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log *gf* values for astrophysically important transitions Fe II

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ABSTRACT

Aims. In a recent measurement, Meléndez & Barbuy (2009, A&A, 497, 611) report accurate log *gf* values for 142 important astrophysical lines with wavelengths in the range 4000 Å to 8000 Å. Their results include both solar and laboratory measurements. In this paper, we describe a theoretical study of these lines.
Methods. The CIV3 structure codes, combined with our "fine-tuning" extrapolation process, are used to undertake a large-scale CI calculation involving the lowest 262 fine-structure levels belonging to the $3d^64s$, $3d^7$, $3d^54s^2$, $3d^64p$, and $3d^54s4p$ configurations.
Results. We find that many of the 142 transitions are very weak intercombination lines. Other transitions are weak because the dominant configurations in the two levels differ by two orbitals.
Conclusions. The comparison between our log *gf* values and the experimental values generally shows good agreement for most of these transitions, with our theoretical values agreeing slightly more closely with the solar than with the laboratory measurements. A detailed analysis of the small number of transitions for which the agreement between theory and experiment is not as good shows that such disagreements largely arise from severe cancellation due to CI mixing.

Key words. atomic data – relativistic processes – methods: numerical

1. Introduction

The Goddard High Resolution Spectrograph (GHRC) and the more recent Space Telescope Imaging Spectrograph (STIS) onboard the *Hubble* Space Telescope (HST) have produced many iron lines, particularly lines of Fe II, over a wide wavelength range. With the ground-based high-resolution fibre-fed echelle spectrograph mounted on the 3.6-m telescope at ESO-La Silla Observatory under the HARPS GTO scheme, new spectroscopic parameters for different ions, including Fe II, are emerging. In one such measurement, Sousa et al. (2008) has reported log *gf* values for 263 Fe I and 36 Fe II weak lines and were subsequently used to determine iron abundances. Meléndez & Barbuy (2009) have presented log *gf* values for weak 142 Fe II lines. These solar and laboratory measurements, claimed to be accurate and precise, included the Fe II lines measured by Sousa et al. (2008). For the transitions in common in these two independent measurements, there is generally good agreement. In the present investigation, we have undertaken a large-scale calculation in which we represent the wave functions of the levels involved in these (and other) transitions by means of configuration interaction (CI) expansions. We are then able to compare our calculated oscillator strengths with the experimental results given by Sousa et al. (2008) and by Meléndez & Barbuy (2009). A preliminary report was given in the proceedings of the XXVIIth ICPEAC conference (Deb & Hibbert 2012).

2. Method of calculation

Our group has undertaken a number of recent CI calculations of transitions in Fe II. There are many similarities in the approaches

we have adopted in these calculations, but the method of optimisation of some of the orbitals has varied from calculation to calculation. Corrégé & Hibbert (2005, 2006) used orbitals up to 7s, 7p, 6d, and 4f to study a number of transitions involving $3d^6nl$ and $3d^54s^2$ or $3d^54s4p$ states. One of the difficulties that arise is the significant variation in the form of the optimal 3d function between different states. For transitions between levels of these configurations, the 3d orbital that appears in the dipole matrix elements is represented best by the Hartree-Fock orbital of the $3d^64s$ ^6D state. Subsequently, we (Deb & Hibbert 2010a,b, 2011) studied forbidden transitions, but since many of the transitions involve the $3d^7$ levels, we chose the 3d function to be the HF function for the $3d^7$ ^4F state. However, in all our calculations, the remaining d-functions were used to account for the variation in the form of the optimal 3d function in different configurations. In the present work we have reverted to the orbitals given by Corrégé & Hibbert (2005), since the transitions reported by Meléndez & Barbuy (2009) mostly have the form $3d^64s$–$3d^64p$.

