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The FERRUM project: Branching ratios and atomic transition probabilities of Fe II transitions from the $3d^6(a^3F)4p$ subconfiguration in the visible to VUV spectral region⋆

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Abstract. We report measurements of the relative intensities of 81 emission lines of Fe II between 160 nm and 350 nm (62 168 cm^{-1} to 28 564 cm^{-1}) from 4 levels by high resolution Fourier transform spectrometry, using a Penning discharge lamp as light source. These relative intensities have been used to determine the line branching fractions, which have then been combined with accurate experimental radiative lifetime measurements reported recently to give absolute transition probabilities and oscillator strengths for 81 lines. The accuracy of these *f*-values is compared with other previous experimental measurements, and with theoretical values. The new transition probabilities will allow accurate determinations of Fe II abundances in a wide variety of astrophysical objects.

Key words. atomic data – line: identification – techniques: spectroscopic – stars: abundances

1. Introduction

Knowledge of the spectrum of singly ionized iron is essential in a wide variety of astrophysical applications. Over the past few years there have been many laboratory studies of the spectra of the abundant iron-group elements driven by the need for new accurate atomic data to interpret astrophysical spectra observed using the new generation of spectrographs on space and ground-based telescopes. Its high abundance and richness of lines means that the spectrum of Fe II is important in objects as diverse as stars and active galaxies, H II regions, the interstellar medium, protostellar disks, supernovae remnants, and quasars. In astrophysical plasmas at about 10 000 K the UV spectra are often dominated by Fe II transitions. The Fe II spectrum is highly sensitive to the physical conditions in the emitting gas and would thus be a good probe of the plasma conditions. However, there are fundamental uncertainties due to the uncertainties in the basic atomic data (Verner et al. 1999). The availability of self-consistent sets of oscillator strengths for Fe II covering a range of transition probabilities would enable Fe II abundances to be investigated over a large dynamic range in column density. The *f*-values of weak stellar lines, i.e. lines that are weak because they have low *f*-values or because they originate from high-lying energy levels, are also needed since the strong lines are often saturated and cannot be used in abundance determinations. Until recently Fe II abundance determination has relied mainly on calculated *f*-values that have the disadvantage of uncertain errors. The work reported in this paper is part of a new collaborative project, the FERRUM project (Johansson 2001; and references therein), in which many *f*-values for Fe II are being measured. The excitation energies of the lower levels in the transitions studied in this work range from 0 to 10 eV.

The experimental transition probabilities for Fe II available in the literature prior to 1988 were reviewed in the critical compilation of Fuhr et al. (1988). The most accurate transition probabilities for the transitions reported

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⋆ Tables 2 and 3 are 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/cgi-bin/qcat?J/A+A/377/361

in this work were those of Moity (1983) and were assigned a "D" rating (accuracies of between 25–50%) by Fuhr et al. (1988). Moity (1983) had reported transition probabilities from laboratory arc measurements in the range 255 nm to 530 nm with typical uncertainties of greater than 20%. Bergeson et al. (1996) reported accurate new laboratory measurements of transition probabilities for transitions between 224 nm and 276 nm having upper levels of the $3d^6(^5D)4p$ subconfiguration in the range 38 000 cm^{-1} to 46 000 cm^{-1}, but they did not consider levels lying higher than 46 000 cm^{-1}. In general, there is a serious lack of accurate experimental transition probabilities for Fe II for transitions covering the UV to VUV (below 200 nm) spectral regions or from high lying energy levels.

Ekberg & Feldman (1993) presented "astrophysical" transition probabilities in the 200 nm to 280 nm region derived from high resolution solar spectra. They report that their values of $g_i A_{ij}$ (where g_i is the statistical weight of upper level i and A_{ij} is the atomic transition probability between levels i and j) have uncertainties less than $\pm 50\%$ and perhaps even less than $\pm 25\%$. More recently Cardelli & Savage (1995) discussed the reliability of a number of transition probabilities of Fe II lines between 114 nm and 260 nm. For one of the lines in the present work, the weak $4s\ ^6D_{9/2} - 4p\ y^4F_{7/2}$ 161.12 nm transition, they determined the f-value to about 15% (one σ) using spectra of β Sco obtained using the Goddard High Resolution Spectrograph aboard the Hubble Space Telescope.

