Atomic Data and the Spectrum of the Solar Photosphere

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Abstract

Even though the solar photospheric abundances are now on the whole in very good agreement with the meteoritic values, some problems remain which will only be solved with a higher level of accuracy in the atomic data, especially the transition probabilities for faint lines. We justify this request for many more very accurate *gf*-values through a few particularly striking points.

1. Introduction

The study of the photospheric spectrum teaches us important aspects of various problems that are suspected to be encountered in other stars as well. Since the Sun is the brightest star, it is the one for which the observations reach the highest signal-to-noise ratio and resolving power.

The interpretation of these data should lead to the refined knowledge of the physical conditions, physical processes and abundances of the elements in the upper layers of the Sun. As long as these problems are not entirely solved for the Sun, we will not be able to handle similar problems for other stars with success.

It is well known that these problems are interconnected and strongly depend on basic atomic data: wavelengths, ionization energies, partition functions, hyperfine structures, line broadening parameters, Landé *g*-values, cross-sections and transition probabilities. These aspects have already been discussed in the past [1–3]. We shall update these reviews, insisting on a few crucial points like the wavelengths and transition probabilities. Other aspects of atomic data, also needed in solar spectroscopy, are covered in the contributions of L. Andersen, R. L. Kurucz and D. L. Lambert to this volume as well as in [3].

2. Wavelengths

2.1. *Line identifications*

Very high quality solar spectra at the center of the solar disk are now available from 300 nm to 16 µm [4–6]. Photospheric UV spectra also exist but they will not be discussed here, as they do not help very much in solving the problems mentioned in the introduction because of too numerous blends below 3000 Å.

Kurucz [7, 8] has drawn attention to the fact that a very large number of solar lines are still unidentified or unclassified in the visible spectrum, even when using his new data which include millions of new lines [9]. On the other hand, using his numerous new results for faint lines of the iron group, he has been able to solve the problem of the "missing UV opacity" [10].

In the infrared, the situation is even worse than in the visible. Geller [11] has recently identified a large number of

lines in the ATMOS solar infrared spectra obtained from space and covering the region from 2.5 to 16 µm (646 to 4798 cm^{-1}). Molecular lines are all attributed without any doubt but among the atomic lines, quite a large number of lines remain unidentified due to the lack of laboratory data for atomic species in the IR.

The solar spectrum has eventually been used as a laboratory source to provide important additional information concerning highly excited levels in C I, Mg I, Si I, Ca I, Fe I [11, 12]. Most of these levels have never been observed from laboratory sources.

2.2. *Precision*

Solar granulation is the evidence of motions in the upper layers of the Sun, hot matter moving upwards while cool matter moves downward. Observations indeed show that lines, after correction for the Sun–Earth motion and for the gravitational redshift, are blue shifted and asymmetric [13–18].

These apparent Doppler shifts are key data and severe constraints for modelling the detailed dynamical structure of the photosphere. As these Doppler velocities vary from a few tens of m/s to a few hundreds of m/s, the accuracy of the laboratory wavelengths of the unblended solar lines used for these diagnostics must accordingly be of the order of $\delta\lambda/\lambda \sim 10^{-7}$, i.e. 30 m/s (see also [19]).

3. Transition probabilities

It is well known that the accuracy of the transition probabilities play a key role not only for solar abundance determinations but also to test the empirical model of the photosphere (see e.g. [2]), to derive accurate values of the microturbulence [20] and to test hypothesis of local thermodynamic equilibrium, LTE (see e.g. [2, 19]).

We shall hereafter discuss the impact of the accuracy of the transition probabilities on the solar abundances and the needs for highly accurate *gf*-values for many more faint lines of neutral and once ionized atomic species present in the solar photospheric spectrum.

3.1. *Need for accurate solar abundances*

Among the many reasons why we continue to refine the solar photospheric abundances (see e.g. [21–24]), are some very important points.