The CIV3 program of Hibbert (1975), Hibbert et al. (1991) has been used to carry out the present structure calculation of Fe II. The form of the CI wave functions is, in LSJ coupling,

$$\Psi(J) = \sum_{i=1}^{M} a_i \Phi_i(\alpha_i L_i S_i J). \tag{1}$$

In (1), Φ_i represents a configuration state function (CSF) which is constructed from a common set of one-electron orbitals of the form

$$\frac{1}{r} P_{nl}(r) Y_l^{m_l}(\theta, \phi) \chi_{m_s}(\sigma) \tag{2}$$

where Y is a spherical harmonic, χ a spin function (often denoted by α or β for $m_s = \frac{1}{2}$ or $-\frac{1}{2}$, respectively), and the radial functions

in (2) are expressed in analytic form as linear combinations of normalised Slater orbitals (STOs):

$$P_{nl}(r) = \sum_{j=1}^{k} c_{jnl} \eta_{jnl}(r), \tag{3}$$

and where the STOs take the form

$$\eta_{jnl}(r) = \left[\frac{(2\xi_{jnl})^{2I_{jnl}+1}}{(2I_{jnl})!} \right]^{1/2} r^{I_{jnl}} \exp(-\xi_{jnl}r). \tag{4}$$

Also in (1), α_i represents the angular momentum coupling scheme and other necessary labelling, and a_i is the corresponding component of the eigenvector, associated with this wave function, of the diagonalised Hamiltonian matrix whose typical element is $H_{ij} = \langle \Phi_i | H | \Phi_j \rangle$.

We have sought to represent the 262 fine-structure levels belonging to the $3d^6 4s$, $3d^7$, $3d^5 4s^2$, $3d^6 4p$, and $3d^5 4s4p$ configurations with energies up to $88\,615$ cm^{-1}. We treat this set of configurations as our reference set. Beyond this energy, levels of the $3d^6 5p$ configuration begin to appear in the spectrum, and some of the wave functions require careful treatment of CI mixing, particularly between $3d^6 5p$ and $3d^5 4s4p$. The work of Corrégé & Hibbert (2005) was specifically focussed on this type of mixing, but the transitions reported by Meléndez & Barbuy (2009) involve levels lying well below any of the $3d^6 5p$ levels. Below energies of $88\,615$ cm^{-1}, there are a few levels that belong to the $3d^6 4d$ and $3d^6 5s$ configurations, but they do not show any significant coupling with the even levels considered in the present calculations. Similarly, because we have not included $3d^6 5p$ in the reference set, the mixing between $3d^6 5p$ and $3d^5 4s4p$ will not be correctly represented.

Corrégé & Hibbert (2005, 2006) were able to include only a few sextet and quartet states, in order to keep the configuration size manageable, and so no doublets were included in their calculation. Nor did they include the $3d^7$ configuration. In the present calculation, we include all doublets, quartets, sextets, and one octet belonging to the above configurations and below $88\,615$ cm^{-1}. The configuration set in the present calculation is therefore significantly larger that those in Corrégé & Hibbert (2005, 2006).

The set of configurations was chosen in two steps: (a) keeping subshells up to 3p filled, we included single and double replacements of orbitals from the outer shells by any of the available orbitals, for each configuration in the reference set; (b) then we included configurations formed by replacing up to two orbitals (in total) from the 3s and 3p subshells by available orbitals up to $n = 6$. This produced a large number of separate configuration state functions (CSFs).

For each LSπ symmetry, we first undertook a calculation in LS coupling. We found that a significant number of the CSFs had very small eigenvector components, so we deleted those whose $|a_i|$ had a value less than 0.001. In previous calculations, we found that such a cut-off made very little difference to the calculated energies or to the eigenvector components of the remaining CSFs.

Relativistic effects were introduced in the Breit-Pauli approximation, with the following operators: mass correction and Darwin terms, and a modified spin-orbit term H_{so} that allows for both the nuclear spin-orbit effect and the main part of the spin-other-orbit effect:

$$H_{so} = \frac{\alpha^2}{2} Z \sum_{i=1}^{N} \frac{\zeta(l)}{r_i^3} (\mathbf{l}_i \cdot \mathbf{s}_i), \tag{5}$$

Table 1. Number of CSFs used.