There is a variety of theoretical work done on transition probabilities for Fe II in the literature. For example, Kurucz (1993) has made extensive semi-empirical calculations using the Cowan code (1981) of energy levels and log gf values for astrophysically important atoms and ions including Fe II. In general, his log gf values agree well with experimental data for strong lines, but are less reliable for weaker lines. Nahar (1995) has made calculations as part of the IRON project based on the R-matrix method including the fine structure according to the LS recipe. Raassen has also calculated transition probabilites using an orthogonal operator technique (Raassen & Uylings 1998a, 1998b; Raassen 1999). In the present work we compare these theoretical calculations with our experimentally determined log gf values.

In this work we report on newly measured absolute transition probabilities for Fe II obtained by combining measurements of normalized relative line intensities from a given upper energy level (branching fractions) with an absolute measurement of the level lifetime. This procedure does not depend on any assumption of the population distribution over different levels, but all significant lines from a particular level must be included in the sum of transition probabilities, and the lines may be spread over a broad wavelength range. The emission branching fractions were measured using the VUV Fourier transform (FT) spectrometer at Imperial College with a Penning discharge lamp (PDL) as source. The lifetimes of the levels studied in this work were measured recently at Lund University (Sikström et al. 1999) as part of the FERRUM project (Li et al. 1999). We have combined our emission branching fractions with the radiative lifetimes of four levels to give oscillator strengths for 81 lines with uncertainties of less than 12% for the majority of the stronger lines (log $gf > -1.5$) and less than 20% for the majority of the weaker lines (log $gf < -1.5$). The upper levels of the transitions belong to the $3d^6(a^3F)4p$ subconfiguration and range in energy from 62 065 cm^{-1} to 64 040 cm^{-1}. The lines studied extend from 158 nm to 380 nm in wavelength (63 291 cm^{-1} to 26 315 cm^{-1}).

2. Experimental procedure

The method of using experimental branching fractions to determine oscillator strengths has been used successfully in recent years. The basic procedure is to record each iron spectrum together with a suitable calibration spectrum using an accurately calibrated intensity standard. This calibration spectrum enables an intensity-calibrated linelist for the iron spectrum to be prepared with intensities of lines on a relative scale. Because of the wide spectral range of the lines in this work several spectra are required. Lines from a given upper level are then grouped together and placed on the same relative intensity scale using lines common to the spectra to give the scaling factor. Finally, the branching fractions are determined from the relative intensities by normalising each set of lines from a particular upper level to unit sum, where necessary allowing for any lines missing from the set. The measured lifetime of the upper level is then combined with the branching fractions to give the absolute transition probabilities and log gf values.

2.1. Experimental measurements

The measurements were carried out using the Imperial College VUV FT spectrometer (Thorne 1996) and a Penning Discharge Lamp (PDL). In previous work at Imperial College on Fe II (Nave et al. 1997) a water cooled hollow cathode had been used and gave a rich spectrum of Fe II through excitation by charge transfer (Johansson & Litzén 1978). Because the energy levels investigated in our work lie at energies too low for effective population through charge transfer with neon, the Fe-Ne hollow cathode was found to be unsuitable as a source. Recently we have been studying the spectrum of Fe III (Pickering et al. 1999; Smith et al. 1998) using a PDL and this source was found to populate the $3d^6(a^3F)4p$ levels of Fe II. The PDL was run with a mixture of Ne and Ar gases at 1.7×10^{-3} mbar pressure and a current of 1.55 A. The cathodes were 99.8% pure iron and were water cooled to reduce the Doppler line widths. The MgF_2 window between the FT spectrometer and the PDL was placed at a sufficient distance from the PDL to ensure that there was no sputtering of metal atoms onto the window from the source which could produce systematic errors in the relative line intensities.