It has been a longstanding problem to know whether there is a difference or not between the solar photospheric abundances and the meteoritic ones. Large discrepancies previously found have progressively disappeared as the accuracy of the transitions probabilities has been increasing. Anders and Grevesse [25] have shown that on the

whole the agreement is remarkably good between photospheric and meteoritic abundances. However, the uncertainties are much larger for the solar results than for the meteorites and it is still impossible to rule out slight differences hidden in the solar photospheric error bars. These error bars (see Section 3.4) essentially come from the uncertainties in the transition probabilities.

Photospheric abundances are essential data in the opacity computations used in models of the external layers of the Sun as well as in evolutionary models of the Sun's interior, if it can be proven that they reflect the chemical composition of the solar nebula. For other stars, the distribution of elements heavier than helium in the metallicity is often assumed to be solarlike. After the pioneering work of computing an Astrophysical Opacity Library by the Los Alamos group [26], gigantic efforts have recently been made to considerably improve the atomic data and the equation of state for stellar interiors as well as for envelopes. Two groups have directed their efforts towards high temperature opacities (OPAL: [27]; Opacity Project: [28, 29]). while Kurucz [9] computed opacities to be used in stellar atmosphere modelling. Such improvements in the opacity computations demand very accurate abundances for all the numerous contributors to these opacities. As an example, the reduction of the iron photospheric abundance to the meteoritic value (see Section 3.2) has a significant influence on the opacities, even at physical conditions typical of the solar central regions [30], and change the calibrated solar model.

It is now well known that there are differences between the photospheric and the coronal abundances due to a fractionation process leading to an overabundance in the corona of the elements which have their first ionization potential lower than about 10 eV. Even more subtle behaviours among different elements are now observed and they must be carefully analysed before being used as constraints in any hydrodynamical envelope model.

There might possibly exist diffusion mechanisms which could lead to slight abundance gradients for some elements in the photosphere. Unfortunately, it is still out of reach to observe such gradients, since the dispersion in the photospheric results is still much too large. It would require much higher accuracy in the gf-values for many more faint lines.

3.2. Photospheric abundance results

Progress made during the last decade or so in our knowledge of the photospheric abundances is essentially due to the availability of accurate gf-values for lines of solar interest. As already mentioned in Section 3.1, past discrepancies between meteoritic and photospheric abundances have disappeared as accurate transition probabilities have progressively become available for many more species and many more lines. Atomic spectroscopists have played a major role in allowing to refine the photospheric abundances and they are co-authors of many papers on solar abundances.

Meteoritic abundances are now known with an accuracy often better than 10% [25]. Photospheric abundances, as reviewed in [25] and in different more recent papers [22–24] still have much larger error bars (see Section 3.4).

The longstanding puzzling problem of the difference between the photospheric and the meteoritic abundance of iron has recently been solved. Let us recall that Blackwell *et*

al. [31, 32], using the very accurate Oxford transition probabilities [33] for low excitation Fe I lines, derived a solar abundance of iron of $A_{Fe} = 7.67 \pm 0.03$ (where $A_{el} = N_{el}/N_H$, the abundance by number relative to hydrogen in the usual logarithmic scale where $\log N_H = 12.00$), larger than the very accurate meteoritic value of $A_{Fe} = 7.51 \pm 0.01$ [25].

New accurate transition probabilities have recently been obtained for lines of higher excitation in Fe I as well as for Fe II lines. Such lines are much less sensitive to departure from LTE and to slight uncertainties in the atmospheric model than the low excitation Fe I lines. Different groups, including the atomic spectroscopists who obtained the new gf-values, have redetermined the photospheric abundance of iron using these new data [34–38]. The new results all converge to the meteoritic value with uncertainties of the order of 10 to 15%. Even if the problem seems to be solved, we claim that more analyses should be done using Fe I as well as Fe II lines. To obtain significant results, we need many more very accurate gf-values for faint Fe I and Fe II lines (see Section 3.4).

Rather puzzling are recent results on Sc [39] and on Ti [40] abundances, obtained using accurate gf-values for both neutral and singly ionized species. These solar abundances are slightly larger than the meteoritic values.

