A comparative analysis of the laboratory and theoretical transition probabilities of the Fe-peak elements for a new release of VALD based on high-resolution high S/N stellar spectra

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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 UVES at the 8-m ESO VLT , can provide S/N>300, R=80,000-100,000 wide spectral coverage echelle spectra of moderately 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 large number of lines without compromising accuracy. This task cannot be achieved without a corresponding development of the laboratory and theoretical spectroscopy which should provide stellar spectroscopists with the accurate atomic data.

Since the last release of the ***Vienna Atomic Line Database*** (VALD2) in 1999 new experimental data for the Fe-peak elements were published. Also, theoretical calculations have been continually improving (Raassen & Uylings orthogonal operator calculations - http://www.wins.uva.nl/pub/orth, henceforth RU; Kurucz calculations - ***http://cfaku5.cfa.harvard.edu/ATOMS/***) providing stellar spectroscopists with the less accurate but much more numerous atomic data necessary for spectral synthesis.

Here we present a comparative analysis of the recently published transition probabilities for the Fe-peak elements (neutral atoms and first ions), and compare them with the data already included in VALD as well as with the theoretical calculations. We also analyse an accuracy of some sets of experimental data using UVES and ESPaDOnS spectra of the normal slow-rotating stars Procyon (T_{eff}=6510 K), HD 73666 (T_{eff}=9380 K), and Ap star HD 133792 (T_{eff}=9400 K) with extreme Cr and Fe overabundances. We also used the NSO solar flux atlas.

Experimental transition probabilities

Here is a list of the publications with the experimental transition probablities analysed in our study and planned to be included to the next release of the ***Vienna Atomic Line Database*** (VALD3).

Ca I
The list of the papers and a verification of the experimental data are published in L. Mashonkina et al. 'A non-LTE study of neutral and singly-ionized calcium in late-type stars'. 2007, A&A 461, 261-275

Ti I (92 lines in 3206 – 9723 A spectral region)
D. E. Nitz, M. E. Wickliffe, & J. E. Lawler. 1998, ApJS 117, 313-317

Ti II (942 lines in 1865 – 5674 spectral region)
J. C. Pickering, A. P. Thorne, & R. Perez. 2001, ApJS 132, 403-409 (IC)

Cr I (263 lines in 2726 – 9735 A spectral region)
J.S. Sobeck, J.E. Lawler, & C. Sneden. 2007, ApJ preprint doi: 10.1086/'519987

Cr II (119 lines in 2055 – 4850 A spectral region)
H. Nilsson, G. Ljung, H. Lundberg,K. E. Nielsen. 2006, A&A 445, 1165–1168 (Lund)

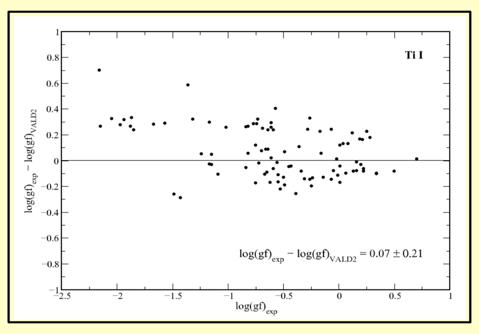
Mn II (187 lines in 1678 – 4810 A spectral region)
R. Kling, U. Griesmann. 2000, ApJ 531, 1173-1178
R. Kling, R. Schnabel, U.Griesmann . 2001, ApJS 134, 173-178

Fe II (158 new lines in 1608 – 3500 A spectral region + 140 improved (Schnabel et al.) in 2249-7711)
C.M. Sikström, M. Schultz-Johanning, M. Kock, Z.S. Li, Nilsson, S. Johansson, H. Lundberg, & A.J.J. Raassen. 1999, J. Phys. B32, 5687-5698 (SSK)
H. Karlsson, C.M. Sikström, S. Johansson, Z.S. Li, & H. Lundberg. 2001, A&A 371, 360-365 (KSJ)
H. Nilsson, C.M. Sikström, Z.S. Li, H. Lundberg, A.J.J. Raassen, S. Johansson, D.S. Leckrone, & S. Svanberg. 2000, A&A 362, 410-418 (NSL)
J.C. Pickering, S. Johansson, & P.L. Smith. 2001, A&A 377, 361-367 (PJS)
L.M. Wiese, G.A. Bonvallet, & J.E. Lawler. J.E. 2002, ApJ, 569, 1032-1036
J.C. Pickering, M.P. Donelly , H. Nilsson, A. Hibbert, & S. Johansson. 2002, A&A 396, 715-722 (PDN)
R. Schnabel, M. Schultz-Johanning, & M. Kock. 2004, A&A 414, 1169-1176 (Schnb)

