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The FERRUM project: Experimental f-values for 4p-5s transitions in Fe II

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Abstract. New measurements of radiative lifetimes of four $3d^65s$ levels in Fe II at about 10 eV are presented along with absolute oscillator strengths for twenty 4p-5s transitions involving the four levels. The experimental measurements are compared with two different sets of theoretical calculations. The lines are of particular interest in the modeling of HLy α pumped fluorescence of Fe II in astrophysical plasmas.

Key words. atomic data – line: identification – methods: laboratory

1. Introduction

This is the fifth paper presenting data on lifetimes and oscillator strengths for Fe II within the FERRUM Project, which aims at extending the existing database of oscillator strengths for iron group elements. Three of the previous papers have been focused on gf -values for lines from two different transition arrays, 4s-4p (Li et al. 1999a, Paper I), (Sikström et al. 1999, Paper II) and 4p-4d (Nilsson et al. 2000, Paper III). Both sets of lines appear in the 2000–3000 Å region but they differ in excitation potential by about 2–3 eV. Thus, by using the new data in abundance analyses they provide a possibility to test the excitation conditions assumed in LTE stellar model atmospheres. The fourth paper (Li et al. 2000a) deals with lifetimes of a particular term at 8 eV, giving ground term transitions around 1600 Å.

The present data set contains 4p-5s transitions which appear in the upper part of the 2000–3000 Å region. The transitions are complementary to the 4p-4d transitions in abundance work as they have the same excitation potential of the lower levels. However, the 4p-5s lines are also of interest in stellar emission line spectra, as they normally appear enhanced in spectra of many objects, e.g. cool star chromospheres, symbiotic stars, η Carinae (see e.g. Johansson & Hamann 1993). The lines are secondary cascades in a fluorescence process in Fe II, where HLy α photons resonantly excite 5p-states, which decay in a primary channel to the 5s states, studied in the present paper. The transition probabilities for the 4p-5s lines are therefore of value in the modelling of this fluorescence process.

2. Laboratory measurements

2.1. Lifetime measurements

Lifetimes of four levels in the $3d^65s$ configuration of Fe II have been measured using the technique of time-resolved laser induced fluorescence (LIF), and the results are presented in Table 1 along with theoretical lifetimes from Raassen & Uylings (2000) and Kurucz (2000). The lifetimes were measured in the VUV laboratory at Lund Laser Centre (LLC). A figure of the experimental setup can be found in Paper III. The free Fe⁺ ions were produced in a laser produced plasma. The frequency doubled radiation from a Nd:YAG laser was focused onto a rotating iron target to create the ablation. By varying the focus of the ablation point and the intensity of the laser beam it is possible to change some plasma parameters, such as the velocity of the ions and the density of the plasma (Li et al. 2000b). Such variation was done in order to check for systematic errors, for example collisional and flight-out-of-view effects, which both tend to shorten the lifetime deduced from the observed decay curves.

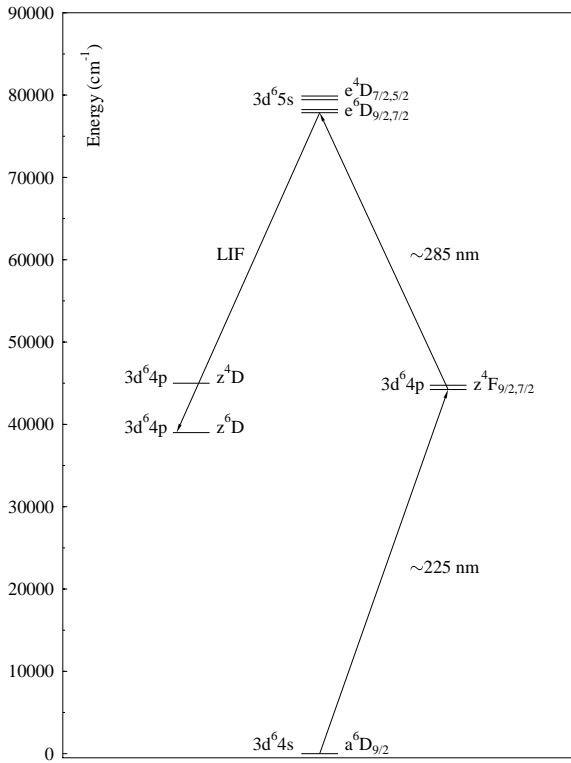
Since the $3d^65s$ configuration has the same parity as the ground configuration, $3d^64s$, it is necessary to have a two photon process to populate $3d^65s$ states from the ground state. This can be done using either a two-step or a two-photon excitation scheme. For a more detailed description of the two methods, see Paper 3. As was the case in the measurements of the 4d states in Paper 3, a two-step excitation provided the most reliable results for the $3d^65s$ states. The two-step excitation scheme and the decays are illustrated in Fig. 1.