Even if the agreement between photospheric and meteoritic abundances on the whole is very good, we still need to use many more faint lines of very good quality with large ranges of excitation energies in order to seek for possible differences between the meteorites and the solar photosphere and to better understand the physical processes in the photosphere.

3.3. gf-values and physical processes

We summarized in [3] the problem of the empirical departures from LTE observed in iron group neutrals thanks to the use of very accurate gf-values (a few %). Figure 1 shows the abundance results obtained from low excitation lines in Fe I [31], Cr I [41], Ti I [41, 42] and V I [43].
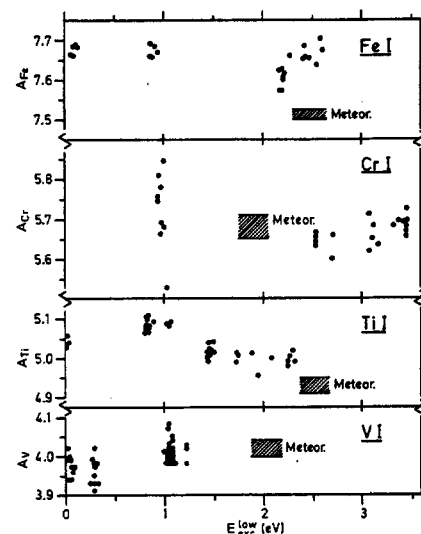

Fig. 1. Solar abundances, as functions of the excitation energy, derived using very accurate gf-values for low excitation lines of Fe I [31], Cr I [41], Ti I [41, 42] and V I [43]. The variations of the abundance with excitation energy are real and correspond to non-LTE effects (see text)

For narrow ranges of the excitation energy, the dispersion of the abundance results is quite small but there is clearly a trend showing some dependence of the abundance on the excitation energy of the lower level. This could possibly be explained as slight and subtle departures from LTE. These peculiar behaviours would totally be masked if less accurate gf-values had been used (see Section 3.4).

3.4. *gf-values and abundances*

We shall hereafter illustrate with a few examples the influence of the accuracy of the gf-values on the dispersion and the mean value of the solar photospheric abundances.

Figure 2 shows the vanadium abundance as a function of the excitation energy as derived by different authors ([44–46], presents results: [43]), using the gf-values available at the time. Note that there is a strong decrease in the dispersion of the results down to the very small dispersion in [43] obtained when using accurate gf-values derived from lifetime and branching fraction measurements.

The iron abundance has followed the same trend with time, as can be seen in Fig. 3 where we have plotted the solar abundances as derived from Fe I lines, using gf-values
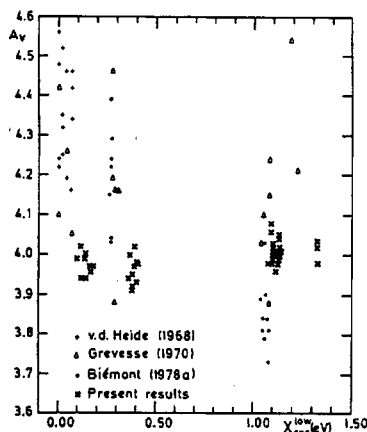

Fig. 2. Abundance of vanadium as a function of the excitation energy derived by different authors [44–46] and present results [43], using different gf-values. The very large dispersion noted for works prior to [43] reduces tremendously when using the accurate gf-values of [43]. It also shows that results prior to [43] were in complete disagreement with the meteoritic abundance, $A_v = 4.02$, essentially because of the use of inaccurate transition probabilities
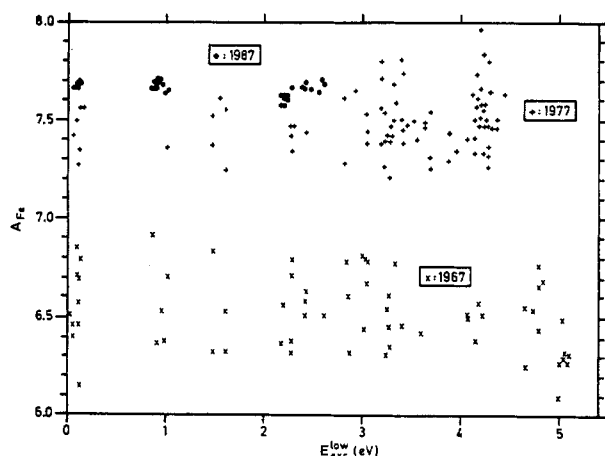

