Physica Scripta. Vol. T83, 162–173, 1999

The Vienna Atomic Line Data Base – a Status Report

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Received October 7, 1998; accepted in revised form December 14, 1998

PACS Ref: 9530Ky, 9530Dr, 3270Cs, 3290+a, 9575Fg

Abstract

Atomic transition parameters are of fundamental importance for many aspects of astrophysical research. But this information is spread over an enormous variety of publications in the fields of, e.g., applied and atomic physics, chemistry, and astronomy. Moreover, they differ in parameters listed and physical units used, as well as in their relative and absolute accuracy. This unfortunate situation led us to create a set of both critically evaluated and more homogeneous lists of astrophysically important atomic transition parameters and of supporting extraction software.

This new data base is called the "Vienna Atomic Line Data Base" (VALD) and contains about 600 000 entries for spectral lines with measured energy levels. VALD includes tools for extracting data and references which are particularly suitable for astrophysical applications such as spectrum synthesis and model atmosphere calculations. They are described in papers by Piskunov *et al.* (1995) and Kupka *et al.* (1999).

We describe in this paper the structure of VALD, present a summary of all available data sets, explain our ranking procedure, in particular for the case of recent data on Fe I and Fe II, and comment briefly on the specific retrieval tools. The electronic-mail interface VALD-EMS allows remote access to VALD and is now extended by the WWW interfaces:
http://www.astro.univie.ac.at/~vald
http://www.astro.uu.se/~vald

1. Motivation

The structure of VALD is illustrated in Fig. 1. The motivation for developing this data base was:

- to compile the most accurate and complete lists of spectral lines relevant to stellar atmospheres (originally we focussed on atomic lines observed in stars of intermediate spectral type);
- 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,
  - provide quality criteria, and
  - extract homogeneous datasets containing the best transition data for spectrum synthesis or model atmosphere calculations.

* supported by grant 2.2.1.5 of the Russian Federal program "Astronomy".
† supported by FWF projects S7303-AST & P11882-PHY.
‡ supported by FWF projects S7303-AST & P11882-PHY.

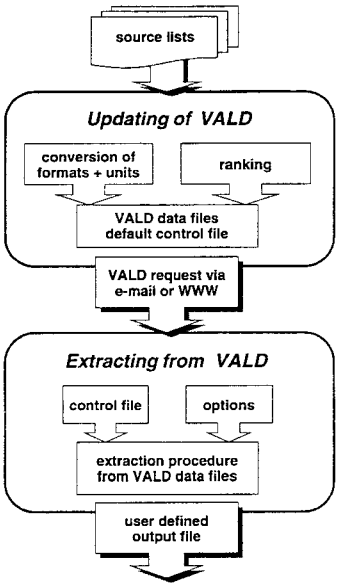

Fig. 1. Block diagram showing the logical structure of VALD. Individual components are described in the text.

2. Structure of VALD

The Vienna Atomic Line Data Base, VALD, was introduced in [79] and its extensions to what is called version VALD-2 are described in [55]. The data base consists of several lists of atomic line data from various providers. These *input lists* (or *source lists*) are ranked according to error estimates, provided with the original data, which in many cases have been verified by astrophysical abundance analysis. Each extracted transition datum is compiled from the highest ranking list. This procedure avoids averaging of data with very different individual errors, like measured and calculated oscillator strengths ($\log gf$-values). However, for the creation of some of the new VALD input lists (see Section 2.2) a weighted average of original data with individual error estimates was performed to obtain a higher accuracy for the data distributed through VALD.

2.1. *VALD standard format*

To store the interesting information for each spectral line archived in VALD we adopted the following format. It is referred to as version 3.0 format, because it already includes all the features necessary to handle molecular line data which will be part of the next VALD release. The format contains the following 16 parameters:

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 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 is 99, if no value can be provided.
9. g_k – Landé factor of the upper energy level; default is 99, if no value can be provided.
10. $\log \Gamma_r$ – logarithm of the radiation damping constant in s^{-1}; default is 0, if no value can be provided.
11. $\log \Gamma_s$ – logarithm of the Stark damping constant at 10 000 K in $(s \cdot N_e)^{-1}$, i.e. per perturber; default is 0, if no value can be provided.
12. $\log \Gamma_w$ – logarithm of the van der Waals damping constant at 10 000 K in $(s \cdot N_H)^{-1}$, i.e. per perturber; default is 0, if no value can be provided.
13. Spectroscopic terms of lower and upper energy levels.
14. Accuracy for $\log gf$ in dex; default is –1, if no value can be provided.
15. Comments, e.g. multiplet number as in [68].
16. Flags, which 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.

The first 12 entries contain numerical data and occupy 52 bytes if they are stored as a sequence of uncompressed IEEE floating point numbers which are common on all modern workstations. The next three parameters provide more than 40 characters altogether.

Field 13 offers 24 characters to store term designations for both lower and upper levels (Greek letters are indicated by a preceeding "\" in analogy to the LaTeX convention).

As more precise estimates of oscillator strengths have become available, the letter-type accuracy identifier for $\log gf$ as in [68] was replaced by an error estimate given in dex (two bytes) in parameter field 14. The next parameter field, "comments" (16 characters), allows for

- accurate source description for input lists compiled with data from different authors,
- multiplet designation (where available), and to
- store additional accuracy descriptors.

Finally, we decided to add two bytes for flag values (parameter field 16). These will be used to cross-reference VALD entries with auxiliary information from other data bases, e.g. Zeeman patterns, Stark and van der Waals broadening, and to indicate hydrogen lines and autoionization lines. Future VALD extraction tools are expected to use these flags when assembling the reply to a request.

Special numerical values are used in VALD to indicate the absence of various atomic parameters. A particular number is chosen such that it is both easy to remember and that it cannot appear as a physical value for this quantity under any known circumstances.

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 (fields 8 to 12) are missing from the source list, *default values* of '0' for the damping constants and '99' for Landé factors are inserted (to avoid confusion with real zero Landé factors).

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.

2.2. *VALD data files*

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

To speed up access for requests on individual species (e.g. elements), source lists for VALD are sometimes split into several files, though the references provided by the data base clearly indicate the original compilation. 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 (or molecular) transition (hereafter simply called "line"). Records are stored sequentially in binary format. Different files can contain data on the same line, but each line of a given file has to be unique. The species (atoms or molecules in a given ionization stage) are identified internally with a number. The unique correspondence between a number and a species is defined in a VALD internal table of species.