In the first excitation step, Fe⁺ ions are excited from the ground state $3d^64s\ a^6D_{9/2}$ to levels in the $3d^64p$

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Table 1. Radiative lifetimes of Fe II levels

Level	Energy	Det. λ^a	Lifetime (ns)		
	(cm^{-1})	(\AA)	This work	Raassen ^b	Kurucz ^c
$3d^6 5s \ e^6 D_{9/2}$	77 861.6	2537.138	2.4 ± 0.2	2.4	3.0
$3d^6 5s \ e^6 D_{7/2}$	78 237.7	2525.919	2.4 ± 0.2	2.4	2.8
$3d^6 5s \ e^4 D_{7/2}$	79 439.5	2856.909	2.7 ± 0.3	2.9	3.9
$3d^6 5s \ e^4 D_{5/2}$	79 885.5	2848.106	2.7 ± 0.3	2.9	3.1

^a Detection wavelength in the LIF measurements.^b Raassen & Uylings (2000).^c Kurucz (2000).**Fig. 1.** Scheme over excitation and de-excitation of the $3d^6 5s$ levels during lifetime measurements. The arrows represent transitions between the upper and lower levels. LIF is the laser induced fluorescent transitions detected in the lifetime measurements

configuration, namely $z^4 F_{7/2}$ or $z^4 F_{9/2}$. Using the ground state as the base for the first step has the advantage of a higher population in the plasma and the possibility to utilize a later part of the plasma, where the particle density, temperature and velocities are lower. The photons required for the first excitation step have an energy of either $44\,233$ or $44\,754 \text{ cm}^{-1}$ depending on the J -value of the intermediate level. The use of different intermediate states made it possible to reach $3d^6 5s$ levels with J -values of $5/2$ to $9/2$. The radiation needed to reach the $z^4 F_{7/2,9/2}$ levels was produced by letting the frequency doubled output of a second Nd:YAG laser with a repetition rate of 10 Hz pump a dye laser which produced visible red light. The dye laser was tuned to either 6782 or 6703 \AA and the output was frequency tripled in a system of non-linear crystals

and polarizers. This produced 8 ns long pulses with wavelengths 2234 or 2261 \AA , which match the Fe II transitions $a^6 D_{9/2} - z^4 F_{7/2}$ and $a^6 D_{9/2} - z^4 F_{9/2}$, respectively.

The energy of the second excitation step from $3d^6 4p \ z^4 F$ to the $e^6 D$ or $e^4 D$ terms in the $3d^6 5s$ configuration is approximately $35\,000 \text{ cm}^{-1}$, or 2850 \AA . With a lifetime of the order of a few ns it was necessary to have sufficiently short pulses ($\approx 1 \text{ ns}$). Therefore, the frequency doubled pulses from the third Nd:YAG laser were time compressed in a Stimulated Brillouin Scattering (SBS) water cell (Li et al. 1999b). The compressed pulses were then used to pump a second dye laser, operated on the Rhodamine 6G dye producing tuneable radiation in the region $5600\text{--}5900 \text{ \AA}$. By frequency doubling the dye laser output at around 5700 \AA , pulses at the desired wavelength in the 2850 \AA vicinity with a pulse length of $\approx 1 \text{ ns}$ can be produced.

All three laser pulses must be synchronized to arrive at the target with a proper time delay. It is especially important for the two excitation pulses to overlap in time, as well as spatially inside the plasma cone created by the ablation laser. The time delay was controlled using two connected external trigger boxes which triggered both the flash lamps and the Q-switches of the three lasers. An appropriate time delay between the three pulses is crucial for measuring the lifetimes correctly and to avoid systematic errors affecting the results. This was carefully investigated by moving the position of three pulses in time and recording and evaluating decay curves at different settings. This is described in some detail in Paper III.