Fig. 3. Evolution of the solar abundance of iron and of the disperson of the results as derived from Fe I lines. The 1987 results are obtained using the very accurate gf-values of Oxford [31]. Earlier results are obtained using solar equivalent widths measured with high accuracy but gf-values available in 1967 and 1977 respectively

available in 1967, 1977 and 1987. The last results have been obtained with the accurate Oxford gf-values [31] (see Section 3.2).

The difference in the mean values and in the dispersion is striking and emphasizes the crucial role played by the accuracy of the transition probabilities.

We must stress that the dispersion observed in solar abundances essentially reflects the level of accuracy of the gf-values used.

This iron problem which is now claimed to be solved (see Section 3.2) has in fact opened a new iron problem namely the behaviour of the abundance derived from Fe I line *vs.* the excitation energy, E_{ex}, for a very large range of E_{ex}, from 0 to 7.5 eV, observed in the solar spectrum. O'Brian *et al.* [47] have recently published quite a large number of transition probabilities for Fe I lines obtained from lifetime and branching fraction measurements. We used their data for about 100 faint Fe I lines in order to avoid the microturbulence and broadening uncertainties. The results are presented in Fig. 4. They are somewhat disappointing in the sense that the dispersion is still quite large. Although the mean value is close to the meteoritic one, the error bar is so large that the agreement could be only apparent. Moreover, because of this large dispersion, nothing definite can be said about the detailed behaviour of the iron abundance in terms of the excitation energy of the lower level. A much smaller dispersion is observed in Fig. 1 (upper panel) obtained with the Oxford gf-values [31]. However, it should be recalled that these results lead to a mean value higher than the meteoritic one.

The dispersion observed in Fig. 4 is intimately related to the uncertainty in the gf-values, essentially coming from the very difficult technical aspects in the branching fraction measurements for faint lines. Once again, it illustrates that the dispersion in the abundance results is really a function of the uncertainty in the gf-values.

When measured branching fractions are missing, some authors turn to Kurucz's semi-empirical gf-values [9], sometimes normalizing them to measured lifetimes. This is not a crucial point as Kurucz's new transition probabilities for the iron group elements are on the whole accurate to within 10–15% for strong lines which are by far the main contributors to the lifetimes. It is well known that the accuracy of Kurucz's data decreases as the intensity or gf-value of the lines decreases (see e.g. [47, 48]). When comparison
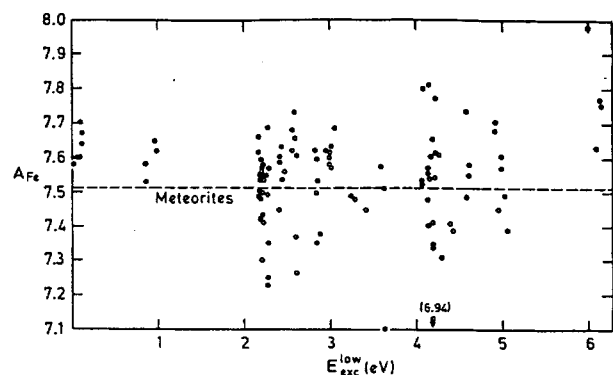