Currently, to add a new source to the data base, 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 in the internal VALD format (see Section 2.1). To increase the efficiency the data files are finally compressed. The compression is based on the Lempel-Ziv-Welch algorithm [104] which was modified to achieve the highest compression ratio and to preserve direct access to the data [78]. Any data extraction in VALD is performed using a pipeline of the corresponding filters or "VALD extraction tools" which are described in the references given in Section 4.

2.3. *Configuration files*

The entire extraction procedure for a given request to VALD is controlled by the configuration file (which is also called "control file" in [79]). An example is given in Table I.

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

- the *wavelength window*, used by VALD to search for identical lines in different files. Two lines are assumed to be the same, if 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

Table I. *An example of a VALD configuration file.*

```
0.02,5,50.
; wavelength window in Angstroem, maximum ionization stage,
; and maximum excitation potential of lower level in eV
;
'/CVALD/Ga2Ba',                    5,31,56,3,3,3,3,0,0,0,0,5,'Bell heavy: Ga to Ba'
'/CVALD/la2lu_all_lan',            6,57,71,2,2,2,2,2,0,0,0,5,'Bell heavy: La to Lu & g_Lande'
'/CVALD/gf26_obs',                 23,26,26,3,3,3,3,3,3,3,3,5,'GFIRON obs. energy level: Fe'
;'/linelists/vald1/gf26_pred',     32,26,26,2,2,2,2,2,2,2,2,1,'GFIRON pred. energy level: Fe'
'/CVALD/iron.nbs',                 40,26,26,0,5,0,0,0,0,0,0,3,'NBS: Iron'
'/CVALD/Ti2',                      44,22,22,0,6,0,0,0,0,0,0,3,'Ti 2 accurate gf-values'
'/CVALD/Cr2',                      45,24,24,0,6,0,0,0,0,0,0,3,'Cr 2 accurate gf-values'
'/CVALD/ree_exp',                  46,57,71,6,6,6,6,6,0,0,0,3,'REE experimental & solar'
'/CVALD/Ga2exp',                   47,31,31,6,6,6,6,0,0,6,0,3,'Ga 2 accurate gf-values'
'/CVALD/Xe2exp',                   48,54,54,6,6,6,6,0,0,0,0,3,'Xe 2 accurate gf-values'
'/CVALD/fe1_cor',                  49,26,26,6,6,6,6,0,0,0,0,3,'FeI NMT Whaling and Bard & Kock'
'/CVALD/la2lu_cow',                50,57,68,4,4,4,4,4,0,0,0,3,'New REE interpolated gf-values'
```

give slightly different wavelengths for the same transition.

- the *maximum spectrum number* (ionization stage + 1), 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, for internal usage only), followed by the range of species covered (in line 12 of Table I, i.e. for the eighth reference given, the string '57,71' indicates that lines of La to Lu are listed in 'ree_exp'). The next nine numbers describe the quality (ranking parameters) of the values given for a line (see Section 2.4) and are followed by a short text describing the source list. This text will also appear in the output files. Each client who uses the data base through remote access facilities has now the possibility to keep a personal copy of the configuration file. The client can choose between the standard configuration, created by VALD experts, or a personal configuration file that is modified only by the owner.

More information about data retrieval, in particular by electronic mail service, is given in Section 4.

2.4. *Ranking parameters and replacement lists*

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 configuration file (Section 2.3).

The ranking of a quantity is defined by a non-negative integer number. Nine ranking parameters are given in the data base control file and provide, in sequence, quality assessments for each of the quantities λ, gf, E_i, E_k, $\bar{g}_{\rm eff}$, Γ_r, Γ_s, Γ_w, and level classification. If entries to the same line in different files are found, the parameters with the highest respective ranking are extracted (for the unusual case of equal ranking the first value found is chosen). The sample control file in Table I addresses files 'gf26_obs' and 'fe1_cor' for which the latter has a higher ranking for data on the (neutral) iron lines contained in both lists. The individual numerical value of a ranking parameter (except for '0' and '1') 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 Section 2.1) is given for that parameter. 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. 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 avoid extraction of an "extra line" due to a wavelength error in the *replacement* list being larger than the wavelength window defined in Section 2.3. Recalibration of such data is part of the VALD project, and examples are given in Section 3.

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 ranking. This low quality ranking is chosen for all files generated directly from the old Kurucz-Peytremann list [61].

A comment sign (before 'gf26_pred' in our example) causes no lines to be extracted from that file, no matter which queries are asked. 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. Alternatively, where specific improvements for a source list with a given ranking are identified, these can be included into VALD through the addition of supplementary source lists (e.g. Section 3.4 or [79]).

2.5. *Referencing by VALD*

An important feature of the VALD output is the listing of references to laboratory spectroscopy work and other input sources for VALD. A list of references is compiled at the