J	Even	Odd
0.5	7862	27 070
1.5	14 180	45 494
2.5	17 132	52 187
3.5	14 514	50 820
4.5	11 141	43 433
5.5	5620	31 340
6.5	1913	17 909
7.5		6569

where $\zeta(l)$ is a parameter that only depends on the l-value of the interacting electrons in the Breit-Pauli Hamiltonian matrix element. The values of the parameters $\zeta(l)$ were chosen so that, for certain key CSFs, the matrix element of H_{so} reproduces the sum of the matrix elements of the full spin-orbit and spin-other-orbit operators. This process is then independent of the numbers or types of the CSFs included in the CI expansions. The most suitable parameters were found to be $\zeta(s) = 0.0$, $\zeta(p) = 0.88$, $\zeta(d) = 0.59242$, and $\zeta(f) = 0.52908$. The number of CSFs included in our calculation, for each J-value, is given in Table 1.

Finally, we adopted our customary practice of "fine-tuning", whereby we make small adjustments to the Hamiltonian matrix elements so as to bring the calculated energy differences (i.e., above the ground state) as closely as possible into line with experimental values.

3. Results and discussions

The oscillator strengths determined by Meléndez & Barbuy (2009) are all weak. Most correspond either to intercombination lines (E1 transitions that in LS coupling would be zero but become non-zero when spin-orbit mixing is introduced, resulting in the upper and lower levels of the transitions being described by wave functions containing CSFs with the same J but different L or S) or to transitions in which the dominant CSFs of the two levels differ by more than one orbital. In the latter case, a single configuration approximation would again result in a zero oscillator strength, assuming orthogonal orbitals, but configuration mixing makes a non-zero result possible. Moreover, in the calculation of many of these transitions, configuration mixing results in cancellation of contributions from different CSFs, and in some cases this cancellation is substantial, lowering the oscillator strength by one or occasionally more orders of magnitude.

An interesting and important example is provided by the three transitions of multiplet 42. These are usually described as $3d^5 4s^2\ ^6S_{5/2}$–$3d^6 4p\ ^6P^o_J$, with $J = 3/2, 5/2, 7/2$: a notionally two-electron change between upper and lower levels. The non-zero nature of the calculated oscillator strength arises because of mixing of the dominant CSF of the lower level with $3d^5 4p^2$ and the dominant CSF of the upper level with $3d^5 4s4p$ CSFs, primarily the latter. These additional CSFs have direct dipole interactions with the dominant CSF of the opposite parity and are the main contributors to the oscillator strengths. The calculated oscillator strengths are therefore very sensitive to the degree of this mixing.

Some comparative results for the three transitions are displayed in Table 2. Our work is in very close agreement with the experimental determinations of Meléndez & Barbuy (2009). The earlier calculations of Raassen & Uylings (1998, 1999) give gf values that are almost a factor of two lower than ours, and are somewhat similar to the values given previously by Kurucz (1988) and in later revisions of his database, though these are

Table 2. log gf values for the multiplet 42 transitions.

Source	Upper state		
	$^6P^o_{3/2}$	$^6P^o_{5/2}$	$^6P^o_{7/2}$
This work	−1.29	−1.12	−1.03
Meléndez & Barbuy (2009)	−1.26	−1.10	−1.00
Kroll & Kock (1987)	−1.24		−0.87
Schnabel et al. (2004)	−1.21		−0.87
Raassen & Uylings (1999)	−1.50	−1.35	−1.25
Kurucz (1988)	−1.56	−1.40	−1.30
Kurucz & Bell (1995)	−1.32	−1.22	−0.87

even lower. On the other hand, the current (2013) tabulation on the CD of Kurucz & Bell (1995) shows values that have been substantially revised; although these are closer to ours, the ratios of the three oscillator strengths (or differences between log gf values) do not match either those of other authors or of the present calculation. Our work therefore shows a clear preference for the results of Meléndez & Barbuy (2009), and the closeness of the agreement is encouraging, given the sensitivity to CI mixing in our work.

