a description of the structure of VALD-2 as well as a description of the information now stored for each transition. Section 3 discusses the VALD-2 software that provides efficient handling of over 50 million lines, offers flexible extraction modes, ensures its portability and supports mirror sites. We also describe the new and more complete referencing system, the new WWW interface and certain provisions made for a future release (VALD-3). Section 4 is dedicated to the new atomic data in VALD with the emphasis on quality checks and ranking of the new lists. The concluding Sect. 5 summarizes the changes introduced with VALD-2 and describes our plans for the future VALD-3 which will also contain molecular lines.

2. Structure and the new format of VALD line data

The basic structure of VALD as described in Paper I remains unchanged: the data base is built from several lists of atomic line data published by various providers. These *input lists* (or *source lists*) are preserved separately and are at first ranked according to their known performance in applications (predominantly in astrophysics), as well as according to error estimates provided by the authors of the original data. Comparisons are made by the VALD team to decide on the final ranking. Lists are also re-ranked according to their actual performance as part of the data base or whenever new data are included which supply information about the same atomic (or, in the near future, also molecular) species.

Each individual request to the data base is handled by merging data from all relevant lists available. The merging procedure is performed by selecting each datum for

an individual spectral line from the most highly ranked list which provides information on the particular atomic parameter (see Paper I). This selection is preferred over averaging of data, because individual errors of line data from different sources can vary dramatically, like oscillator strengths ($\log gf$ -values) obtained from semi-empirical calculations (cf. Fig. 2) which would then be mixed up with high accuracy laboratory data. Moreover, for most of the line data individual error estimates are not available. Weighted averaging is recommended only when such estimates are known for all individual lines from two or more line lists which are supposed to be merged. On several occasions this has been done to create new VALD line lists which appear to the merging procedure of a VALD request as a single line list, although they were composed from several individual source lists (see Sect. 4). Sometimes, line data had to be corrected for systematic deviations (usually but not always known from the literature) before becoming part of the VALD archive. Thus, it was possible to enlarge, for instance, the number of lines for which reliable oscillator strengths with individual error estimates are available.

The data base can be accessed by extraction programs (tools) described in Paper I. At the time of publication, VALD had already been upgraded substantially in comparison with its original installation (cf. the overview of Piskunov 1996). Besides of adding new line data this upgrade also included the application of compression techniques to some of the VALD tools and provision to treat an archive of many million spectral lines with limits only set by disk space and the speed of the host computer. More details about these and related improvements are given below. These enhancements have been indispensable for the computation of opacity distribution functions (Kupka & Piskunov 1998; Piskunov & Kupka 1999) and provide the basis for including molecules into the data base for both spectroscopic work and opacity calculations. In addition, more detailed information on the accuracy of oscillator strengths has become available for many spectral lines. As a consequence, it became necessary to extend the information stored with each spectral line archived in VALD and a spectral line now is characterized by the following parameters (we refer to the introduction in Paper I):

1. Central wavelength in Å.
2. Species identifier. Provides element (or molecule) name and ionization stage.
3. $\log gf$ – logarithm of the oscillator strength f times the statistical weight g of the lower energy level.
4. E_i – excitation energy of the lower level (in eV).
5. J_i – total angular momentum quantum number of the lower energy level.
6. E_k – excitation energy of the upper level (in eV).
7. J_k – total angular momentum quantum number of the upper energy level.
8. g_i – Landé factor of the lower energy level; default value is 99, if no value can be provided.

9. g_k – Landé factor of the upper energy level; default value is 99, if no value can be provided.
10. $\log \Gamma_r$ – logarithm of the radiation damping constant in s^{-1} ; default value is 0, if no value can be provided.
11. $\log \Gamma_s$ – logarithm of the Stark damping constant in $(s N_e)^{-1}$ (i.e. per perturber) at 10 000 K; default value is 0, if no value can be provided.
12. $\log \Gamma_w$ – logarithm of the van der Waals damping constant in $(s N_H)^{-1}$ (i.e. per perturber) at 10 000 K; default value is 0, if no value can be provided.
13. Spectroscopic terms of lower and upper energy levels.
14. Accuracy for $\log gf$ in dex (where available).
15. Comments, e.g. multiplet number as in Martin et al. (1988).
16. Flags. Will be used to provide a link to information on Zeeman patterns, on autoionization lines, to information available for computing more accurate Stark and van der Waals broadening parameters, to supplement the main quantum numbers for hydrogen lines, and more.

We refer to this new format as “version 3.0 format”, because it already includes all the features necessary to handle molecular line data. The first 12 entries contain numerical data and occupy 52 bytes if they are stored as a sequence of uncompressed IEEE floating point numbers¹. The new species identifier allows for more flexibility and avoids a cumbersome extension of the ion identifier used in previous versions of VALD when molecules are included at a later stage (see Sect. 5). Following the 12 numerical parameters the next three parameters originally consisted of plain (ASCII) text fields for a total of 30 characters. Field 13 was enlarged to provide 24 characters altogether for both lower and upper energy levels to ensure that term designations for molecules can be stored properly (Greek letters will be indicated by a preceding \). As more precise estimates of oscillator strengths have become available since the first release of VALD, it was decided to replace the letter identifier for the accuracy of $\log gf$ as used in Martin et al. (1988) by indicating the error $\Delta \log gf$ in dex. Hence, the associated parameter field 14 now holds a numerical value (two bytes). Also, the “comments field”, now number 15, had to be enlarged significantly from 6 to 16 characters. It is used to provide

- accurate source descriptions for input lists compiled with data from different authors,
- multiplet designation (where available), and also to
- store now outdated, but still commonly used accuracy descriptors, like letters which were provided by the previous VALD version.

The parameter fields 13 and 15 are filled with blanks when no information is available. A value of -1 is inserted for the accuracy descriptor (parameter field 14) when no information is available. Finally, we decided to add two bytes

for flag values. These will be used to indicate the availability of additional information in external databases like, for example, Zeeman patterns, Stark and van der Waals broadening, and to mark special cases (as, for example, Hydrogen lines where Stark and van der Waals constant fields are actually used to store energy levels, or autoionization lines for which the same fields contain parameters of the Fano profile). Typically, such information is available or needed for a small sub-set of lines. Thus, instead of an unnecessary increase of the data base or change of its internal format, we will provide a link to other data bases. Future VALD extraction tools are expected to use these flags when assembling the reply to a request but this transition will be transparent for the end user.

The impact of all these changes on the default output for VALD-EMS requests is minimal and guarantees as much continuity for the users as possible.

3. Software improvements

VALD has been in operation for more than four years. Its success was largely determined by the choice of the data base architecture. Individual line lists are pipelined through a merging and filtering software which can be configured according to the type and parameters of a request.

The upgrade of the VALD software was driven by our intention to handle additional information requested by users, to accommodate larger data sets and to reduce the response time of the data base.

3.1. Internal data format and data flow in VALD

Currently, each VALD line list is stored on magnetic disk as one of several compressed files. Each file consists of binary records (one record per transition). When a new line list is to be included to VALD, it is first converted to the internal VALD format (see Sect. 2) and then compressed. In preparation for the future inclusion of molecular lines (in VALD-3) two changes to the internal record format have been made already now. First, the species are identified internally with a number rather than by the atomic number and ionization stage. This unique correspondence between a number and a species is defined in the VALD internal table of species. Second, each record has been extended with two new fields that contain the quality parameter and additional reference (see Sect. 2). Both of these fields are extracted by the `SHOW LINE` extraction option of VALD which is used to obtain all the data on a particular transition from all lists included in the data base (see Paper I).

