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On the determination of the solar iron abundance using Fe II lines*

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Abstract. Transition probabilities of lines related to odd terms based on the lowest (^{5}D) parent of Fe II have been calculated using the orthogonal operator approach for both the odd and the even energy levels. The obtained log(gf) values are used to calculate the solar Fe-abundance. The result, A_{Fe} = 7.59 ± 0.06, is the average of the two abundance values proposed in recent literature.

Key words: atomic data – Sun: abundances

1. Introduction

Over the last decade, there has been a lively discussion on the issue of the solar iron abundance. Two conflicting values have been advocated, a 'high' value of 7.67 ±0.03 (Blackwell et al. 1984, Pauls et al. 1990, Blackwell et al. 1995a: BLS, 1995b) and a 'low' value of 7.50±0.07 (Holweger et al. 1990, Biémont et al. 1991: BBKAP, Hannaford et al. 1992, Milford et al. 1994, Holweger et al. 1995). The situation is pictured in Fig. 1, where no attempt has been made to show error bars, as the quoted errors are of different origin (internal v. external) and often not directly comparable.

The investigations are based on faint lines of both neutral and singly ionized iron originating from the solar atmosphere. BLS suggests that in Fe I, the discrepancy can be traced to the use of different line parameters entering the atmospheric model; the important parameters are listed by BLS as A [equivalent width], B [log(gf)], C [micro-turbulence velocity] and D [damping parameter]. A similar explanation for the low abundances obtained using Fe II lines (BBKAP, Hannaford et al. 1992), however, could not be given. The sensitivity to effects A, C and D seems larger in the case of Fe I than for Fe II (BLS, BBKAP), for which non-LTE effects are supposed to be less important as well. Therefore we concentrate on effect B as the main cause of uncertainty in Fe II.

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* The full Table 1 is only available in electronic form at the CDS via anonymous ftp to cdsarc.u-strasbg.fr (130.79.128.5) or via http://cdsweb.u-strasbg.fr/Abstract.html.

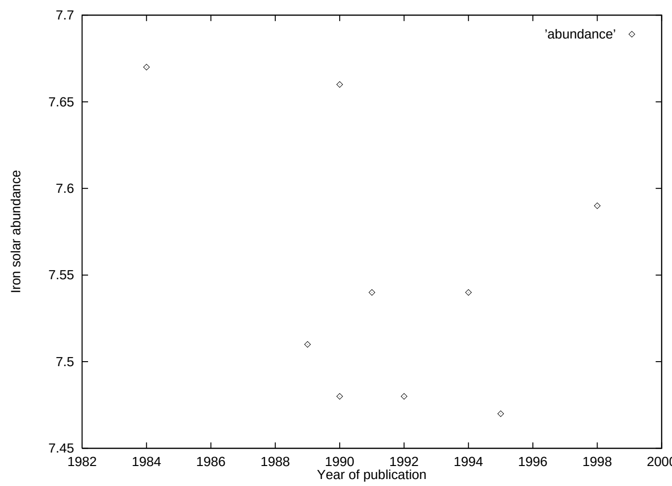

Fig. 1. Overview of recent values for the solar iron abundance

2. Calculational method and the use of orthogonal operators

Transition probability calculations of such complex systems as transition metals with their many closely lying energy levels, require highly accurate eigenvectors. A semi-empirical approach, in which parameters of a model Hamiltonian are adjusted to yield eigenvalues as closely as possible to the experimental energies, is an obvious tool for this purpose. For the production of large quantities of reliable data, Cowan's RCN/RCG suite of programs (Cowan 1981) has gained widespread acceptance; the method is based on the traditional Slater-Condon theory of atomic spectra.

The orthogonal operator method can be seen as a next step in the semi-empirical description of complex spectra. Orthogonal operators (Hansen et al. 1988), have the marked advantage that the parameters in a least squares fit of model Hamiltonian eigenvalues to observed energy levels are as independent and stable as possible. Therefore small (and traditionally neglected) higher order magnetic and electrostatic effects can be introduced in the fitting procedure as well. As a result, the mean error σ of the fit is reduced by an order of magnitude in a physically significant way. In spite of the sometimes large number of parameters, the number of parameters actually $varied$ is in