The full comparison between our results and the experimental results of Meléndez & Barbuy (2009) is shown in Table 3. The close agreement between theory and experiment seen for the multiplet 42 continues for many of the 142 transitions displayed in Table 3, even though the calculated values involve substantial CI mixing and often CI cancellation. For some transitions, the agreement between calculated and experimental oscillator strengths is within 10%, though for many transitions the results differ by around 25%, which is still good for such weak transitions. In any case for some transitions, this size of difference occurs between the results of Meléndez & Barbuy (2009) and of Sousa et al. (2008). For some, though, there is a difference of about a factor of two, while in two cases, there are greater discrepancies: at $\lambda6433$, the difference is two orders of magnitude; at $\lambda6508$, the difference is more than four orders of magnitude.

We briefly examine three specific transitions, to see why such a variation in difference occurs.

3.1. $\lambda6416.91$ Å

For this transition, our result is almost identical to that of Meléndez & Barbuy (2009). It corresponds to the transition $3d^6(^3D)4s\ ^4D_{5/2}$–$3d^6(^5D)4p\ ^4P^o_{5/2}$, with the levels labelled by the dominant CSF in each case. With the assumption of orthogonal orbitals, the oscillator strength would be zero, because of the different resultant angular momenta of the two $3d^6$ cores. The actual non-zero result of our calculations arises through the mixing of $3d^6(^5D)4p\ ^4P^o_{5/2}$ with $3d^6(^3D)4p\ ^4P^o_{5/2}$, even though the a_i^2 for the second CSF is only 0.02. This second CSF in the odd parity state has a direct dipole interaction with the dominant even parity CSF. All other such interactions are minor in comparison. The agreement with the experimental result suggests that our fine-tuning process is successful in obtaining mixing coefficients that are reasonably accurate.

3.2. $\lambda4515.33$ Å

This transition corresponds to $3d^6(^3F2)4s\ ^4F_{5/2}$–$3d^6(^5D)4p\ ^4F^o_{5/2}$. Our oscillator strength is more than double the value of Meléndez & Barbuy (2009). The lower level exhibits strong

mixing with $3d^6(^3F1)4s\ ^4F_{5/2}$ (the 3d cores can also be written in terms of seniority as ^3_4F and ^3_2F). This mixing gives contributions to the dipole matrix element that are additive, and if the strength of the mixing were in error, there would be little effect on the total. However, these contributions arise from the mixing of both $3d^6(^3F2)4p\ ^4F^o_{5/2}$ and $3d^6(^3F1)4p\ ^4F^o_{5/2}$ in the wave function for $3d^6(^5D)4p\ ^4F^o_{5/2}$. Again, this mixing has an additive effect on the oscillator strength, which makes it less sensitive to errors in the CI mixing coefficients. Other mixing in the lower level with $3d^6(^5D)4s\ ^4D$ and $3d^7\ ^4F$ has a smaller but again non-cancelling effect on the oscillator strength. It would seem that the calculated oscillator strength could only be reduced through the CI mixings being too strong, though changes by a factor of two would be surprising.

3.3. $\lambda6508.12$ Å

This is the transition for which our oscillator strength is four orders of magnitude below the experimental value determined by Meléndez & Barbuy (2009). It corresponds to the transition $3d^6(^5D)4p\ ^4F^o_{5/2}$–$3d^54s^2\ ^4D_{3/2}$. There are two orbitals that are different in the dominant CSFs of the two levels so that again the single configuration result for the oscillator strength would be zero: the non-zero result is obtained through CI mixing.

To compare the effects of mixing arising from different CSFs, it is convenient to define

$$F_{ij} = \left(\frac{2\Delta E}{3g_l}\right)^{1/2} a_i^l a_j^u \left\langle \Phi_i^l | \text{Op} | \Phi_j^u \right\rangle$$

where l and u denote the lower and upper levels of the transition, ΔE is the transition energy, and Op is the appropriate dipole operator. Then the oscillator strength is given simply by

$$f = \left(\sum_i \sum_j F_{ij}\right)^2.$$

For this particular transition, the main contributions to the dipole integral are displayed in Table 4.