The data compression is based on the Lempel-Ziv-Welch algorithm (Welch 1984) which was modified to achieve the highest compression ratio (files are compressed to less than 46% of the original size) and to preserve direct

¹ Which are common for most modern workstations.

access to the data. A high compression ratio is achieved by taking advantage of the fixed record length of the internal data format. To speed up the response time we created a special descriptor file that allows starting decompression of a given list within less than 1000 spectral lines from the requested wavelength rather than from the start of a file.

Any data extraction in VALD is performed using a pipeline of the corresponding filters or “VALD extraction tools”. Presently, two tools can initiate a pipeline: PRESELECT and SHOW LINE (the PRESELECT tool is used to extract the best data for each transition in a certain wavelength range, see Paper I). Both of them are calling special routines to access data base files (open, close and read/decompress functions) which helps to make VALD independent of computer systems, because the content of external files is interpreted as a stream of bits while the components of the pipeline exchange ASCII messages. The success of this strategy was confirmed by porting VALD between DEC and Hewlett-Packard workstations, as well as running VALD over the network in a mixed environment, when different pipeline components are running on different computers. The extraction and merging of data from different lists is directed (as before) by the VALD configuration file (cf. Paper I). The format of this file has been extended to accommodate to the possibility to choose term designations from a specific list. Moreover, each client who uses the data base through remote access facilities (VALD EMS and WWW) has now a possibility to keep a personal copy of the configuration file (see Sect. 3.3).

3.2. Mirror site support

Creation of mirror sites is a logical way to distribute the work load and reduce VALD response time. It is particularly important for massive extraction which is performed, e.g. for model atmosphere calculations. Two VALD mirror sites became operational in 1998: Uppsala Astronomical Observatory (vald@astro.uu.se) and Astrophysics Data Facility at NASA Goddard Space Flight Center (vald@hypatia.gsfc.nasa.gov). In order to achieve coherence of all VALD servers we developed an additional layer of the software that runs automatically on top of the VALD email service and ensures the synchronization of all sites. Currently, synchronization is performed twice a day which means that within less than a day after registration a new client will have EMS access to all VALD sites.

3.3. Changes to the user interface and extracted data format

As described in Paper I the VALD-EMS (email service) remains the main user interface, but now it offers several additional options. A VALD-EMS request still consists

of two parts: the type of request (SHOW LINE, EXTRACT ALL, EXTRACT ELEMENT and EXTRACT STELLAR) and the parameters of extraction. VALD-2 offers the possibility to specify additional options for a better control of the data extraction. The following options can be specified with all request types except for SHOW LINE, where only the PERSONAL CONFIGURATION option is allowed:

SHORT FORMAT	default extraction format;
LONG FORMAT	extract term description for each transition;
PERSONAL CONFIGURATION	use a personal VALD configuration file (see below) instead of the standard VALD configuration;
HAVE RAD	select lines with known radiative damping constant;
HAVE STARK	select lines with known Stark damping constant;
HAVE WAALS	select lines with known van der Waals damping constant;
HAVE LANDE	select lines with known Landé factor;
HAVE TERM	select lines for which VALD contains term designations.

Multiple options can be combined in arbitrary sequence. For example, the following request will extract all neutral iron lines in a given spectral range for which the van der Waals damping constant is known and provide term description for upper and lower levels:

```
begin request
extract element
long format
have waals
6170,6190
Fe 1
end request
```

The resulting extraction procedure will create a list similar to (some of the columns “...” have been omitted):

```

... Damping parameters
Elm Ion WL(A) log($gf$) ... Rad. Stark Waals
'Fe 1', 6170.5040, -0.654, ... 8.243,-5.588,-7.590,
'(4F)4p y3D(4F)4d ... 1 1 1 1 1'
'Fe 1', 6171.0060, -1.788, ... 8.377,-4.676,-7.749,
'(4F)4p y3D(4F)4d ... 1 1 1 1 1'
'Fe 1', 6172.2130, -3.916, ... 8.275,-5.181,-7.808,
'(4F)4p z5Gs6D)4d ... 1 1 1 1 1'
'Fe 1', 6173.0050, -6.670, ... 4.057,-6.272,-7.878,
'(4F)4s a5F(5D)sp ... 1 1 1 1 1'
'Fe 1', 6173.0280, -5.957, ... 7.799,-6.335,-7.833,
's2 b3D (3P)sp ... 1 1 1 1 1'
'Fe 1', 6173.3410, -3.081, ... 8.223,-6.194,-7.815,
'(4P)4s a5P(4F)4p ... 1 1 1 1 1'
'Fe 1', 6173.6420, -3.413, ... 8.237,-6.069,-7.631,
'(4F)4p z5Gs4D)5s ... 1 1 1 1 1'
...

```

References:

1. FeI NMT Whaling and Bard & Kock

On top of the VALD-EMS, a World-Wide-Web interface was developed. This interface allows interactive creation of a request to VALD-EMS. It notifies the user of inconsistencies or omissions of input data before converting them to an ordinary VALD-EMS request. Just as for VALD-EMS, access to the WWW interface is limited to registered clients only. The interface will resolve the hostname of the connecting computer and attempt to match the combination of the provided username and resolved hostname against the list of email addresses in the client register. If this is successful, access is granted to the WWW interface. In this way, the interface also determines the client's email address to which VALD-EMS will send the result of the request. It is therefore *important* that the client provides `user@host` addresses to the client register at which the client can receive email.

Another addition to the user interface is the personal configuration file which was primarily dictated by the quick evolution of the content of our data base. With the addition of new line data of higher accuracy it is often impossible to reproduce the same selection with the standard VALD configuration file that controls the merging of different line lists according to the ranking system. One can still get the same selection with the old configuration file, but until VALD-2 a user had no control over the content of the configuration file when using the EMS interface to access the data base. Now each client can choose between the standard configuration, created by VALD experts, or a personal configuration file that is modified only by the owner. A personal configuration file is first created as a copy of the standard configuration in response to the VALD-EMS request that contains the “**personal configuration**” option or via the WWW interface. The WWW interface also provides a convenient editing tool. The VALD client can select a subset of the line lists that will be searched for extraction requests, set the ranking of different parameters that determines the merging procedure etc. (see Paper1). The latest copies of the personal configuration files are automatically distributed to all VALD servers as part of the synchronization procedure.

Two changes have been introduced to the format of extracted data: case sensitivity for names of species and the new referencing system. The first one is part of preparation for VALD-3 which will include molecular line lists of astrophysical interest. We intend to keep conventional notations for the names of molecules, therefore case sensitivity is crucial to distinguish e.g. between CO (Cobalt) and CO (carbon oxide). The second change will simplify acknowledgement of laboratory spectroscopy work as was suggested by several of the VALD contributors and users. VALD-2 now also compiles a list of references at the end of every extraction where the source of each item in each transition is given in the line reference field. For example, a response to a particular request may contain:

```

                                Damping parameters
Elm Ion WL(A)   Excit(eV) log($gf$)   .... Waals
```

```

Lande factor   References
'Fe 1', 4804.5190, 3.5730, -2.590, .... -7.824,
1.170, ' 1 1 1 .... 2 2 '
```

...