The fluorescence was collected in a direction perpendicular to both the two excitation beams and to the ablation beam using a lens which focused the light onto the entrance slit of a $1/8 \text{ m}$ monochromator (64 \AA/mm resolution). This made it possible to use a channel different from the excitation to record the LIF. The signal was recorded using a fast detection system, consisting of a photo-multiplier tube (PMT) (rise time 200 ps) and a digital transient recorder (1 GHz bandwidth) and 2 GSamples/s sampling rate. The second step excitation laser pulse was used to trigger the oscilloscope, and 1000 decays were averaged to produce each decay curve.

The lifetime was evaluated by fitting a convolution of an exponential decay and the recorded second step laser pulse to the recorded LIF curve with the lifetime of the

best fit taken as the result. About 20 decay curves were averaged to determine each lifetime. Both the quality as well as the general shape of the LIF curves closely resemble the shape of the curves shown in Paper III.

The measured lifetimes of the four 3d⁶5s levels are given in Table 1. As predicted by Raassen & Uylings (2000) calculations, there is a small difference in the lifetimes for the quartet and sextet levels, whereas levels with the same multiplicity have the same value. The uncertainties given in the table include both statistical and systematic uncertainties. The statistical uncertainties are smaller, with $\sigma < 0.05$ ns.

2.2. Branching fractions

A branching fraction (BF) is the ratio between the transition probability of one transition divided by the sum of all transition probabilities from the same upper level. The transition probability of a line is proportional to the measured intensity of the same line in a spectrum. The intensities measured need to be corrected for the response curve of the instrument due to detector efficiency and optical response of the components in the instrument. To get a good measurement of BF the spectrum recorded needs to have a good signal-to-noise ratio (SNR) and a large free spectral range, so that all prominent lines of an upper level can be detected.

Spectra of iron in the region 22 000–50 000 cm⁻¹ (4500–2000 Å) were recorded at the Lund Atomic Spectroscopy Laboratory using a Chelsea Instruments VUV FT500 Fourier transform spectrometer (FTS). The spectral range was recorded in two separate regions, since the detectors used are not sensitive throughout the whole spectral range required. The first region covered 33 000–50 000 cm⁻¹ and the second 22 000–40 000 cm⁻¹. The first spectrum contained all strong lines from the 5s e⁶D_{7/2,9/2} levels and the second all strong lines from the 5s e⁴D_{5/2,7/2} levels.

The spectra were recorded from a hollow cathode discharge lamp (HCD) and from a Penning discharge lamp (PD). In general, we use HCD lamps to produce second spectra, and the 4p-5s transitions showed a higher SNR in the HCD spectrum than in the PD spectrum. However, some of the 4p-5s lines of interest are blended by Fe I lines, and for that reason we used the PD lamp spectrum. The excitation is different in the PD lamp and the lines from the neutral atom are suppressed or absent. Thus, by using data from the PD lamp spectrum we managed to solve the problems with blends from Fe I and derive branching fractions for all lines except one, which is blended with another Fe II line, see Table 2.

The carrier gas used in the light source was in the first spectral region (33 000–50 000 cm⁻¹) both Ne and Ar in different runs. The Fe-Ne spectrum has stronger lines from the 5s levels than the Fe-Ar spectrum due to charge transfer collisions in the HCD (Johansson & Litzén 1978), and the Fe-Ne spectrum were used in the final analysis.

However only Fe-Ar spectrum were used in the second spectral region (22 000–40 000 cm⁻¹). The reason for this choice of gas is the need of internal gas lines for the intensity calibration of the spectra in the second spectral region. The PD lamp was run at 1.5 A and the pressure of the gas flow of Ar was 0.67 Pa (5 mTorr) and 6.7 Pa (50 mTorr) for Ne. To check for influence of self absorption in the lines a number of spectra were recorded at different currents. As the lower levels in the 4p-5s transitions have opposite parity to the ground configuration they have very short lifetimes and fast decay channels, and, as expected, we did not observe any sign of self absorption.

