A comparative analysis of the laboratory and theoretical transition probabilities of the Fe-peak elements for a new release of VALD

T Ryabchikova¹, R Kildiyarova², N Piskunov³, U Heiter³, L Fossati⁴ and W W Weiss⁴

¹Institute of Astronomy RAS, Moscow, Russia
²Institute of Spectroscopy RAS, Troitsk, Russia
³Department of Astronomy and Space Physics, Uppsala University, Uppsala, Sweden
⁴Department of Astronomy, Vienna University, Vienna, Austria

E-mail: ryabchik@inasan.ru

Abstract. We carried out a comparative analysis of the recent atomic data for iron-peak elements, mainly Ti, Cr and Fe, for a new release of the Vienna Atomic Line Database (VALD3). New data were compared with those available in VALD2 and were checked using high-resolution, high signal-to-noise spectra of sharp-lined chemically normal stars including the Sun, and the zero-rotation extremely Cr- and Fe-rich chemically peculiar star HD 133792. The observed spectrum of the latter star allowed for comparison with transition probability calculations based on the orthogonal operator technique with the Cowan code for Cr II and Fe II lines for lower level energies between 2 eV and 11 eV in the wavelength region 3100 to 9000 Å.

In general, the agreement between the new experimental transition probabilities and those currently available in VALD2 is fairly good, which helps to validate the stellar abundance data derived with the VALD2 atomic parameters. We also found that, for a few important Ti II and Fe II lines in the visible spectral region, new transition probabilities are not consistent within their quoted accuracy.

In a series of recent works on experimental f-values for Fe II it was shown that calculations based on the orthogonal operator technique agree better with the experimental data than the Cowan code calculations and, hence, should have preference for stellar spectroscopy. Our analysis of the Ap star HD 133792 spectrum clearly demonstrates that there are quite a number of high-excitation Cr II and Fe II lines which are fitted reasonably well when using the transition probabilities calculated with the Cowan code. As a rule these lines have their upper energy levels classified differently in both methods of calculations.

1. Introduction
Recent major improvements in the quality of spectroscopic observations stimulated a surge of interest in detailed model atmosphere and chemical abundance studies. Modern spectrographs, such as Ultraviolet-Visible Echelle Spectrograph (UVES) at the European Southern Observatory 8 m Very Large Telescope (VLT), can provide high signal-to-noise ratio (S/N>300) and high resolving power (R=80 000 – 100 000) spectra of rather faint stars. Availability of new observational material has to be matched by the corresponding development of new analysis techniques, capable of handling large spectral regions and a large number of lines without
compromising accuracy. This task cannot be achieved without an extensive production of accurate atomic data.

Since the latest release of the Vienna Atomic Line Database (VALD2 - [1]), new experimental data for the iron-peak elements have been published. Also, calculations have been continuously improving (Raassen & Uylings orthogonal operator calculations [2] – http://www.wins.uva.nl/pub/orth; Kurucz calculations – http://cfaku5.cfa.harvard.edu/ATOMS), providing stellar spectroscopists with more numerous atomic data that are necessary for spectral synthesis. Here we present a comparative analysis of the recently published transition probabilities for the iron-peak elements (neutral atoms and first ions), and we compare them with the data already included in VALD as well as with results from calculations. We analyse the accuracy of some sets of experimental data using spectra obtained from UVES and ESPaDOnS (Echelle SpectroPolarimetric Device for Observation of Stars, mounted at the Canada-France-Hawaii-Telescope (CFHT)) of the chemically normal slow-rotating stars Procyon ($T_{\text{eff}}=6510$ K) and HD 73666 ($T_{\text{eff}}=9380$ K), and an Ap star HD 133792 ($T_{\text{eff}}=9400$ K) having extreme chromium and iron overabundances. We have also made use of the National Solar Observatory solar flux atlas [3].

2. Transition probabilities
2.1. Experimental data
We present here a listing of the publications having experimental transition probabilities which have been analysed in our study and are planned to be included into the next release of the VALD (VALD3).

Ca\textsc{i}

The list of the papers and a verification of the experimental data are given in [4], where non-local thermodynamic equilibrium (NLTE) analysis of Ca\textsc{i} and Ca\textsc{ii} line formation is performed.