References:

1. FeI NMT Whaling and Bard & Kock
2. GFIRON obs. energy level: Fe

where reference numbers ' 1 1 1 1 2 2 2 ' correspond to wavelength, excitation potential of the lower level, oscillator strength, 3 damping constants and Landé factor(s). One more reference number for term designation will appear in the *long* output format. It will be useful in case one develops an automatic term interpretation system since the designations are (unfortunately) not standardized across the lists.

In some cases a single line list may contain a compilation from different sources (like the reference 1 in the example above). For such lists the VALD-2 SHOW LINE request returns a label pointing to the original publication for each datum of each transition. The description of the labels can be found in the reference section of the VALD-EMS electronic document. This document is regularly sent to VALD clients to inform them about new extraction capabilities and/or changes of the user interface. It can also be obtained from the WWW sites of VALD. A label description which compiles all the lists within VALD-2 (as of December 1998) can also be found in Ryabchikova et al. (1999b).

4. New atomic line data and their evaluation

The new line lists for VALD-2 primarily consist of laboratory data and data improved or derived from astrophysical applications. For some species not present in the previous version of our data base we include new calculations. In the following subsections we report on the new data (essentially element by element) and we also explain our ranking when several data sources are available for the same transitions. A survey of all ions for which data has been acquired for VALD in addition to the Kurucz (1993b,c) lists is given in Fig.1 (all the ions discussed in this Section are marked). To improve both old line lists (such as BELLHEAVY from Kurucz 1993b) and new lists described in Sect.4.4 Landé factors for the neutral and first ions of all rare earth elements were added (this includes Tb and is not specifically marked in Fig.1).

The following lists were already part of the first installation of VALD: BELLLIGHT, BELLHEAVY, and NLTE LINES from Kurucz (1993b), the GFIRON data on iron peak elements from Kurucz (1993c), lines with observed energy levels taken from Kurucz & Peytremann (1975, not distributed any more), and a list on rare earth elements based on Meggers et al. (1975). They are part of the VALD-2 installation as well but will not be discussed here except for comparison with new data. A few additional lists with highly accurate oscillator strength data

had been included into VALD-1 which were redistributed to new VALD-2 line lists. The latter have been compiled separately for each element. The line data redistributed to new lists are compared here with new data and references are given to both the original sources and Paper I.

To make the ensuing discussion more readable we use abbreviations for the references. The same abbreviations are also used in the “reference field” (number 15) of the VALD extraction output and consist of up to four letters derived from the initials of the respective authors. Uniqueness of these references is guaranteed within an individual element, which is sufficient as all the new line lists of VALD-2 are grouped according to elements and a compact reference format is mandatory when dealing with millions of lines.

4.1. Light elements

While this paper was being refereed, we implemented new atomic data for C, N, and O (Wiese et al. 1996) into VALD which were provided by NIST. A detailed description of these data sets has to be postponed to a paper on the next implementation of the data base (VALD-3). Already before this extension, we had included new data for 62 lines of Si II and P I into the data base.

Silicon. Experimental transition probabilities for Si II lines were measured by Bergeson & Lawler (1993a – BLa), by Calamai et al. (1993 – CSB) and by Blanco et al. (1995 – BBC). BLa used a combination of the lifetimes measured by time-resolved laser-induced fluorescence (LIF) and emission branching ratios. CSB measured transition probabilities of $3s^23p(^2P^0) - 3s3p(^4P)$ intersystem lines with an ion-trapping technique. BBC measurements were based on emission line intensities from laser-produced plasma. The accuracy (relative error) of the experimental oscillator strengths lies between 10 and 20%. For two lines in the near ultraviolet and three lines in the red region the experimental data were obtained for the first time. The new list contains 35 spectral lines and for 15 of them we included calculated Stark damping constants taken from Lanz et al. (1988).

Phosphorus. Radiative lifetimes for the 4p excited states of neutral phosphorus were measured experimentally for the first time by Berzinsh et al. (1997). Measurements for 6 levels were combined with calculations for another 7 levels and with theoretical branching ratios to deduce oscillator strengths for 27 lines belonging to the $4s - 4p$ transition of P I. Using this set of oscillator strengths a new value for the solar phosphorus abundance of 5.49 ± 0.04 was obtained which decreases the discrepancy between earlier determinations and the meteoritic value (Berzinsh et al. 1997).

4.2. Iron group elements

From the near ultraviolet to the near infrared, iron peak elements contribute the bulk part of line opacity in most stars of spectral types B to K. In VALD-1 most of the experimental data was based on the NBS compilations by Martin et al. (1988) and by Fuhr et al. (1988) in the revised version by A. Gulliver — with Fe I as the only major exception (see Paper I for details). Meanwhile, for most species of lower ionization stage new atomic data of high accuracy and — in many cases — with individual error estimates have become available. Consequently, we were able to include new data for almost 12 000 lines from iron peak elements into VALD-2.

Scandium. New absolute transition probabilities for 182 Sc I and for 64 Sc II lines were measured by Lawler & Dakin (1989–LD) combining emission branching ratios with radiative lifetimes from time-resolved laser-induced fluorescence (LIF) with a relative error not more than 10%. These data include 141 new Sc I and 25 new Sc II lines in addition to the NIST compilation (Martin et al. 1988). The overall agreement between the new and the NIST data is within 0.1 dex, although the absolute scale is slightly shifted. A few lines show a larger discrepancy, for example 3 lines of the $^4F - ^4D^0$ multiplet of Sc I, two weak lines of Sc I at 2719.13 Å and 6306.0 Å, and two lines of Sc II at 3645.31 Å and 3666.53 Å. The two last lines have an accuracy of about 50% in the NIST list. If we ignore the latter, we obtain the following difference between NIST and LD transition probabilities:

$$\begin{aligned} \text{Sc I: } \log gf_{\text{NIST}} - \log gf_{\text{LD}} &= -0.04 \pm 0.04 \text{ (27 lines)} \\ \text{Sc II: } \log gf_{\text{NIST}} - \log gf_{\text{LD}} &= +0.04 \pm 0.08 \text{ (37 lines)}. \end{aligned}$$

We also checked the new data with abundance calculations for the Sun using Kurucz’s (1993a) standard solar atmosphere model with $T_{\text{eff}} = 5777$ K, $\log g = 4.44$, and $\xi_t = 1.5 \text{ km s}^{-1}$ (for the actual line calculations a value of $\xi_t = 0.85 \text{ km s}^{-1}$ was used). The equivalent widths of the solar lines were taken from the solar atlas of Moore et al. (1966). The mean solar scandium abundance deduced from 21 very weak (1–14 mÅ) Sc I lines is 3.12 ± 0.24 , and from 26 Sc II lines it is 3.22 ± 0.14 . No weights were introduced for calculating the standard deviations. The corresponding values obtained for the same sample of solar lines with the available NIST oscillator strengths are 3.24 ± 0.33 (12 Sc I lines), and 3.19 ± 0.17 (10 Sc II lines). The adopted solar abundance is 3.17 ± 0.10 (Grevesse et al. 1996). The new data are in good agreement with the Kurucz (1993c) semi-empirical calculations. Note that in the NIST compilation Sc I $\lambda 5301.96$ has a wrong wavelength (5302.98 Å).

