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Original scientific paper

ON THE MODIFICATIONS OF OSCILLATOR STRENGTHS AND DAMPING CONSTANTS OF Fe I SPECTRAL LINES FROM 500 nm TO 510 nm

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SUMMARY: We modified oscillator strengths and enhancement factors of van der Waals damping constants for 84 moderately strong and weak neutral iron spectral lines between 500 nm and 510 nm, by fitting the solar synthetic spectrum to the observed one. We have found significant difference between the oscillator strengths and damping constants taken from an extensive spectral line list, frequently used for spectral synthesis, and their modified values. Our findings include: (1) the mean value of the distribution of the difference between our and listed oscillator strengths is -0.31dex and its width is 0.42 dex, (2) a decrease of this difference with increasing equivalent width of spectral lines, (3) unusually high values of the obtained enhancement factors in comparison with the results of other authors, (4) a decrease of enhancement factor with increasing excitation potential for lines with equivalent width greater than 7.5 pm, (5) a decrease of enhancement factors with increasing equivalent width and (6) a decrease of enhancement factors with increasing oscillator strengths.

Key words. Atomic data - Line: profiles - Techniques: spectroscopic

1. INTRODUCTION

For comparison and interpretation of the observed high - resolution solar spectral line profiles we usually use synthetic spectral line profiles calculated under LTE conditions (e.g. Vince and Vince 2003, Vitas and Vince 2003). We took the atomic data for these calculations from extended atomic data tables published at different web sites (e.g. Kurucz Atomic Data Files[1]). Often we found that the calculated and observed spectra are very different, i.e. there are spectral lines in calculated spectra that do not exist in observed ones and vice versa. More often the observed line profiles differ very much from calculated profiles. These discrepancies are independent of the employed solar atmospheric models. We also noticed that for a good fit of the calculated to the observed line profiles the values in atomic data tables must be changed: usually the oscillator strength (gf) and van der Waals enhancement factor (E). Therefore, one can conclude that these discrepancies are caused by erroneous atomic data used for calculation of line profiles. These problems with atomic

[1]http://cfa-www.harward.edu/amdata/ampdata/kurucz18/kurucz.html

data motivated us to modify their tabulated values by fitting the calculated solar spectral line profiles to the observed ones, supposing that the solar atmospheric models are well known and that the LTE assumption is good enough for not too strong lines. In this paper we present the modified atomic data (gf and E) for weak and moderately strong iron lines from 500 to 510 nm. We do not consider very weak lines because their profiles are often very deformed by unrecognized blends and can cause large statistical uncertainties. Since the theoretical spectra are synthesized adopting LTE conditions, we also avoid very strong iron lines for which the influence of non - LTE effect could be significant.

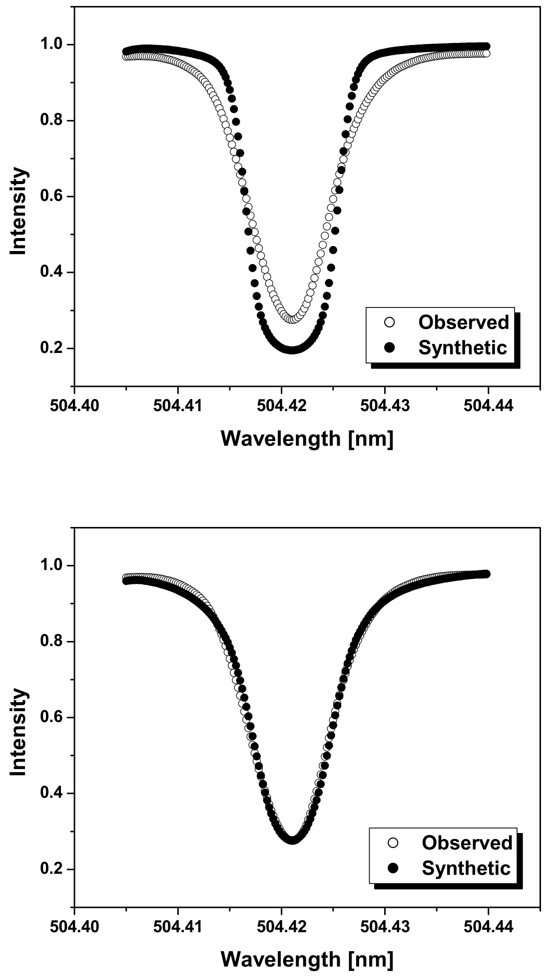

Fig. 1. *Fe I line at 504.421 nm with original parameters: log(gf)=-2.146 and E=1 (above), and after our corrections: log(gf)=-2.54 and E=15 (below).*