There is severe cancellation within the final four interactions owing to the interaction between $3d^6(^5D)4p\ ^4F$ with $3d^6(^5D)4p\ ^4D$, resulting in a net contribution of 0.009 to the total of $100F_{ij}$. A similar degree of cancellation occurs amongst the first three interactions listed, with a combined contribution of −0.049, resulting in a total of −0.040 for these seven interactions, which is a factor of more than 20 smaller than the largest of the individual contributions. At this point, other contributions of a similar magnitude to the total of these seven make a significant contribution: with the seven alone, the oscillator strength would be 1.6×10^{-7}, whereas when all contributions are included, the oscillator strength reduces still further to 2.1×10^{-9}.

One possible source of error in the calculation is therefore the loss of significant figures arising from these cancellations. Moreover, the relevant mixing coefficients are themselves small. Their values are shown in Table 5.

The magnitude of at least one of the a_i in each of the key interactions is itself very small, and is perhaps open to change if more CSFs were to be added to the wave function expansions. In view of the extent of the cancellation effects, the calculated oscillator strength for this particular transition is much less reliable than those of other transitions in Table 3.

Table 3. Comparison of our log gf values with solar (S) and laboratory (L) measurements of Meléndez & Barbuy (2009).

λ (Å)	MB	Present	λ (Å)	MB	Present	λ (Å)	MB	Present
4648.94	−4.58[S]	−4.45	6371.12	−3.13[S]	−4.19	4549.47	−2.09[L]	−1.95
4670.18	−4.09[S]	−4.08	6383.72	−2.24[S]	−2.39	4555.89	−2.40[L]	−2.14
4720.15	−4.48[S]	−3.92	6385.45	−2.59[S]	−2.58	4576.34	−2.95[L]	−3.19
4825.74	−4.87[S]	−4.83	6416.91	−2.64[S]	−2.63	4582.83	−3.18[L]	−2.95
4831.13	−4.89[S]	−4.79	6433.81	−2.37[S]	−4.41	4583.83	−1.93[L]	−1.78
4833.19	−4.64[S]	−4.55	6442.95	−2.44[S]	−2.45	4601.37	−4.48[L]	−4.34
4833.86	−5.11[S]	−5.02	6446.41	−1.97[S]	−1.84	4620.52	−3.21[L]	−3.67
4839.99	−4.75[S]	−4.66	6455.83	−2.92[S]	−3.06	4625.89	−2.35[L]	−2.41
4855.55	−4.46[S]	−4.27	6456.38	−2.05[S]	−1.94	4629.33	−2.34[L]	−2.19
4871.27	−4.25[S]	−3.93	6482.20	−1.78[S]	−1.71	4635.31	−1.42[L]	−1.75
4893.82	−4.21[S]	−4.11	6491.24	−2.76[S]	−2.84	4656.98	−3.60[L]	−3.51
4924.92	−4.90[S]	−4.80	6493.03	−2.55[S]	−2.61	4666.75	−3.28[L]	−3.03
4991.12	−4.55[S]	−4.05	6506.33	−2.68[S]	−2.66	4731.45	−3.10[L]	−2.98
4993.35	−3.62[S]	−3.50	6508.12	−3.45[S]	−7.90	4923.92	−1.26[L]	−1.29
5000.74	−4.61[S]	−4.00	6517.01	−2.73[S]	−2.74	5018.44	−1.10[L]	−1.12
5036.92	−4.67[S]	−4.53	6562.20	−2.83[S]	−2.84	5169.03	−1.00[L]	−1.03