Titanium and Manganese. Raassen & Uylings (1997 – RU) and Uylings & Raassen (1997 – UR) published new calculations of the transition probabilities for Ti III and Mn III. The authors used the orthogonal operator description for odd and even energy levels. This method

	Ia	IIa	IIIb	IVb	Vb	Vlb	VIIb	VIII					lb	IIb	IIIa	IVa	Va	Vla	VIIa	0
1	1 H																		2 He	
2	3 Li	4 Be		N element I II III									5 B	6 C	7 N	8 O	9 F	10 Ne		
3	11 Na	12 Mg										13 Al	14 Si	15 P	16 S	17 Cl	18 Ar			
4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr		
5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 J	54 Xe		
6	55 Cs	56 Ba	57-71 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn		
7	87 Fr	88 Ra	89-103 Ac	104 Ku	105 Ha															

Rare earth elements	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
Lanthanides														
Actinides	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

Fig. 1. Within the VALD project data for about 23 000 lines from 58 different ions have been collected, compared, and tested in order to extend the Kurucz (1993bc) compilations. We have marked the spectrum number (from neutral, I, to doubly ionized, III) for each element for which improvements have been achieved either in VALD-1 or VALD-2 (this paper) or both. Work to include data on C, N, O was finished while this paper was being refereed, while work on S is still in progress. Note that all line lists for rare earth elements also have been supplemented by Landé factors as far as possible (not specifically marked here)

allows a more accurate evaluation of the wave functions which leads to an order of magnitude better accuracy for the transition probabilities in comparison with the semi-empirical method used by Kurucz (1993c). Not surprising, the new calculations for Ti III agree better with the experimental intensities (Raassen & Uylings 1997). Both data sets are included in VALD-2 with higher ranking than older lists.

Vanadium. New measurements of lifetimes and transition probabilities for V II were performed by Biémont et al. (1989 – BGF) based on LIF lifetime measurements and emission branching fractions. They measured 147 lines of which 85 are in common with the NIST compilation (Martin et al. 1988). Most of the V II data in the NIST table are coming from Karamatskos et al. (1986). A comparison of NIST and BGF lists shows an agreement within 15% ($\log gf_K - \log gf_{BGF} = -0.014 \pm 0.065$) with the exception of 6 lines which were taken from Wujec & Musielok (1986) and from Roberts et al. (1973). For these lines the difference exceeds 0.2 dex and amounts to up to 0.6 dex. Both groups, Karamatskos et al. and BGF, claim identical accuracies ($\leq 10\%$) in most of the cases. We prefer the BGF line list, because it contains more lines with accurate transition probabilities.

Chromium. New measurements of the transition probabilities for 12 Cr II lines from the $3d^4(5D)4p z^6P^0$ levels were published by Bergeson & Lawler (1993b – BL) with an estimated accuracy of about 10%. Only one of

these lines was previously included in the NIST compilation (Martin et al. 1988). The determinations are based on the combination of emission branching ratios with LIF lifetime measurements.

Ekberg (1997) analyzed a spectrum of doubly ionized chromium with a low voltage spark discharge and the normal incidence spectrograph at NIST. He observed 143 new energy levels of the $3d^3 4d$ and $3d^3 5s$ configurations leading to a classification of 721 new Cr III lines. Using the Cowan (1981, 1995) codes Ekberg calculated transition probabilities for 1893 lines in the wavelength region from 736 Å to 2675 Å. Figure 2 compares Kurucz’s semi-empirical calculations with Ekberg’s results. A large dispersion of ± 3 dex is observed for the lines with lower level excitation energy between 8 and 9 eV. We prefer the new calculations by Ekberg, because they are based on a larger sample of observed energy levels and therefore provide more accurate wavelengths and transition probabilities.

Iron. New accurate measurements of the transition probabilities for neutral iron became available after the NIST compilation by Fuhr et al. (1988) appeared. The most extensive set of measurements, which contains 1814 lines in the range of 2250 – 26660 Å, was produced by O’Brian et al. (1991 – BWL) and already included into VALD-1. They used their LIF lifetime measurements in combination with emission branching fractions. For 640 lines transition probabilities were found by

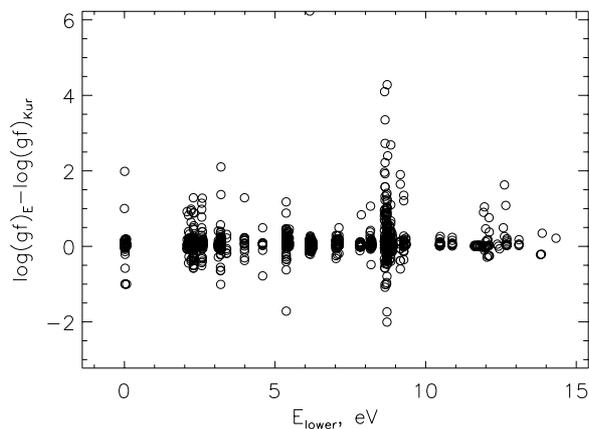


Fig. 2. Dependence of the differences in $\log(gf)$ calculated by Ekberg and by Kurucz for Cr III lines on the excitation energy of the lower level

interpolating level populations in the inductively coupled plasma source (ICP). For most of these lines the accuracy is better than 10%, which is supported by a comparison with the high accuracy Oxford absorption oscillator strengths. Bard et al. (1991 – BKK) and Bard & Kock (1994 – BK) measured transition probabilities for 230 Fe I lines using the same technique. Both works have 80 lines in common with O’Brian et al. (1991). There is no difference in the absolute scale of both sets and they agree within 25%.

We merged all three sets in one new VALD line list and averaged data with the same accuracy (according to the authors); otherwise we tabulated the oscillator strengths with the higher accuracy. We also included in the new list theoretical $\log gf$ -values calculated for neutral iron lines in the IR which were classified by Johansson et al. (1994b – JNG) and by Schoenfeld et al. (1995 – SCG) based on laboratory and solar analyses. These lines belong to the $4f - 5g$ supermultiplet (25445 Å – 25700 Å), to the $4f - 5g$ supermultiplet (38730 Å – 39280 Å), and to the $5g - 6h$ supermultiplet (73700 Å – 74100 Å) of the $3d^6 4s(^6D)$ configuration. All theoretical calculations were compared to $\log gf$ -values derived from the solar spectrum and they were in good agreement. The new file contains latest data on wavelengths, level energies and classification – when available – from the New Fe I Multiplet Tables (Nave et al. 1994). The final VALD-2 file consists of 2962 Fe I lines of which half have a relative error in $\log gf$ of not more than 10%.

Likewise, accurate LIF lifetime measurements with an uncertainty of less than 5% are now available for Fe II (Biémont et al. 1991; Guo et al. 1992; Hannaford et al. 1992). They were used to transform high precision emission branching ratios to absolute transition probabilities. The most recent work by Bergeson et al. (1996 – BMW) includes 67 lines from the $3d^6(^5D)4p$ subconfiguration in the

spectral region from 2249 Å to 2762 Å. All but four lines have an accuracy between 3 and 10%. Another work by Mullman et al. (1997 – MSL) provides absolute absorption oscillator strengths for 7 vacuum-UV lines of Fe II in the 1608 Å – 1640 Å spectral region with an accuracy better than 10%. We decided to use the BMW list as a reference for the comparison between different lists of Fe II transition probabilities. First, we compared BMW with the data by Bridges (1973), by Whaling (1985 – W), by Kroll & Kock (1987 – KK), and by Pauls et al. (1990 – PGH). The last list has only two lines in common with BMW and they agree within 12%. The list of Bridges contains three lines in common with BMW and the agreement is better than 10%. A comparison between BMW and W data is shown in Fig. 3a, and between BMW and KK in Fig. 3b. The 46 lines which are in common with Whaling’s list agree within 12%. The only systematic difference between both sets is a shift of -0.04 dex in the absolute scale of Whaling’s $\log gf$ -values. Therefore, we apply this shift to all Whaling data. BMW and KK data agree within 10% with no difference between the absolute scales, but there is a systematic dependence of the $\log gf$ -difference on the oscillator strength which causes an error of less than 25% for the whole range of $-2.0 \leq \log gf \leq 0.5$. As a result, we give the highest priority in the spectral region of 1600 Å to 3000 Å to MSL and BMW data. We supplement them with Whaling’s data corrected by $+0.04$ dex, with Bridges’ data (second priority), and with PGH and KK data (third and fourth priority). For a few lines we averaged KK and PGH oscillator strengths.