2. DATA AND RESULTS

We compared the calculated and observed spectra using ISAAC, an interactive program developed specifically for this purpose (Latković et al. 2002). It displays the two spectra and their difference, and allows quick changing of atomic line parameters. The new parameters are passed then to "Spectrum" (written by R. O. Gray), which does the calculations. The lines we worked on are a part of a list compiled by R. O. Gray from various sources[2]. A Kurucz solar atmosphere model with microturbulent velocity of 1 km/s and iron abundance of 7.5 was employed. For comparison, we used photometric atlas of the solar spectrum observed at Jungfraujoch Observatory (Delbouille et al. 1973).

As we expected, we found significant disagreement between the synthetic and observed spectra. A typical example is presented in Fig. 1. Assuming that this disagreement is a result of imprecise atomic parameters that "Spectrum" uses, we modified these values for a selected group of neutral iron lines from 500 to 510 nm. The list contains 176 neutral iron lines in this range. We disregarded very weak lines (central depth less than 0.1). Also, we left some lines in superposition for later, more detailed consideration. We treated 84 lines varying their log(gf) and E-factor values until a good fit was achieved. In most cases, this means that after applying our corrections, the difference between corresponding line profile points is less than 0.03 expressed in units of the local continuum (see Fig. 1, below). This is not so with a number of stronger lines (equivalent width greater than 8 pm) where a specific problem appeared: while we were able to match the wings, the core of the synthetic line remained considerably wider than in the observed line. This problem will remain for further investigation.

In Table 1 the old and the modified oscillator strengths and enhancement factors for van der Waals broadening are presented. The original values for enhancements factors in Gray's list are all equal to 1.0, so they are omitted. Equivalent widths are taken from Moore et al. (1966). Missing equivalent widths mean that in Moore et al. (1966) these lines are not identified as iron lines or the iron line is in an unresolved overlap with other spectral lines.

2.1. Oscillator strengths

We compared our data with the list compiled by Gray, and with the data from NIST web site[3]. In Fig. 2 this comparison is presented as the difference of tabulated and corrected log(gf) values versus corrected log(gf) values. The differences show large scattering. Maximum deviation between our and Gray's data is about -1.9 dex, and about -1.3 dex between our data and the data from NIST. The distribution function of differences for our and Gray's

[2]ftp `pencaer.phys.appstate.edu/spectrum`

[3]`http://physics.nist.gov/cgi-bin/AtData/display.ksh`

log(gf) values is presented in Fig. 4. The distribution of differences is slightly asymmetric and shifted toward the negative values. The shift (mean value of the distribution) is -0.31 dex and the average deviation (rms) is 0.42 dex. This means that our values are systematically smaller than the values of other authors (sampled in Gray's list).

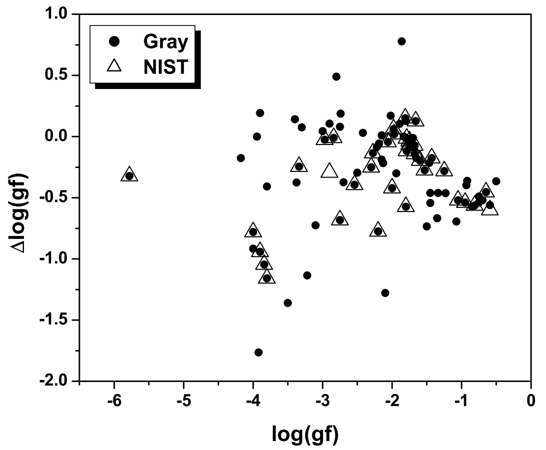

Fig. 2. *The difference of the modified and tabulated values (Gray and NIST) of log(gf) vs. the modified values.*

