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## THÈSE <br> Pour obtenir le grade de Docteur

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## Le rôle des collisions inélastique avec l'hydrogène dans la détermination hors-ETL de l'abondance du fer dans les étoiles froides

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# Non-LTE Iron abundance determination in cool stars: The role of Hydrogen collisions 

Rana Ezzeddine

December, 2015


#### Abstract

Résumé

La détermination d'abondances stellaires très précises est un objectif majeur de la plupart des études spectroscopiques. L'hypothèse de l'équilibre thermodynamique local (ETL), largement utilisée dans les analyses spectroscopiques, est souvent inadéquate pour déterminer les abondances et les paramètres stellaires, particulièrement pour les étoiles géantes ou pauvres en métaux, où les effets hors-ETL dominent. C'est pourquoi, une modélisation hors-ETL des spectres stellaires est cruciale afin de reproduire les observations et ainsi déterminer avec précision les paramètres stellaires. Cette modélisation hors-ETL nécessite l'utilisation d'un grand jeu de données atomiques, qui ne sont pas toujours connues avec certitude. Les taux de collisions avec l'hydrogène sont une des sources d'incertitudes les plus fortes dans le cas des étoiles froides. Ces taux sont souvent approximés en considérant une approche classique (l'approximation de Drawin), et ceci seulement dans le cas de transitions permises liée-liée et d'ionisations. Cette approche classique, tend à surestimer le taux de collision et ne reproduit pas correctement le comportement en fonction de l'énergie de la transition. Je démontre dans cette thèse l'incapacité de l'approximation de Drawin à décrire le taux de collisions avec l'hydrogène. Je présente une nouvelle méthode empirique pour estimer ce taux, par le biais d'ajustement sur des taux quantiques existant pour d'autres éléments. Je montre ensuite que cette méthode d'ajustement quantique (que je nomme QFM) permet de reproduire les résultats des modélisations hors-ETL effectuées avec des taux quantiques existants (cas du Si ). J'utilise ensuite cette nouvelle méthode, avec mon propre modèle d'atome de fer, sur des étoiles de référence issues du "Gaia-ESO survey", ce qui me permet de déterminer empiriquement les taux de collision avec l'hydrogène. En partant de paramètres photosphériques non-spectroscopiques, je détermine les abondances en fer de ces étoiles de référence dans le cas ETL comme hors-ETL. Les résultats dans le cas hors-ETL montrent un très bon accord entre les abondances de fer neutre et ionisé avec de faibles écarts raie à raie, particulièrement dans le cas des étoiles pauvres en métaux. Finalement cette méthode est validée par une comparaison avec des calculs quantiques très récents et encore non publiés.


#### Abstract

Determination of high precision abundances has and will always be an important goal of all spectroscopic studies. The use of LTE assumption in spectroscopic analyses has been extensively shown in the literature to badly affect the determined abundances and stellar parameters, especially in metal-poor and giant stars which can be subject to large non-LTE effects. Non-LTE modeling of stellar spectra is therefore essential to accurately reproduce the observations and derive stellar abundances. Non-LTE calculations require the input of a bulk of atomic data, which may be subject to uncertainties. In cool stars, hydrogen collisional rates are a major source of uncertainty, which are often approximated using a classical recipe (the Drawin approximation) for allowed bound-bound, and ionization transitions only. This approximation has been shown to overestimate the collisional rates, and does not reproduce the correct behavior with energies. I demonstrate in this dissertation the inability of the Drawin approximation to describe the hydrogen collisional rates. I introduce a new method to estimate these rates based on fitting the existing quantum rates of several elements. I show that this quantum fitting method (QFM) performs well in non-LTE calculations when detailed quantum rates are not available, and is able to reproduce the results obtained with the quantum rates (the case of Si ). I test the newly proposed method, with a complete iron model atom that I developed, on a reference set of stars from the "Gaia-ESO survey". Starting from well determined non-spectroscopic atmospheric parameters, I determine 1D, non-LTE, and LTE iron abundances for this set of stars. The non-LTE results show excellent agreement between Fe I and Fe II abundances and small line-by-line dispersions, especially for the metal-poor stars. The method is validated upon comparison with new preliminary Fe I + H quantum calculations, whose fits show an excellent agreement with ours.


"And you run and you run to catch up with the sun but it's sinking. Racing around to come up behind you again.
The sun is the same in a relative way, but you're older.
Shorter of breath and one day closer to death."
— Pink Floyd

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## 1 Introduction

The chemistry of the stars holds clues to how the Galaxy was formed and how it evolved through time. The primordial nebulous clouds that formed into the Milky Way consisted merely of the Big Bang elements (Hydrogen, Helium and Lithium), while most other elements were created by the stars (Burbidge et al., 1957). This process involves a chain of fusion of lighter elements, in which several nuclear processes are involved, depending on the mass of the star, which will determine the types of different assortment of elements that will be formed. The answer to when and how these processes take place is largely of the chemical elements that it will contribute to the interstellar medium at the end of its life, which will then create the next generation of stars. By studying the chemical composition of stars in different environments and ages, we can trace this cosmic recycling process.

The total metal content of a star, comprising of all elements except hydrogen and helium, is denoted as its metallicity ( $[\mathrm{Fe} / \mathrm{H}]$ ), whose value increase with time. Hence, old stars are more metal poor than younger ones, since the stellar chemical factories from which these stars were born were in their early stages, and there was not enough time to create a great abundance of metals that could be incorporated into the stellar formation from its gaseous nebulae.

The chemical elemental content (abundances) of a star is deciphered from its spectrum, originating from its stellar atmosphere. A significant progress in the field of stellar atmospheres has been achieved in the past few years, making use of rapid advances in multiple areas of astrophysics. Telescopes and detectors became larger, making increasingly precise observations of progressively fainter and more distant objects more feasible, and the analysis of the datasets has surged due to increasing capabilities of computers and networked systems.

With the launch of Gaia spacecraft in December 2013, which will chart our Galaxy and provide a large catalog of the positions and motions of a billion of stars, complementary large-scale studies (Gaia-ESO, SDSSIII-APOGEE, RAVE, ...) have started to take place in order to trace the history of stellar populations and the Galaxy. In this context, an important need to characterize in details the chemical composition of these stars, with the highest accuracies possible, has arisen.