Fig. 4. Solar abundance of iron as derived from a large number of Fe I lines as a function of the excitation energy up to rather high excitations. The transition probabilities of these essentially faint lines are from [47] (see text)

can be made, the dispersion obtained with Kurucz's data is much larger than when using measured values. This is illustrated in Fig. 5 which shows the iron abundance derived from Fe II lines with Kurucz's data normalized to the best lifetime values in the upper panel [36] and measured data in the lower one [38]. The mean iron abundance obtained using gf-values derived from accurate lifetimes and branching fractions [38] is $A_{Fe} = 7.48 \pm 0.09$ (s.d.) [Fig. 5(A)] whereas using Kurucz's branching fractions [Fig. 5(B)] leads to $A_{Fe} = 7.66 \pm 0.18$ (s.d.). Not only the dispersion of the results is much larger but the mean iron abundance is also much higher. It was only when deleting some lines with high iron abundances that Biémont *et al.* [36], using Kurucz's gf-values [9], obtained a solar abundance in agreement with the meteoritic value.

This is even more striking in Fig. 6 where the Ti abundance derived from Ti II lines is shown using Kurucz's data, normalized to the lifetime of [40] (upper panel B), and gf-values obtained from accurate lifetime and branching fraction measurements (lower panel A) [40]. The solar abundance of Ti is $A_{Ti} = 5.04 \pm 0.04$ [Fig. 6(A)]; it becomes $A_{Ti} = 4.97 \pm 0.30$ with Kurucz's data.

These results are not shown to criticize Kurucz's gf-values [9]. Kurucz's data have been computed for opacity purposes and not for a line by line analysis. The same type of remark could be made concerning the Opacity Project gf-
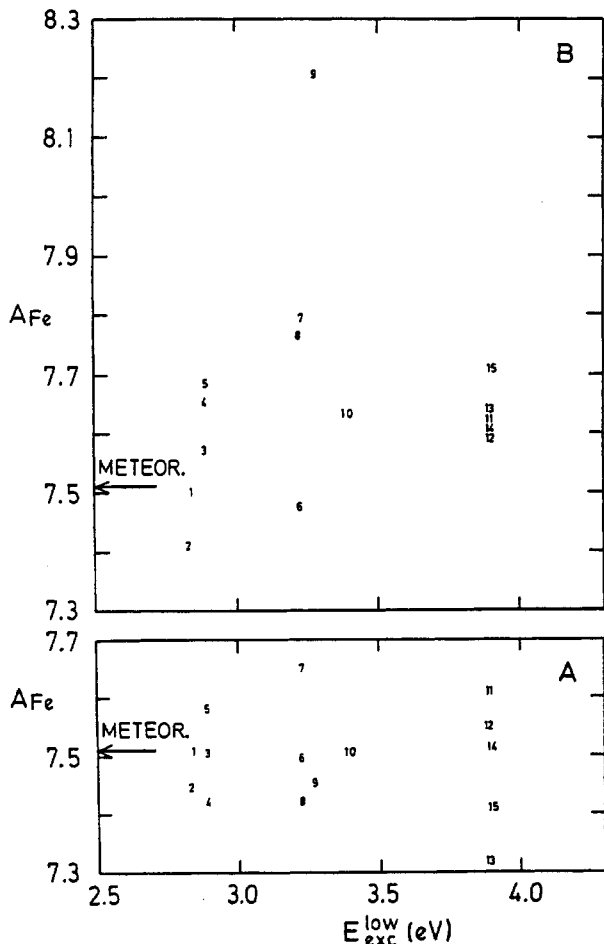

Fig. 6. Solar abundance of titanium as derived from Ti II lines as a function of the excitation energy. Panel A shows the results obtained using measured gf-values from [40]. Panel B displays the same lines but using Kurucz's semi-empirical gf-values [9] (see text)

values [28, 29]. Using these data for abundance determinations from faint lines might be seriously misleading.