end of the extraction while the source of each item in each transition is given in the line reference field. For example:

```
                                    Damping param.
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 2 2 2 2 ' correspond to wavelength, excitation potential of the lower level, oscillator strength, 3 damping constants and Landé factor(s). These reference numbers refer specifically to the compilation given at the end of a reply to a VALD request and are related to the "name" of an individual line list used in the VALD configuration file. The complete list of references is contained in the VALD–EMS electronic documentation, but for the VALD–2 release as described in [55] it can also be found in Table II given below.

3. Line data and evaluation

VALD uses source lists of very different origin. Thus, we encountered the problem of homogeneity. 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 Section 3.1). Lists with more accurate gf-values are continually being added to VALD.

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 [94] and basically relies on an a priori accepted abundance value and an optimum fit of spectral lines to observations, where the gf-value is a free parameter.

In the following subsections we also explain our ranking preferences when several data sources are available for a transition. 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.[1] Uniqueness of these references is guaranteed by their context as is evident from the following discussion of individual species, because each datum refers to a particular VALD line list for which the reference is always unique.

Most of the spectral lines in VALD are extracted from four large line lists: BELLLIGHT, BELLHEAVY, GFIRON and NLTElines [57]. These lists are used as the primary source for wavelengths, energy levels, J-values, damping constants and Landé factors. These compilations have been extended by transition parameters for about 23 000 lines during the last four years. Many of these lines cannot be found in the Bell, GFIRON, and NLTElines lists. In the sequel, we survey the most recent improvements and focus, in particular, on iron.

3.1. *Light elements up to Ca*

The need for improving the data on light elements was already evident during the first extensive use of a VALD prototype (at that time called VLDB) described in [54]. Several obviously incorrect entries in source lists were identified during early tests of the data base. Particularly, the NLTE source list [58] 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. With atomic parameters from "NLTElines" [59] the Si I line at λ 6029.869 Å produces a distinct feature in the spectrum of a solar abundant star with $T_{\rm eff}$= 7900 K and log g= 4.2, but contrary to the other synthesized Si lines this feature cannot be found in α Cir (CP2, SrEuCr) spectra.[2] Other examples for controversial Si II lines can be found at wavelengths of 4002.585, 4028.459, and 4035.272 Å. They are very strong in the synthetic spectrum for the extremely Si–rich star ET And (HD 219749), but cannot be detected in the stellar spectrum (cf. [62] for an abundance analysis).

In the mean time, we have included new atomic data on light elements in VALD. Experimental transition probabilities for Si II lines, for example, were measured by Bergeson and Lawler [9], by Calamai *et al.* [29] and by Blanco *et al.* [24]. The accuracy 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. Hence, a new list for Si lines was created which contains 35 spectral lines, and for a subset of 15 lines we included calculated Stark damping constants taken from [64].

In turn, radiative lifetimes for the 4p excited states of neutral phosphorus were measured experimentally for the first time by Berzinsh *et al.* [13] and were used to derive oscillator strengths for 27 lines. A new solar phosphorus abundance of 5.49 ± 0.04 was obtained with this subset of P I lines which decreases a difference between earlier determinations and the meteoritic value and thus proves our preference for the new data [13].

New atomic data for C, N, and O [109] will be provided by NIST. These data probably will be available to VALD users by the end of 1998.

3.2. *Iron group elements*

Below, we report rather briefly on improvements for Sc to Mn and Ni, but provide a detailed discussion for Fe I and Fe II. Additional results are also presented for the cases of Co I and Co II, whereas for the other species more details are published by [55].

3.2.1. *Sc to Mn*

New absolute transition probabilities for 182 Sc I and for 64 Sc II lines were measured by Lawler and Dakin [65] who combined emission branching ratios with radiative lifetimes from time-resolved laser-induced fluorescence (LIF) with an accuracy of 10% and better. These data include 141

[1] For publications with more than four authors not more than the first four initials are used to keep the SHOW LINE output (cf. Section 4) within a reasonable size.

[2] parameters taken from [56], where Si was actually found to be even slightly overabundant.

Table II. *The current VALD source lists. Note that some spectral lines may appear in several of these lists. The first set of lists contains line data either collected, distributed, or produced by R.L. Kurucz. The second set, separated by a horizontal line, contains additional data for VALD–1, followed by the third set which contains new line data for VALD–2 and some VALD–1 line data which were revised or assigned to new line lists (cf. Piskunov* et al. *[79], Kupka* et al. *[55]). Abbreviations used for referencing and the method of log* gf *determination for new line data of VALD–2 are indicated.*

Source List	Elements/Ions	Number of Lines	abbr.	meth.	References
Bell light:	Li to K	66794			[59] Kurucz CDROM 18 (1993)
Bell heavy:	Cu to U	38453			[59] Kurucz CDROM 18 (1993)