Most models of stellar atmospheres adopt the assumption of Local Thermodynamic Equilibrium (LTE). Departures from LTE conditions in the atmospheres of cool stars, however, may significantly affect determinations of chemical abundances, in particular the determinations based on spectral lines of minority species. This deviation from LTE grows toward lower metallicities and extended atmospheres, due to decreasing number of electrons donated by metals and decreasing collisional rates. Thus non-LTE modeling of the stellar spectra of these stars becomes important, which in turn requires a good knowledge of a bulk of atomic data for each atom under consideration.

Homogeneous stellar parameters, including effective temperatures, surface gravities and metallicities of the stars are a fundamental cornerstone in any non-LTE study. The iron abundance ( $[\mathrm{Fe} / \mathrm{H}]$ ) is a key ingredient, due to its wealth of lines in most stellar spectra, and its common use as a proxy to the total metal content of the star (i.e. its metallicity).

Though stellar parameters determinations are becoming more reliable and less model dependent, lagging far behind in non-LTE modeling of stellar spectra, are the necessary laboratory astrophysics data. A common problem for calculating non-LTE abundances is that they can be subject to errors from uncertainties in the underlying atomic data. Line parameters for the iron atom are a particularly important case. While energy levels, wavelengths, transition probabilities ( $g f$-values) and collisional cross-sections can often be theoretically derived for light, simple atoms, the case is more difficult for atoms as complex as iron.

The influence of inelastic neutral hydrogen collisions on non-LTE spectral line formation remains the most significant source of uncertainty for stellar abundance analysis (Barklem et al., 2011; Osorio et al., 2015). Quantum calculations for hydrogen collisional rates have recently been calculated for a small number of elements including Li (Belyaev and Barklem, 2003), Na (Barklem et al., 2010), Mg (Belyaev et al., 2012), Al (Belyaev, 2013), and Si (Belyaev et al., 2014). For iron and other elements, however, no quantum calculations have been published yet ${ }^{1}$. In the lack of quantum calculations, the tendency is to approximate the hydrogen collisional rates using the classical Drawin (Drawin, 1968, 1969) approximation which is a modified version of Thomson (1912) classical $e^{-}+$atom ionization rate equation.

Upon comparison with quantum calculations, the Drawin approximation has been shown to overestimate the collisional rates by several orders of magnitude (Barklem et al., 2011; Lambert, 1993). This is commonly treated by applying a multiplicative scaling fudge factor $\mathbf{S}_{\mathbf{H}}$ to the Drawin rate equation by using different calibration methods on different reference stars. This method however, has been shown to give different scaling factors for different types of stars. This contradicts the fact that collisional cross-sections of an element with an impact species should be model and stellar parameters independent. The failure of the Drawin approximation is clearly seen upon comparison with the quantum calculations for elements like $\mathrm{Na}, \mathrm{Al}, \mathrm{Mg}$ and Si , where the cross-section - transition energy dependence trends are quite different. Thus a multiplicative scaling factor to the Drawin approximation cannot reproduce quantum calculations.

In the light of the inefficiency of the Drawin approximation, a new method to calculate the H -collisional rates is introduced in this dissertation. It is based on fitting the existing quantum data of few elements such as $\mathrm{Na}, \mathrm{Mg}, \mathrm{Al}$ and Si . The aim is to apply this quantum fitting method (QFM) for iron.

[^1]
## Summary

The following dissertation is organized as follows:
Chapter 2 recaps a brief description of the theory of radiative transfer in stellar atmospheres with a focused concentration on non-Local Thermodynamic Equilibrium.

Chapter 3, reviews a brief history of treatment of inelastic hydrogen collisions with atoms in cool stellar atmospheres, where both the classical and quantum approaches are explained.

Chapter 4 describes a newly developed iron model atom which was used in the calculations.
In Chapter 5, a set of benchmark stars upon which the different methods have been tested are presented with their corresponding atmospheric fundamental parameters which were determined mostly via non-spectroscopic model independent methods.

The Drawin approach to calculating the hydrogen collisional rates, with their results are presented in Chapter 6.

Chapter 7 introduced the quantum fitting method to calculating the hydrogen collisional rates, which was tested on 30 benchmark stars.

## 2 Investigating stellar atmospheres

Astellar atmosphere is the transition region from the stellar interior to the interstellar medium. It can be divided into many layers depending on different temperature gradient behaviors (Fig. 2.1). The major part of the visible spectrum originates from the stellar "Photosphere". Higher layers are typically studied at shorter and longer wavelengths.

Everything we know about the stars and systems of stars is derived from the analysis of the radiation emitted by their atmospheres. A great amount of information can be deciphered from the electromagnetic radiation of stars. In order to understand stellar atmospheres, we need to establish the fundamental physics of the energy transport, which is giving rise to the actual thermodynamical stratification in the surface layers of stars. Two intrinsically distinct regimes for the transport of energy can be identified at the boundaries of late-type stars: one convective, where the hydrodynamic equations govern the physics, and another radiative, which is described by the radiative transfer equation.
The main goal of modeling the stellar atmosphere is to calculate an emergent flux of a star for a given temperature, surface gravity and chemical composition. Such models can then be used to compare with observations and ultimately to determine relevant properties of the star. The models allow us to go from observable quantities, e.g. stellar fluxes, spectral energy distributions, and photometric magnitudes, to physical parameters of stars, such as the effective temperature $T_{\text {eff }}$, the surface gravity $g$, the metallicity $[\mathrm{Fe} / \mathrm{H}]$, abundances, rotation and turbulent velocities ${ }^{1}$...

I will overview in this chapter the basics of the theory of radiative transfer in the first Section 2.1, where I will outline the general approach used in modeling the radiative contribution to the stellar flux. In the second Section 2.2, I will describe the non-Local thermodynamic equilibrium approach to solving the radiative transfer problem. In the third Section 2.3, I will describe briefly the hydrostatic and hydrodynamic approaches to describe the radiative and convective stratification of the stellar atmosphere, in which physical parameters such as temperature, density, micro- and macro- turbulent velocities are expressed as a function of optical or geometric depths.
Unless specified otherwise, what follows is mainly from the work of Rutten (2003), Mihalas (1978) \& Gray (2008), in addition to the exhaustive reading and help of the PhD dissertation of Thibault Merle (Merle, 2012).