\begin{align*}
\text{Ti\textsc{i}} & (92 \text{ lines from 3206 to 9723 }\AA) \\
& \underline{\text{NWL}} – \text{Nitz et al. (1998) [5]} \\
\text{Ti\textsc{ii}} & (942 \text{ lines from 1865 to 5674 }\AA) \\
& \underline{\text{PTP}} – \text{Pickering et al. (2001a) [6]} \\
\text{Cr\textsc{i}} & (263 \text{ lines from 2726 to 9735 }\AA) \\
& \underline{\text{SLS}} – \text{Sobeck et al. (2007) [7]} \\
\text{Cr\textsc{ii}} & (119 \text{ lines from 2055 to 4850 }\AA) \\
& \underline{\text{NLLN}} – \text{Nilsson et al. (2006) [8]} \\
\text{Mn\textsc{ii}} & (187 \text{ lines from 1678 to 4810 }\AA) \\
& \underline{\text{KG}} – \text{Kling & Griesmann (2000) [9]} \\
& \underline{\text{KSG}} – \text{Kling et al. (2001) [10]} \\
\text{Fe\textsc{ii}} & (158 \text{ new lines from 1608 to 3500 }\AA \text{ and } 140 \text{ lines from 2249 to 7711 }\AA) \\
& \underline{\text{SSK}} – \text{Sikström et al. (1999) [11]} \\
& \underline{\text{KSJ}} – \text{Karlsson et al. (2001) [12]} \\
& \underline{\text{NSL}} – \text{Nilsson et al. (2000) [13]} \\
& \underline{\text{PJS}} – \text{Pickering et al. (2001b) [14]} \\
& \underline{\text{WBL}} – \text{Wiese et al. (2002) [15]} \\
& \underline{\text{PDN}} – \text{Pickering et al. (2002) [16]} \\
\end{align*}
2.2. Theoretically derived oscillator strengths
The following calculations were used in our comparative study. Both are included in the current VALD2 database.

- **RU** – calculations based on the orthogonal operator technique for Fe II ([20]) and Co II ([21]); also, Raassen & Uylings 1998, unpublished data for Cr II available at ftp://ftp.wins.uva.nl/pub/orth/chromium/
- **KuruczXX** – calculations using the Cowan code, where XX stands for the year of the calculations for a specific ion.

3. Comparison of experiment with calculations and stellar spectra

**Ti I**
84 out of 92 lines in VALD2 are from Kurucz88 calculations. The agreement on the absolute scale is encouraging and the new data set will certainly improve the accuracy of the titanium abundance determinations in late-type stars.

**Ti II**
692 lines from [6] have accuracy estimates. Comparison with the Kurucz99 calculations reveals a difference of more than |0.9| dex for 13 lines. Spectral synthesis made for Procyon and HD 133792 in the region 3100 to 5700 Å allows us to check the stated accuracy for nine out of 13 Ti II lines. For seven lines the fit to the observed stellar features confirms the quoted accuracy, while for the lines λλ3361.06, 3411.67 Å the experimental data are inconsistent with the observations (see Figure 1).

Also, for a few lines PTP gives the upper limits for transition probability, which are too small to fit the observed stellar lines (for example, A4589.95). New wavelength measurements by PTP provide a better fit to the Ti II lines observed in stellar spectra.

**Cr I**
Sobeck et al. (2007) [7] gives a detailed comparison of their experimental transition probabilities with other measurements. The accuracy of the [7] data is supported by the analysis of the solar spectrum in the visible spectral region. However, there is an indication that transition probabilities of the IR lines (longer than 9000 Å) may be underestimated.

**Cr II**
Nilsson et al. (2006) [8] derived experimental transition probabilities for 119 Cr II lines to an accuracy of 3 to 10 % for the strongest lines and 10 to 25 % for the weaker lines. Comparison of these experimental data with the calculations of RU and Kurucz88 show that of the two theoretical sets the RU values appear to differ the least from the experimental results. Synthetic spectrum calculations with new transition probabilities show that for three lines in the visible region, λλ4558, 4588 and 4592 Å, experimental transition probabilities may be slightly underestimated.

**Fe II**
Experimental transition probabilities for 158 new lines became available since 1999. Most of the lines lie in the ultraviolet region below 3000 Å. Schnabel et al. (2004) [17] provided improved absolute oscillator strengths in the spectral region between 2249 and 7711 Å. Comparison of the new experimental data with the calculations are shown in Figure 2. We also compare the
Figure 1. Comparison of the observed line profiles of Ti II 3411.67 Å (dots) with synthetic spectra calculated with the experimental log\((gf)\) from PTP (dashed line) and theoretical log\((gf)\) from Kurucz (solid line).

Experimental data from VALD2 with both sets of calculations. Figure 2 demonstrates that the RU calculations agree slightly better with the experimental results. It is worth noting that there are significant improvements in the Kurucz calculations compared with those from 1988 and 2003.

However, not all experimental values confirm the assigned accuracy. The largest deviation of the experimental data from the calculated is observed for the weak transitions in the ultraviolet region, but a few ‘outliers’ also exist in the visible spectral region, and our stellar spectra allow us to check the accuracy given for these particular lines. A comparison between synthetic spectra in the region of two ‘outliers’ (Fe II 5325, 5607 Å) with the observed stellar spectra is shown in Figure 3. For both lines as well as for Fe II 4173, an accuracy between 13 and 24 % is given in Schub but it is not confirmed by the observations.