Table 1. Details of the spectra observed.

spectrum number	wavenumber range (cm^{-1})	detector	filter	resolution (cm^{-1})	number of coadded interferograms
I	31 596 – 41 700	R1220	270 nm	0.08	24
II	39 000 – 52 000	R1220	220 nm	0.08	16
III	31 596 – 61 000	R1220	180 nm	0.09	16
IV	35 000 – 63 100	R1220	156 nm	0.09	24
V	51 000 – 66 000	R1259	-	0.11	28
VI	24 000 – 47 000	1P28	UG5	0.06	14

The FT spectrometer used is a Chelsea Instruments FT500, based on the laboratory prototype designed and built at Imperial College (Thorne et al. 1987), but with a magnesium fluoride beamsplitter that gives a short wavelength limit of about 135 nm (Thorne 1996; Thorne et al. 1994). The spectral range covered was from 24 000 cm^{-1} (4167 Å) to 66 000 cm^{-1} (1515 Å), and the detectors, bandpass filters, resolution used in the various regions, and the number of coadded interferograms are summarised in Table 1.

Three broad band spectra were recorded: the visible to UV (spectrum VI) was defined by a Hamamatsu 1P28 photomultiplier tube (PMT) with an Oriel UG5 filter; the UV to VUV region (spectrum IV) was recorded with a Hamamatsu R1220 PMT and 156 nm filter, and the VUV region (spectrum V) was recorded with a Hamamatsu R1259 PMT which has a MgF_2 window and no filter was used. Three further spectra (spectra I, II, III) were recorded with narrower bandpass filters in order to improve the signal-to-noise ratio (SNR) for some of the weaker lines. For each spectrum several interferograms were coadded to improve the SNR, with total acquisition times for a spectrum being typically between one and two hours. Intensity calibration spectra were recorded immediately prior to and after each Fe II spectrum acquisition (see Sect. 2.2). The Doppler widths of the PDL lines ranged from about 0.18 cm^{-1} at 36 000 cm^{-1} to 0.30 cm^{-1} at 61 000 cm^{-1}, and the interferograms were recorded with resolutions to give at least 3 points per linewidth in the resulting spectra.

The GREMLIN program developed by Brault (Brault & Abrams 1999) was used to produce Fe II linelists from the phase-corrected spectra. For each line a least squares fit to a Voigt profile was performed, and the relative intensity of the line in wavenumber units was given by the integral over this profile, ie the equivalent width. The Voigt fits to the lines were examined to ensure that self-absorption was not a problem for the stronger lines.

2.2. Intensity calibration of the Fe II spectra

The Fe II linelist described in Sect. 2.1 was intensity calibrated taking all precautions necessary to avoid potential systematic errors. The instrument response in FT spectroscopy depends on the detector characteristics, the transmissivity and reflectivity of the optical components, and also on the modulation achieved in the interferogram. The modulation is limited by the errors in the recombining wavefronts, and it is always wavelength-dependent. The modulation usually decreases slowly with time, falls off more rapidly at shorter wavelengths, and depends on the area of the beamsplitter that is illuminated. One method of determining the instrument response involves using argon lines generated in the source itself to determine the instrument response (Bizzarri et al. 1993; O'Brian et al. 1991), but in our case this was not possible because the Ar lines were too weak and did not cover our entire spectral range.

Therefore to determine the instrument response directly we have used a D_2 lamp with a MgF_2 window, calibrated for spectral radiance by the Physikalisch-Technische Bundesanstalt (PTB), Berlin, Germany to within 8% (two standard deviations (2 σ)) in the range 166 nm to 358 nm, to within 12% in the range 113 nm to 166 nm, and to within 10% in the range 360 nm to 410 nm.

The PDL and the deuterium calibration lamp were placed at equal distances from the FT spectrometer entrance aperture, and the path between the lamps and the FT spectrometer was evacuated to prevent absorption of the UV and VUV light in air. A mirror was used to switch between the lamps. Any potential modulation drifts were allowed for by ensuring that calibration spectra were recorded immediately before and after each set of coadded Fe interferograms. These calibration spectra were compared to check that there had been no change in instrument response during the course of that particular interferogram acquisition.

The molecular deuterium spectrum is a quasi continuum spectrum with some line structure, and, thus our calibration spectrum must have the same spectral resolution as used by PTB to calibrate the lamp. Three values of relative spectral radiance are given by PTB at each wavelength corresponding to measurements at resolutions of 0.4, 0.8, and 1.6 nm. The values at 1.6 nm resolution were used for all but the VUV runs (spectra IV and V), where significant line structure meant that a more reliable response curve could be obtained using the 0.4 nm resolution data. Using the GREMLIN program

(Brault & Abrams 1999) we interpolated our lamp spectrum onto a linear wavelength scale, convolved it with a function equivalent to a 1.6 nm or 0.4 nm slit, and then divided through by the scaled PTB values to yield the FT spectrometer response on a wavelength scale. The response curve was then interpolated back onto a wavenumber scale to give the response curve to be used for the Fe intensity calibration. Figure 1 shows typical relative response curves for the six spectral regions.