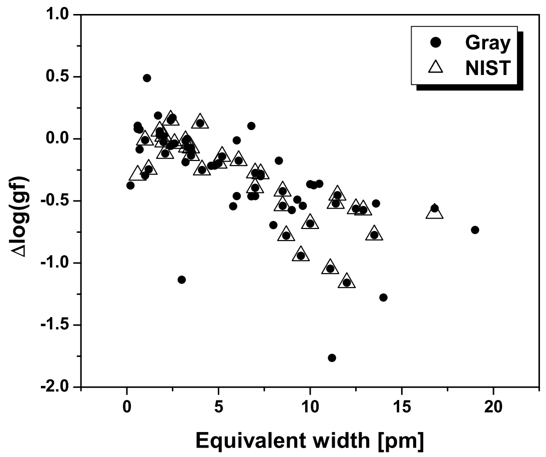

Fig. 3. *The difference of the modified and tabulated values (Gray and NIST) of log(gf) vs. the equivalent width.*

We do not have definite explanation for negative shift of the mean value of distribution. It is possible that the adapted microturbulent velocity of 1 km/s is too high for the used solar atmosphere model and systematically lowers our log(gf) values. The other possibility is that the negative shift is due to very high values of our estimated enhancement factors (see discussion later). Namely, high values of enhancement factors can have significant influence on the far wings of synthetic line profiles (redistributing line intensity from the core to far wings of the line profile). The far wings of synthesized lines are difficult to compare with observations because they are usually blended with the wings of neighboring lines. This idea is supported by the result of comparison of the difference of our and Gray's log(gf) values with equivalent width of spectral lines. This comparison is given in Fig. 3. As one can see, there is a significant correlation between the difference of our and Gray's log(gf) values and equivalent width: the difference decreases with equivalent width.

The scattering of 0.42 dex is very high in comparison with the scattering of differences between different laboratory measurements, but it is comparable with the scattering of differences between semi-empirical calculations and laboratory values (see e.g. Bard et al. 1991). We obtained this high scattering since Gray's list mostly contains calculated values. Large scattering might be partly due to selection rules. Namely, for laboratory measurements usually the most favorable lines are selected. For instance, Bard et al. (1991) data set has only 114 Fe I lines (for comparison with other data they never used more than 40 lines) from the wavelength range of 910 nm (260-1170 nm). Our data set contains 84 (also selected) lines from a much narrower wavelength range of 10 nm (500-510 nm) and only two lines are common with the Bard et al. (1991). We plan to apply our method for simultaneous determination of log(gf) and enhancement factors on these 114 FeI spectral lines and compare our results with results of Bard et al. (1991).

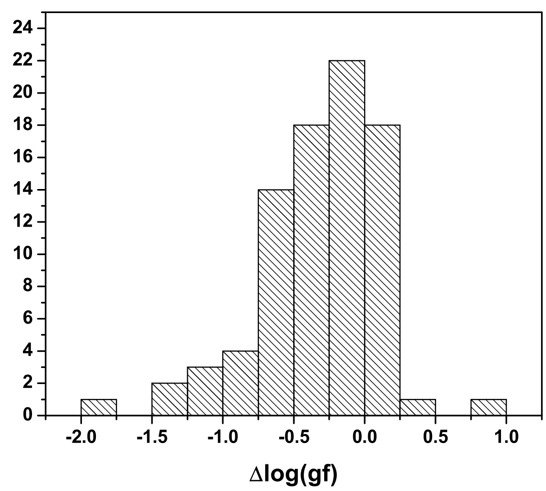

Fig. 4. *The distribution of the differences between our values for log(gf) and the values taken from Gray's table.*