For $\lambda \geq 3000$ Å the main sources for Fe II oscillator strengths are: Bridges (1973), Baschek et al. (1970, corrected by $+0.16$ according to Fuhr et al. 1988), Whaling (1985), Hannaford et al. (1992 – HLG), Kroll & Kock (1987), Heise & Kock (1990 – HK), Pauls et al. (1990), and Blackwell et al. (1980 – BSS). The HK and PGH data were slightly corrected to fit the best available lifetime measurements by HLG. The solar oscillator strengths obtained by BSS have a good relative accuracy, but they were based on a solar iron abundance of $\log(\text{Fe}/\text{H}) = -4.31$. The best present estimate gives $\log(\text{Fe}/\text{H}) = -4.50$ (e.g. HLG) and we therefore applied a $+0.19$ dex correction to the BSS oscillator strengths. A comparison of the corrected data with the data from other sets showed a good agreement. In total we obtained 84 lines in the 3000 Å – 7712 Å spectral region with oscillator strengths having an accuracy of 25% or better. For roughly half of the lines oscillator strengths from 2 to 4 different sources were averaged and they may be considered as the most reliable.

We corrected oscillator strengths for the forbidden ($\Delta S = 2$) transitions of Fe II, which stem from an anomaly originating from an indirect level mixing of $w^2P_{3/2}$ and $x^6P_{3/2}$ (Johansson et al. 1995 – JBL). We also included new oscillator strengths for 222 lines of the $4f - 5g$ supermultiplet of Fe II calculated with the Cowan code (Rosberg

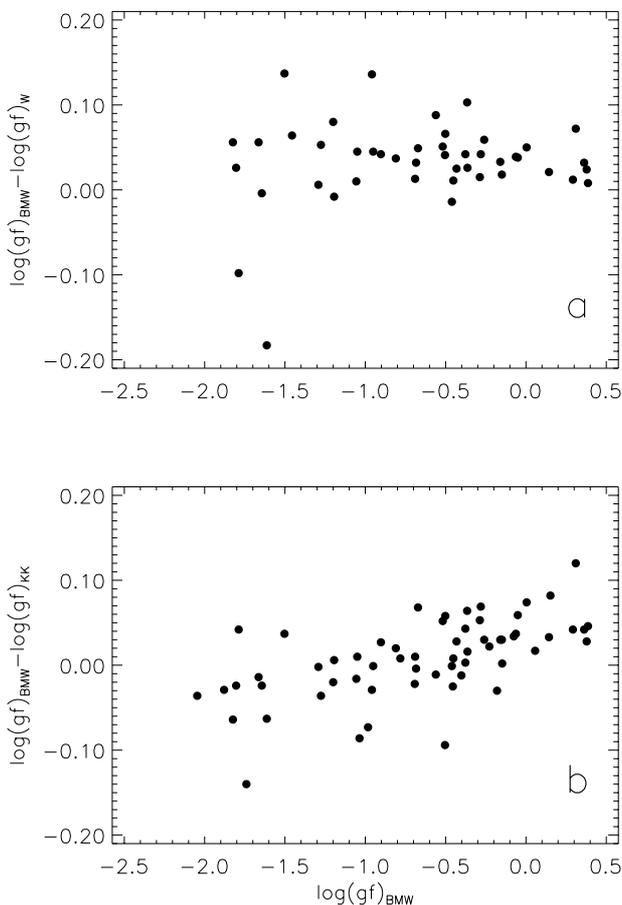


Fig. 3. A comparison between Fe II oscillator strengths measured by Bergeson et al. and by Whaling a), and by Bergeson et al. and by Kroll & Kock b)

& Johansson 1992 – RJ) and for 76 lines of the lowest 5g – 6h supermultiplet of Fe II calculated in the framework of the relativistic Hartree-Fock approximation by Biémont et al. (1997 – BJP). The final VALD-2 list contains 522 lines of Fe II. Further information on the input data for iron can be found in Ryabchikova et al. (1999b).

Cobalt. Accurate transition probabilities for 15 Co I lines with $w^4D_{3/2}$ as the upper level were published by Lawler et al. (1990 – LWG). The measurements were based on LIF lifetime measurements and on emission branching ratios. They have an accuracy of 10 – 12%. Previously, only Kurucz’s semi-empirical data were available for these lines.

Two new experiments on Co II transition probabilities were published since the paper by Salih et al. (1985) which was the only source for this ion in the NIST compilation. Crespo López-Urrita et al. (1994b – CUNJ) measured emission branching ratios and converted them into absolute transition probabilities using the lifetimes published by Salih et al. (1985) and by Pinnington et al. (1973). A comparison between the oscillator strength measurements

of CUNJ and of Salih et al. (1985) shows a remarkable agreement in the absolute scale within 1% and with a standard deviation of 10% for 26 lines with $\log(gf) > -1.0$. Only one line, $\lambda 2694.68 \text{ \AA}$, is significantly outside these error limits. For weaker lines we find $\log gf$ -values from CUNJ to be systematically larger by 0.22 dex. There are a few lines from Salih et al. which were not included in the NIST compilation due to their apparently low accuracy. Mullman et al. (1998 – MCL) reported transition probabilities for 28 lines combining LIF and emission branching ratio measurements. The error estimates for most of these lines do not exceed 10%. They have 8 lines in common with CUNJ and after correcting the latter for new lifetime measurements they agree within 22%. We attributed the highest rank to MCL data and trusted the error estimates provided by the authors. Based on our comparisons we averaged for most of the lines data from Salih et al. and from CUNJ and compiled them to a new VALD-2 file, together with the MCL and the other new lines from CUNJ. For the lines with $\log gf > -1.0$ we estimate the error to be 10% (0.04 dex), and for the rest of the lines we give the errors as quoted by the authors. In total, the new list contains 89 Co II lines.