2.2.1. Intensity calibration of broad band spectrum IV (35 000 cm^{-1} to 63 100 cm^{-1})

Fe spectrum IV was needed for a few cases where there were no suitable overlap lines that could be used to link together lines of a set (ie lines from the same upper level) in the VUV with lines at much longer wavelengths in the UV. The 156 nm filter ensured that both the VUV Fe II lines around 60 000 cm^{-1} and the lines around 40 000 cm^{-1} could be simultaneously observed. The response of the FT spectrometer falls off rapidly at shorter wavelengths, so the SNR of the VUV lines is enhanced by using a 156 nm filter to cut down the instrument response for the strong longer wavelength Fe II lines. The filter also allows a little light through at longer wavelengths so that the strong Fe II lines around 40 000 cm^{-1}, where the modulation of the FT spectrometer is naturally higher, may also be observed. However, over the spectral range of this broad band spectrum (35 000 cm^{-1} to 63 100 cm^{-1}) the relative spectral radiance of the deuterium lamp varies by a factor of about 500 with the lamp being most intense at the shortest wavelengths. Consequently it was found that initially the recorded deuterium calibration spectrum only contained information in the short wavelength part of the spectrum since the noise level resulting from this portion dominated the longer wavelengths where the deuterium intensity was too low to be detected in the same scan. This problem was overcome by placing a 170 VBB filter (Acton Research Corp.) in front of the deuterium lamp modifying its emission in the VUV so that the light intensity was of the same order of magnitude throughout the spectrum range. The transmission of this filter was provided by Acton Research, and so the combined relative spectral radiance of the deuterium lamp and 170 VBB filter could be calculated and used to determine the instrumental response of the FT spectrometer for spectral range IV.

2.3. Determination of the branching fractions, absolute transition probabilities and log gf's

At this stage in the analysis there are six spectra, each of which has been intensity calibrated using the instrument response determined separately for each individual spectrum. Each spectrum has a fitted linelist giving wavenumber, SNR, line width, and relative intensity for all the lines. The next step was to group together all lines from each particular upper level from the six spectra and put them on a common intensity scale. The calculations of Raassen (1999) defined the linelist for each set of lines from a particular upper level, with an intensity cut-off of log $gf = -3.0$.

Lines in the different spectra were related using scaling factors determined by using lines from the same upper level in the spectra overlap regions. It is preferable that the transfer lines used have the same upper level, or at least an upper level in the same multiplet, as the two sets of lines they are connecting. It is likely that the relative excitation is the same for levels only a few hundred cm^{-1} apart. In some cases this was not possible because of the way the Fe II lines are grouped with a rather large gap between the UV and VUV lines. However, as the PDL was run in the same conditions for all the spectra, the scaling factor was expected to be the same. To within the measurement uncertainties the scaling factors in the overlap regions showed no variation with upper energy level of the transition used to determine the scaling factor.

The integrated area of each calibrated line is proportional to its intensity Φ_{ij} in photons per second, and the branching fraction of the line BF_{ij} is given by:

$$BF_{ij} = \frac{\Phi_{ij}}{\Sigma_j \Phi_{ij}} \quad (1)$$

where the sum is taken over all lines from a given upper level i. The calculations of Raassen (1999) defined the complete set of lines from the upper level, and enabled an estimation of the contribution from missing lines to be carried out. Lines are described as missing if they fall outside the spectral region of observation or if they are blended with another line (Fe I, Ar, or Ne) or doubly identified. For most of the levels the fraction α of the total transition probability that is missing is less than 1%, which is smaller than the uncertainty in the sum of the transition probability of all the observed lines in a set. Where the missing fraction is greater a correction factor $(1 + \alpha)$ to the sum in Eq. (1) has been applied to give the best estimate of the true value of each BF_{ij}.

