

# **Evaluation of the Recent Atomic Data for Fe I Lines Based on Solar and Stellar Spectra**

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**Abstract** We performed an extensive comparative analysis of the recent experimental data on Fe I transition probabilities (TP) based on the observed solar and stellar spectra. This work is part of the Vienna Atomic Line database (VALD) activities. Our motivation is to keep the VALD line list as complete as possible and provide VALD users with substantiated recommendations for the most accurate atomic data. For assessment of data quality we choose the "normal" (as opposed to peculiar and/or magnetic) Main Sequence sharpline stars of different effective temperatures with accurately known atmospheric parameters: Sun, Procyon, HD 32115, and 21 Peg. Theoretical spectra of these stars were synthesized for 1D plane-parallel model atmospheres accounting for non-local thermodynamic equilibrium (NLTE) effects, and then they were compared with the observations. For all of the stars we derived atmospheric abundances based on the new and previous experimental TP. When using the new TPs the best agreement for iron is achieved with the TP of the Hannover group (Bard, Kock, and Kock, *Astron. Astrophys.* **248**, 315, [1991;](#page-8-0) Bard and Kock, *Astron. Astrophys.* **282**, 1014, [1994\)](#page-8-1). The Hannover set is recommended as the primary source of transition probabilities in stellar abundance analysis. The new TP data significantly increase the number of spectral lines of Fe I in the optical and red spectral regions available for accurate abundance analysis of stars in a wide range of temperatures and metallicities. Comparison with the observed stellar spectra invalidates some new experimental data despite the

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small given uncertainty of the laboratory measurements. Finally, we note the importance of accurate line-broadening data.

**Keywords** Solar irradiance · Spectrum, visible · Spectral line, intensity and diagnostics

## **1. Introduction**

Iron is one of the most important chemical elements in astronomical spectroscopy.  $[Fe/H]$ <sup>[1](#page-1-0)</sup> serves as a metallicity index of various astronomical objects and is the basis for studying the chemical evolution of the Galaxy and other galaxies both observationally (see, for example, Mashonkina *et al.*, [2017](#page-9-0)) and theoretically (for example, Kobayashi, Karakas, and Umeda, [2011\)](#page-8-2). The special role of Fe motivates the theoretical and laboratory studies of its atomic properties to increase the accuracy of iron-abundance determination. At present, about 130,000 spectral lines of Fe I are classified and have accurate wavelengths. For all of these lines, theoretical transition probabilities (hereafter TP) are calculated by Kurucz ([kurucz.harvard.edu/atoms/2600/](http://kurucz.harvard.edu/atoms/2600/)). These massive but not very accurate data (see Figure 4 in Ryabchikova, Pakhomov, and Piskunov, [2018\)](#page-9-1) play an important role in atmospheric modelling through line-opacity calculations. Laboratory studies provide more accurate atomic parameters but they are available for a much smaller number of spectral lines and are often restricted to a few small spectral regions. Here we present an overview of the recent experimental Fe I transition probabilities, comparison with the previously known experimental data, and quality assessment based on the observed solar and stellar spectra.

## <span id="page-1-1"></span>**2. Experimental Transition Probabilities of Fe I Lines**

Until recently, stellar Fe abundance determinations were performed with the experimental transition probabilities from four main sources:

- i) A series of articles by the Oxford group from Blackwell *et al.* [\(1979](#page-8-3)) to Blackwell *et al.* ([1986\)](#page-8-4) based on absorption-furnace technique measurements described by Blackwell and Collins ([1972\)](#page-8-5). Hereafter we refer to this set as "Oxford". A total number of 231 lines in the range of excitation energies  $0-2.6$  eV were measured. The claimed uncertainty of absolute transition probabilities varies from 2.5% (0.01 dex) for strong lines to 7% (0.03 dex) for weak lines.
- <span id="page-1-0"></span>ii) Experimental data produced by the Wisconsin group (O'Brian *et al.*, [1991](#page-9-2)), hereafter referred to as "BWL". This group used a combination of laser-lifetime measurements and emission branching fractions measured with a high-resolution Fourier-transform spectrometer. The total number of lines is 1814; the average claimed uncertainty of absolute transition probabilities is  $13 \pm 8\%$  (0.05  $\pm$  0.03 dex).
- iii) Experimental data produced by the Hannover group (Bard, Kock, and Kock, [1991](#page-8-0); Bard and Kock, [1994](#page-8-1)), hereafter "Hannover". The same technique as used by O'Brian *et al.* ([1991\)](#page-9-2) was employed. The total number of lines is 232, and the average claimed uncertainty of absolute transition probabilities is  $10 \pm 4\%$  (0.04  $\pm$  0.02 dex).