A Voigt profile was fitted to each individual line, and the area under the fitted profile was taken as the intensity. The PD lamp gives almost a pure Gaussian line profile due to Doppler broadening. It is not possible to measure every branch from a given upper level, either because it is very weak and disappears in the noise or because it is outside the accessible spectral range of the instrument. Therefore, we do not actually measure the BF:s but the branching ratios (BR). For the missing branches we derive BR:s from the calculated transition probabilities. In this way we can get a sum of all the branches and derive the BF:s for each line. The sum of the BF:s for the missing branches is treated as a residual. In our case we use theoretical values from Raassen & Uylings (2000), as these calculations have shown to be good for other transition arrays (Papers II and III). We see in Tables 2 and 3 that the residual is just a few percent, except for the level 5s e⁶D_{7/2}, where the strongest line at 2767.512 Å is blended with one Fe II line and two Fe I lines. Even if the Fe I lines were suppressed in the PD spectrum it was not possible to resolve the blend with the other Fe II line. Thus, we have used the calculated transition probability from Raassen & Uylings (2000) for that line to get the BF. The uncertainty in the BF for the other lines from that upper level is determined by the uncertainties in the measurement and assuming that the theoretical gf -value of the transition 2767.512 Å is correct.

The calibration of the line intensities was done in two different ways. The spectrum between 33 000–50 000 cm⁻¹ was calibrated with a deuterium (D₂) lamp that gives a continuous spectrum with a known spectral intensity distribution. The D₂ lamp has been calibrated at the Physikalisch-Technische Bundesanstalt, Berlin, Germany, to a 2 σ (2 standard deviation) accuracy of 8% in the spectral range 33 000–60 000 cm⁻¹. The calibration was independently checked against Ar II lines with known branching ratios (Siems et al. 1995), and an agreement within 10% was found.

The spectrum in the region 22 000–40 000 cm⁻¹ was calibrated by means of Ar II lines from the carrier gas. The branching ratios in Ar II are well known (Whaling et al. 1993; Hashiguchi & Hasikuni 1985), and a curve giving the optical response of the instrument was constructed from Ar II lines. The response curve was applied to the measured Fe II lines to get the correct intensity.

Table 2. Absolute oscillator strength of Fe II transitions, intensity calibrated with a D₂ lamp

Level		λ_{air}	BF	gA	log gf			Unc. ^a
upper	lower	(Å)		(s ⁻¹)	Exp.	Raassen ^b	Kurucz ^c	
5s e ⁶ D _{9/2}	4p z ⁶ D _{9/2}	2537.138	0.345	1.44 10 ⁹	0.142	0.093	0.130	12
	4p z ⁶ D _{7/2}	2550.152	0.094	3.91 10 ⁸	-0.419	-0.421	-0.410	15
	4p z ⁶ F _{11/2}	2785.192	0.367	1.53 10 ⁹	0.250	0.268	0.070	12
	4p z ⁶ F _{9/2}	2796.628	0.048	2.01 10 ⁸	-0.626	-0.728	-0.920	20
	4p z ⁶ P _{7/2}	2839.800	0.140	5.81 10 ⁸	-0.153	-0.092	-0.300	14
	<i>residual</i>		0.006					
5s e ⁶ D _{7/2}	4p z ⁶ D _{9/2}	2513.151	0.060	1.99 10 ⁸	-0.724	-0.792	-0.806	15 ^d
	4p z ⁶ D _{7/2}	2525.919	0.178	5.93 10 ⁸	-0.246	-0.294	-0.311	13 ^d
	4p z ⁶ D _{5/2}	2538.680	0.177	5.90 10 ⁸	-0.244	-0.345	-0.362	13 ^d
	4p z ⁶ F _{9/2}	2767.512	blend			0.132	0.118	
	4p z ⁶ F _{7/2}	2776.908	0.098	3.27 10 ⁸	-0.423	-0.399	-0.560	15 ^d
	4p z ⁶ P _{7/2}	2809.783	0.075	2.48 10 ⁸	-0.532	-0.606	-0.810	19 ^d
	4p z ⁶ P _{5/2}	2856.377	0.106	3.53 10 ⁸	-0.364	-0.397	-0.580	18 ^d
	<i>residual</i>		0.307					

^a Uncertainty in the f -value in %.^b Raassen & Uylings (2000).^c Kurucz (2000).^d Assuming the theoretical gf -value of the transition 2767.512 Å to be correct.**Table 3.** Absolute oscillator strength of Fe II transitions, intensity calibrated with Ar II lines