The lifetimes τ_i measured recently by Sikström et al. (1999) using the technique of time-resolved laser-induced fluorescence were used together with our measured branching fractions to give absolute transition probabilities A_{ij} and log gf values using the following relation:

$$A_{ij} = \frac{BF_{ij}}{\tau_i}. \quad (2)$$

Lines that are not seen in our spectra as they lie below the noise level of the spectra, and which have a predicted log gf that is greater than -3.0, are also "missing". However we have assigned these lines an experimental maximum log gf value. This can be done because the noise level in FT spectroscopy is independent of wavelength, and, as there are about 3 spectral resolution elements per line width the detection limit corresponds to a peak value of about 2.5 times the rms noise. Using nearby lines this detection limit can be converted to an

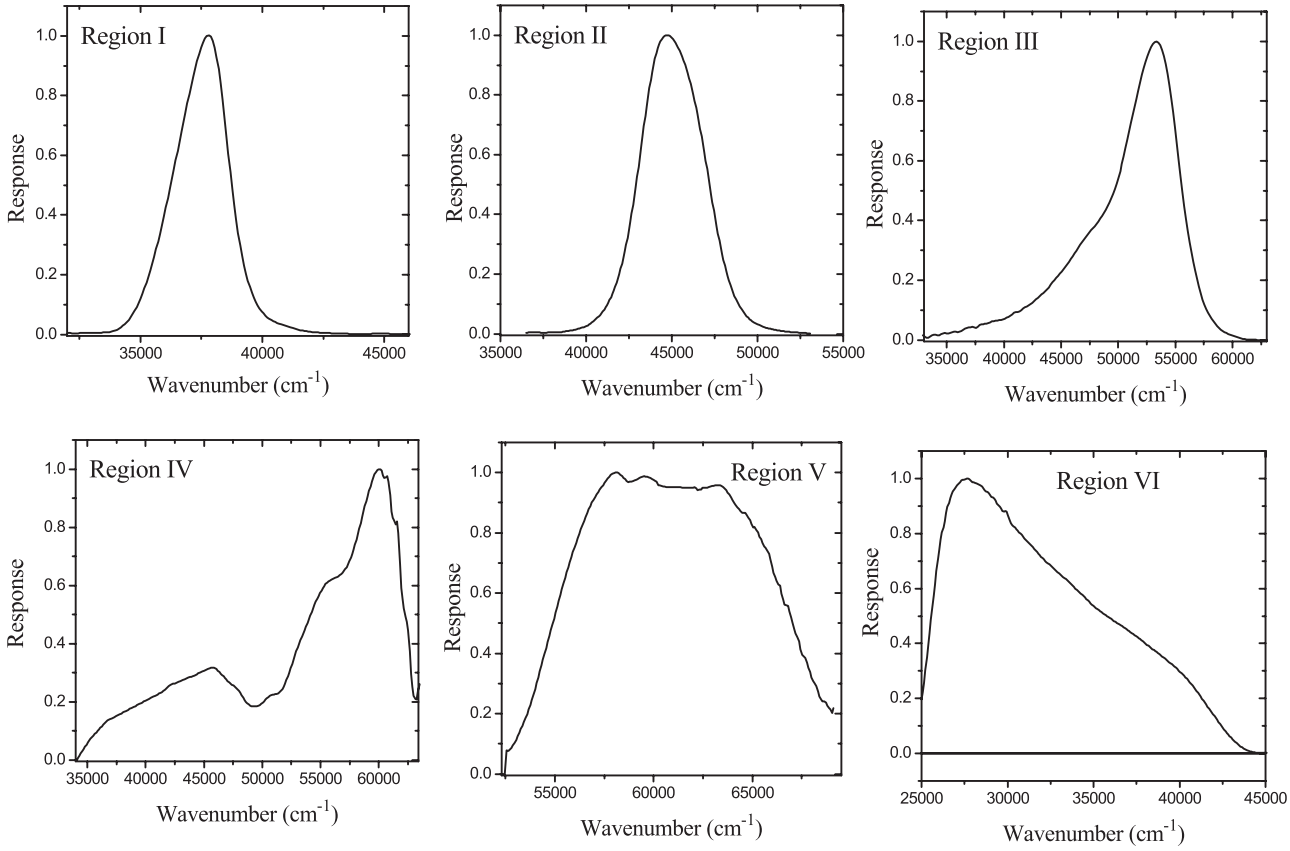

Fig. 1. Relative instrument response curves for the six spectra regions.

integrated line intensity to give an upper limit for the branching fraction and log gf value. The upper limits for these weak lines fall within the uncertainties of the sum in Eq. (1).