 $1[Fe/H] = \log(N_{Fe}/N_{H})_{star} - \log(N_{Fe}/N_{H})_{\odot}$ , where  $N_{Fe}$  and  $N_{H}$  are the number density of iron and hydrogen, respectively.



<span id="page-2-0"></span>**Figure 1** Difference between the new experimental log*(gf )* (IC+W: Imperial College London and University of Wisconsin, Madison) and the previous ones (Oxford, Hannover, BWL, and MRW) as a function of log*(gf )* of IC+W. Data for the lines common with the Oxford ones are shown by *filled red diamonds* in the *bottom panels*, while data for the lines common with the Hannover ones are shown by *filled green squares*. The mean difference between two sets (*dashed line*) with the standard deviation is given in *each panel*.

iv) Experimental data produced by May, Richter, and Wichelmann [\(1974](#page-9-3)), hereafter "MRW". TP were determined for more than 1000 weak Fe I lines from an emission low-current arc. The errors quoted by the authors range between 0.1 and 0.2 dex.

These data listed above form the basis of the NIST Atomic Spectra Database (Kramida *et al.*, [2018](#page-8-6)) and Vienna Atomic Line Database (VALD: Kupka *et al.*, [1999](#page-8-7)). MRW data were renormalized in NIST ASD to a different scale, which leads to a decrease of the original TPs by 0.05 dex on average.

New laboratory measurements of the TP for Fe I lines were performed by the joint efforts of the spectroscopic groups at the Imperial College London and at the University of Wisconsin, Madison (Ruffoni *et al.*, [2014;](#page-9-4) Den Hartog *et al.*, [2014;](#page-8-8) Belmonte *et al.*, [2017](#page-8-9), hereafter "IC+W"). The experimental oscillator strengths were derived for 465 Fe I lines from branching fractions and level lifetimes. For 166 lines, experimental data were obtained for the first time. The average claimed uncertainty of absolute transition probabilities is  $0.04 \pm 0.03$  dex with a clear trend to increase towards smaller TPs. In general, the error distribution in new measurements is identical to that in the Hannover data. The new measurements were performed with a technique similar to BWL and Hannover, but different from Oxford and MRW. Figure [1](#page-2-0) shows the comparison between the new and the previous TP measurements expressed as  $log(gf)$ , where *f* is an oscillator strength, and *g* is the lower-level statistical weight.

Inspecting Figure [1](#page-2-0) one notices a very good agreement between the new measurements and those made in Oxford and Hannover and a rather large dispersion with BWL and MRW

$T_{\rm eff}$ [K]	$\log g$	$v_e \sin i$ [km s <sup>-1</sup> ]	$\mathrm{km}\,\mathrm{s}^{-1}$	$V_{\text{mac}}$ $\mathrm{km}\,\mathrm{s}^{-1}$ ]	Reference
5777	4.44	1.7	0.9	3.2	
6615	3.89	1.5	2.0	7.4	
7376	4.14	4.1	2.5	12.2	
10,400	3.55	3.8	0.5	0.0	3

<span id="page-3-0"></span>**Table 1** Atmospheric parameters of stars selected for TP evaluation.

1 – Ryabchikova *et al.* [\(2016\)](#page-9-5).

2 – Ryabchikova, Piskunov, and Shulyak ([2015\)](#page-9-6).

3 – Fossati *et al.* ([2009\)](#page-8-10).

data comparisons even though we see no systematic shift. In a few cases, the deviation exceeds 0.6 dex in absolute value. Moreover, a comparison of the  $IC+W$  data with the recent theoretical calculations by Kurucz ([kurucz.harvard.edu/atoms/2600/](http://kurucz.harvard.edu/atoms/2600/)) when fitting the observations clearly shows significant errors in laboratory measurements (see Figure 5 of Ryabchikova, Pakhomov, and Piskunov, [2018](#page-9-1)). Therefore, in extreme cases, we need to verify the superiority of the new data. This can be done by synthesis of spectra for stars with reliable atmospheric parameters.