2.2. Enhancement factors for van der Waals broadening parameters

Our estimated enhancement factors (E-factors) are unexpectedly high in comparison with the results of other authors. For example, Gurtovenko et al. (1982) determined enhancement factors for 75 neutral iron lines. The distribution of these enhancement factors is given in Fig. 5. The mean value of the enhancement factors is 3.3 with average deviation of 2.4. The minimum and maximum values are 0.4 and 14, respectively. The distribution is asymmetric toward the higher values of E-factors. The distribution of our E-factors is presented in Fig. 6. It is very different from the previous one. The mean value is about 15 and the average deviation is about 9. If several extreme values (larger than 25) are excluded, the distribution becomes rather symmetrical. Among 25 articles (listed in Table IA of the article by Gurtovenko and Kondrashova 1980) dealing with E-factors, only the value of 20 obtained by Sacotte and Bonnet (1972), exceeds our mean value of 15.

Unusually high values of our enhancement factors are not completely understood. We suspect that a part of this discrepancy is due to the fact that different authors use different methods for van der Waals broadening parameters calculation. These different approaches can lead to different values for van der Waals broadening parameters and systematic differences between E-factors. For example, spectral synthesis program "Spectrum" that we employed for our line profile calculations, uses van der Waals broadening parameters obtained from theory of Barklem et al. (1998), while Gurtovenko et al. (1982) use another approximation. We proved this hypothesis by comparing the enhancement factors obtained by Gurtovenko et al (1982) and Anstee and O'Mara (1995). Anstee and O'Mara (1995) applied their broadening parameters in the synthesis of three strong solar lines: sodium (589.592 nm), calcium (616.218 nm) and iron (526.954 nm). Synthetic profiles of these lines corrected by E-factors of 1.93, 2.39 and 2.11 respectively give consistent solar abundances of these elements with the meteoritic values and an excellent fit to wings (but not to cores) of the observed line profiles. Since these enhancement factors are very similar to the mean value (1.27) of 19 stronger (EW>15 pm) iron lines obtained by Gurtovenko et al. (1982), our hypothesis is incorrect for strong lines. It is possible that this discrepancy is a consequence of the fact that our set of spectral lines contains mostly moderately strong and weak spectral lines, in contrast to other authors who mainly study stronger spectral lines. In order to check this assumption we plotted the E-factors versus equivalent widths (Fig. 7). There is correlation between equivalent widths and E-factors: E-factors decrease with increasing equivalent widths, confirming the results published by Gurtovenko et al. (1982). They argued that the observed increase of E-factors with decreasing equivalent widths is due to peculiarities of deep photospheric velocity fields but not to errors in the theory of van der Waals broadening. Although there is a quantitative agreement between our results and results of Gurtovenko et al. (1982) our E-factors are systematically larger. We believe that the neglecting of the depression of the observed local continuum level in synthetic spectrum calculation can lead to this systematic effect. Weaker lines are more influenced by this effect than stronger ones. This is also supported by the correlation between E-factors and oscillator strengths (Fig. 8): E-factors decrease with increasing oscillator strengths. This is probably the reason why our log(gf) values are systematically smaller than the values of other authors. In the future work this correlation has to be taken into account since it can cause systematic errors in determination of E-factors and oscillator strengths.

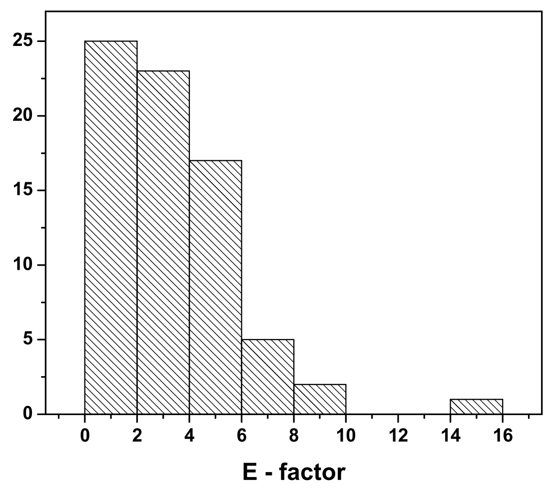

Fig. 5. *The distribution of enhancement factors published by Gurtovenko at al. (1982).*