Ni II (63 lines in 1454 – 2545 A spectral region)
J. A. Fedchak, & J. E. Lawler. 1999, ApJ 523, 734-738
J. A. Fedchak, L.M. Wiese, J. E. Lawler. 2000, ApJ 538, 773-776

Comparison with the theoretical calculations and with stellar spectra

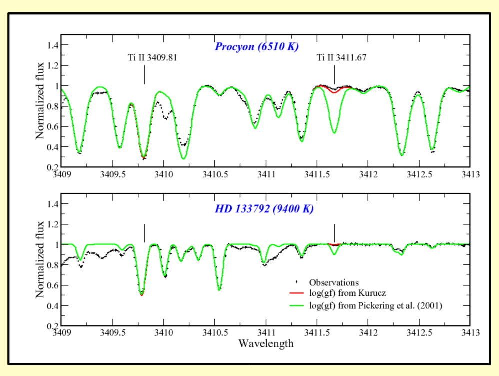
Fig.1



Ti I

Fig.1 shows a comparison between the new experimental data and the current VALD2 data for Ti I. 84 out of 92 lines in VALD2 are from Kurucz88 calculations. An agreement in the absolute scales is encouraging and new data set will certainly improve an accuracy of the Ti abundance determinations in late-type stars.

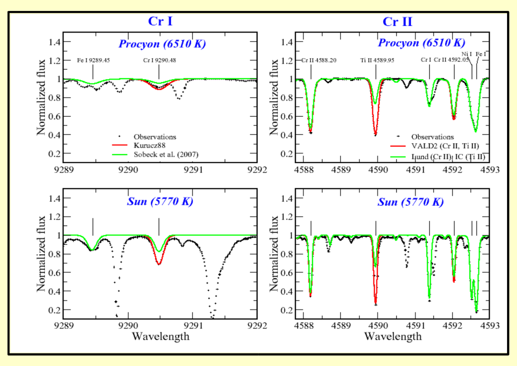
Fig.2



Ti II

692 lines from Pickering et al. (2001 – IC) list have an accuracy estimates. Comparison with the Kurucz (1999) calculations reaveals a difference above |0.9| dex for 13 lines. Spectral synthesis made for Procyon and HD 133792 in 3100-5700 A allows to check a given accuracy for 9 out of 13 Ti II lines. For 7 lines the fit to the observed stellar features confirms the quoted accuracy, while for 2 lines (see an example in Fig.2) experimental data are inconsistent with the observations. Also for a few lines IC gives the upper limits for log(gf), which are too small to fit the observed stellar lines (see an example of 4589 line in Fig.3 - right panels).
New wavelength measurements fit better to the Ti II lines observed in stellar spectra.

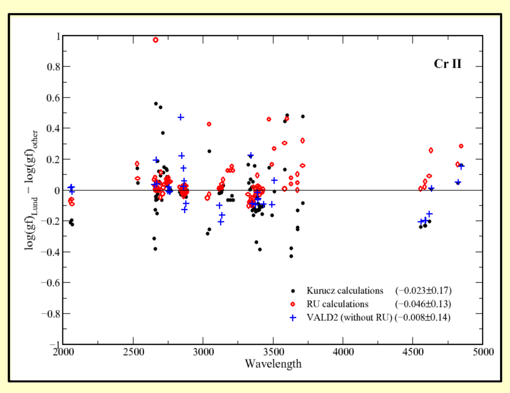
Fig.3



Cr I

Sobeck et al. (2007) gives a detailed comparison of their experimental transition probabilities with the other measurements. The accuracy of Sobeck et al. data is supported by the analysis of the solar spectrum in visible spectral region. However, there is an indication that transition probabilities of the IR lines (longer than 9000 A) may be underestimated (Fig.3 - left panels).