### 2.1 Radiative transfer

The dominant mechanism of energy transport throughout the surface layers of a star is radiation, in addition to convection which comes into play in some stars (giants, cool dwarfs and metal-poor stars). Radiation is not only a probe of the physical state of the atmosphere,

[^2]Figure 2.1: Temperature distribution in Kelvin as a function of geometrical height above a zero-point where $\tau_{5000}=1$ (in kilometers) in the outer layers of the Sun, adapted from Vernazza et al. (1973).

but in fact determines its structure. Thus the knowledge of the processes of interaction between the radiation and the gas in the stellar atmosphere allows us to better understand the physical properties of the medium through which light travels. Hence, we should define some basic physical quantities which help us demonstrate this interaction, leading us to the derivation of the radiative transfer equation which may be viewed as the kinetic equation for photons.

### 2.1.1 Intensity and Flux

If we consider a radiating surface of area $\mathrm{d} A$ of a star (Fig. 2.2), situated at position $\vec{r}$, we can define the specific intensity $I(\vec{r}, \vec{k}, \nu, t)$ (hereafter denoted $\left.I_{\nu}\right)^{2}$ traveling in direction $\vec{k}$ as the radiative energy transported through this surface per frequency interval $\mathrm{d} \nu$, per solid angle $\mathrm{d} \Omega$, per unit time $\mathrm{d} t$ as:

$$
\begin{equation*}
I_{\nu}=\frac{\mathrm{d} E_{\nu}}{\mathrm{d} A \cos \theta \mathrm{~d} \Omega \mathrm{~d} \nu \mathrm{~d} t} \tag{2.1}
\end{equation*}
$$

where $\theta$ is the angle of propagation of the light with the normal $\vec{n}$ to the surface $\mathrm{d} A$.
$I_{\nu}$ represents the energy transported by a bunch of identical photons along a single "ray of light". Thus it is the basic macroscopic quantity to use in formulating radiative transfer.
Equation 2.1 describes the monochromatic intensity emitted from the surface $\mathrm{d} A$ at a frequency $\nu$. The intensity emitted in the full spectral range is:

$$
\begin{equation*}
I=\int_{0}^{\infty} I_{\nu} \mathrm{d} \nu=\int_{0}^{\infty} I_{\lambda} \mathrm{d} \lambda \tag{2.2}
\end{equation*}
$$

$\overline{2}$ expressed in units of erg $\cdot \mathrm{s}^{-1} \cdot \mathrm{~cm}^{-2} \cdot \mathrm{rad}^{-2} \cdot \mathrm{~Hz}^{-1}$

From the specific intensity, other useful quantities can be calculated. The mean intensity $J_{\nu}{ }^{3}$ is defined as the directional average of $I_{\nu}$ :

$$
\begin{equation*}
J_{\nu}=\frac{1}{4 \pi} \int I_{\nu} \mathrm{d} \Omega=\frac{1}{4 \pi} \int_{0}^{2 \pi} \int_{0}^{\pi} I_{\nu} \sin \theta \mathrm{d} \theta \mathrm{~d} \phi \tag{2.3}
\end{equation*}
$$

where $\mathrm{d} \Omega=\sin \theta \mathrm{d} \theta \mathrm{d} \phi$ in spherical coordinates (See Fig. 2.2). It is interesting to use when only the presence of the radiation is of interest, regardless of its origin, i.e. when calculating the radiative ionization and excitation of atoms in the atmosphere (explained explicitly in Sec. 2.1.4.1).


Figure 2.2: A radiation beam of specific intensity $I_{\nu}$ traversing a surface area $\mathrm{d} A$ within a solid angle $\mathrm{d} \Omega$ and with an angle $\theta$ to the normal of the surface.

Another quantity of interest is the monochromatic flux $F_{\nu}{ }^{4}$, which describes the net flow of energy across the area $\mathrm{d} A$, over a time $\mathrm{d} t$, in a spectral range $\mathrm{d} \nu$, which can be written as:

$$
\begin{equation*}
F_{\nu}=\oint \frac{\mathrm{d} E_{\nu}}{\mathrm{d} A \mathrm{~d} t \mathrm{~d} \nu}=\int I_{\nu} \cos \theta \mathrm{d} \Omega=\int_{0}^{2 \pi} \int_{0}^{\pi} I_{\nu} \cos \theta \sin \theta \mathrm{d} \theta \mathrm{~d} \phi \tag{2.4}
\end{equation*}
$$

It is to be noted that while $I_{\nu}$ is independent on the distance from the source, $F_{\nu}$ obeys the standard inverse square law with respect to distance. Specific intensity can only be directly measured if we can resolve the radiating surface (which is usually not the case for stars other than the Sun).

Setting $\mu=\cos \theta$, and assuming axial symmetry about the z -axis (i.e. plane-parallel geometry) (Fig. 2.2), the monochromatic flux can be written as:

$$
\begin{equation*}
F_{\nu}=2 \pi \int_{-1}^{1} I_{\nu} \mu \mathrm{d} \mu \tag{2.5}
\end{equation*}
$$

[^3]Electromagnetic radiation has a momentum equal to its energy divided by the velocity of light c. The component of momentum, normal to the surface $\mathrm{d} A$, thus transferred by the beam of light, per unit time, per unit frequency is called the radiation pressure ${ }^{5}$, which can be written as:

$$
\begin{equation*}
p_{\nu}=\frac{1}{c} \int I_{\nu} \cos ^{2} \theta \mathrm{~d} \Omega \tag{2.6}
\end{equation*}
$$

### 2.1.2 Absorption and emission coefficients

The radiative transfer equation describes the change in the radiation field due to its interaction with matter in the atmosphere. To illustrate this interaction, phenomenological quantities which define the absorption and emission in the layers of the stellar atmosphere must be introduced.

The radiation can be absorbed by an amount $\mathrm{d} I_{\nu}$ due to the interaction with charged particles, atoms, ions, molecules or dust particles present in the atmosphere, and can be expressed as:

$$
\begin{equation*}
\mathrm{d} \mathrm{I}_{\nu}=-\kappa_{\nu} \rho I_{\nu} \mathrm{d} x \tag{2.7}
\end{equation*}
$$

where $\kappa_{\nu}$ is the monochromatic absorption coefficient ${ }^{6}$ per unit mass, referred to as opacity, $\rho$ is the density of the gas and $\mathrm{d} x$ the geometrical path length along the beam.