5100.66	−4.17[S]	−4.07	6586.69	−2.74[S]	−2.73	5197.57	−2.22[L]	−2.17
5120.35	−4.24[S]	−4.12	6598.30	−3.05[S]	−3.09	5234.62	−2.18[L]	−2.16
5132.66	−4.08[S]	−3.87	7301.56	−3.63[S]	−3.41	5264.81	−3.13[L]	−2.79
5136.80	−4.43[S]	−4.25	7479.69	−3.61[S]	−3.34	5276.00	−2.01[L]	−2.08
5146.12	−3.91[S]	−3.87				5316.61	−1.87[L]	−1.85
5150.94	−4.48[S]	−4.38	4087.28	−4.57[L]	−4.23	5316.78	−2.74[L]	−2.38
5154.40	−4.13[S]	−4.08	4122.66	−3.26[L]	−2.94	5325.55	−3.16[L]	−3.28
5161.18	−4.47[S]	−4.42	4128.74	−3.63[L]	−3.54	5337.73	−3.72[L]	−3.42
5171.64	−4.54[S]	−4.70	4173.46	−2.65[L]	−2.59	5362.86	−2.57[L]	−2.28
5238.62	−5.11[S]	−5.12	4178.86	−2.51[L]	−2.30	5414.07	−3.58[L]	−3.35
5256.93	−4.06[S]	−4.07	4233.17	−1.97[L]	−1.94	5425.25	−3.22[L]	−3.30
5284.10	−3.11[S]	−3.07	4258.15	−3.33[L]	−3.26	5525.12	−3.97[L]	−3.72
5432.96	−3.38[S]	−3.34	4273.32	−3.38[L]	−3.18	5627.49	−4.10[L]	−3.95
5534.84	−2.75[S]	−2.56	4278.76	−3.73[L]	−3.60	5657.93	−4.03[L]	−3.76
5591.36	−4.44[S]	−4.36	4296.57	−2.92[L]	−2.61	5725.96	−4.76[L]	−4.56
5991.37	−3.54[S]	−3.52	4303.17	−2.56[L]	−2.45	5732.72	−4.60[L]	−4.38
6084.11	−3.79[S]	−3.72	4351.76	−2.25[L]	−2.15	5813.67	−2.51[L]	−2.46
6113.32	−4.14[S]	−4.08	4369.41	−3.65[L]	−3.09	6238.39	−2.60[L]	−2.51
6116.05	−4.67[S]	−4.63	4384.31	−3.44[L]	−3.39	6369.46	−4.11[L]	−4.06
6129.70	−4.64[S]	−4.55	4385.38	−2.66[L]	−2.59	6432.68	−3.57[L]	−3.51
6147.74	−2.69[S]	−2.59	4413.60	−3.79[L]	−3.74	6516.08	−3.31[L]	−3.25
6149.25	−2.69[S]	−2.62	4416.83	−2.65[L]	−2.52	7222.39	−3.26[L]	−3.16
6150.09	−4.73[S]	−4.69	4472.92	−3.36[L]	−3.19	7224.48	−3.20[L]	−3.06
6179.38	−2.62[S]	−2.57	4489.18	−2.96[L]	−2.55	7308.07	−3.03[L]	−2.92
6184.92	−3.72[S]	−3.45	4491.40	−2.71[L]	−2.47	7310.21	−3.37[L]	−3.31
6233.53	−2.51[S]	−2.85	4508.28	−2.44[L]	−2.22	7320.65	−3.23[L]	−3.13
6239.95	−3.41[S]	−3.34	4515.33	−2.60[L]	−2.24	7449.33	−3.27[L]	−3.33
6247.35	−1.98[S]	−2.15	4520.22	−2.65[L]	−2.31	7462.40	−2.74[L]	−2.68
6247.55	−2.30[S]	−2.19	4522.63	−2.25[L]	−2.06	7515.83	−3.39[L]	−3.39
6248.90	−2.67[S]	−2.63	4534.16	−3.28[L]	−3.08	7655.48	−3.56[L]	−3.55
6317.98	−1.96[S]	−2.08	4541.52	−2.98[L]	−2.96	7711.72	−2.50[L]	−2.49
6331.95	−1.88[S]	−1.97	4549.19	−1.62[L]	−1.86			

4. Conclusions

In the previous section we discussed three exemplars of transitions, all of which (as E1 transitions) might normally be expected to be strong but which in fact are weak, sometimes very weak. The type of accuracy that can be expected of theoretical results depends, not on the wavelength of the transition, but on the make-up of the wave functions of the levels involved in each transition and, in particular, on the angular momenta of the $3d^n$ cores.