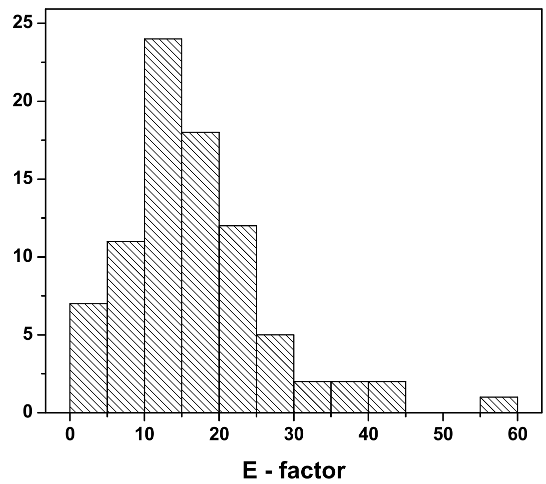

Fig. 6. *The distribution of our enhancement factors.*

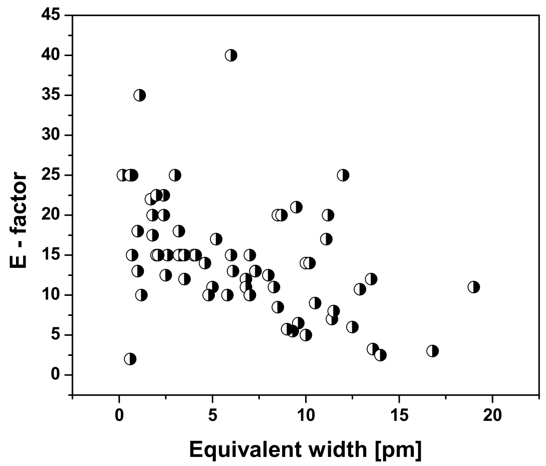

Fig. 7. *The dependence of the enhancement factor on the equivalent width.*

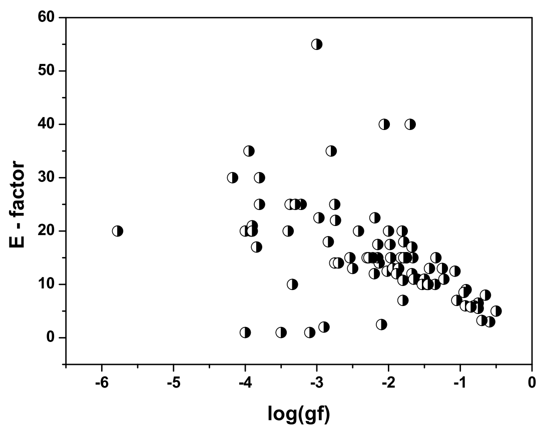

Fig. 8. *The correlation between enhancement factors and oscillator strengths.*

We also investigated if there were any correlation between excitation potential of lower energy level of line transition and the obtained enhancement factors. For this purpose we divided our data into two groups according to equivalent width: lines with EW $<$ 7.5 pm and EW $>$ 7.5 pm. For the first group there is no correlation (see Fig. 9). The second group shows decreasing enhancement factor with increasing lower energy level (see Fig. 10). This result is in contradiction with results of Gurtovenko et al. (1982). They did not find any significant systematic dependence between E-factors and lower-level excitation potential.

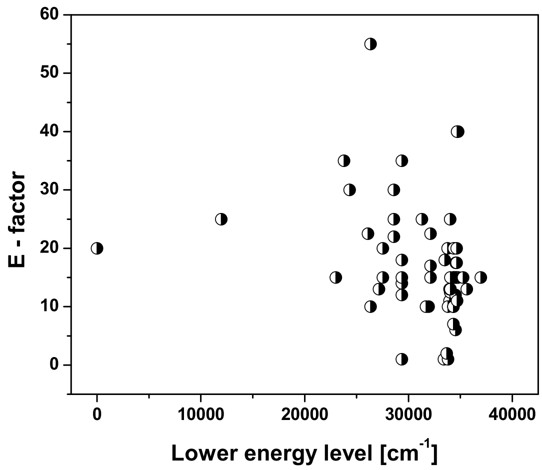

Fig. 9. *The dependence of the enhancement factor on lower-level excitation potential for lines with EW less than 7.5 pm.*