In addition photons can be emitted into the direction being considered. This can be expressed as:

$$
\begin{equation*}
\mathrm{d} I_{\nu}=j_{\nu} \rho \mathrm{d} x \tag{2.8}
\end{equation*}
$$

where $j_{\nu}$ is the monochromatic emission coefficient ${ }^{7}$.
The ratio of the emission to the absorption is called the source function $\mathrm{S}_{\nu}{ }^{8}$ :

$$
\begin{equation*}
S_{\nu}=\frac{j_{\nu}}{\kappa_{\nu}} \tag{2.9}
\end{equation*}
$$

### 2.1.3 Transport equation

Using the above definitions, we can write the radiation transfer equation representing the absorption, emission and scattering along a geometrical path $\mathrm{d} x$ in the propagation direction as:

$$
\begin{equation*}
\frac{\mathrm{d} I_{\nu}}{\mathrm{d} x}=j_{\nu} \rho-\kappa_{\nu} \rho I_{\nu} \tag{2.10}
\end{equation*}
$$

Eqn. 2.10 can also be written as:

$$
\begin{equation*}
\frac{\mathrm{d} I_{\nu}}{\kappa_{\nu} \rho \mathrm{d} x}=S_{\nu}-I_{\nu} \tag{2.11}
\end{equation*}
$$

Hence it is appropriate to define the monochromatic optical thickness $\tau_{\nu}$ (unitless) as a measure of the "optical transparency" of the medium, as:

$$
\begin{equation*}
\mathrm{d} \tau_{\nu}=\kappa_{\nu} \rho \mathrm{d} x \tag{2.12}
\end{equation*}
$$

[^4]and the monochromatic optical thickness of a medium of total path length (thickness) $L$ as:
\[

$$
\begin{equation*}
\tau_{\nu}(L)=\int_{0}^{L} \kappa_{\nu} \rho \mathrm{d} x \tag{2.13}
\end{equation*}
$$

\]

And so the radiative transfer (RT) equation can finally be written in terms of the optical thickness of the medium as:

$$
\begin{equation*}
\frac{\mathrm{d} I_{\nu}}{\mathrm{d} \tau_{\nu}}=S_{\nu}-I_{\nu} \tag{2.14}
\end{equation*}
$$

## The concept of optical depth (thickness):

In reality, the definition of the "border" of a star is not trivial at all, and so there is no definitive way to determine the actual extent of the stellar atmosphere. Going from the center of the star outwards, the density of the gas decreases and eventually reaches values as low as the surrounding interstellar medium. At some point in the stellar atmosphere, the density becomes low enough that photons can escape and be observed by our instruments. Therefore, using the term "radial optical depth" is then a reasonable approach to defining different regions in the stellar atmosphere, which can be defined at a given geometrical position $z_{0}$ as:

$$
\begin{equation*}
\tau_{\nu}\left(z_{0}\right)=\int_{z_{0}}^{\infty} \kappa_{\nu} \rho \mathrm{d} z \tag{2.15}
\end{equation*}
$$

which measures the optical depth along the radial line of sight with $\mu=1$ at $z_{0}$, from $\tau_{\nu}=0$ which is the optical depth at the observer's eye located at $z=\infty$. This can be helpful to allow us to answer the question: From which atmospheric depth does the radiation come from? In order to answer that, we first have to define a solution to the (RT) equation to better understand the propagation of radiation throughout the stellar atmosphere.

### 2.1.4 Solution of the radiative transfer equation

In order to simplify the solution to the (RT) equation, we assume that the radiation is monochromatic, and that our atmosphere is static (time-independent) and plane parallel which is a valid assumption as long as the atmospheric thickness is much smaller than the stellar radius $R_{\star}{ }^{9}$. The geometric distance traveled by the beam between two consecutive parallel shells $\mathrm{d} z$ apart in the atmosphere, is then:

$$
\begin{equation*}
\mathrm{d} x=\frac{\mathrm{d} z}{\cos \theta} \tag{2.16}
\end{equation*}
$$

Hence the (RT) equation can then be written in the standard form in terms of the optical depth as:

$$
\begin{equation*}
\mu \frac{\mathrm{d} I_{\nu}}{\mathrm{d} \tau_{\nu}}=I_{\nu}-S_{\nu} \tag{2.17}
\end{equation*}
$$

The solution to Eqn. 2.17 can be expressed by:

$$
\begin{array}{ll}
I_{\nu}^{-}\left(\tau_{\nu}, \mu\right)=-\int_{0}^{\tau_{\nu}} S_{\nu}\left(\tau_{\nu}^{\prime}\right) e^{-\left(\tau_{\nu}^{\prime}-\tau_{\nu}\right) / \mu} \mathrm{d} \tau_{\nu}^{\prime} / \mu & (\mu<0) \\
I_{\nu}^{+}\left(\tau_{\nu}, \mu\right)=+\int_{\tau_{\nu}}^{\infty} S_{\nu}\left(\tau_{\nu}^{\prime}\right) e^{-\left(\tau_{\nu}^{\prime}-\tau_{\nu}\right) / \mu} \mathrm{d} \tau_{\nu}^{\prime} / \mu & (\mu>0) \tag{2.18}
\end{array}
$$

[^5]which represent the sums of source functions $\mathrm{S}_{\nu}$ originating at points $\tau_{\nu}^{\prime}$, and exposed to absorption through the optical thickness ( $\tau_{\nu}-\tau_{\nu}^{\prime}$ ) by a factor $e^{-\left(\tau_{\nu}-\tau_{\nu}^{\prime}\right)}$, for the cases of inward ( $\mu<0$ ) and outward $(\mu>0)$ directed intensities respectively.

### 2.1.4.1 Special case

- Local Thermodynamic Equilibrium (LTE) approximation: It is the approximation widely and most often used in the description of emitted radiation field from stellar atmospheres and in the interpretation of stellar spectra, as it vastly simplifies the calculations as will be demonstrated below. The basic criteria for the LTE approximation to hold, is to have a finite volume in the stellar atmosphere with a uniform temperature $T$, in which the gas material is assumed to be in equilibrium with the radiation field. Hence, the majority of the interaction between photons and gas particles can be viewed as occurring between particles in thermodynamic equilibrium. This state allows the properties of the gas to be determined by the local temperature $T$ of this volume alone and is known as Local Thermodynamic Equilibrium (LTE).