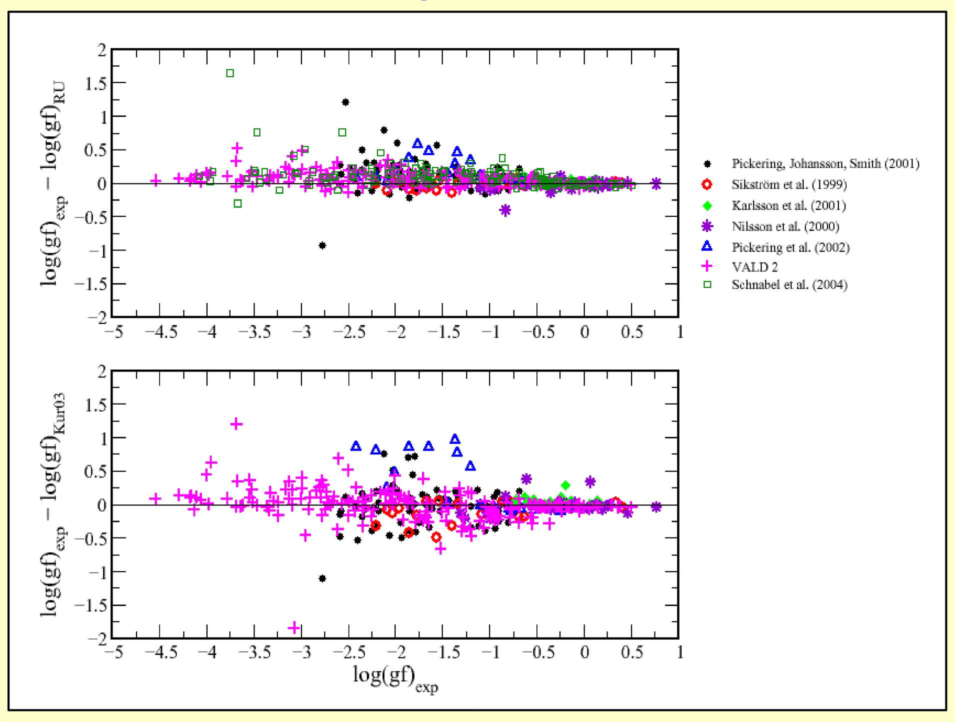
Fig.4



Cr II

Nilsson et al. (2006 – Lund) derived experimental transition probabilities for 119 Cr II lines with the accuracy 3-10 % for the strongest lines and 10-25 % for the weaker lines. Comparison of these experimental data with the theoretical calculations by RU and by Kurucz88 as well as with the data included in VALD2 (besides RU) is given in Fig.4. Of two theoretical sets RU values appear to differ the least from the experimental results. Synthetic spectrum calculations with new log(gf)'s show that for 3 lines in the visible region, 4558, 4588 and 4592 experimental transition probablities may be slightly underestimated (see Fig.3 – left panels).

Fig.5



Fe II

Experimental transition probabilities for 158 new lines became available since 1999. Most of the lines are lying in the ultraviolet region below 3000 A. Schnabel et al. (2004 – Schnb) provided improved absolute oscillator strengths from 2249 to 7711 A. Comparison of the new experimental data with the theoretical calculations are shown in Fig.5 (RU – top; Kurucz2003 – bottom). We also compare the currently used experimental data from VALD2 with both sets of calculations. Figure 5 demonstrates that RU theoretical calulations agree better with the experimental results. However, not all experimental values correspond to the given accuracy. Figure 6 shows a comparison between the experimental data and RU calculations as a function of the wavelength. The greatest deviation of the experimental data from the calculated ones is observed for the weak transitions in UV region, but a few 'outliers' exist in the visible spectral region, too, and our stellar spectra allow to check the accuracy given for these particular lines.