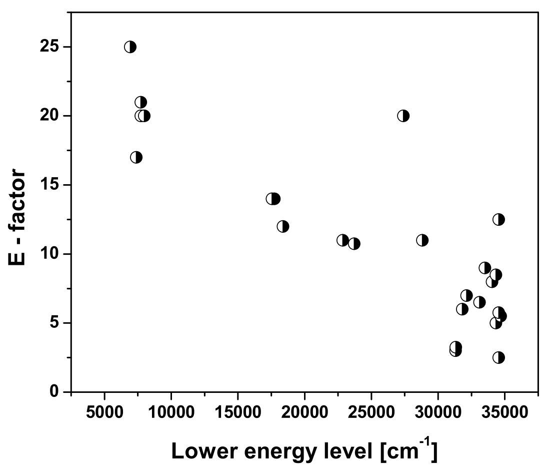

Fig. 10. *The dependence of the enhancement factor on lower-level excitation potential for lines with EW greater than 7.5 pm.*

Table 1. The tabulated and our modified values for oscillator strengths (log(gf)) and enhancement factors (E) as well as equivalent widths (EW) for a number of FeI lines. The columns containing our modified values are marked with asterisk.

$\lambda[nm]$	$log(gf)$	$log(gf)*$	$E*$	$EW[pm]$
500.1862	-0.030	-0.590	3	16.8
500.2582	-2.450	-2.420	20	1.8
500.2789	-1.579	-2.000	20	8.5
500.4037	-1.404	-1.600	11	5
500.5711	-0.180	-0.700	3	13.6
500.6117	-0.767	-1.500	11	19
500.7293	-0.210	-0.750	7	9.6
500.7728	-1.830	-1.830	15	3.3
501.1213	-4.000	-4.175	30	
501.1239	-3.000	-3.375	25	0.2
501.2067	-2.642	-3.800	25	12
501.2153	-0.908	-1.450	10	5.8
501.2683	-1.786	-1.660	15	4
501.4941	-0.247	-0.810	6	12.5
501.6476	-1.683	-1.750	15	3.3
501.9660	-2.375	-3.100	1	
501.9732	-2.134	-2.190	23	2.4
502.0816	-2.927	-2.740	22	1.7
502.1602	-1.250	-1.465	10	4.8
502.1675	-2.190	-2.020	13	2.5
502.2236	-0.530	-1.050	7	11.4
502.3198	-1.602	-1.675	12	3.5
502.3489	-1.712	-1.750	15	2.6
502.5080	-1.990	-1.970	15	2
502.5318	-2.041	-1.980	17	1.8
502.7120	-0.559	-0.920	9	10.5
502.7226	-1.914	-2.130	14	4.6
502.7299	-3.083	-4.000	1	
502.7341	-1.963	-2.150	15	3.2
502.7756	-1.254	-1.430	13	6.1
502.8126	-1.474	-1.650	11	8.3
502.9621	-2.050	-2.300	15	4.1
503.0779	-2.944	-2.970	23	2
503.1213	-3.290	-2.800	35	1.1
503.1915	-1.672	-1.790	15	2.1
503.9250	-1.640	-1.940	13	7.3
504.0252	-2.205	-2.500	13	1
504.0853	-0.682	-1.350	10	
504.0901	-0.533	-0.930	6	
504.1071	-2.156	-3.920	20	11.2
504.1755	-2.086	-3.220	25	3
504.1847	-0.822	-2.100	3	14