## - Radiation in LTE:

Under the LTE approximation, it is required that as much energy be emitted as is absorbed and this can be expressed by Kirchhoff-Planck's law as:

$$
\begin{equation*}
\mathrm{j}_{\nu}=\kappa_{\nu} B_{\nu}(T) \tag{2.19}
\end{equation*}
$$

where $B_{\nu}(T)$ is the Planck function which describes the photon distribution as a function of temperature only.
From Eqn. 2.19 and under the LTE assumption, the source function of radiation is then equal to the Planck function:

$$
\begin{equation*}
\left[S_{\nu}\right]_{\mathrm{LTE}}=B_{\nu}(T)=\frac{2 h \nu^{3}}{c^{2}} \frac{1}{e^{h \nu / k_{\mathrm{B}} T}-1} \tag{2.20}
\end{equation*}
$$

where $h$ is the Planck constant and $k_{\mathrm{B}}$ is the Boltzmann constant.

## - Matter in LTE:

## * Maxwell velocity distribution:

Which describes the velocity distribution of gas particle species of mass $m$ :

$$
\begin{equation*}
f(v) \mathrm{d} v=\left[\frac{\mathrm{N}(v)}{\mathrm{N}_{\text {total }}} \mathrm{d} v\right]_{\mathrm{LTE}}=\left(\frac{m}{2 \pi k_{\mathrm{B}} T}\right)^{3 / 2} 4 \pi v^{2} e^{-(1 / 2) m v^{2} / k_{\mathrm{B}} T} \mathrm{~d} v \tag{2.21}
\end{equation*}
$$

where $\mathrm{N}(v)$ is the number of gas particles, per unit volume, of velocity $v . \mathrm{N}_{\text {total }}$ is the total particles density per unit volume. The left-hand-side of the equation is evaluated under LTE conditions, where the kinetic local electron temperature $T_{\mathrm{e}}$ is estimated as equal to all other material temperatures ( $T=T_{\mathrm{e}}$ ). The most probable velocity of the particles can be evaluated at $v_{\mathrm{p}}=\sqrt{2 k_{\mathrm{B}} T / m}$.

* Energy level populations: The Boltzmann distribution

The fraction of atoms excited to the $i$ th level is:

$$
\begin{equation*}
\mathrm{N}_{i}=g_{i} \frac{e^{-\chi_{i} / k_{\mathrm{B}} T}}{u(T)} \tag{2.22}
\end{equation*}
$$

where $g_{i}=2 J+1$ is the statistical weight of the level $i$, in which $J$ is the total quantum angular momentum, $\chi_{i}$ is the energy ${ }^{10}$ of level $i$ and

$$
\begin{equation*}
u(T)=\sum g_{i} e^{-\chi_{i} / k_{\mathrm{B}} T} \tag{2.23}
\end{equation*}
$$

is the partition function of the level $i$.
Hence the Boltzmann distribution gives the ratio of populations between two levels $j$ and $i$ :

$$
\begin{equation*}
\frac{\mathrm{N}_{i}}{\mathrm{~N}_{j}}=\frac{g_{i}}{g_{j}} e^{-\Delta \chi / k_{\mathrm{B}} T} \tag{2.24}
\end{equation*}
$$

where $\Delta \chi=\chi_{i}-\chi_{j}$

* Ionization fraction distribution: The Saha Equation

For collisionally dominated gas, the ionized to neutral species ratio $N_{1} / N_{0}$ is described by the Saha equation as:

$$
\begin{equation*}
\left[\frac{N_{1}}{N_{0}} P_{e}\right]_{\mathrm{LTE}}=\frac{\left(2 \pi m_{\mathrm{e}}\right)^{3 / 2}\left(k_{\mathrm{B}} T\right)^{5 / 2}}{h^{3}} \frac{2 u_{1}(T)}{u_{0}(T)} e^{-\chi_{0}^{\infty} / k_{\mathrm{B}} T} \tag{2.25}
\end{equation*}
$$

where $P_{e}$ is the electron gas pressure, $m_{e}$ is the electron mass, $\chi_{0}^{\infty}$ is the ionization energy of the ground neutral state.

* Saha-Boltzmann distribution: The combination of the two distribution equations above (Boltzmann and Saha) allows to calculate the ratio of the population $n_{i}$ of a level $i$ in a neutral atom to the number $n_{c}$ of ions in an ionized state $c$ :

$$
\begin{equation*}
\left[\frac{n_{c}}{n_{i}}\right]_{\mathrm{LTE}}=\frac{1}{N_{\mathrm{e}}} \frac{2 g_{c}}{g_{i}}\left(\frac{2 \pi m_{\mathrm{e}} k_{\mathrm{B}} T}{h^{2}}\right)^{3 / 2} e^{-\chi_{c i} / k_{\mathrm{B}} T} \tag{2.26}
\end{equation*}
$$

where $N_{\mathrm{e}}$ is the electron density and $\chi_{c i}$ is the ionization energy from level $i$ to c.

### 2.1.4.2 Breakdown of LTE:

The assumption of LTE is valid in the interior of the stellar atmosphere where the gas particle density is large enough to induce thermodynamic equilibrium, however in the upper reaches of the atmosphere, the density decreases to such a point that collisions between gas particles will be insufficient for the establishment of LTE. Also, as we move outwards, the photon mean free path becomes large, i.e. larger than the scale height of material, and thus the decoupling between radiation and matter increases, radiation becomes non-local, anisotropic, and strongly non-Planckian.
The radiative excitation and ionization rates dominate over collisional ones, and thus the assumption of LTE fails.

[^6]In order to quantify the deviation of the populations from those calculated under the LTE assumption using the Saha-Boltzmann distributions, it is convenient to introduce the departure coefficient $b_{i} \equiv n_{i} / n_{i}^{\mathrm{LTE}}$ where $n_{i}$ is the actual population density of energy level $i$ and $n_{i}^{\mathrm{LTE}}$ is the corresponding population density under LTE.

Therefore, when LTE conditions break down, it is necessary to solve for level populations and line strengths using non-Local Thermodynamic Equilibrium approach (hereafter non-LTE) where all possible radiative and collisional transitions are treated in the line formation analysis.