Level		λ_{air}	BF	gA	log gf			Unc. ^a
upper	lower	(Å)		(s ⁻¹)	Exp.	Raassen ^b	Kurucz ^c	
5s e ⁴ D _{7/2}	4p z ⁴ F _{9/2}	2839.513	0.396	1.17 10 ⁹	0.152	0.131	-0.020	13
	4p z ⁴ D _{7/2}	2856.909	0.358	1.06 10 ⁹	0.113	0.045	-0.070	13
	4p z ⁴ D _{5/2}	2884.765	0.067	1.97 10 ⁸	-0.609	-0.686	-0.840	16
	4p z ⁴ P _{7/2}	3078.680	0.150	4.44 10 ⁸	-0.200	-0.164	-0.320	15
	<i>residual</i>		0.029					
5s e ⁴ D _{5/2}	4p z ⁴ F _{7/2}	2845.596	0.424	9.43 10 ⁸	0.059	0.036	0.060	12
	4p z ⁴ D _{5/2}	2848.106	0.267	5.93 10 ⁸	-0.142	-0.211	-0.290	14
	4p z ⁴ D _{3/2}	2869.313	0.109	2.42 10 ⁸	-0.524	-0.638	-0.609	15
	4p z ⁴ P _{5/2}	3036.963	0.060	1.33 10 ⁸	-0.734	-0.705	-0.870	16
	4p z ⁴ P _{3/2}	3076.435	0.101	2.25 10 ⁸	-0.496	-0.445	-0.620	15
	<i>residual</i>		0.038					

^a Uncertainty in the f -value in %.^b Raassen & Uylings (2000).^c Kurucz (2000).

The uncertainty in the BF:s is mainly due to the intensity calibration and the line profile fitting. The uncertainty in the fitting procedure is strongly related to the SNR, and a weak line causes a larger uncertainty. This uncertainty, which is estimated by a computer code (Blom 2000) that derives the standard deviation of a Gaussian profile fitted to a line with a certain SNR, is less than 15% for the weakest lines. The uncertainty of the intensity calibration, which arises from the calibration of the D₂ lamp and the uncertainties of the Ar II lines used for calibration, is estimated to be 10%.

3. Oscillator strengths

By combining the BF:s and the radiative lifetimes from Table 1 we get the Einstein coefficients A , and as the lines appear in emission in astrophysical spectra we have

inserted the gA -values in Tables 2 and 3. The oscillator strengths (f), also given in the tables, are derived from the A -values. For each line we give the upper and lower level in column one and two and the wavelength in air in column three. In column four the BF:s from an upper level are given with the residual, and in column five the gA -values are listed. In column six the experimental log gf -values are presented, and they are compared in columns seven and eight with theoretical values from Raassen & Uylings (2000) and Kurucz (2000). The uncertainty of the gf -value in the last column is the combined uncertainties from the lifetime and BF measurements. These uncertainties are considered to be conservative estimates.

We have compared the experimental data with the two sets of theoretical log gf -values included in Tables 2 and 3 by plotting the difference between the

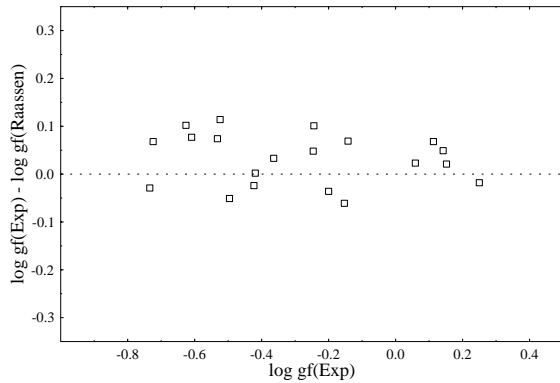


Fig. 2. Experimental $\log gf$ -values compared to theoretical $\log gf$ -values calculated by Raassen & Uylings (2000). The difference is plotted against the experimental $\log gf$