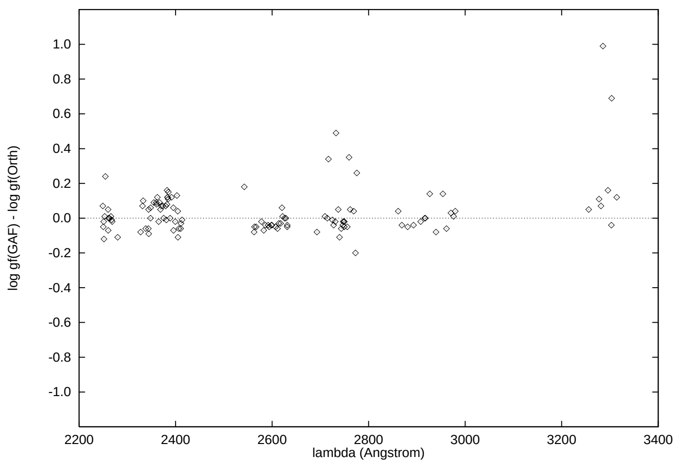

Fig. 2. Difference between experimental (GAF) and our calculated log(gf) values

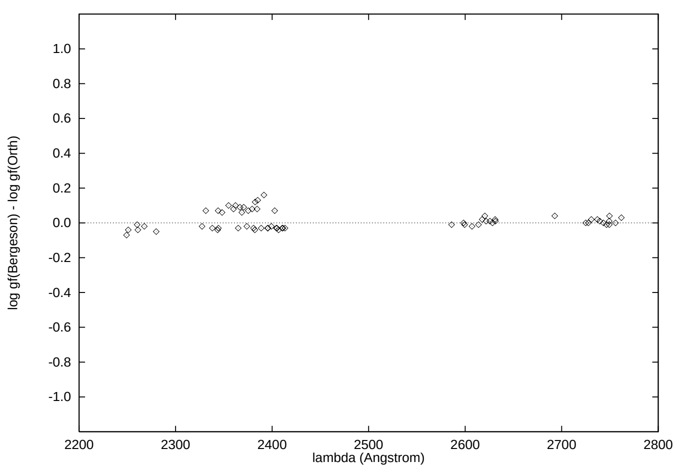

Fig. 3. Difference between experimental (Bergeson et al.) and our calculated log(gf) values

many cases about the same as in the traditional Slater-Condon method. Even without varying the remaining additional parameters, the orthogonal operator method still provides an improved description of complex spectra (Raassen and Uylings 1996). In a critical evaluation of experimental and computational transition probabilities in singly ionized transition elements (Raassen & Uylings 1998) the orthogonal operator method is shown to have good agreement with the most recent experimental data.

Angular coefficients of the transition matrix in pure LS coupling are found from straightforward Racah algebra, and multiplied with the transition integrals (after correction for core polarization, generally yielding a reduction of 5-10%) obtained from a relativistic Hartree-Fock program (MCDF from Parpia et al. 1996). Then the pure but unphysical LS transition matrix is transformed into the actual intermediate coupling by means of the eigenvectors obtained from the orthogonal operator approach. The squared matrix elements of this final transition matrix yield the line strengths and thereby the log(gf) or the A-values (Raassen & Uylings 1997, Uylings & Raassen 1997). Computational details of the method can be found in the above references.

The agreement between experiment and our method is exemplified in Figs. 2 and 3. Numerical details can be found in Table 1; a specimen of the full table available at CDS is included in the paper. The experimental data for Fig. 2 are taken from the critical compilation by Giridhar and Ferro 1995 using data from Kroll and Kock 1987. The difference between the log(gf) values given by Giridhar and Ferro 1995 and our log(gf) values is displayed. In Fig. 2, there are eight lines for which the difference between the experimental value and our value is ≥ 0.2. Only for one of these lines the experimental transition probability is lower than our calculated value, while for the others the experimental transition probabilities are constantly higher than our calculated values. This is not expected when the calculations fail. For one of them (the line at 328.541 nm, showing the largest difference between experiment and our value) Kroll and Kock 1987 mentioned already that the line behaves as a Fe I and that 80% of the line intensity is due to the Fe I line. The same (i.e. blending) might be true for the other lines for which the experimental value is far stronger than the calculated one.

The most recent experimental data by Bergeson et al. 1996 are taken for Fig. 3 which shows the difference between the log(gf) values of Bergeson et al. 1996 and our values. The list of Bergeson et al. contains less data and covers a smaller wavelength range; lines from Giridhar and Ferro exhibiting large deviations were not measured by Bergeson et al.