### 2.2 Non-Local Thermodynamic equilibrium:

The non-LTE level population densities are calculated under the assumption of statistical equilibrium (SE) where the sum of all transition rates to and out of an atomic energy level must be equal to zero. This assumption is valid when considering a time-independent atmosphere, where the radiation field and level populations do not vary with time. The term "population equations" introduced earlier under the LTE assumption are more conveniently replaced by the term "rate equations". The statistical equilibrium rate equation for a level $i$ can then be written as:

$$
\begin{equation*}
\frac{\mathrm{d} n_{i}}{\mathrm{~d} t}=\sum_{j \neq i}^{N} n_{j} P_{j i}-n_{i} \sum_{j \neq i}^{N} P_{i j}=0 \tag{2.27}
\end{equation*}
$$

where $n_{i}$ is the population of a particular level $i, P_{i j}$ is the transition probability of a transition from level $i$ to $j$, and $N$ is the total number of levels which can be coupled through transitions to level $i$. The transition rates $P_{i j}$ and $P_{j i}$ are the sum of radiative $R_{i j}$ and collisional $C_{i j}$ processes rates per particle that contribute to the transitions from and to level $i$ respectively:

$$
\begin{equation*}
P_{i j}=R_{i j}+C_{i j} \tag{2.28}
\end{equation*}
$$

The following important continuous and line absorption and emission processes that may contribute to these rates will be considered in our calculations:

- Radiative processes:
- bound-bound radiative processes, which are due to electron excitation and deexcitation transitions by photon emission or absorption.
- bound-free radiative processes, i.e. photoionization where an atom or ion loses an electron due to a photon absorption, and its counterpart photorecombination.
- free-free radiative processes ${ }^{11}$, which are due to accelerating electrons passing close to ions, thus emitting radiation.
- Collisional processes
- bound-bound collisional processes which correspond to electron excitation and de-excitation in atoms and ions due to collisions with $e^{-}$, atoms or ions.

[^7]- bound-free collisional processes which correspond to the ionization of an atom or ion, or its recombination with an electron, due to collisions with $e^{-}$, atoms or ions.

Figure 2.3: A schematic energy diagram for possible atomic transition processes.


To correctly reproduce the emergent stellar spectrum from a star, the radiative and collisional rates from all the processes that have the ability to populate and depopulate the energy levels of the atoms and ions present in the stellar atmosphere have to be included in the calculation of the level populations.

### 2.2.1 Radiative rates:

The bound-bound radiative rates can be due to radiative excitation (absorption), spontaneous radiative de-excitation and stimulated radiative de-excitation (emission).

- The rate of spontaneous radiative de-excitations per atom from an upper level $j$ to a level $i$ per atom is $A_{j i}$, where $A_{j i}$ is the Einstein coefficient for spontaneous emission and is defined as the probability per second per atom that an electron in level $j$ will spontaneously decay to level $i$.
- The probability to have a radiative excitation transition from level $i$ to level $j$ per atom per second in a radiation field of mean intensity $\bar{J}_{\nu}$ is equal to $4 \pi \bar{J}_{\nu} B_{i j}$, where $B_{i j}$ is the Einstein coefficient for excitation, and $\nu=E_{j i} / h$ where $E_{j i}=E_{j}-E_{i}$ is the energy difference between levels $i$ and $j$. Here $\bar{J}_{\nu}=\int_{0}^{\infty} J_{\nu} \phi(\nu) \mathrm{d} \nu$, where $\phi(\nu)$ is the line profile function which represents the probability that a photon is absorbed at frequency $\nu$ within the line, and which is normalized ${ }^{12}$ to 1 (See Appendix A for details on the line profile function).
- Similarly, the probability of a stimulated radiative de-excitation from a level $j$ to a level $i$ is $4 \pi \bar{J}_{\nu} B_{j i}$.

[^8]The Einstein coefficients are coupled by the Einstein relations:

$$
\begin{equation*}
\frac{B_{i j}}{B_{j i}}=\frac{g_{j}}{g_{i}} \quad \frac{A_{j i}}{B_{j i}}=\frac{2 h \nu^{3}}{c^{2}} \tag{2.29}
\end{equation*}
$$

The Einstein coefficients are calculated using quantum mechanics by solving for the wave function of the lower and upper levels $\left|\psi_{i}\right\rangle$ and $\left|\psi_{j}\right\rangle$ respectively. In spectroscopic analysis, it is customary to introduce the dimensionless oscillator strength $f_{i j}$ to describe the probability of a given radiative absorption transition which is related to the absorption Einstein coefficient by:

$$
\begin{equation*}
\frac{h \nu}{4 \pi} B_{i j}=\frac{\pi e^{2}}{m_{e} c} f_{i j} \tag{2.30}
\end{equation*}
$$

The oscillator strength of a given transition line is usually combined with the lower level statistical weight value $g_{i}$ to give a "gf-value", a product which is commonly used to define the effective transition probability which is needed to calculate the line extinction and emission coefficients.

To express the radiative rates of radiative transitions in terms of Einstein coefficients, we first have to express the source function $S_{\nu}$ in terms of these latter. Assuming complete redistribution, the number of spontaneous emissions per unit time, volume and frequency is $n_{j} A_{j i} \phi(\nu)$. Since each emission coefficient contributes an energy equal to $h \nu$ over a solid angle $4 \pi$, the line emission coefficient is:

$$
\begin{equation*}
j_{\nu}^{l}=(h \nu / 4 \pi) n_{j} A_{j i} \phi(\nu) \tag{2.31}
\end{equation*}
$$

Similarly, the line extinction coefficient per unit path length $\alpha_{\nu}=\kappa_{\nu} \rho$ can be expressed as:

$$
\begin{align*}
\alpha_{\nu}^{l} & =\frac{h \nu}{4 \pi}\left[n_{i} B_{i j} \phi(\nu)-n_{j} B_{j i} \phi(\nu)\right]  \tag{2.32}\\
& =\frac{h \nu}{4 \pi} n_{i} B_{i j} \phi(\nu)\left[1-\frac{n_{j} g_{i}}{n_{i} g_{j}}\right]
\end{align*}
$$

Hence the line source function $S_{\nu}^{l}$ can be written using the Einstein relations (Eqn. 2.29) as:

$$
\begin{align*}
S_{\nu}^{l} & =\frac{j_{\nu}^{l}}{\alpha_{\nu}^{l}} \\
& =\frac{n_{j} A_{j i}}{n_{i} B_{i j}-n_{j} B_{j i}}  \tag{2.33}\\
& =\frac{2 h \nu^{3}}{c^{2}} \frac{1}{\frac{g_{j} n_{i}}{g_{i} n_{j}}-1}
\end{align*}
$$

The radiative rates for radiative transitions can then be written as:

- Bound-bound radiative excitation rate per unit volume:

$$
\begin{align*}
n_{i} R_{i j} & =n_{i} B_{i j} \bar{J}_{\nu} \\
& =n_{i} \int_{0}^{\infty} B_{i j} J_{\nu} \phi(\nu) \mathrm{d} \nu  \tag{2.34}\\
& =4 \pi n_{i} \int_{0}^{\infty} \frac{\sigma_{\nu}^{l}}{h \nu} J_{\nu} \mathrm{d} \nu
\end{align*}
$$

where $\sigma_{\nu}^{l}=\frac{h \nu}{4 \pi} B_{i j} \phi(\nu)$ is introduced as the line extinction coefficient per particle.