#### **3. Stellar Spectra and Abundance Determinations**

Ideally, in a stellar atmosphere with a uniform element abundance distribution, all of the observed lines should be fitted with the same element abundance. Abundance dispersion may be caused by uncertainties in atmospheric structure and in atomic-line parameters; therefore different sets of TP were checked and evaluated using the observed spectra of sharp-line stars with accurately defined atmospheric parameters. Our primary target was the Sun, which has the most accurate fundamental parameters: effective temperature [T<sub>eff</sub>], surface gravity [log g], microturbulent [*ξ*t], and macroturbulent [*V*mac] velocities. Since the most part of stellar abundance studies are based on the observed flux spectra, we used the well-known Solar Flux Atlas by Kurucz *et al.* ([1984\)](#page-8-11) in our testing procedure. Many lines of Fe I with the best laboratory TP are very strong in the solar spectrum, and their intensity depends not only on TP, but also on different collisional effects with the van der Waals (VdW) broadening being the most important. Unfortunately, VdW damping constants are often not accurate, preventing us from using some of the lines with the most accurate TPs for abundance determinations. Therefore we extended our testing procedure towards the hotter stars, where VdW broadening is much less important. As additional targets, we used Procyon (F5IV–V), HD 32115 (A9V), and 21 Peg (HD 209459 – B9.5V).

Fundamental parameters of the sample stars are collected in Table [1,](#page-3-0) where the last column contains a corresponding reference. We used high-resolution, high signal-to-noise spectra, obtained with the *UV-Visual Echelle Spectrograph* (UVES) at the ESO VLT (Procyon), with the *Echelle SpectroPolarimetric Device for Observations of Stars* (ESPaDOnS) at the Canada–France–Hawaii Telescope (HD 32115), and with the high-resolution *FIbrefed Echelle Spectrograph* (FIES) at the Nordic Optical Telescope (21 Peg). The resolving power of ESPaDOnS and FIES is  $R = 65,000$ , that of UVES is  $R = 80,000$ . The details of observations and data reduction are given by Ryabchikova *et al.* ([2016\)](#page-9-5) and

Fossati *et al.* ([2009\)](#page-8-10). The ESPaDOnS spectrum is extracted from the ESPaDOnS archive ([www.cfht.hawaii.edu/Instruments/Spectroscopy/Espadons/](http://www.cfht.hawaii.edu/Instruments/Spectroscopy/Espadons/)). All selected objects are Main Sequence (MS) stars with approximately solar abundances of the iron-peak elements (not magnetic chemically peculiar Ap or metallic-line Am stars), which are supported by the previous abundance analysis (Bikmaev *et al.*, [2002](#page-8-12); Fossati *et al.*, [2009\)](#page-8-10).

To determine iron abundance, we employ the synthetic-spectrum method, taking into account the non-local thermodynamic equilibrium (NLTE) effects. Atmospheric parameters of our sample stars span a wide range, from spectral type G to late B. Due to a difference in atmospheric conditions of late and early spectral type stars, we use slightly different methods of NLTE calculations, designed for each of these ranges of effective temperatures. The NLTE atomic-level populations were calculated with the DETAIL code (Butler and Giddings, [1985\)](#page-8-13) with the opacity package updated by Mashonkina *et al.* ([2011\)](#page-8-14) and Przybilla, Nieva, and Butler [\(2011](#page-9-7)) for late-type and early-type stars, respectively. For the Sun and Procyon, NLTE calculations were performed with Fe I – II model atom from Mashonkina *et al.* [\(2011](#page-8-14)) with the scaling coefficient for inelastic collisions with hydrogen atoms of  $S_H = 0.5$  as calibrated by Sitnova *et al.* [\(2015](#page-9-8)). Fe I is a minority species and levels of Fe I are underpopulated compared to their LTE populations due to an overionization, while Fe II is a majority species and the departures from LTE are minor for the levels of Fe II in the atmospheres of late-type stars. NLTE effects increase with increasing temperature and decreasing surface gravity. For early-type subgiants, the level populations of not only Fe I but also Fe II deviate from LTE. For HD 32115 and 21 Peg, the NLTE calculations were performed with the extended model atom of Fe I – II from Sitnova *et al.* ([2015\)](#page-9-8). The key difference between the Fe I – II model atom of Mashonkina *et al.* [\(2011](#page-8-14)) and Sitnova *et al.* [\(2015](#page-9-8)) is the inclusion of all available experimental and theoretical energy levels data for Fe II. It can be used for NLTE calculations in early-type stars. Departure coefficients  $b_i = n_{\text{NLTE}}/n_{\text{LTE}}$ , where  $n_{\text{NLTE}}$ and  $n_{\text{LTE}}$  are the NLTE and LTE populations of the level *i*, computed with the DETAIL code are then employed by the synthV\_NLTE code for synthetic-spectrum calculations (Tsymbal, Ryabchikova, and Sitnova, [2019\)](#page-9-9). Finally, an integration of the synthV\_NLTE with the IDL visualization code BinMag6 written by Kochukhov ([2018\)](#page-8-15) allows us to determine the best fit to the observed line profile. Element abundance, line position, and broadening parameters  $v_e \sin i$  and  $V_{\text{mac}}$  were tuned by the fitting procedure for each spectral line. Table [1](#page-3-0) provides the averaged values of microturbulent  $[\xi_t]$ , macroturbulent  $[V_{\text{mac}}]$ , and surface rotational  $[v_e \sin i]$  velocities for the Sun, Procyon, HD 32115, and 21 Peg. Average values of these velocities in the Sun were derived by spectral fitting of six 100 Å-wide intervals in the 4500 – 6600 Å region of the Solar Flux Atlas (see Ryabchikova *et al.*, [2016\)](#page-9-5). Model atmospheres were calculated with the LLmodels code (Shulyak *et al.*, [2004](#page-9-10)). An exception is the Sun, whose model atmosphere was taken from the MARCS model grid (Gustafsson *et al.*, [2008](#page-8-16)).