Fig. 2 supports the suggestion above that some of the stronger lines might be affected by blending. Focusing on differences between -0.2 and +0.2 the spread in values is smaller for the more recent Bergeson et al. data.

In most cases the magnetic effects within one particular configuration are dominant but configuration interaction cannot be neglected. Apart from the effective operators that take into account higher order correlation, the energy matrices were built from the configurations

($3d^7$+$3d^6 4s$+$3d^5 4s^2$+$3d^6 4d$+$3d^6 5s$+$3d^6 5d$+$3d^6 6s$+$3d^5 4p^2$ +$3d^5 4s4d$+$3d^5 4s5d$) for the even system and from the configurations ($3d^6 4p$+$3d^5 4s4p$+$3d^4 4s^2 4p$+$3d^6 5p$+$3d^6 4f$) for the odd system.

Everyone further interested in orthogonal operators is invited to contact the authors or to visit our Internet address ftp://nucleus.phys.uva.nl in the directory pub/orth.

3. Results

In this paper we focus on BBKAP: 'The solar abundance of iron: a "final" word!'. Reason for this limitation is two-fold: firstly, in BBKAP the iron abundance is obtained from Fe II lines and secondly, calculated log(gf) values given in that paper play a crucial role in the abundance determination; this agrees with our report in both respects. We show in Table 2 the lifetimes given by Guo et al. 1992 and Biémont et al. and values obtained using the orthogonal operator technique. Our calculated values give better agreement with experiment than the values given

Table 1. Comparison of recent experimental log(gf) values and values obtained by means of the orthogonal operator technique. An * in front of the orthogonal log(gf) values means a difference between the experimental and our calculated log(gf) value ≥ 0.2.

λ(Å)	log(gf) GAF[a]	log(gf) Bergeson[b]	log(gf) Orth[c]	J_f	E_f(cm^{-1})	even	J_i	E_i(cm^{-1})	odd
2260.860	−2.01	−2.05	−2.01	1.5	862.61	$2\|^5_4D)^6D$	2.5	45079.88	$1\|^5_4D)^4F$
2260.240	−2.36		−2.29	.5	977.05	$2\|^5_4D)^6D$	.5	45206.45	$1\|^5_4D)^4D$
2260.081	−1.55	−1.61	−1.60	4.5	.00	$2\|^5_4D)^6D$	4.5	44232.51	$1\|^5_4D)^4F$
2254.406	−2.85		*−3.09	1.5	862.61	$2\|^5_4D)^6D$	.5	45206.45	$1\|^5_4D)^4D$
2253.127	−1.60		−1.61	3.5	384.79	$2\|^5_4D)^6D$	3.5	44753.80	$1\|^5_4D)^4F$
2251.556	−2.48		−2.36	3.5	384.79	$2\|^5_4D)^6D$	2.5	44784.76	$1\|^5_4D)^4D$
2250.936	−1.85	−1.87	−1.83	2.5	667.68	$2\|^5_4D)^6D$	2.5	45079.88	$1\|^5_4D)^4F$
2250.176	−2.34		−2.29	1.5	862.61	$2\|^5_4D)^6D$	1.5	45289.80	$1\|^5_4D)^4F$
2249.180	−1.60	−1.74	−1.67	4.5	.00	$2\|^5_4D)^6D$	3.5	44446.88	$1\|^5_4D)^4D$

[a] Giridhar and Ferro 1995
[b] Bergeson et al. 1996
[c] This work

Table 2. Lifetime values (in ns) as measured and calculated by Biémont (sextet terms) and Guo (quartet terms) and calculated in this work

Term	J-value	Theory[a]	Exp.[a]	Theory[b]
z^6D	9/2	3.41	3.70(6)	3.66
	7/2	3.43	3.68(7)	3.69
	5/2	3.44	3.63(8)	3.71
	3/2	3.45	3.83(10)	3.71
	1/2	3.45	3.76(10)	3.71
z^6F	11/2	2.83	3.19(4)	2.97
	9/2	2.89	3.24(6)	3.03
	7/2	2.92	3.26(10)	3.06
	5/2	2.93	3.33(9)	3.07
	3/2	2.94	3.34(10)	3.08
z^6P	7/2	3.28	3.73(5)	3.43
	5/2	3.26	3.83(7)	3.41
Term	J-value	Theory[c]	Exp.[c]	Theory[b]
z^4D	7/2	2.43	3.02(7)	3.21
	5/2	2.44	3.10(8)	3.22
z^4F	9/2	3.34	3.87(9)	3.92
	7/2	3.22	3.63(11)	3.74
	5/2	3.26	3.75(14)	3.78
z^4P	5/2	2.97	3.43(9)	3.54
	3/2	2.96	3.44(11)	3.54