Nickel. Fuhr et al. (1988) give the highest priority to two sets of experimental transition probabilities for Ni I presented by Huber & Sandeman (1980) and by Doerr & Kock (1985). In the mean time, two new sets of experimental measurements were published. Blackwell et al. (1989 – BBPL) used the Oxford spectroscopic furnace to measure relative oscillator strengths for 75 low-lying lines with a very high precision of 0.7%. They converted them to an absolute scale using lifetimes mainly from Becker et al. (1974, 1981). Wickliffe & Lawler (1997a – WLa) reported transition probabilities for 76 lines connected to high-lying, even-parity levels, using emission branching ratios and new LIF lifetime measurements (Bergeson & Lawler 1993c). WLa also checked the Oxford absolute scale with the new lifetimes and found it to be accurate to within 2% after applying an offset of 0.015 dex. Hence, one may expect an accuracy for individual lines of the “Oxford measurements” by BBPL of about 5%. The same accuracy is reported for most lines from WLa. Thus, both lists combined give a total of 151 lines with accurate transition probabilities which we included in VALD-2 with a high ranking. A comparison of the WLa list with the NIST compilation (35 lines in common) shows good agreement. If we reject 3 lines for which the accuracy is marked with a “D” in the NIST table, we obtain $\Delta \log gf_{\text{NIST-WLa}} = -0.05 \pm 0.04$. A similar comparison of NIST and BBPL is less comforting. For 74 common lines we obtain $\Delta \log gf_{\text{NIST-BBPL}} = 0.06 \pm 0.13$. The excess scatter probably is due to the Doerr & Kock’s data, because for lines with $\log gf > -2.0$ the transition probabilities from Huber & Sandeman are in excellent agreement with BBPL measurements. Even for weaker lines the differences are still within the errors quoted by Huber

& Sandeman (see Blackwell et al. 1989 for a discussion). We used 38 lines from the solar spectrum with equivalent widths from 3 to 110 mÅ and the same solar model atmosphere as in the case of scandium to check the new data. Without attributing weights to individual lines we obtain $\log(\text{Ni}/\text{H}) = -5.74 \pm 0.10$ which agrees perfectly with the solar and meteoritic value of -5.75 (Grevesse et al. 1996).

4.3. Elements of the fourth and fifth periods

For elements of the fourth and fifth periods the data for the previous release of VALD has almost entirely been taken from the BELLHEAVY compilation (Kurucz 1993b). New experiments and calculations for these species allow improvement and extension of the contents of VALD for about 1000 spectral lines. For several of these ions no data was available before.

Copper. Most of the data for Cu II described in Paper I were taken from the BELLHEAVY line list (Kurucz 1993b) and actually date back to the compilation of Kurucz & Peytremann (1975). In the meantime, experimental absolute transition probabilities were derived by Kono & Hattori (1982) using the delayed-coincidence technique, and by Crespo López-Urritia et al. (1994a) with special high frequency hollow electrode discharge and emission measurements. The results from the last two groups agree within the expected errors and we merged them into the new file for Cu II after averaging oscillator strengths for the lines which were in common. The final list contains data for 71 spectral lines with an accuracy for the $\log gf$ -values of the order of 15 – 25%. Old VALD and the new data agree within 25%, without any shift in absolute scales. We recommend to use the new data also because they have individual error estimates.

Zinc. New absolute transition probabilities for 2 resonance lines of Zn II at 2025.5 Å and 2062.0 Å were measured by Bergeson & Lawler (1993b) combining emission branching ratios and LIF lifetime measurements. The accuracy of the new data is 7%. The new oscillator strengths are higher by 0.08 dex than those available in VALD-1.

Yttrium and Zirconium. Previously, there was no information in VALD on the second ions for any of the elements of the Sr-Y-Zr group. However, transition probabilities for the most prominent lines of Y III and Zr III were calculated by Redfors (1991) using the Cowan code with estimated uncertainties of about 10%. Later on, Reader & Acquista (1997 – RA) measured and classified 482 Zr III spectral lines in the 630 – 4610 Å region. For 4 lines they gave double or multiple classifications. The observed energy levels were interpreted theoretically with the Cowan code and the oscillator strengths were calculated for all observed transitions. Maniak et al. (1994) measured the lifetimes of five levels of Y III which were converted to oscillator strengths using their theoretical calculations of the branching ratios. Both sets of data for Y III agree quite

well for 5p – 5d and 5p – 6s lines, while the experimental values on average are smaller by 25% for 5s – 5p and 4d – 5p lines than those from Redfors (1991). Our final list consists of 39 Y III lines in the 1280 Å to 3020 Å spectral region for which the oscillator strengths were taken from Maniak et al. (1994) and supplemented by the data from Redfors (1991).

The Reader & Acquista (1997) line list for Zr III has 75 lines in common with Redfors' list. A comparison between both sets of data shows that, with the exception of a few lines for which RA oscillator strengths are smaller by 0.3 dex, the agreement for most of the lines is within 10–15%. We prefer the RA list for VALD-2, supplemented by 3 lines from Redfors (1991). The final list contains 493 Zr III lines.

Ruthenium. Accurate transition probabilities for 482 Ru I lines were derived by Wickliffe et al. (1994). They combined LIF lifetime measurements with the emission branching ratios. For most of the measurements the precision is better than 10%. The new data included in VALD-2 show systematically lower gf -values than the Corliss & Bozman (1962) data. For 114 Ru I lines we had no oscillator strength values in the previous version of VALD. Absolute transition probabilities for 18 UV lines of Ru II were determined by Johansson et al. (1994a). The accuracy of the measurements is better than 25%, which could be confirmed by the Ru abundance analysis in the atmosphere of the HgMn star χ Lup (Johansson et al. 1994a).

Xenon. The energy level classification of Xe II lines in VALD (see Paper I) was checked and when necessary corrected according to the extensive analysis of Xe II by Hansen & Persson (1987).

4.4. Rare earth elements (REE)

The atomic data for neutral atoms and first ions of REE included in the first version of VALD were mainly based on the BELLHEAVY line list supplemented with experimental data from Komarovskij (1991) and data based on Meggers et al. (1975) for some of the first ions. A new set of experimental data for Pr I, Sm I, Eu I, Ho I, and Yb I was created from the compilation of Komarovskij (1991) and included into VALD-2. No information was available for the second ions which are dominant among rare earth elements in stellar atmospheres with a T_{eff} greater than 7500 K. In particular, for Ap stars with overabundant REE the second ions may contribute significantly to the total line absorption. Lines of the REE appear prominently in spectra of magnetic Ap stars which implies the necessity to include Zeeman splitting parameters. For the neutral atoms and the first ions of all REE, except for Pr II and Nd II, Landé factors of the lower and upper levels determined by experiments were extracted from the AEL section of the NIST atomic line data base (Martin et al. 1978) and included into VALD-2. For Pr II and Nd II the

measurements by Ginibre (1989) and by Blaise & Wyart (1984) were used. Moreover, new $\log gf$ -values as well as improved wavelength calibrations and level classifications for 1 800 lines from rare earth elements have been included into the data base, which we describe in the following.

Lanthanum. A new calibration of the intensities published by Meggers et al. (1975) was proposed by Bord et al. (1996). They provide oscillator strengths in agreement with the laser-beam results by Arnesen et al. (1977). The latter was used by Gratton & Sneden (1994) for the recent solar lanthanum abundance determination. Hence, the intensity calibration of Bord et al. (1996) was adopted to compile a new list of La II lines for VALD.

Cerium. Bord et al. (1997) calculated the transition probabilities for Ce III lines using the atomic structure code of Cowan and they found good agreement between Ce II and Ce III abundances for the silicon star HD 200311. While the relative accuracy of the calculations can be estimated as ± 0.15 dex, the absolute scale may be too large by 0.25 dex. A total of 43 Ce III lines in the 2840 Å to 6061 Å spectral region was added to VALD.

Neodymium. For Nd I we again used the compilation of Komarovskij (1991). Oscillator strengths for Nd III lines became available from calculations by Cowley & Bord (1998) based on the Cowan code. The authors provide data for 54 lines in the 3280 Å to 6870 Å spectral region. The estimated relative and absolute errors are similar to Ce III.