NLTE lines:	H, He, B, C, O, Na, Mg, Al, Si, K, Ca	39791			[59] Kurucz CDROM 18 (1993)
KP–1975:	He to U	265587			[61] Kurucz and Peytremann (1975) (observed levels)
GFIRON ext.	Ca to Ni	406889			[60] from Kurucz CDROM 20–22 (1994)
NBS/NIST:	Sc to Ni	8124			[68] Martin, Fuhr and Wiese (1988), A. Gulliver (included in Kurucz, 1993), [38] Fuhr, Martin and Wiese (1988)
NBS Mono 145:	La II, Ce II, Pr II, Nd II, Sm II, Er II	4367			[70] Meggers *et al.* (1975)
VALD 2: Si 2	Si II	35	CSB	exp	[29] Calamai *et al.* (1993),
			BBC	exp	[24] Blanco *et al.* (1995),
			BLa	exp	[9] Bergeson and Lawler (1993), [64] Lanz *et al.* (1988, Stark damp. const.)
VALD 2: P 1	P I	27	BSB	exp	[13] Berzinsh *et al.* (1997)
VALD 2: Sc	Sc I, Sc II	246	LD	exp	[65] Lawler and Dakin (1989)
VALD 2: Ti	Ti II, Ti III	281	BHN	exp	[18] Bizzarri *et al.* (1993, Ti 2),
			BMP	exp	[20] Blackwell *et al.* (1982, Ti 2),
			RHL	ast	[90] Ryabchikova *et al.* (1994, Ti 2),
			RU	calc	[82] Raassen and Uylings (1997, Ti 3)
VALD 2: V 2	V II	147	BGF	exp	[15] Biemont *et al.* (1989)
VALD 2: Cr	Cr II, Cr III	1961	BLb old: BL	exp	[10] Bergeson and Lawler (1993b, Cr 2),
			SLd	ast	[98] Sigut and Landstreet (1990, Cr 2),
			PGBH	exp	[77] Pinnington *et al.* (1993, Cr 2),
			E	calc	[37] Ekberg (1997, Cr 3)
VALD 2: Mn 3	Mn III	7442	UR	calc	[100] Uylings and Raassen (1997)
VALD 2: Fe	Fe I, Fe II	3483			for details see text
VALD 2: Co	Co I, Co II	104	LWG	exp	[66] Lawler *et al.* (1990, Co 1),
			CUNJ	exp	[34] Crespo L.-U. *et al.* (1994b, Co 2),
			SLW	exp	[96] Salih *et al.* (1985, Co 2)
			MCL	exp	[72] Mullman *et al.* (1998, Co 2)
VALD 2: Ni 1	Ni I	151	WLa	exp	[106] Wickliffe and Lawler (1997a),
			BBPL	exp	[19] Blackwell *et al.* (1989)
VALD 2: Cu 2	Cu II	71	CKNJ	exp	[33] Crespo L.-U. *et al.* (1994a),
			KH	exp	[52] Kono and Hattori (1982)
VALD 2: Zn 2	Zn II	2	BLb old: BL	exp	[10] Bergeson and Lawler (1993b)
VALD 2: Ga 2	Ga II	16	RSb	e+a	[94] Ryabchikova & Smirnov (1994b),
			LADM	calc	[63] Lanz *et al.* (1993)
VALD 2: Y 3	Y III	39	R	calc	[87] Redfors (1991),
			MCT	exp	[67] Maniak *et al.* (1994)
VALD 2: Zr 3	Zr III	493	R	calc	[87] Redfors (1991),
			RA	calc	[84] Reader and Acquista (1997)
VALD 2: Ru	Ru I, Ru II	502	WSL	exp	[108] Wickliffe *et al.* (1994, Ru 1),
			JJL	exp	[45] Johansson *et al.* (1994a, Ru 2)
VALD 2: Xe 2	Xe II	33	RSa	exp	[93] Ryabchikova and Smirnov (1989),
			WM		[110] Wiese and Martin (1980),
			HP		[42] Hansen and Persson (1987)
VALD 2: Ce	Ce II, Ce III	73	sol	sol	solar averaged *gf*-values (Ce 2, sol., cf. Piskunov *et al.* 1995),
			BCN	calc	[27] Bord *et al.* (1997, Ce 3)
VALD 2: Pr	Pr I, Pr II	52	K	exp	[48] Komarovskij (1991)
VALD 2: Nd	Nd I, Nd II, Nd III	121	K	exp	[48] Komarovskij (1991, Nd 1 & Nd 2),
			CB	calc	[32] Cowley and Bord (1998, Nd 3)

Table II. *continued.*

Source List	Elements/Ions	Number of Lines	abbr.	meth.	References
VALD 2: Sm	Sm I, Sm II	367	K	exp	[48] Komarovskij (1991)
VALD 2: Eu	Eu I, Eu II, Eu III	74	K	exp	[48] Komarovskij (1991, Eu 1 & Eu 2),
			RPS	ast	[92] Ryabchikova *et al.* (1998, Eu 3)
VALD 2: Gd	Gd I, Gd II	110	KSa	exp	[49] Komarovskij and Smirnov (1992, Gd 1),
			BBLP	exp	[12] Bergstrom *et al.* (1988, Gd 2)
VALD 2: Dy	Dy I, Dy II	105	BL	exp	[17] Biemont and Lowe (1993, Dy 2),
			KSc	exp	[51] Komarovskij and Smirnov (1994)
VALD 2: Ho 2	Ho II	4	K	exp	[48] Komarovskij (1991)
VALD 2: Er	Er I, Er II, Er III	427	KSb	exp	[50] Komarovskij and Smirnov (1993, Er1),
			K	exp	[48] Komarovskij (1991, Er 2),
			WBBC	calc	[112] Wyart *et al.* (1997, Er 3)
VALD 2: Tm	Tm I, Tm II	522	WLb	exp	[107] Wickliffe and Lawler (1997b)
VALD 2: Yb 1	Yb I	19	K	exp	[48] Komarovskij (1991)
VALD 2: Lu	Lu I, Lu II	31	K	exp	[48] Komarovskij (1991, Lu 1),
			BCM	calc	[26] Bord *et al.* (1998, Lu 2),
			DCWL	exp	[35] Den Hartog *et al.* (1998, Lu 2)
VALD 2: Re 2	Re II	1	WJL	exp	[102] Wahlgren *et al.* (1997)
VALD 2: Pt	Pt I, Pt II, Pt III	799	WLJ	calc	[103] Wahlgren *et al.* (1995, Pt 1),
			WB	calc	[111] Wyart and Blaise (1995, Pt 2),
			DSJ	ast	[36] Dworetsky *et al.* (1984, Pt 2),
			RWJ	calc	[95] Ryabtsev *et al.* (1993, Pt 3)
VALD 2: Au	Au II, Au III	672	RW	calc	[89] Rosberg and Wyart (1997, Au 2),
			WLJ	L+c	[103] Wahlgren *et al.* (1995, Au 2, LIF & calc)
			WJT	calc	[113] Wyart *et al.* (1996, Au 3)
VALD 2: Hg 3	Hg III	42	URJ	calc	[99] Uylings *et al.* (1993)
VALD 2: Pb 2	Pb II	37	AMa	exp	[1] Alonso-Medina (1996)
			AMb	exp	[2] Alonso-Medina (1997)

new Sc I and 25 new Sc II lines in addition to the NIST compilation [68]. Note that in the NIST compilation Sc I λ 5301.96 has a wrong wavelength (5302.98 Å).

Bizzarri *et al.* [18] measured transition probabilities for 100 Ti II lines in the λ 3050–10000 Å spectral region with an average accuracy of 0.04 dex. A comparison of these measurements with the astrophysical *gf*-values extracted from Ryabchikova *et al.* [90] shows a good correlation between both data sets, with a correlation coefficient of 0.995 and a dispersion of 0.08 dex. Slightly larger dispersion exists in the comparison between the Bizzarri *et al.* [18] data and the NIST compilation [68]. We combined the data from [18] and [90] to create a single replacement list for Ti II oscillator strengths. Furthermore, precise measurements from the Oxford group [20], corrected by +0.09 dex, as proposed by Bizzarri *et al.* [18], were added to this list, which finally contains 185 Ti II lines.

Transition probabilities for Ti III and Mn III were calculated by Raassen and Uylings [82] and Uylings and Raassen [100] who used the orthogonal operator description for odd and even energy levels. This method 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 [60]. Both data sets are included in VALD–2 with a higher ranking than the corresponding line lists of Kurucz [60].