## - Bound-bound radiative de-excitation rate per unit volume:

$$
\begin{align*}
n_{j} R_{j i} & =n_{j} A_{j i}+n_{j} B_{j i} \bar{J}_{\nu} \\
& =n_{j} \int_{0}^{\infty} A_{j i} \phi(\nu) \mathrm{d} \nu+n_{j} \int_{0}^{\infty} B_{j i} J_{\nu} \phi(\nu) \mathrm{d} \nu \\
& =n_{j} \frac{g_{i}}{g_{j}} \int_{0}^{\infty} B_{i j} \phi(\nu)\left(\frac{2 h \nu^{3}}{c^{2}}+J_{\nu}\right) \mathrm{d} \nu  \tag{2.35}\\
& =4 \pi n_{j} \frac{g_{i}}{g_{j}} \int_{0}^{\infty} \frac{\sigma_{\nu}^{l}}{h \nu}\left(\frac{2 h \nu^{3}}{c^{2}}+J_{\nu}\right) \mathrm{d} \nu
\end{align*}
$$

## - Bound-free photoionization rate per unit volume:

Similarly the photoionization rate of an electron in an energy level $i$ to a continuum level $c$ can be expressed in terms of the mean radiation field $J_{\nu}$ and the bound-free frequency dependent extinction coefficient per particle (photoionization cross-section) $\sigma_{i c}(\nu)$ as:

$$
\begin{equation*}
n_{i} R_{i c}=4 \pi n_{i} \int_{\nu_{0}}^{\infty} \frac{\sigma_{i c}(\nu)}{h \nu} J_{\nu} \mathrm{d} \nu \tag{2.36}
\end{equation*}
$$

where $\nu_{0}$ is the threshold frequency corresponding to the ionization energy of level $i$ equal to $h \nu_{0}$. As the photoionization cross-sections become more difficult to calculate for complicated atomic systems (atoms and ions with a large number of electrons, Fe-like atoms), a semi-classical approximation, Kramer's law (Travis and Matsushima, 1968), can be used to calculate the photoionization cross-section for Hydrogen like atoms:

$$
\begin{equation*}
\sigma_{\nu}^{i c}=\sigma_{\nu 0}^{i c}\left(\frac{\nu}{\nu_{0}}\right)^{-3} \tag{2.37}
\end{equation*}
$$

where $\nu_{0}$ and $\sigma_{\nu 0}^{i c}$ are respectively the threshold frequency and cross-section (in $\mathrm{cm}^{-2}$ ) and where:

$$
\begin{equation*}
\sigma_{\nu 0}^{i c}=7.91 \times 10^{-22} \frac{n}{Z^{2}} g_{\mathrm{rad}}^{i c} \tag{2.38}
\end{equation*}
$$

where $Z$ is the atomic number of the element in consideration, $n$ is the principal quantum number of the level $i$ from which the level is ionized. $g_{\text {rad }}^{i c}$ is called the Gaunt factor and is a correction factor of the order unity. For complex atoms, the cross-sections are shown from laboratory calculations not to a have a simple $\nu^{-3}$ dependence but instead possess "resonance" peaks caused by other electrons in the same shell.

- Bound-free radiative recombination rate per $\mathrm{cm}^{3}$ :

Under thermal equilibrium each process is balanced by its reverse counterpart (detailed balance):

$$
\begin{equation*}
\left[n_{c} R_{c i}\right]_{\mathrm{TE}}=\left[n_{i} R_{i c}\right]_{\mathrm{TE}} \tag{2.39}
\end{equation*}
$$

The recombination rate can then be deduced from the photoionization rate assuming the velocity distribution of free electrons to be Maxwellian (Eqn. 2.21). The (single) continuum level can then be considered to be in thermal equilibrium (TE), i.e. $n_{c}$ can be calculated under the assumption of LTE. Using the Boltzmann distribution equation (Eqn. 2.24), the radiative recombination rate can be written as:

$$
\begin{equation*}
n_{c} R_{c i}=4 \pi n_{c}\left[\frac{n_{i}}{n_{c}}\right]_{[\mathrm{LTE}]} \int_{\nu_{0}}^{\infty} \frac{\sigma_{i c}(\nu)}{h \nu}\left(\frac{2 h \nu^{3}}{c^{2}}+J_{\nu}\right) e^{-h \nu / k_{\mathrm{B}} T} \mathrm{~d} \nu \tag{2.40}
\end{equation*}
$$

## note:

The rates $P_{i j}$ and $P_{j i}$ in Eqn. 2.27 depend on $\bar{J}_{\nu}$ which in turn depends on $I_{\nu}$ in all directions, whereas the source function $S_{\nu}$ depends on the populations $n_{i}$ and $n_{j}$ of the lower and upper levels involved in the transition at frequency $\nu$. These populations may depend on other transitions and therefore on other populations as well, which are in turn dependent on the radiation fields at other frequencies. Thus a given transition may be influenced by many other transitions in other atoms and molecules which possess transitions at overlapping frequencies. This coupling between populations and radiation is thus non-linear and non-local!