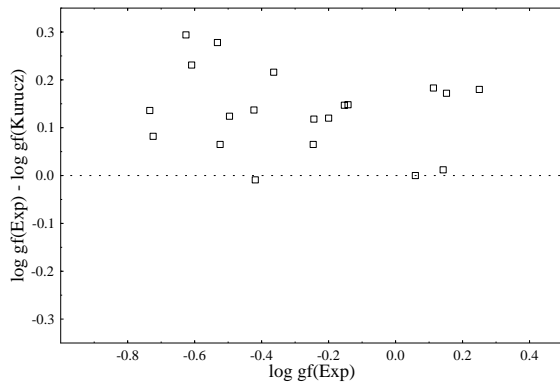


Fig. 3. Experimental $\log gf$ -values compared to theoretical $\log gf$ -values calculated by Kurucz (2000). The difference is plotted against the experimental $\log gf$

experimental and calculated $\log gf$ -values in Figs. 2 and 3 as a function of the experimental $\log gf$ -value. In Fig. 2 we see that the agreement between Raassen & Uylings (2000) values and the experimental values are within 0.1 dex for all the measured lines and if we adopt a slight offset of 0.03 all values are within ± 0.07 dex, which corresponds to 17%. In the comparison with Kurucz's (2000) data in Fig. 3 the scatter is larger, and there seems to be an offset of about 0.15 dex. The offset in the two comparisons goes in the same direction and may imply an uncertainty in the dipole moment used in the calculations of the 4p-5s transition. There is also the possibility of a systematic error in the lifetime measurements which would affect all gf -values in the same direction. However, in the previous work in Papers II and III we also found a slight offset between the experimental values and the calculated values by Raassen & Uylings (2000), but in the opposite direction. This implies that the offset is due to the calculated values and not to the experimental lifetimes. Due to the good agreement with the calculations by Raassen & Uylings (2000) we recommend the use of this database for other 4p-5s transitions not measured in the present work.

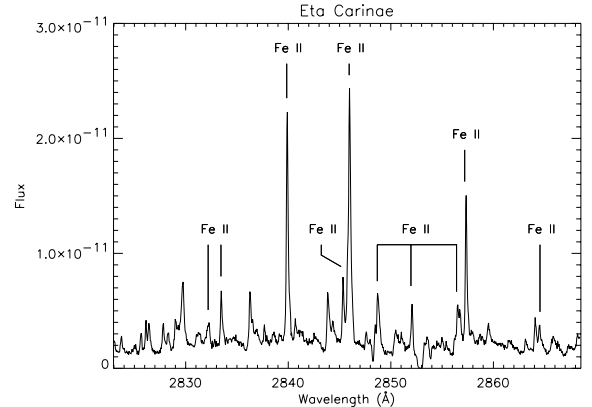


Fig. 4. GHRs spectrum of η Carinae where the 4p-5s transitions are marked with Fe II

4. Astrophysical applications

As mentioned in the introduction the $3d^6(^5D)4p-3d^6(^5D)5s$ transitions appear in emission in many astrophysical objects, as first observed by the International Ultraviolet Explorer (IUE) in spectra of cool stars. Brown et al. (1981) pointed out the possibility that these lines could be a secondary decay channel in the depopulation of highly excited 5p states, pumped by HLy α . The same lines also appeared enhanced in the IUE spectrum of RR Tel (Penston et al. 1983) due to the same reason as their appearance in cool stars. Johansson & Jordan (1984) verified this pumping by doing a systematic study of fluorescence lines in the solar spectrum and RR Tel, and later work, see e.g. (Hartman & Johansson 2000), has confirmed this pumping process. The primary decay from the pumped 5p levels feeds the 5s levels, and a great number of 5s-5p transitions have been observed in the near-infrared region in e.g. η Carinae (Hamann et al. 1994). The secondary decay (4p-5s) around 2850 Å shows up as narrow lines in the spectrum of gaseous condensations close to the central star of η Carinae (Zethson 2001). An extract of the *Hubble Space Telescope* (HST)/Goddard High Resolution Spectrograph (GHRs) spectrum is shown in Fig 4, where the 4p-5s transitions are very prominent.

By using the gA -values in this work and in the Raassen & Uylings (2000) database it is now possible to derive the relative enhancement in the 4p-5s transitions appearing in emission in various astrophysical spectra, work is in progress also on the 5s-5p transitions, which will make it possible to model the HLy α pumping of Fe II to the 5p states around 11 eV.

5. Conclusion

We have measured absolute oscillator strengths for twenty transitions within the $3d^64p-3d^65s$ supermultiplet, and we estimate the uncertainty of the f -values to be 12–20%. The experimental data are compared with two sets of theoretical data, and we find a good agreement with the

calculations by Raassen & Uylings (2000). We therefore recommend the use of this database of f -values for other transitions, for which no experimental values are available. The data presented in this paper can, together with the theoretical data recommended, be used when modelling HLy α induced fluorescence in various types of emission line objects.

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