## **4. Evaluation of the Laboratory Sets of Transition Probabilities**

We perform abundance determinations for individual Fe I lines using three sets of TP laboratory data: Oxford, Hannover, and  $IC+W$ . The results of our analysis are presented in Figure [2,](#page-5-0) where we indicate the average Fe abundance derived with each set of TP for every star. The average iron abundance, derived using the whole list of lines, is given as well. Iron abundances are expressed on a logarithmic scale relative to the total number of atoms.

The following conclusions can be drawn:

i) Our sample of MS stars has an average Fe abundance consistent with the solar one within the uncertainty of abundance determination without any signature of abundance



<span id="page-5-0"></span>**Figure 2** Individual Fe I line abundances as a function of the excitation energy for three sets of laboratory TP measurements. Linear regression for each TP set is indicated by coloured *solid line*, while the linear regression for the unified data is shown by *dashed black line*. The averaged Fe abundance with the standard deviation is indicated for each TP data set.

anomalies, which proves their usefulness as spectral standards for TP quality assessment.

- ii) The quality of the abundances derived with one-dimensional plane-parallel (1D) models using solar and stellar flux spectra is consistent with the results based on a 3D model,  $log(N_{Fe}/N_{tot}) = -4.57 \pm 0.04$ , derived with the solar-centre intensity spectrum (Scott *et al.*, [2015](#page-9-11)).
- iii) It is evident that there is a shift in abundance derived using the Oxford set of TP for cool stars, and this shift disappears in hotter stars.

The Oxford TP are derived for lines of the lower excitation energy, which are rather strong in the solar and cool-star spectra. These lines also show extended wings. It means that they are sensitive to VdW broadening. Therefore we looked at the dependence of individual line abundances on the line intensity (equivalent width: EqW), which may be caused both by inaccuracies in TP and in VdW data. Figure [3](#page-6-0) shows this dependence for solar abundances.

There are no laboratory measurements of VdW broadening for Fe I lines. The best present-to-day parameters were calculated by Barklem, Piskunov, and O'Mara [\(2000](#page-8-17): hereafter BPM) based on the line-broadening theory developed by Anstee and O'Mara [\(1991](#page-8-18)). The results presented in Figure [3](#page-6-0) do not reveal any significant dependence of the individual line abundances on the EqW for Hannover and IC+W TP sets in large range of line intensities. In particular, it refers to the abundances calculated using the Hannover TP, which means that this set of TP may be recommended as the primary source for accurate Fe abundance determinations in the atmospheres of cool stars of different metallicities. The new set of TP  $(IC+W)$  may provide supplementary data in abundance analyses although the dis-

<span id="page-6-0"></span>

persion in individual line abundances is higher, in particular in the EqW range  $0 - 100$  mÅ, which is considered to be the best for abundance determinations due to smaller sensitivity to broadening. It is interesting to note a jump in the abundances derived with the Oxford data at EqW  $= 100$  mÅ. For stronger lines, the Oxford TP provide the same abundances as the Hannover and IC+W ones, while for the line with EqW  $\leq 100 \text{ Å}$ , a systematic shift occurs. The fact that for the strong lines in the solar spectrum all experimental TP data provide consistent abundances is very important for studies of the metal-poor stars. There, only these lines are available for abundance analysis. It also explains the vanishing of the abundance shift in a hotter star, 21 Peg, because only strong Fe I lines remain in the stellar spectrum.