New measurements of lifetimes and transition probabilities for V II were performed by Biémont *et al.* (BGF) [15] based on LIF lifetime measurements and emission branching fractions. They measured 147 lines, of which 85 are in common with the NIST compilation [68]. The NIST compilation mainly consists of the data from Karamatskos *et al.* [47]. Both groups, Karamatskos *et al.* and BGF, claim identical accuracies ($\leq$ 10%) in most of the cases. For VALD–2 we have preferred the BGF line list, because it contains more lines with accurate transition probabilities.

For the Cr II lines three new sets of measurements are available which form the basis for our Cr II replacement list in VALD–2: experimental transition probabilities by Pinnington *et al.* [77] and by Bergeson and Lawler [10], and astrophysical *gf*-values extracted from Sigut and Landstreet [98]. A comparison between [77] and [98] data shows a close correlation between both sources, which is again better than for the NIST data. The final replacement list for Cr II lines contains 69 entries.

Ekberg [37] analyzed a spectrum of doubly ionized chromium. 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 [30,31] codes Ekberg calculated transition probabilities for 1893 lines in the wavelength region from 736 Å to 2675 Å. A comparison of the new calculations with the semi-empirical data by Kurucz shows a large dispersion of ±3 dex, mainly for the lines with lower level excitation energy between 8 and 9 eV. Ekberg's calculations replace the Kurucz data in VALD–2, because they are based on a larger sample of observed energy levels.

3.2.2. *Iron*

Due to a special interest at this conference in the accuracy of Fe I and in particular of Fe II transition probabilities we give now a more detailed description of recent VALD input data for these species.

Specifically, new accurate measurements of the transition probabilities for neutral iron became available after the NIST compilation by Fuhr *et al.* [38] appeared. For the

optical region they are taken from O'Brian *et al.* [75], from Bard *et al.* [4] and from Bard and Kock [5]. We merged all three sets in one new VALD line list and averaged the 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 infrared [46,97]. For the lines of the new VALD replacement file we took wavelengths, energies and classifications – when available – from the Fe I multiplet tables of Nave *et al.* [74]. The final VALD–2 file consists of 2962 Fe I lines of which half have a $\log gf$ accuracy of about 10%.

Moreover, new measurements of transition probabilities have appeared for ionized iron since the publication of the NIST compilation [38]. Accurate LIF lifetime measurements with an uncertainty of better than 5% are available now for Fe II [14,40,41] which were used to transform high precision emission branching ratios to absolute transition probabilities. The most recent paper by Bergeson *et al.* (BMW) [11] describes 67 lines from the $3d^6(^5D)4p$ subconfiguration in the spectral region from 2249 to 2762 Å with all but four lines having an accuracy between 3 and 10%. Another work by Mullman *et al.* (MSL) [73] provides absolute absorption oscillator strengths with an accuracy better than 10% for seven vacuum UV Fe II lines between 1608 and 1640 Å.

We decided to use the BMW list as a reference for the comparison of different lists with Fe II transition probabilities which were provided by Bridges (B) [28], Whaling (W) [105], Kroll and Kock (KK) [53], and Pauls *et al.* (PGH) [76]. The last list has only two lines in common with BMW which agree within 12%, whereas the list of Bridges has three lines in common with BMW in agreement of better than 10%. The 46 lines which are common to both Whaling's and BMW's lists agree to within 12%; however, the $\log gf$-values from Whaling have an off-set of −0.04 dex relative to those in BMW's list. We therefore applied a correction of +0.04 dex to the entire Whaling-dataset. BMW and KK data have an overall agreement to within 10%, with no off-sets but a systematic dependence of the $\log gf$-difference on the oscillator strength value. This dependence contributes to the error budget of less than 25% for $-2.0 \leq \log gf \leq 0.5$.

In conclusion, we attribute the highest priority in the spectral region of 1600 to 3000 Å to the MSL and BMW data and 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.

Raassen and Uylings (RUa) [83] made new calculations of Fe II transition probabilities using the orthogonal operator approach for odd and even energy levels. This method allows better accuracy for the wave functions which leads to an order of magnitude better accuracy for the transition probabilities compared to the semi-empirical method used by Kurucz [58]. These new $\log gf$-values agree to better than ± 0.1 dex (see Fig.3 in [83]) with the BMW measurements. This success encouraged us to check other data, especially in the $\lambda \geq 3000$ Å spectral region, with the RUa calculations.

The main references for Fe II oscillator strengths for $\lambda \geq$ 3000 Å are: Bridges (B) [28], Baschek *et al.* (BGHR) [6] corrected by +0.16 according to [38], Whaling (W) [105], Hannaford *et al.* (HLGN) [41], Kroll and Kock (KK) [53], Heise and Kock (HK) [43], Pauls *et al.* (PGH) [76], and Blackwell *et al.* (BSS) [21]. The HK and PGH data were slightly corrected to fit the best lifetime measurements by HLGN. The solar oscillator strengths obtained by BSS have a good relative accuracy, but they were based on a solar iron abundance of log(Fe/H) = –4.31. Presently, the best estimate is log(Fe/H) = –4.50 (see, for example, HLGN), therefore we applied a +0.19 dex correction to the BSS oscillator strengths.