The characteristic feature of transitions such as the 6416.91 Å line (Sect. 3.1) is that the $3d^6$ cores, while having different LS symmetries in the 4s and 4p states, are mixed mainly with CSFs containing the other symmetry. That is, the main mixing in the $3d^6(L_1S_1)4s$ level is with $3d^6(L_2S_2)4s$, while the one for $3d^6(L_2S_2)4p$ is with $3d^6(L_1S_1)4p$. The close agreement

Table 4. Main contributions F_{ij} to the dipole integral in line $\lambda 6508.12$ Å.

Lower level CSF	Upper level CSF	$100F_{ij}$
$3d^6(^5D)4p\ ^4F$	$3d^6(^5D)4s\ ^4D$	0.232
$3d^5(^4D)\ 4s4p(^1P)\ ^4F$	$3d^54s^2\ ^4D$	–0.863
$3d^5(^4D)\ 4s4p(^1P)\ ^4D$	$3d^54s^2\ ^4D$	0.582
$3d^6(^5D)4p\ ^4F$	$3d^6(^5D)4s\ ^4D$	–0.115
$3d^6(^5D)4p\ ^4F$	$3d^5(^4D)4p^2\ ^4D$	–0.163
$3d^6(^5D)4p\ ^4D$	$3d^6(^5D)4s\ ^4D$	0.119
$3d^6(^5D)4p\ ^4D$	$3d^5(^4D)4p^2\ ^4D$	0.168

Table 5. Significant CI mixing coefficients relevant to the line $\lambda 6508.12$ Å.

CSF	a_i
$3d^6(^5D)4p\ ^4D$	–0.43918
$3d^5(^4D)\ 4s4p(^1P)\ ^4D$	0.02559
$3d^6(^5D)4p\ ^4F$	0.83224
$3d^5(^4D)\ 4s4p(^1P)\ ^4F$	0.02124
$3d^6(^5D)4s\ ^4D$	0.00894
$3d^6(^5D)4d\ ^4D$	0.00110
$3d^5(^4D)4s^2\ ^4D$	–0.92205
$3d^5(^4D)4p^2\ ^4D$	0.16055

between our oscillator strengths and those of Meléndez & Barbuy (2009) encourages us to believe that, for such lines, we have obtained this mixing accurately and therefore also the oscillator strengths.

The characteristic feature of transitions such as 4515.33 Å (Sect. 3.2) is that, in addition, the core angular momenta L_1S_1 and/or L_2S_2 can occur with more than one seniority, and this introduces a further CI mixing that is usually very strong (in that case $^3F2$ and $^3F1$). Our experience is that such mixing is

difficult to achieve accurately. When this occurs, we would be more hesitant about the accuracy of the oscillator strengths.

Lines such as 6508.12 Å (Sect. 3.3) are characterised by a two-electron change between the main CSFs of the two levels $(3d4p \rightarrow 4s^2)$. Frequently for such lines there is severe cancellation in the dipole matrix elements due to strong CI mixing, giving rise to calculated oscillator strengths that can be abnormally low (by several orders of magnitude). Then, different calculations may give very different results, pointing to a need to undertake more extensive and perhaps more focussed calculations for such lines.

In Table 3 we have not given the usual labels for the levels involved in the transitions. In the near future, we plan to submit for publication our full set of results, comprising oscillator strengths of all transitions between levels of the configurations $3d^64s$, $3d^7$, $3d^54s^2$, $3d^64p$, $3d^54s4p$, and also $3d^65p$. The labels of the lower and upper levels of each transition will then be specified.

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