Europium. An abundance analysis of this element forced us to implement oscillator strengths data in VALD which were determined from stellar and/or solar spectra. A few lines of Eu III were identified in spectra of magnetic Ap stars by Ryabchikova et al. (1999a). For 4 lines they determined astrophysical oscillator strengths with a relative accuracy of ± 0.2 dex. The absolute scale could be more inaccurate, because of the dependency of the present determination on the ionization balance in stellar atmospheres.

Gadolinium. Komarovskij & Smirnov (1992) revised transition probabilities for Gd I on the basis of new lifetime and branching ratio measurements and extended the list of lines with experimentally measured oscillator strengths. Similar measurements by Bergstrom et al. (1988) provide accurate oscillator strengths for 23 lines of Gd II which were used to improve the solar abundance of gadolinium. The authors give an error estimate for the stronger lines of 10%.

Dysprosium. Komarovskij & Smirnov (1994) deduced absolute oscillator strengths for 35 Dy I and 28 Dy II lines using lifetime and branching ratio measurements with an estimated accuracy of 25%. For 13 Dy I lines the experimental data were obtained for the first time. The new Dy I list of VALD contains 42 lines and it also includes data extracted from the compilation of Komarovskij (1991).

Similar to Komarovskij & Smirnov (1994 – KS) absolute oscillator strengths measurements for Dy II

were carried out by Biémont & Lowe (1993 – BL) on the basis of LIF lifetime measurements and relative intensities taken from Kusz (1992). A total number of 63 lines was measured and with two exceptions the lifetimes determined by KS and BL agree very well. The oscillator strengths from BL are considered to be slightly more accurate, because the branching ratios used by BL were measured on spectra with higher resolution than those used by KS. Smirnov (private communication) corrected a few lines which showed the largest difference (in addition to those, for which lifetime measurements in KS were certainly wrong), and after this correction the difference between KS and BL measurements reduced to 0.01 dex with a dispersion of 0.1 dex. This dispersion corresponds exactly to the 25% accuracy claimed by KS. For the final list of oscillator strengths we used data from BL and one additional line from KS.

Erbium. Absolute experimental transition probabilities for 41 Er I lines were obtained by Komarovskij & Smirnov (1993) with an accuracy of about 25% using lifetimes and branching ratio measurements. For 22 lines experimental data were presented for the first time.

The spectrum of Er III was re-analyzed by Wyart et al. (1997), who argued for new energy levels and transition probabilities based on a comparison of their line list with the spectrum of the Ap star HR 465. The number of known energy levels was increased from 45 to 115 and the number of classified lines to 470. Oscillator strengths for 304 lines calculated with the Cowan code are included in VALD-2.

Thulium. New LIF lifetime measurements (Andersen et al. 1996) together with the emission branching ratios resulted in oscillator strengths for 376 lines of Tm I and 146 lines of Tm II in the 2500 Å to 10000 Å spectral region (Wickliffe & Lawler 1997b). The new measurements increase the existing data by 241 Tm I and by 30 Tm II lines and yield a significant improvement of $\log gf$ -values over the BELLHEAVY list. A new classification was possible for 3 lines of Tm II, and for most of the measured lines the typical uncertainty is less than 10%. A comparison between BELLHEAVY and the new oscillator strengths is shown in Fig. 4. The new data provide systematically lower $\log gf$ -values than the old ones and the difference increases for weaker lines. For the Tm II lines at 3362.6 Å and 3462.2 Å, used for the determination of the solar abundance of thulium (Andersen & Sørensen 1974), the new oscillator strengths agree within the claimed accuracy with the old values.

Lutetium. Bord et al. (1998) reported oscillator strengths calculations for 24 lines of Lu II using the Cowan code. They found on average their $\log gf$ -values to be smaller by 0.27 dex than those given by Corliss & Bozman (1962) for $\lambda < 3000$ Å, while for three lines with $\lambda > 5400$ Å their $\log gf$ -values are larger by ≈ 0.5 dex. Den Hartog et al. (1998) reported oscillator strengths for 3 lines of Lu II at 3507.4 Å, 5983.9 Å and 6221.9 Å obtained from LIF lifetime measurements combined with emission

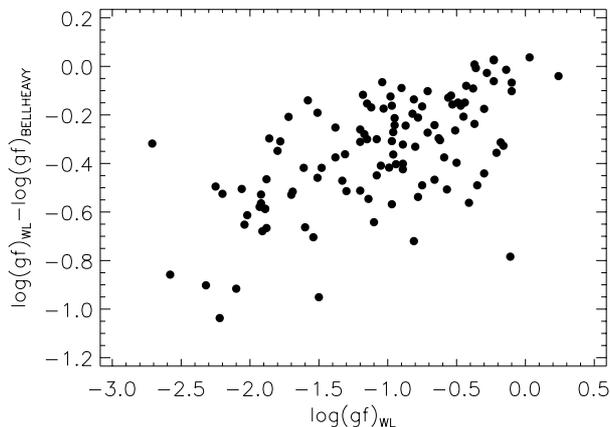


Fig. 4. A comparison of the experimental oscillator strengths for Tm II determined by Wickliffe & Lawler (1997b) with the BELLHEAVY data

branching ratios with an accuracy of 0.06 dex or better. Only the last line is in common with the list of Bord et al. (1998) and its measured oscillator strength is smaller by 0.16 dex than the calculated value. A comparison between the new measurements and those by Corliss & Bozman proved the new $\log gf$'s to be larger by about 0.4 dex for red and blue lines. On the other hand, the results of Bord et al. (1998) agree rather well with theoretical calculations of Migdalek & Baylis (1988). We therefore included the experimental oscillator strengths by Den Hartog et al. (1998) in the new list and supplemented it with the data from Bord et al. (1998). The expected errors of the latter data are at least 0.1 dex with a possible shift of their absolute scale of about +0.15 dex.

4.5. Elements heavier than Lu ($Z > 71$)

Heavy elements such as Au, Pt, and Hg are important tracers for the study of diffusion processes in chemically peculiar stars, in particular for those of HgMn type. Recent laboratory data and new theoretical calculations allow now for more reliable abundance analyses using several ions of the same element. A total of about 1600 lines for elements heavier than Lu has been included into VALD-2.

Rhenium. The oscillator strengths for singly ionized rhenium used for VALD-1 were based on Corliss & Bozman (1962) data. Wahlgren et al. (1997) determined an accurate oscillator strength for one (2275.25 Å) out of three lines of the Re II UV1 multiplet, using LIF lifetime measurements and emission branching ratios. The new value of $\log gf$ is included in VALD-2. It is smaller by 0.6 dex than the corresponding value from Corliss & Bozman (1962). This fact has to be kept in mind, because we do not propose any corrections for the other lines from Corliss & Bozman (1962). Wahlgren et al. (1997) provide

for all three lines of the UV1 multiplet also wavelength and intensity data for the hyperfine components of both stable isotopes of rhenium.