[a] Biémont et al. 1991
[b] This work
[c] Guo et al. 1992

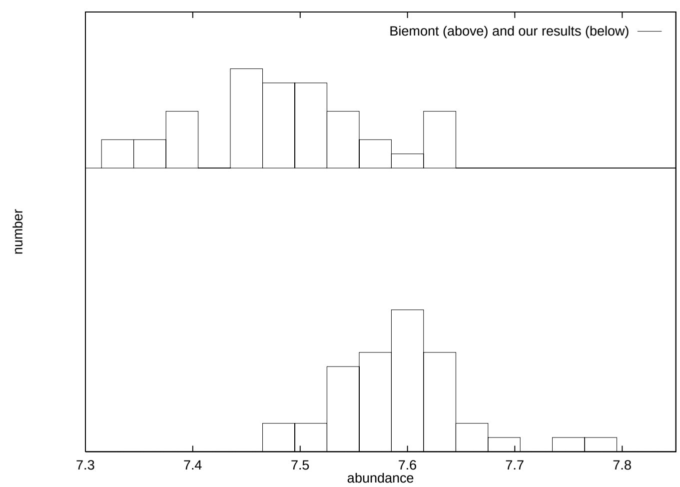

Fig. 4. Counts per abundance for the solar iron abundance, based on the data by Biémont and our results

by BBKAP which were calculated by Kurucz using the Cowan RCN/RCG suite mentioned above. Biémont et al. corrected for the average deviation between calculated and experimental lifetimes in a global way by introducing a correction of 0.05 dex in the determination of the solar Fe II abundance.

Lifetimes are mainly obtained from strong transitions, while solar abundances are determined from weak lines to avoid saturation and broadening mechanisms. In the calculation, strong and weak line strengths have quite different sources of error, the latter being predominantly determined by small admixtures in the pertinent eigenvectors. As the acquisition of accurate eigenvectors is a strong point of the orthogonal operator technique, it can be expected that our calculated weak transitions are better than those given by BBKAP. Based on their calculated log(gf) values BBKAP support the 'low' abundance case. It is interesting, however, that if we substitute our new calculated log(gf) values into Table 3 of BBKAP, a considerably higher value of 7.59 is obtained. The Fe II lines, log(gf) values and abundances (corrected for log N_H = 12) are given in Table 3. From the mean deviations in the abundances shown in Table 3, 0.08 for BBKAP and 0.06 in this work, an additional argument in support of the correctness of our approach is obtained.

To explain why the abundances of BBKAP are generally lower, we would need more detailed information on their calculations. Apparently, their global correction of 0.05 dex does not suffice. We expect that apart from a different eigenvector composition, larger radial transition integrals were adapted by