Table III lists the comparison between the RUa calculations and some of the line lists mentioned above. Evidently, in the $\lambda \geq 3000$ Å spectral region practically all measurements produce higher gf-values than the best calculations, while this is not the case for shorter wavelengths. This explains the higher solar iron abundance of log(Fe/H) = –4.41 obtained by RUa from Fe II lines in the 4100 – 7720Å spectral region, compared to log(Fe/H) = –4.50 derived from the same set of lines using experimental data [41].

In Fig. 2 we compare four experimental data sets with the RUa calculations as a function of wavelength. Only the KK data produce a significant trend with λ which again justifies the lower priority given by us to this data set.

In total we find 84 lines in the 3000–7712 Å spectral region with oscillator strengths having an accuracy of 25% or better. For roughly half of them the oscillator strengths were averaged using two to four different sources, and they may be considered as reliable.

We corrected oscillator strengths for the forbidden ($\Delta S = 2$) transitions of Fe II in all multiplets that include the $w^2P_{3/2}$ and $x^6P_{3/2}$ levels, following Johansson *et al.* [44]. They showed that the observed anomaly originates from an indirect mixing of the above mentioned levels. We also included new oscillator strengths for 222 lines of the 4f-5g supermultiplet of Fe II calculated with the Cowan code [88], 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.* [16]. Hence, we finally included data for 522 lines of Fe II in the new Fe line list created for VALD–2.

3.2.3. *Co and Ni*

Accurate transition probabilities for 15 Co I lines (Lawler *et al.* [66]) and for 89 Co II lines [96,34], and [72] (abbreviated as SLW, CUNJ, and MCL) are included in VALD–2. Most of them are based on LIF lifetime measurements and on emission branching ratios. They have an accuracy of 10–12%. A comparison shows that the SLW and CUNJ data agree within 10% for lines with $\log gf > -1.0$. Therefore we

Table III. *Off-sets of log* gf *values for Fe II lines for experimental data relative to RUa [83] calculations.*

Reference	Wavelength region	N	Δ	σ
W – RUa	2900 – 4930	14	0.08	0.09
KK – RUa	2880 – 5330	43	0.15	0.15
B – RUa	3180 – 5020	10	0.12	0.08
PGH – RUa	3170 – 7520	14	0.05	0.12
BSS – RUa	4170 – 7720	32	0.19	0.08
BGHR – RUa	4500 – 5000	13	0.13	0.08

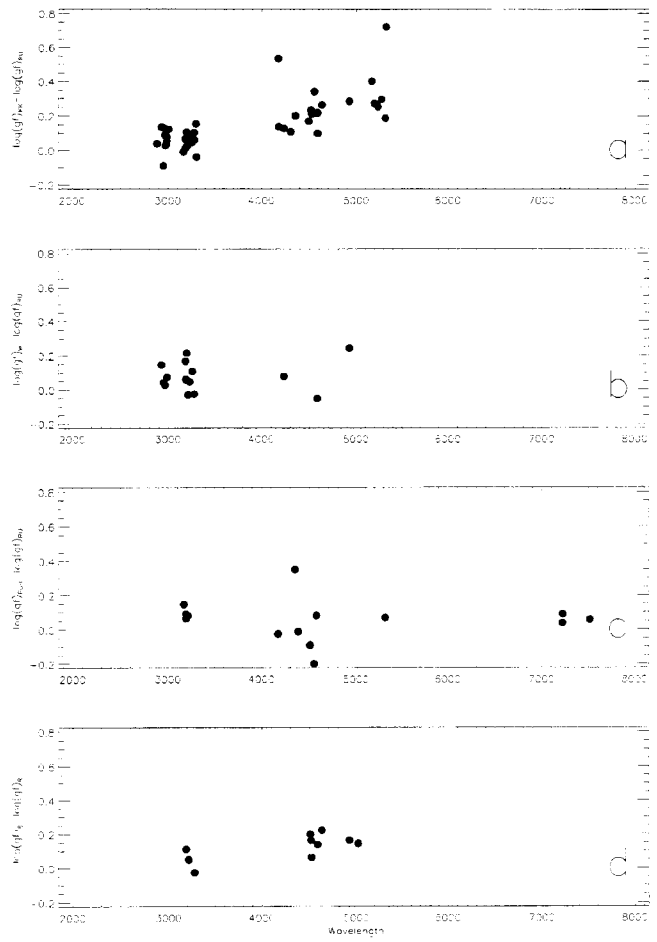

Fig. 2. A comparison between Fe II oscillator strengths calculated by Raassen & Uylings [83] and measurements by Kroll and Kock [53] (a), by Whaling [105] (b), by Pauls *et al.* [76] (c), and by Bridges [28] (d) as a function of wavelength.

compiled the averaged data for these lines in a new line list for VALD–2, together with the MCL data to which we give the highest priority. For the weaker lines the CUNJ data are systematically higher by 0.22 dex than the SLW gf-values. A comparison of all three data sets with the best calculations made for Co II by Raassen *et al.* (RPU) [81] showed that for weaker lines the SLW data agree better with the calculations, and we prefer to use them in VALD–2. 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. A comparison of the data compiled in the VALD–2 line list with the RPU calculations is shown in Fig. 3.

In turn, new input data for Ni I were created from two new sets of experimental measurements. Blackwell *et al.* [19] 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.* [7,8]. Wickliffe and Lawler (WLa) [106] reported transition probabilities for 76 lines. 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 measurements by Blackwell *et al.* [19] of about 5%. The same accuracy is reported for most lines from WLa. Thus, both lists com-

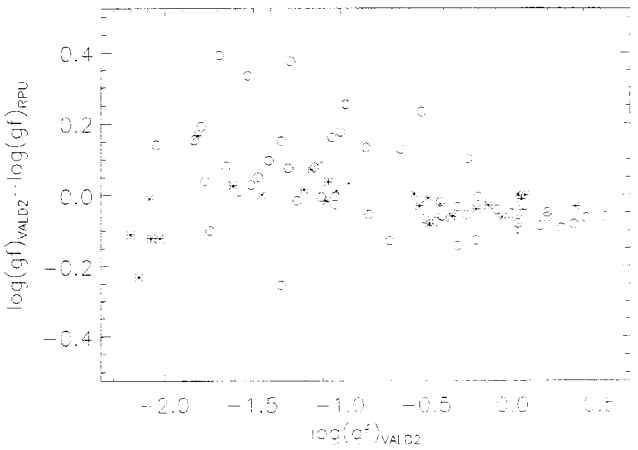

Fig. 3. A comparison between Co II oscillator strengths calculated by Raassen et al. [81] and the VALD–2 compilation. Data from Mullman et al. [72] are shown by asterisks.

bined give a total number of 151 lines with accurate transition probabilities which we included in VALD–2 with a higher ranking than previous data from NIST and Kurucz' GFIRON line lists (cf. Table II).

3.3. *Elements of the Fourth and Fifth periods*

The data for Cu II originally included in VALD were entirely taken from the BELLHEAVY line list [59] and date back to the compilation of Kurucz and Peytremann [61]. In the meantime, experimental absolute transition probabilities were derived by Kono and Hattori [52] and by Crespo López-Urritia *et al.* [33]. Their results agree within the expected errors. Thus, we merged them into a new list for Cu II after averaging oscillator strengths for those lines found in both publications. The final list contains data for 71 spectral lines with an accuracy for the $\log gf$-values of the order of 15–25%. Previous and new VALD data agree within 25%, without any shift in absolute scales. We recommend to use the new data, because they have individual error estimates.

As an example for our interest in compilations for specific (even single) transitions we mention the inclusion of $\log gf$-values from new absolute transition probabilities for 2 resonance lines of Zn II at 2025.5 Å and 2062.0 Å which were measured by Bergeson & Lawler [10]. The accuracy of the new data is 7%. The new oscillator strengths are higher by 0.08 dex than previous data available from BELLHEAVY [59].

The inclusion of data on the third spectra of "intermediate" and "heavy" elements has always been an important goal of the VALD team, in particular, as the data base was originally created to facilitate the study of chemically peculiar (CP) stars for which the second ionization stage frequently corresponds to the dominant species. For example, there was no information available on the second ions for any of the elements of the Sr-Y-Zr group in the BELLHEAVY lists. However, transition probabilities for the most prominent lines of Y III and Zr III were calculated by Redfors [87] using the Cowan code with estimated uncertainties of about 10%. Maniak *et al.* [67] measured the lifetimes of five levels of Y III which were converted to oscillator strengths using their theoretical calcu-