Platinum. Calculations of the transition probabilities for Pt I lines in the 1730 Å to 2540 Å spectral region using the Cowan code were carried out by Wahlgren et al. (1995). Wavelengths and energy levels were taken from Blaise & Wyart (1992). In the same paper, Wahlgren et al. report on calculated oscillator strength for the Pt II line at 2144.25 Å which turned out to be slightly larger than the relative astrophysical $\log gf$ -value derived by Dworetsky et al. (1984). Soon after, Wyart & Blaise (1995) published an extensive study of the Pt II spectrum based on the atlas of Sansonetti et al. (1992). Wyart & Blaise calculated the transition probabilities for 112 lines in the 1380 Å to 2800 Å spectral region and also provided theoretical Landé factors for the odd energy levels. Their $\log gf$ -value for the 2144.25 Å line agrees nicely with the value of Dworetsky et al. and we therefore included all the data from Wyart & Blaise (1995) into VALD-2 together with the astrophysical $\log gf$ -values from Dworetsky et al. (1984) for lines in the optical spectral region. For Pt I the new list contains the oscillator strengths from Wahlgren et al. (1995). Ryabtsev et al. (1993) classified more than 800 Pt III lines in the range of 559 Å to 2020 Å and provided the transition probabilities for 666 lines, calculated with the Cowan code. Oscillator strength data for the Pt lines in three ionization stages were used in the abundance analysis of the HgMn star χ Lup and gave a satisfactory agreement for the platinum abundance obtained from the lines of the different ions (Wahlgren et al. 1995). In total, we have included new line data for 14, 119, and 666 lines of Pt I, Pt II, and Pt III, respectively.

Gold. Similar to Pt, VALD contained information only for the lines of neutral gold. At the same time, lines of Au II and Au III were also observed in the spectra of HgMn stars. The oscillator strength for the Au II 1740 Å line was obtained by combining theoretical branching ratios with measured lifetimes (Wahlgren et al. 1995).

Rosberg & Wyart (1997) performed an extensive study of the Au II spectrum in the 800 Å to 8000 Å spectral region. They identified more than 500 spectral lines and calculated oscillator strengths for 497 lines using the Cowan codes. Their $\log gf$ -value for the 1740 Å line is higher by 0.3 dex than the corresponding experimental value from Wahlgren et al. (1995). Using Rosberg & Wyart data for the optical lines Ryabchikova (1998a) recalculated the Au abundance in the atmosphere of χ Lup A and obtained $\log(\text{Au}/\text{H}) = -6.69$ which agrees with the $\log(\text{Au}/\text{H}) = -6.74$ deduced by Wahlgren et al. (1995). It means that the absolute oscillator strength scale for the optical Au II lines agrees better with the experimental oscillator strength for the 1740 Å line than the scale for the UV lines. The reason for the 0.3 dex difference is not clear yet. Thus, we included in VALD-2 all the data from Rosberg & Wyart with the exception of the Au II line at

1740 Å for which we used the experimental $\log gf$ -value from Wahlgren et al. (1995).

Wyart et al. (1996) identified more than 1000 lines of Au III and calculated transition probabilities for 175 lines in the 800 Å to 2000 Å spectral region. Their $\log gf$ -value for the 1746 Å line is lower by 0.18 dex than the corresponding value from Wahlgren et al. who have calculated the oscillator strength for this line. For VALD-2 we preferred the data from Wyart et al. (1996).

Mercury. The previous VALD version provided data for Hg I and Hg II extracted from the BELLHEAVY line list. During the analysis of HgMn stars we found substantial inaccuracies of the wavelengths used in BELLHEAVY. Therefore, we produced a correction file for Hg II lines with wavelengths taken from Reader & Sansonetti (1986) measured for the terrestrial mixture of Hg isotopes. In the new list of Hg III lines we included oscillator strengths for 42 spectral lines in the 740 – 3100 Å spectral region calculated by Uylings et al. (1993) using the orthogonal operator method with configuration interaction.

Lead. VALD originally contained 11 lines of Pb II with theoretical oscillator strengths mainly taken from Migdalek (1976). Meanwhile, Miller et al. (1979) and Alonso-Medina (1996, 1997) provided experimental measurements of the Pb II oscillator strengths using emission branching ratios and lifetime measurements. Two different experiments of Alonso-Medina (hollow-cathode discharge and laser induced plasma) gave oscillator strengths which agree within 10%. The cited accuracy of Miller et al. data is lower. Five out of nine lines common to both lists agree within 15% while for 4 lines the difference in transition probabilities may be 2 – 3 times larger. We included in the VALD-2 list 37 Pb II lines for which oscillator strengths were taken from Alonso-Medina (1996, 1997). Two lines, at 3665.5 Å and 3945.7 Å were rejected, because their wavelengths do not correspond to the proposed classification. Because the accuracy of the wavelengths is not good in Alonso-Medina, we used central wavelengths from Reader & Corliss (1980) whenever possible. Atomic energy levels and experimental Landé factors were taken from Moore (1958).

5. Conclusions

More than 4 years of operation have proven the usefulness of the VALD concept as it was described in Paper I. Two mirror sites and more than 240 users from all around the world confirm the need for such a data base. Most of the proposed improvements listed at the end of Paper I have been implemented to various degrees in VALD-2. Only the compilation of telluric line lists has not yet been started. In particular, we have reported the following achievements:

- More than 16 000 individual lines have been processed in preparation of VALD-2. It took an enormous amount of work not only to collect the data but to

compare and establish the relative ranking between different lists, as described in Sect. 4.

- References to primary sources for any measured or computed parameter value extracted by VALD are included to the output. Besides the proper referencing to sources, which is fundamental in scientific publication policy, this new feature also provides an important incentive to contributors of these much needed data to communicate their results to VALD.
- First steps towards including complete information on Zeeman pattern, Stark and van der Waals broadening constants have been made. In collaboration with specialized institutions (e.g. M.S. Dimitrijević and L. Popović, Belgrade Observatory; S. Sahal-Bréchet, Observatoire de Paris-Meudon; R.K. Janev, International Atomic Energy Agency) VALD will significantly improve quality and quantity of such data.
- Access to VALD has been simplified by providing two WWW interfaces,
 - HTTP://WWW.ASTRO.UU.SE/~VALD
 - HTTP://WWW.ASTRO.UNIVIE.AC.AT/~VALD
 and turn around time has been reduced by implementing two mirror sites
 - VALD@ASTRO.UU.SE
 - VALD@HYPATIA.GSFC.NASA.GOV
 in Uppsala and at NASA-GSFC which are synchronized every 12 hours with the main site
 - VALD@ASTRO.UNIVIE.AC.AT
 The Vienna site also continues to take responsibility for registration (at VALDADM@ASTRO.UNIVIE.AC.AT).
- Flexibility of data extraction has been increased by providing personal configuration files which allow optimization of extractions for specific scientific requirements of each user. In addition, usage of personal configuration files will ensure identical outputs even for future versions of the data base and new default settings for data extraction chosen by the VALD team.

Extensive plans have been made for the future development of VALD (VALD-3) and we already started working with the prototype software and test datasets. The main goals are to extend the applicability of VALD to stars with lower effective temperatures and to include additional line data such as Stark broadening and wavelength shift parameters which can be crucial e.g. for proper synthesis of Helium lines. A similar approach will be used for hyperfine structure and isotopic splittings as well as for Zeeman patterns (when the LS coupling approximation is not applicable).

A major new step towards VALD-3 is the inclusion of molecules. Recent progress in molecular spectroscopy resulted in line lists of diatomic molecules that can be compared with high resolution astronomical spectroscopic observations on a line-by-line basis (Valenti et al. 1998). VALD-3 will in the beginning contain a few best lists of diatomic molecules that can be reliably used for spectrum

synthesis. The new internal and the extracted data format provide the capability to accommodate this new data while a molecular equilibrium solver has been developed for the selection procedures.

Last, but not least we call on the community of users to provide us with critical comments on what should be changed and suggestions on what should be included in the next version of VALD. In particular, we are grateful for any references to data we have not yet been aware.

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