4. Comparison between the two sets of theoretical calculations

In a series of recent works on experimental \(f\)-values for Fe II (see, for instance, [14]) it was shown that calculations based on the orthogonal operator technique (RU) agree better with the experimental data than did the Cowan code calculations (Kurucz) and, hence, should be used for stellar spectroscopy. Our comparisons (see Figure 2) generally support this conclusion. However, experimental data are available for the transitions having upper energy levels below 85 000 cm\(^{-1}\) (10.5 eV). According to Kurucz’s calculations, there are about 1000 spectral lines in the 4000 to 10 000 Å interval with lower energy levels above 80 000 cm\(^{-1}\) (10 eV) and with
Figure 2. Comparison of the experimental oscillator strengths for Fe\n\nlines with the theoretical calculations by RU (upper panel) and Kurucz07 (lower panel).

$\log(gf) > -1.1$. The same is valid for Cr\n
Most of the high-excitation lines are not observed in spectra of normal stars, but all of them may be detected in spectra of CrFe-rich chemically peculiar stars. We have observations of one of these stars, HD 133792, with large atmospheric overabundances of iron and, in particular, chromium. HD 133792 has almost zero rotation and a very weak magnetic field, which helps to minimize the effects of blending. The spectrum of this star was used to compare the RU and Kurucz07 theoretical transition probabilities for Cr\n
and Fe\n
While the RU transition probabilities are better than the Kurucz07 values for the transitions with low or intermediate excitation energies, our analysis of the Ap star HD 133792 spectrum shows that there are quite a number of high-excitation Cr\n
and Fe\n
lines which are fitted reasonably well only when using the transition probabilities calculated with the Cowan code. As a rule these lines have their upper energy levels classified differently in both methods and number of calculations. According to our comparative analysis of the RU and Kurucz Cr\n
and Fe\n
linelists, 50 and 67 levels, respectively, have different configurations and/or term classifications. This difference is probably caused by the strong level mixing. The Cowan code appears to treat these better than the orthogonal operator technique.
Figure 3. Comparison of the observed line profile of Fe II $\lambda$5325 Å (upper panels) and of Fe II $\lambda$5607 Å (lower panels) with calculations utilizing the experimental log($gf$) values from Schnb (dashed line) and the theoretical log($gf$) values from RU (solid line). Observations are shown by dots.
Acknowledgments
Our work was financially supported by the Swedish Royal Academy of Sciences (grant No. 11630102), the Russian Foundation for Basic Research (grant No. 06-02-16110a), and the Austrian Science Fund (FWF-P17580).

References
[1] Kupka F, Piskunov N, Ryabchikova T, Stempels H C and Weiss W W 1999, A\&AS 138 119
[2] Uylings P H M and Raassen A J J 1995 J Phys B 28 L209
[3] Kurucz R L, Furenlid I, Brault J and Testerman L 1984, NSO Atlas No. 1: Solar Flux Atlas from 296 to 1300 nm, Sunspot, NSO
[4] Mashonkina L, Korn A J and Przybilla N 2007 A&A 461 261
[5] Nitz D E, Wickliffe M E and Lawler J E 1998 ApJS 117 313
[6] Pickering J C, A. P. Thorne A P and Perez R 2001a ApJS 132 403
[7] Sobeck J S, Lawler J E and Sweden C 2007 ApJ 667 1267
[8] Nilsson H, Ljung G, Lundberg H and Nielsen K E 2006 A&A 445 1165
[9] Kling R and Griesmann U 2000 ApJ 531 1173
[10] Kling R, Schnabel R and Griesmann U 2001 ApJS 134 173
[11] Sikström C M, Schultz-Johanning M, Kock M, Li Z S, Nilsson H, Johansson S, Lundberg H and Raassen A J J 1999, J Phys B 32 5687
[12] Karlsson H, Sikström C M, Johansson S, Li Z S and Lundberg H 2001 A&A 371 360
[13] Nilsson H., Sikström C M, Li Z S, Lundberg H, Raassen A J J, Johansson S, Leckrone D S and Svanberg S 2000 A&A 362 410
[14] Pickering J C, Johansson S and Smith P L 2001b A&A 377 361
[15] Wiese L M, Bonvallet G A and Lawler J E 2002 ApJ 569 1032
[16] Pickering J C, Donelly M P, Nilsson H, Hibbert A and Johansson S 2002, A&A 396 715
[17] Schnabel R, Schultz-Johanning M and Kock M 2004, A&A 414 1169
[18] Fedchak J A and Lawler J E 1999 ApJ 523 734
[19] Fedchak J A, Wiese L M and Lawler J E 2000 ApJ 538 773
[20] Raassen A J J and Uylings P H M 1998 A&A 340 300
[21] Raassen A J J, Pickering J C and Uylings P H M 1998 A&AS 130 541