3. Results and analysis

Our results are presented in Table 2 which gives the groups of lines from four upper energy levels, each level being designated by its energy and LS assignment. For each level the lifetime measurement of Sikström et al. (1999) is given along with its uncertainty. The percentage completeness of the set of transitions is also indicated. For each transition we give: the air wavelength; vacuum wavelength; vacuum wavenumber; the measured branching fraction, with relative uncertainty, the absolute transition probability and its uncertainty, the log gf value with uncertainty in dex, and the theoretical log gf's of Raassen (1999), Kurucz (2000), and Nahar (1995). The "missing" lines also are listed for each level with the theoretical log gf's of Raassen, Kurucz, and Nahar, together with maximum values of branching fraction, transition probability and log gf for the lines in our spectral range that fall below the detection limit. To avoid having two sets of line wavenumbers in the literature we give the Ritz wavenumbers that can be derived from the experimental energy level values obtained in the complete and unpublished term analysis of Fe II being carried out by S. Johansson at Lund University. These were determined using spectra recorded with the Imperial College VUV FT spectrometer (Nave et al. 1997), with the FT spectrometers at Lund and Kitt Peak, and with interferometric measurements by Norlén (private communication). Wavelength calibration (Learner & Thorne 1988) was carried out using a set of 26 Ar II standard lines measured interferometrically by Norlén (1973). The wavenumbers in Tables 2 and 3 have been rounded from eight significant figures to seven.

For lines that are missing from both the Lund and Imperial College linelists (marked with an "x") we have given the Ritz wavenumbers. Since the values of A and log gf for these "missing" lines are maximum values it may be preferable to use the theoretical values for these lines. Blended lines are indicated with "b".

For each measured line in Table 2 we give the uncertainty in the branching fractions determined from the uncertainty in the relative intensities. This uncertainty comprises the uncertainty in the individual line intensity measurement and in the calibration of the standard lamp. The uncertainty in line intensity measurement is set by the SNR of the line itself and also the uncertainty in any transfer ratios used to put lines from different spectra onto a common scale (see Sect. 2.3).

The uncertainty in deuterium lamp calibration (one standard deviation) is quoted by PTB as 6% (113–166 nm), 4% (166–358 nm) and 5% (360–410 nm). Because we are considering only relative intensities we

have assigned $1/\sqrt{2}$ of the relevant calibration uncertainty to each line. The uncertainty in the absolute transition probabilities and log *gf* values for each line includes the uncertainties for the normalization constant $\Sigma_j \Phi_{ij}$ and the lifetime τ_i for the particular upper level involved. The normalization uncertainty $d\Sigma$ is found by summing the uncertainties in relative intensity in quadrature for all observed lines in a set, and $d\Sigma$ it is dominated by the uncertainty in the strongest lines. The uncertainty in the unobserved fraction α is negligible since α is comparable with or less than $d\Sigma/\Sigma$.

In Table 3 we give a finding list for the transitions in Table 2, including the log *gf* values from the present work and the LS labels of the energy levels involved in each transition.

In Fig. 2 we compare our log *gf* values with those calculated by Raassen (1999), Kurucz (2000), and Nahar (1995). Of these three sets of calculations the log *gf* values calculated by Raassen (1999) appear to differ the least from our experimental results. In all three cases it is clear that there is greatest deviation from our measurements for the weaker transitions, and that this deviation is greater than the uncertainty in our experimental measurements.