Table 3. Solar Fe II lines, log(gf) values and modified abundances

λ(Å)	log(gf)[a]	log(gf)[b]	A^a_{Fe}	A^b_{Fe}	J_f	E_f(cm^{-1})	LS-name	J_i	E_i(cm^{-1})	LS-name
4128.748	−3.470	−3.576	7.40	7.51	2.5	20830.58	$2\|^3_4$P)^{4}P	1.5	45044.17	$1\|^5_4$D)^{4}D
4491.405	−2.684	−2.761	7.54	7.62	1.5	23031.30	$2\|^3_4$F)^{4}F	1.5	45289.80	$1\|^5_4$D)^{4}F
4508.288	−2.312	−2.344	7.44	7.47	1.5	23031.30	$2\|^3_4$F)^{4}F	.5	45206.45	$1\|^5_4$D)^{4}D
4576.340	−2.822	−2.960	7.40	7.54	2.5	22939.36	$2\|^3_4$F)^{4}F	2.5	44784.76	$1\|^5_4$D)^{4}D
4582.835	−3.094	−3.223	7.45	7.58	2.5	22939.36	$2\|^3_4$F)^{4}F	3.5	44753.80	$1\|^5_4$D)^{4}F
4620.521	−3.079	−3.290	7.35	7.56	3.5	22810.36	$2\|^3_4$F)^{4}F	3.5	44446.88	$1\|^5_4$D)^{4}D
4635.316	−1.275	−1.579	7.37	7.66	2.5	48039.09	$1\|^2_1$D)	3.5	69606.55	$1\|^3_4$G)^{2}F
4656.981	−3.552	−3.656	7.44	7.54	2.5	23317.63	$3\|^6_5$S)^{6}S	2.5	44784.76	$1\|^5_4$D)^{4}D
4670.182	−3.904	−4.110	7.40	7.61	2.5	20830.58	$2\|^3_4$P)^{4}P	3.5	42237.03	$1\|^5_4$D)^{6}F
4720.149	−4.525	−4.814	7.49	7.78	1.5	25787.60	$2\|^3_4$P)^{2}P	2.5	46967.44	$1\|^5_4$D)^{4}P
4993.358	−3.485	−3.695	7.33	7.54	4.5	22637.21	$2\|^3_4$F)^{4}F	3.5	42658.22	$1\|^5_4$D)^{6}P
5000.743	−4.390	−4.611	7.32	7.54	.5	22409.85	$2\|^3_4$P)^{4}P	1.5	42401.30	$1\|^5_4$D)^{6}F
5100.664	−4.135	−4.222	7.47	7.56	4.5	22637.21	$2\|^3_4$F)^{4}F	3.5	42237.03	$1\|^5_4$D)^{6}F
5132.669	−3.901	−4.125	7.40	7.62	4.5	22637.21	$2\|^3_4$F)^{4}F	4.5	42114.82	$1\|^5_4$D)^{6}F
5136.802	−4.323	−4.366	7.50	7.54	2.5	22939.36	$2\|^3_4$F)^{4}F	1.5	42401.30	$1\|^5_4$D)^{6}F
5197.577	−2.233	−2.342	7.49	7.60	2.5	26055.42	$2\|^3_4$G)^{4}G	1.5	45289.80	$1\|^5_4$D)^{4}F
5234.625	−2.151	−2.273	7.45	7.57	3.5	25981.63	$2\|^3_4$G)^{4}G	2.5	45079.88	$1\|^5_4$D)^{4}F
5325.553	−3.222	−3.315	7.53	7.62	3.5	25981.63	$2\|^3_4$G)^{4}G	3.5	44753.80	$1\|^5_4$D)^{4}F
5414.073	−3.750	−3.645	7.64	7.53	3.5	25981.63	$2\|^3_4$G)^{4}G	3.5	44446.88	$1\|^5_4$D)^{4}D
5425.257	−3.372	−3.382	7.64	7.65	4.5	25805.33	$2\|^3_4$G)^{4}G	4.5	44232.51	$1\|^5_4$D)^{4}F
5732.724	−4.667	−4.632	7.54	7.51	3.5	27314.92	$2\|^3_4$F)^{2}F	3.5	44753.80	$1\|^5_4$D)^{4}F
5991.376	−3.557	−3.663	7.50	7.61	5.5	25428.78	$2\|^3_4$G)^{4}G	4.5	42114.82	$1\|^5_4$D)^{6}F
6084.111	−3.808	−3.892	7.52	7.60	4.5	25805.33	$2\|^3_4$G)^{4}G	3.5	42237.03	$1\|^5_4$D)^{6}F
6149.258	−2.724	−2.837	7.48	7.59	.5	31368.45	$2\|^3_4$D)^{4}D	.5	47626.08	$1\|^5_4$D)^{4}P
6179.384	−2.602	−2.686	7.51	7.59	3.5	44915.05	$2\|^1_4$F)^{2}F	2.5	61093.41	$1\|^3_4$P)^{2}D
6239.953	−3.439	−3.570	7.46	7.59	.5	31368.45	$2\|^3_4$D)^{4}D	1.5	47389.78	$1\|^5_4$D)^{4}P
6247.557	−2.329	−2.431	7.48	7.58	2.5	31387.95	$2\|^3_4$D)^{4}D	1.5	47389.78	$1\|^5_4$D)^{4}P
6369.462	−4.253	−4.251	7.56	7.56	2.5	23317.63	$3\|^6_5$S)^{6}S	1.5	39013.21	$1\|^5_4$D)^{6}D
6383.722	−2.271	−2.413	7.60	7.74	2.5	60445.28	$3\|^4_5$D)^{4}D	2.5	44784.76	$1\|^5_4$D)^{4}D
6416.919	−2.740	−2.874	7.56	7.69	2.5	31387.95	$2\|^3_4$D)^{4}D	2.5	46967.44	$1\|^5_4$D)^{4}P
6432.680	−3.708	−3.708	7.63	7.63	2.5	23317.63	$3\|^6_5$S)^{6}S	2.5	38858.96	$1\|^5_4$D)^{6}D
6446.410	−2.073	−2.087	7.58	7.59	3.5	50187.81	$2\|^3_2$F)^{4}F	4.5	65696.04	$1\|^3_4$G)^{4}G
6456.383	−2.075	−2.182	7.46	7.57	3.5	31483.18	$2\|^3_4$D)^{4}D	2.5	46967.44	$1\|^5_4$D)^{4}P
6516.081	−3.450	−3.455	7.64	7.64	2.5	23317.63	$3\|^6_5$S)^{6}S	3.5	38660.04	$1\|^5_4$D)^{6}D
7222.394	−3.295	−3.395	7.54	7.64	1.5	31364.44	$2\|^3_4$D)^{4}D	.5	45206.45	$1\|^5_4$D)^{4}D
7224.487	−3.243	−3.351	7.52	7.63	.5	31368.45	$2\|^3_4$D)^{4}D	.5	45206.45	$1\|^5_4$D)^{4}D
7479.694	−3.588	−3.627	7.44	7.48	2.5	31387.95	$2\|^3_4$D)^{4}D	3.5	44753.80	$1\|^5_4$D)^{4}F
7515.832	−3.432	−3.542	7.51	7.62	3.5	31483.18	$2\|^3_4$D)^{4}D	2.5	44784.76	$1\|^5_4$D)^{4}D
7711.724	−2.543	−2.674	7.48	7.61	3.5	31483.18	$2\|^3_4$D)^{4}D	3.5	44446.88	$1\|^5_4$D)^{4}D
Mean	value		7.49(8)	7.59(6)						