Fig.6

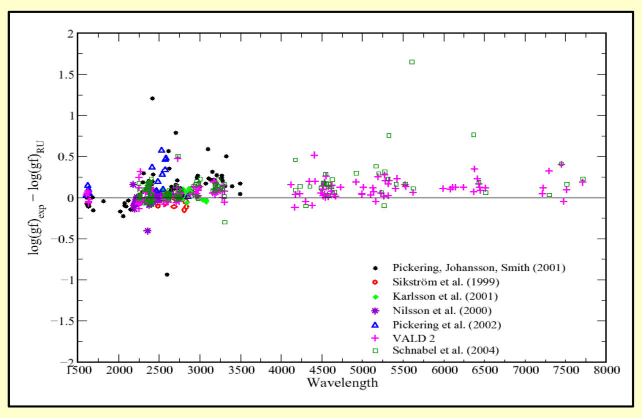
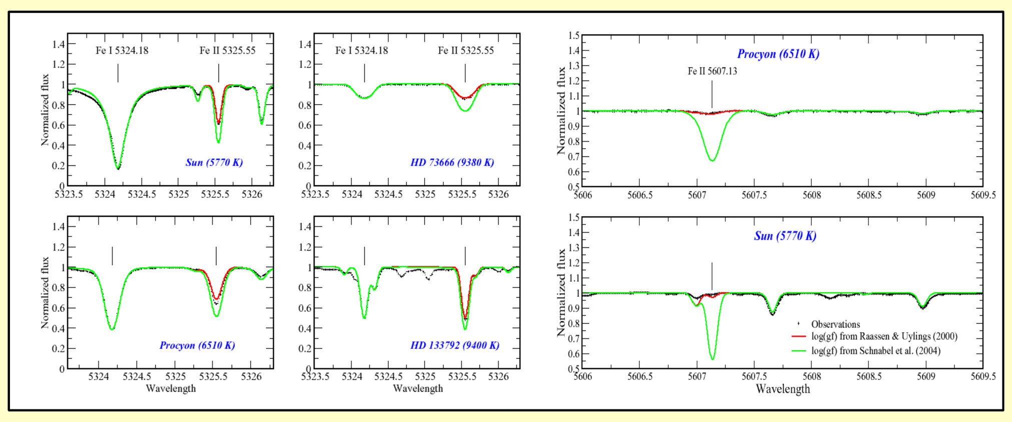


Fig.7



Comparison between synthetic spectrum calculations in the region of two 'outliers' (Fe II λλ 5325, 5607 lines) and the observed stellar spectra is shown in Fig. 7. For both lines as well as for the Fe II λ 4173 line the accuracy between 13 and 24 % is given in Schnb, and it does not correspond to the observations.

Comparison between two sets of the theoretical calculations

In a serie of the recent works on experimental f-values for Fe II it was shown that theoretical calculations based on the orthogonal operator technique (RU) agree much better with the experimental data than the Cowan code calculations (Kurucz) and hence have the preference for stellar spectroscopy. Our comparisons (see Fig.4 and Fig.5) support this conclusion. However, experimental data are available for the transition probabilities with the upper level energy below 85000 cm^{-1} (10.5 eV). According to Kurucz calculations we have about 1000 spectral lines in 4000 – 10000 A interval with the lower level energy above 80000 cm^{-1} (~10 eV) and with log(gf) > -1.1. The same is valid for Cr II. Most of 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 Fe and, in particular, Cr. HD 133792 has almost zero rotation and very small magnetic field, which allows us to minimize blending effects. The spectrum of this star was used to compare RU and Kurucz theoretical transition probabilities for Cr II and Fe II spectral lines.