Together with the overall comparisons between the new and previous sets of TP we performed comparative abundance calculations for individual lines in the cases where the new data deviate significantly from the previously published experimental and theoretical TP (see Section [2\)](#page-1-1).

Figure [4](#page-7-0) demonstrates two cases where TP differences exceed 0.5 dex; however, the quoted errors of TP in corresponding data sets are practically the same:  $\approx 0.05$  for Fe I *λ*3264*.*51 Å, and ≈0*.*12 for Fe I *λ*4276*.*68 Å lines. One needs to increase the Fe abundance by more than 0.3 dex to fit the observed line profiles with the new  $IC+W$  transition probabilities. In these cases the TP from previous sets of laboratory measurements provide a better fit to the observed solar flux spectrum.

As was mentioned before, the spectral line profile is defined by a combination of TP and broadening. In some cases, it is difficult to make a conclusion in favour of a particular TP data due to uncertainty in broadening parameters. Figure [5](#page-7-1) presents an example of a profile fit for the *λ*7937*.*14 Å line using theoretical TP by Kurucz and experimental TP from the IC+W set. The difference between two values is  $\Delta \log(gf) = 0.26$  dex. For this spectral line, no VdW calculations based on the broadening theory by Anstee and O'Mara [\(1991](#page-8-18)) exist except for calculations by R.L. Kurucz. Using the Kurucz VdW broadening parameter we get a better fit to observations with the theoretical TP than with the experimental one in the solar spectrum. However, in the spectrum of a hotter star, HD 32115, where the line does not have extended wings, the observed profile is fitted well with the experimental TP and solar Fe abundance. Increasing the Kurucz VdW value by 0.3 dex we get the same quality fit of the solar line with experimental TP from  $IC+W$ , at least in the line wings. This example clearly shows the importance of broadening parameters in abundance calculations, in particular, for strong high-excitation lines ( $E_{\text{exc}} > 4 \text{ eV}$ ) in the red and IR spectral regions.

<span id="page-7-0"></span>

<span id="page-7-1"></span>**Figure 5** Comparison between the observed (*filled black circles*) and synthesized Fe I *λ*7937*.*14 Å line in the solar spectrum (*left panel*) and in the spectrum of a hotter star HD 32115 (*right panel*). Calculations with the TP and VdW from Kurucz are shown by *solid blue line*, those with TP from IC+W and VdW from Kurucz are shown by *dashed red line*. Calculations with experimental TP and increased VdW are shown by *solid green line*.

## **5. Conclusions**

We performed an extensive comparison study of different sets of experimental TP for Fe I. The recent laboratory measurements produced by the Imperial College London and Wisconsin University groups were checked against the results of the previous experiments by Oxford, Hannover, BWL, and MRW. All of the comparisons were based on the abundance calculations performed for four stars including the Sun in the effective temperature range 5780 – 10,400 K using high-resolution, high S/N spectra. Our analysis gives a preference for experimental data produced by the Hannover group (Bard, Kock, and Kock, [1991](#page-8-0); Bard and Kock, [1994\)](#page-8-1). Iron abundances in the atmospheres of the program stars derived with

the recent  $TP$  data produced by  $IC+W$  groups are consistent with those derived with the Hannover TP. For the first time the laboratory TP were derived for 166 Fe I lines. In a few cases, new laboratory TP happened to be worse than the previously known laboratory or theoretical data. Our analysis is a basis for creating an extended Fe I line list with the accurate experimental TP data for the Vienna Atomic Line Database widely used by stellar spectroscopists.

<span id="page-8-18"></span>**Disclosure of Potential Conflicts of Interest** The authors declare that they have no conflicts of interest.

<span id="page-8-1"></span><span id="page-8-0"></span>**Publisher's Note** Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.

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