lations 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 [87]. Thus, 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 [67] and supplemented by the data from [87]. Later, Reader and Acquista [84] measured and classified 482 Zr III spectral lines in the 630–4610 Å region. The [84] line list for Zr III has 75 lines in common with the list of [87]. A comparison between both sets of data shows that with a few exceptions most of the lines agree within 10–15%. Again we used the data from Reader and Acquista [84] and just supplemented them by those from Redfors [87]. The final set contains 493 Zr III lines.

Due to the work of Wickliffe *et al.* [108] and Johansson *et al.* [45] it was possbile to include a new list with 502 lines of Ru I and Ru II into VALD–2. Also, the line data on Xe II available in VALD–1 could be improved using the energy level classification of Hansen and Persson [42]. Details are given by Kupka *et al.* [55] while for a description of the data on Ga II and Xe II in VALD we also refer to Piskunov *et al.* [79].

3.4. *Rare earth elements (REE)*

In the first version of VALD the data for neutral atoms and the first ions of REE were mainly based on the BELLHEAVY list and supplemented for some of the first ions with experimental data from Komarovskij [48]. BELLHEAVY contains oscillator strengths based on different calibrations of intensities published by Meggers *et al.* [70] which are known to be quite incomplete. In Fig. 4 we reproduce the spectrum of the roAp star HD 24712 (Ryabchikova *et al.* [91]) in a small, but for normal stars well studied spectral region. Even here we find a few unidentifiable lines which most likely belong to the first or second REE ions, because their intensity variations are in phase with the intensity variations of identified REE lines. The number of unidentified features in the spectra of Ap stars increases towards the red region as well as in the UV.

Due to the enormous number of spectral lines of rare earth elements they can contribute substantially to the line opacities of cool CP2 stars. Especially the lines of the second ions may be important, because they dominate in the atmospheres of chemically peculiar stars with $T_{\rm eff}$ = 7500 – 8500 K. The missing opacities lead to incorrect upper atmospheric structures for cool Ap stars and influence the boundary for roAp star pulsation models (Audard *et al.* [3]). Recent experimental measurements of the oscillator strengths for Tm I and Tm II published by Wickliffe and Lawler [107] for the 2500 – 10000 Å spectral region increase significantly the data on Tm available within VALD by 241 Tm I and by 30 Tm II lines. This clearly demonstrates the need for new measurements and/or calculations of atomic data for lines of the first three ionization stages of REE. It was shown by Quinet *et al.* (this conference) that the Cowan code may provide fairly accurate data for singly ionized REE which are sufficient for opacity calculations, while more accurate experimental data, including isotopic and hyperfine structure, are needed for the lines used in abundance analyses.

VALD provides *gf*-data for Ce III, Nd III, Eu III, and Er III which previously were not included in any data base. Ce III and Nd III oscillator strengths were calculated by Bord *et al.* [27] and by Cowley and Bord [32] using the atomic structure code of Cowan. The estimated relative accuracy of the calculations is within ±0.15 dex, the absolute scale may be systematically too large by 0.25 dex. Oscillator strengths for 304 Er III lines were calculated by Wyart *et al.* [112] using again the Cowan code. Spectra of cool Ap stars (Ryabchikova *et al.* [92]) allowed to estimate *gf*-values of four Eu III lines, which illustrates the potential of this

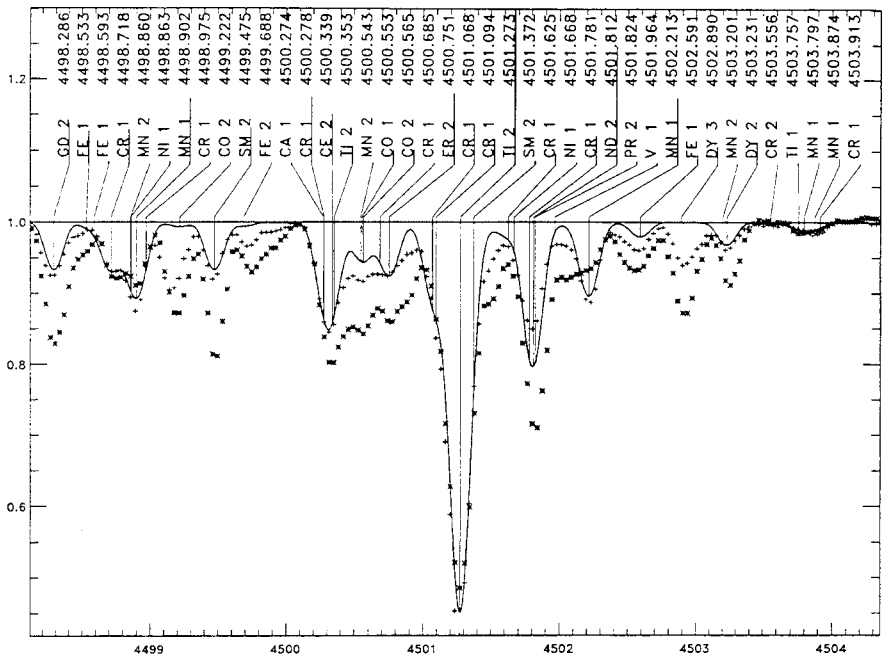

Fig. 4. Comparison of two spectra of HD 24712 taken at phase 0.551 (pluses, magnetic minimum) and at phase 0.952 (asterisks, magnetic maximum). The synthetic spectrum is shown as a solid line.

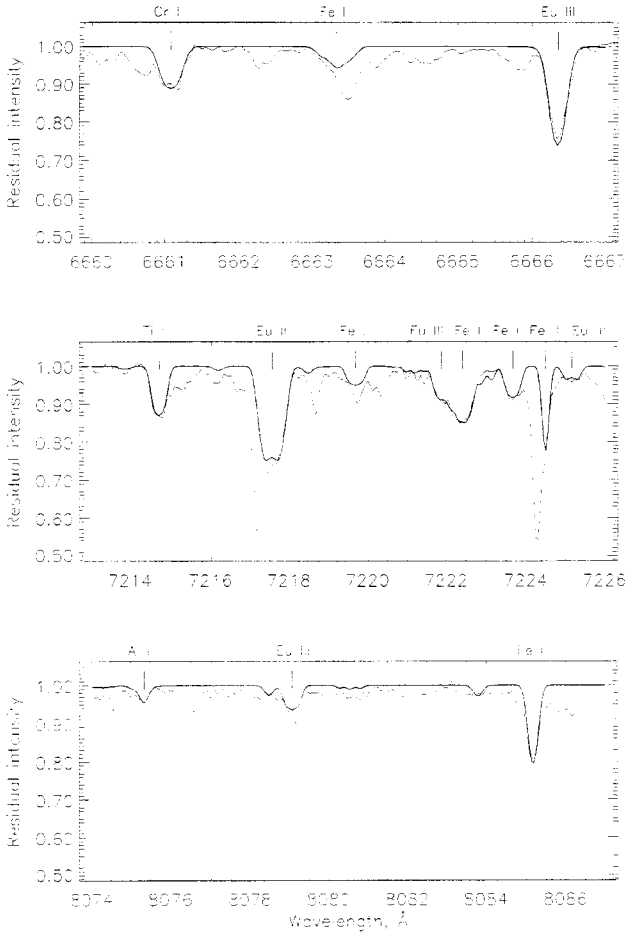

Fig. 5. A comparison between observations (thin line) and synthesized lines of Eu II, Eu III, Al I, Ti II, Cr I, Fe I, and Fe II (thick line) in the spectrum of β CrB. A few additional strong and narrow telluric lines are seen in the spectrum.

group of stars for astrophysical determinations of oscillator strengths for the lines of REE ions. However, horizontal and possibly vertical inhomogeneities in Ap star atmospheres can cause problems for such procedures. Fig. 5 shows sections of the spectrum of the cool Ap star β CrB with newly identified Eu III lines.

The relative accuracy of the *gf*-values for Eu III lines is within ± 0.2 dex, but the absolute values are less well known, because the astrophysical determination depends on the ionization balance in real stellar atmospheres.

It was stressed again in this conference by Wahlgren *et al.* [101] how hyperfine structure influences the abundances derived from REE lines. The Lu abundance obtained for a few roAp stars had to be decreased by about 1.0 dex after taking into account the hyperfine structure. These kind of considerations have to be included in future VALD releases to provide a possibility for a detailed abundance analysis of Ap star atmospheres.

Wherever possible, line lists for RE elements are now supplemented by experimental Landé factors taken from Blaise and Wyart ([22] – Nd II lines), from Ginibre ([39] – Pr II lines), and from Martin *et al.* ([69] – NIST atomic line database, AEL section for other REE). Detailed information on the sources of *gf*-data for rare-earth elements is given in Table II and in [55].

3.5. *Heavy elements (with $Z > 71$)*