4. Conclusion

We have used the Imperial College VUV FT spectrometer with its wide free spectral range, high resolution, and linear response to record spectra of Fe II in the range 152 nm to 416 nm (24 000 cm^{-1} to 66 000 cm^{-1}) using a Penning discharge lamp. Branching fractions of sets of lines from four energy levels were determined and combined with level lifetimes recently measured at Lund University to give absolute transition probabilities and log *gf* values for 81 lines. Typical uncertainties in the transition probabilies are less than 12% for strong lines and better than 20% for the majority of weaker lines. Our measurements are compared with the theoretical calculations of Kurucz (2000), Raassen (1999), and Nahar (1995), where good agreement is found for stronger lines but a larger scatter is found for the weaker transitions. As expected experimental measurements are essential for the medium to weaker transitions. This work represents the first complete measurement of oscillator strengths of transitions from the four $3d^6(a^3F)4p$ levels: $y^4F_{7/2}$, $x^4D_{7/2}$, $y^4G_{9/2}$, and $y^4G_{7/2}$, and provides accurate oscillator strengths for astrophysical applications.

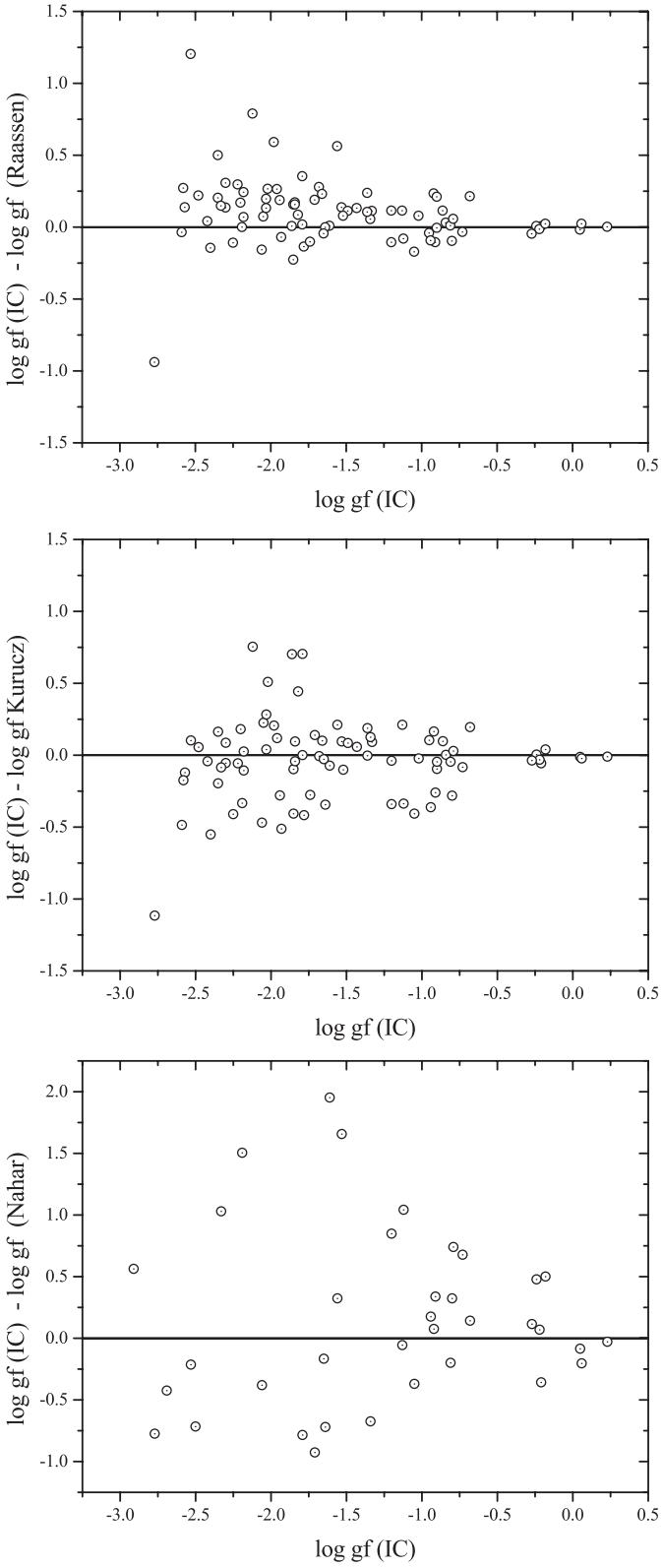

Fig. 2. Comparison of the experimentally determined log *gf* values of this work with those calculated by Raassen (1999), Kurucz (2000), and Nahar (1995).

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