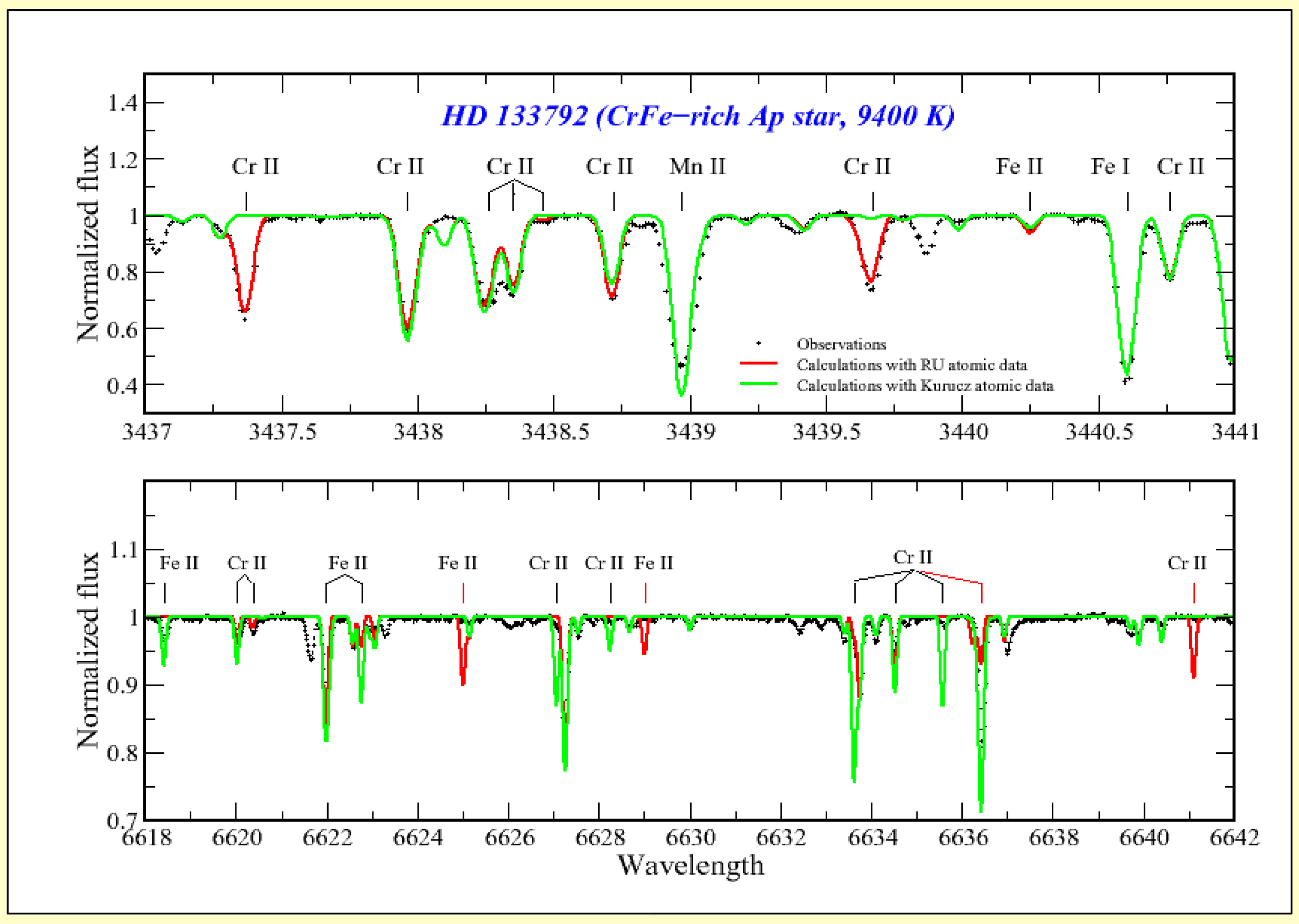


Fig.8

Figure 8 shows a comparison between the observed and synthesized spectra of HD 133792 in short and long wavelength regions. While RU theoretical transition probabilities are better than the Kurucz' values for the transitions with low or intermediate excitation energies (upper panel in Fig.8) , 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 resonably well only using the transition probabilities calculated with the Cowan code (lower panel in Fig.8). As a rule these lines (marked by the red ticks in Fig.8) have the upper energy levels classified differently in both methods of calculations. According to our comparative analysis of the RU's and Kurucz' Cr II and Fe II linelists 50 and 67 levels respectively has different configuration and/or term classification. This difference is probably caused by the strong level mixing. The Cowan code appears to treat it better than the orthogonal operator technique.

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