One of the most important inputs in VALD–2 was the Pt-Au-Hg sequence of elements. For the first time users get the possibility to extract oscillator strengths of the lines of these elements in three ionization stages, which is important in abundance analyses of HgMn stars. Calculations of the transition probabilities for Pt I lines in the 1730 Å to 2540 Å spectral region were carried out by Wahlgren *et al.* [101]. For the Pt II lines we used calculations by Wyart and Blaise [111] who also provided theoretical Landé factors for the odd energy levels. These data were supplemented by astrophysical *gf*-values from Dworetsky *et al.* [36]. Ryabtsev *et al.* [95] published theoretical transition probabilities for 666 lines of Pt III in the range of 559 Å to 2020 Å. 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.* [103]).

As for 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. We included in VALD–2 new measurements of the oscillator strength for the Au II 1740 Å line (Wahlgren *et al.* [103]) and calculations for 497 Au II lines by Rosberg and Wyart [89]. Wyart *et al.* [112] identified more than 1000 lines of Au III and calculated transition probabilities for 175 of them in the 800 Å to 2000 Å spectral region.

We corrected wavelengths of Hg II lines contained in VALD–1 according to the measurements by Reader and Sansonetti [86] made for the terrestrial mixture of Hg isotopes. A new line list for Hg III consists of oscillator strengths calculated for 42 spectral lines by Uylings *et al.* [99].

We also increased the existing list for Pb II from 11 to 37 spectral lines. The corresponding experimental measurements were taken from Alonso-Medina [1,2]. Atomic energy levels and experimental Landé factors were taken from Moore [71]. For a more detailed description of the new data on heavy elements included into the second release of VALD we refer again to [55].

4. Access to VALD

VALD Electronic Mail Service (**VALD–EMS**) is the main interface for accessing VALD by external users. It 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 species in a given spectral window
EXTRACT STELLAR	extracts all spectral lines (with best parameters) which produce significant absorption in an atmosphere with given $T_{\rm eff}$ and log g.

The volume of information to be extracted is defined by the following options (except for SHOW LINE):

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	... with Stark damping constant;
HAVE WAALS	... with van der Waals damp. con.;
HAVE LANDÉ	... with Landé factor;
HAVE TERM	... with term designations.

Multiple options can be combined in arbitrary sequence. The options for personal configuration and for the selective inclusion of only those data which satisfy certain criteria are now available also for VALD–EMS users.

On top of the VALD–EMS (see also Piskunov *et al.* [79] for more details and Kupka *et al.* [55] for recent improvements), a World–Wide–Web interface was developed at Uppsala Astronomical Observatory. However, for both interfaces registration is required to obtain full access. To do so an e-mail message has to be sent to the VALD manager at the address:

VALDADM@ASTRO.UNIVIE.AC.AT

including the full name and the e-mail address(es) at which one intends to receive data requested from VALD.

Furthermore, a manual and tutorial to the registration procedure is available at:

HTTP://WWW.ASTRO.UU.SE/~VALD

HTTP://WWW.ASTRO.UNIVIE.AC.AT/~VALD

Serving more than 200 users all over the world – and their number is continuously rising – VALD became an increasingly used service offered to the community by a team consisting of volunteers. Creation of mirror sites is a logical way to distribute the work load and reduce response time. Two VALD mirror sites became operational in 1998: Uppsala Astronomical Observatory (VALD@ASTRO.UU.SE) and the Astrophysics Data Facility at NASA Goddard Space Flight Center (VALD@HYPATIA.GSFC.NASA.GOV). Synchronization is performed twice a day which means that within less than a day a new client will have EMS access to all VALD sites. Besides distributing the workload this also enhances the availability of the data base for the user community.

5. Conclusions

We have developed a data base of transition parameters of astrophysical interest. Today it includes over 600 000 atomic lines with (mostly) good quality experimental or theoretical oscillator strengths and more than 40 million predicted transitions. New line lists with data of higher quality are continuously added to VALD. Data extraction from VALD is done according to a ranking of the different source lists included into the data base. The decision on a proper ranking is based on detailed comparisons between original data, in particular on error estimates available for individual transitions. In this report we mainly focussed on the oscillator strength data available for Fe I and Fe II, which have been of special interest at this conference, and we partially covered improvements for Co and rare earth elements while a survey was provided for the most recent improvements for other species. To accommodate ever increasing amounts of data they are stored in efficiently compressed format allowing future expansion and quick access to specific wavelength regions and elements. Multiple extraction tools allow data selection and merging according to typical astrophysical applications, e.g. spectrum synthesis or model atmosphere calculations. The data base can be accessed locally or remotely via e-mail or the new WWW interface. The main site in Vienna and two mirror sites in Uppsala and at Goddard Space Flight Center are offering VALD services for free. The change to the new internal format (VALD-3 format) opens the way to future inclusions of the most reliable lists of molecular lines.

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