[a] Biémont et al. 1991
[b] This work

BBKAP. As mentioned earlier, the general effect of including core polarization is to reduce the radial integrals, but the reduction is not the same for different transitions and can therefore not be corrected for in a global way, especially in the case of weak lines.

A more detailed study of the data is given in the Figs. 4 and 5. The Fig. 4 shows the number of spectral lines resulting in a specific abundance in the form of two histograms. The upper one is taken from Biémont and the lower one is based on our results. Apart from a shift it is clear that our distribution is far more pronounced, while the one taken from Biémont shows an unexpected minimum around 7.42 and a value around 7.63 which is too high.

In the Fig. 5 the relation between the abundance and the wavelength is given. From this figure it can be seen that below 5300 Å the values given by Biémont are considerably lower than above 5300 Å. Averaging Biémonts values for the two wavelength regions yields an abundance of 7.43(6) in the region below 5300 Å and 7.54(6) above 5300 Å. Of course both values have to be augmented again with 0.05 dex. This results in values for Biémonts model and Kurucz data of 7.48 and 7.59 respectively, resulting in an average abundance of 7.54 as given

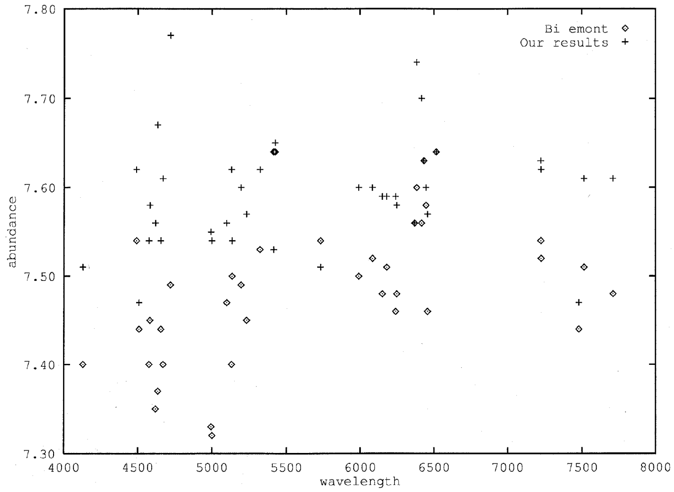

Fig. 5. Solar iron abundances relative to the wavelength range

by Biémont. His value above 5300 Å (with correction at 7.59) agrees very well with our value. It should be noticed that the discrepancy between the low wavelength value and high wavelength value of Biémont is 0.11 dex. This is about the same value as the whole discussion is about (the difference between the “low” and “high” abundance).

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