$\lambda[nm]$	$log(gf)$	$log(gf)*$	$E*$	$EW[pm]$
504.4210	-2.146	-2.540	15	7
504.7130	-2.134	-2.220	15	0.7
504.8433	-1.256	-1.530	10	7
504.9819	-1.426	-2.200	12	13.5
505.1634	-2.794	-3.840	17	11.1
505.2966	-3.044	-3.000	55	
505.4642	-2.140	-2.275	15	3.5
505.5993	-2.015	-2.060	40	
505.6841	-1.961	-1.810	20	2.4
505.7480	-2.638	-1.860	13	
505.7498	-2.140	-3.500	1	
505.8496	-2.830	-2.840	18	1
506.0049	-1.688	-1.700	40	6
506.0078	-5.457	-5.780	20	
506.4955	-1.928	-1.800	7	
506.5014	-0.134	-0.500	5	10
506.5194	-1.994	-1.890	12	6.8
506.7151	-0.969	-1.250	13	7.3
506.8765	-1.227	-1.800	11	12.9
506.9422	-2.160	-2.150	17	
507.2076	-0.380	-1.075	13	8
507.2668	-0.880	-1.340	15	6
507.4748	-0.196	-0.650	8	11.5
507.6262	-0.767	-1.230	11	6.8
507.8528	-3.375	-3.300	25	0.7
507.8972	-0.260	-0.750	5	9.3
507.9224	-2.067	-2.750	14	10
507.9739	-3.220	-4.000	20	8.7
508.0792	-3.946	-3.946	35	
508.0943	-3.094	-3.340	10	1.2
508.1864	-2.831	-2.750	25	0.6
508.3338	-2.958	-3.900	21	9.5
508.5677	-3.005	-2.900	2	0.6
508.8166	-1.775	-1.790	18	3.2
509.0767	-0.410	-0.950	9	8.5
509.1715	-3.541	-3.400	20	
509.1725	-3.392	-3.800	30	
509.1729	-4.093	-3.900	20	
509.6998	-0.277	-0.850	6	9
509.857	-0.990	-1.450	10	7
509.8699	-2.327	-2.700	14	10.2
509.9075	-1.534	-1.675	17	5.2

3. CONCLUSIONS

We confirmed once more that theoretical van der Waals damping constants are insufficient for good fitting of observed line wings in stellar spectra.

According to our results the oscillator strengths and enhancement factors in existing atomic data tables are not suitable for precise line profile calculations. These data have to be improved before they can be used for calculation of synthetic spectra. One of the possible ways to improve these data: the method of comparison of the observed and synthetic spectra, is presented in this paper. We believe that these improved data are precise enough for calculation of medium and low-resolution spectra of (solar like) stars. As we believe that these improved atomic data can be helpful for better interpretation of some spectroscopic observations, we plan to continue this work by taking other spectral lines into consideration and by extending the spectral range to the larger part of the spectrum. This could help us to solve the problems that remain unanswered in this article too.

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О ПОПРАВКАМА АПСОРПЦИОНИХ ОСЦИЛАТОРНИХ ЈАЧИНА И КОНСТАНТИ ШИРЕЊА КОД СПЕКТРАЛНИХ ЛИНИЈА НЕУТРАЛНОГ ГВОЖЂА ОД 500 nm ДО 510 nm

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UDK 523.9
Оригинални научни рад

Одредили смо апсорпционе осцилаторне јачине и поправке за константе ван дер Валсовог ширења за 84 спектралне линије неутралног гвожђа у опсегу од 500 nm до 510 nm, фитовањем синтететизованог спектра према посматраном. Вредности које смо добили значајно се разликују од полазних (које потичу из једне опсежне листе спектралних линија која се често користи за синтезу спектара). Установили смо следеће: (1) расподела разлика између наших и полазних вредности за силе осцилатора има средњу вредност од -0.31 и ширину од 0.42, (2) опадање ових разлика са повећањем еквивалентне ширине, (3) наше поправке за константе ван дер Валсовог ширења су необично велике у односу на резултате других аутора, (4) ове поправке опадају са порастом ексцитационог потенцијала доњег нивоа код линија са еквивалентном ширином већом од 7.5 pm, (5) смањење фактора поправке са растом еквивалентне ширине линија и (6) смањење фактора поправке са растом апсорпционе осцилаторне јачине линија.