Sometimes, only one line is available to derive the solar abundance of an important element. As an example, thorium shows only one Th II line, at 4019.13 Å. Now, the abundance of this element, as derived from this single line that is present in solar and stellar spectra, is a chronometer for determining the age of the Galaxy [49]. It has been shown that this line is blended with a Co I line whose gf-value has been measured with accuracy [50]. The contribution of this Co I line to the Th II feature is not at all negligible and affects the age determination of the Galaxy. Now, even taking this known blend into account, the solar abundance of thorium is about 40% larger than the meteoritic abundance. As thorium is a refractory element, there is no reason why such a difference should exist [25]. One possible explanation is the presence of another blend. A likely candidate is the intercombination line of $VI(a^2 D_{5/2} - w^4 P_{5/2})$ with $\log gf = -1.999$ as computed by Kurucz [9]. With such a strength, the solar contribution of the VI line to the Th II feature is too small to bring the thorium abundance down to the meteoritic value. However, it has been shown [43] that Kurucz's results for intercombination lines in VI might be much too small. Solar and stellar spec-

Fig. 5. Solar abundance of iron as derived from Fe II lines as a function of the excitation energy. Panel A shows the results obtained using measured gf-values from [38]. Panel B displays the same lines but using Kurucz's semi-empirical gf-values [9]. The lines are numbered as they appear in Table 4 of [38] (see text)
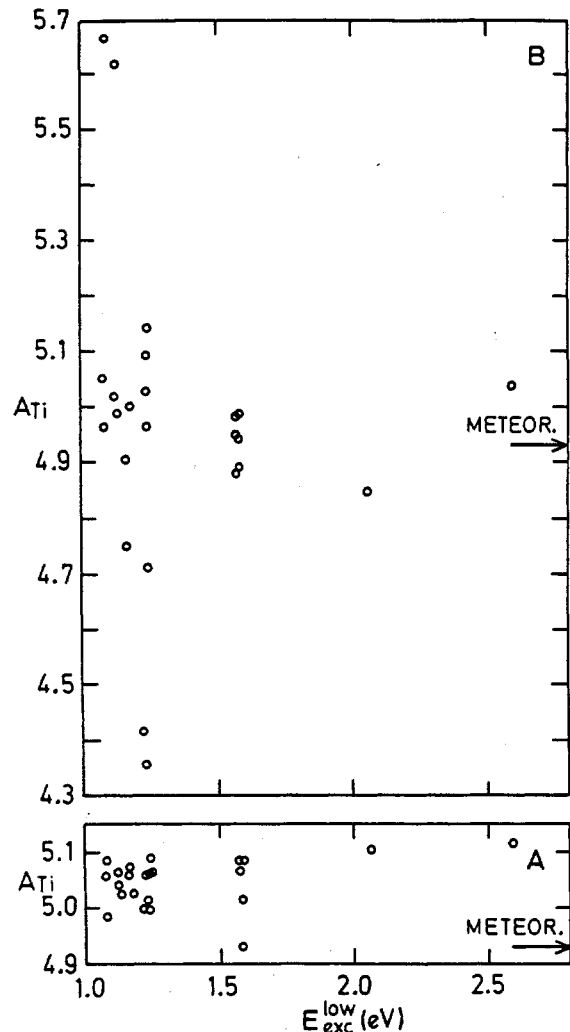
troscopists urgently need accurate measurements of this single VI line.

4. Conclusions

It is now generally accepted that the solar photospheric abundances agree with the meteoritic values thanks to the increase in the number and accuracy of measured transition probabilities for many species. However, this does not mean that the atomic data available at present allow us to fully understand the solar photospheric spectrum.

- Quite a large number of lines are still unidentified or unclassified.
- A higher accuracy in the laboratory wavelength is needed.
- Some problems remain in the photospheric abundances of some species which are still different from the meteoritic values.
- As the accuracy of the *gf*-values increases further, more and more sophisticated informations will be extracted from the solar spectrum.
- Even when the solar photospheric abundances agree with the meteoritic values, the dispersion of the solar results is generally rather large; this could hide some extremely valuable informations on the physics of the photosphere.
- The dispersion observed in solar photospheric abundances essentially reflects the level of accuracy of the *gf*-values used. Astronomers urgently need higher accuracy measurements of branching fractions for faint lines.

Many more high accuracy *gf*-values for a larger number of lines are certainly needed for Mg I, Al I, P I, S I, Mn I, Mn II, Fe I, Fe II, Cu I, Zn I, Ba II and the rare earths.

Acknowledgements

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