### 2.2.2 Collisional rates:

The collision of a free particle $p$ of mass $m_{p}$ and velocity $v_{p}$ with kinetic energy $E_{p}^{k}=1 / 2 m_{p} v_{p}^{2}$ greater than the excitation energy of an electron between two bound levels $i$ and $j$ may excite the atom or ion. Considering a Maxwellian velocity distribution for the free colliding particles, the collisional excitation rate per unit volume can be expressed by:

$$
\begin{equation*}
n_{i} C_{i j}=n_{i} N_{p} \int_{v_{0}}^{\infty} \sigma_{i j}^{p}\left(v_{p}\right) v_{p} f\left(v_{p}\right) \mathrm{d} v_{p}=n_{i} N_{p}\left\langle\sigma_{i j}^{p} v_{p}\right\rangle \tag{2.41}
\end{equation*}
$$

where $\mathrm{C}_{i j}$ is the collisional excitation rate, which is equal to the number of collisional excitations from level $i$ to level $j$ per second, $N_{p}$ is the free colliding particle density, $\sigma_{i j}^{p}(v)$ is the particle collisional cross-section, which is a property of the particles, $f(v)$ is the normalized Maxwell velocity distribution, and $v_{0}$ is the threshold velocity of the particle equal to $\sqrt{2 E_{i j} / m_{p}}$ The Einstein coefficients for excitation and de-excitation are related by the Einstein relation:

$$
\begin{equation*}
\frac{C_{j i}}{C_{i j}}=\frac{g_{i}}{g_{j}} e^{E_{j i / k_{\mathrm{B}} T}} \tag{2.42}
\end{equation*}
$$

which holds in the case of "detailed balance" ${ }^{13}$. This is true since the particles velocity distribution in the stellar atmospheres is considered Maxwellian (Eqn. 2.21).
In the solar atmosphere, Plaskett (1955) considered that the two main candidates to consider in collisional rates are inelastic ${ }^{14}$ collisions with electrons and neutral hydrogen atoms in their ground state. The importance of electron collisions arises from the fact that electrons are the most abundant charged particles in the stellar atmosphere and have a much higher thermal velocity than atoms. In terms of atoms, neutral hydrogen is the most abundant perturbers in cool stars as it outnumbers helium by a 10:1 ratio. In hot stars, the H atoms will be almost completely ionized and thus electrons will be the dominant perturbers. Very cool dwarf atmospheres, on the other hand, are mostly rich with $\mathrm{H}_{2}$ molecules (Lambert, 1993). In this thesis, we are mostly interested by cool stars, and thus we will only consider inelastic collisions with electrons and neutral hydrogen in our calculations.

## Electron $e^{-}$impact collisional rates:

In calculating the electron impact excitation or ionization collisional cross section, Hebb and Menzel (1940) conveniently introduced the dimensionless collision strength ${ }^{15} \Omega_{i j}$, which under

[^9]the assumption of detailed balancing is symmetric with respect to the initial and final states ( $\Omega_{i j}=\Omega_{j i}$ ) and is related to the collisional cross-section as follows:
\[

$$
\begin{equation*}
\sigma_{i j}^{e}=\frac{\pi a_{0}^{2}}{E_{e} g_{i}} \Omega_{i j} \tag{2.43}
\end{equation*}
$$

\]

Where $a_{0}$ is the Bohr radius and $E_{e}$ is the electron impact energy in Rydberg (Ry). Being inversely proportional to the electron energy $\left(E_{e}\right), \Omega_{i j}$ varies slowly with energy making it easier to compare values for different transitions within an atom/ion, or between different atoms/ions.

Seaton (1953) defined the Maxwellian averaged collision strength (or effective collision strength) $\Upsilon_{i j}^{e}(T)$ as a function of the local temperature of the electrons $T_{e}$, which does not vary as strongly with resonances ${ }^{16}$ as $\Omega_{i j}$ (Fig. 2.4):

$$
\begin{equation*}
\Upsilon_{i j}^{e}=\int_{0}^{\infty} \Omega_{i j}(E) e^{-E / k_{\mathrm{B}} T} \mathrm{~d}\left(\frac{E}{k_{\mathrm{B}} T}\right) \tag{2.44}
\end{equation*}
$$

where $E \equiv E_{e}$. The electron excitation/ionization rate per unit volume can finally be expressed as:

$$
\begin{align*}
n_{i} C_{i j} & =n_{i} N_{e} \pi a_{0}^{2}\left(\frac{8\left(\chi_{\mathrm{H}}^{\infty}\right)^{2}}{\pi m_{e} k_{\mathrm{B}}}\right)^{1 / 2} \frac{1}{g_{i} T^{1 / 2}} \Upsilon_{i j}^{e} e^{-E_{j i} / k_{\mathrm{B}} T} \\
& =n_{i} N_{e} \frac{8.63 \times 10^{-6}}{g_{i} T^{1 / 2}} \Upsilon_{i j}^{e} e^{-E_{j i} / k_{\mathrm{B}} T} \tag{2.45}
\end{align*}
$$

On the other hand, the collision of an atom with an electron of any energy may cause the de-excitation or re-combination of the atomic electron from a higher to a lower energy level. Using the Einstein relation for collisions, $n_{i} C_{i j}=n_{j} C_{j i}$, the de-excitation collision rate by electrons can be expressed as:

$$
\begin{equation*}
n_{j} C_{j i}=n_{j} N_{e} \frac{8.63 \times 10^{-6}}{g_{j} T^{1 / 2}} \Upsilon_{j i}^{e} \tag{2.46}
\end{equation*}
$$

[^10]

Figure 2.4: Collision strength for FeII bound-bound transition ${ }^{6} \mathrm{D}_{9 / 2}-{ }^{6} \mathrm{D}_{7 / 2}$ (upper panel) and ${ }^{4} \mathrm{~F}_{3 / 2}$ ${ }^{4} \mathrm{D}_{7 / 2}$ (lower panel) at $\mathrm{T}=10000 \mathrm{~K}$ showing strong resonance peaks (Pradhan and Zhang, 1993).

The inverse process of electron impact ionization is the three-body recombination (2 electrons and ion). It has a low rate, except at high plasma densities, as it scales as $n_{e}^{2}$ (Pradhan and Nahar, 2011).
Theoretically, the study of bound-free impact collisions is more complicated than the boundbound impact, since the two outgoing final electrons must be accounted for in the presence of the residual atom/ion, which makes calculations much more difficult. Fortunately, experimental measurements of the total ionization impact cross-sections are easier to carry out than the excitation/de-excitations ones, since the latter requires information on both the initial and final states.

In the past few decades, considerable progress has been made in theoretical calculations of the collision cross-sections and effective collision strengths for electron impact transitions (the IRON project collaboration ${ }^{17}$, Hummer et al. (1993)). However large-scale calculations involving many atomic states are complex and require extensive computing resources and effort. Quantum mechanically, the basic problem is to describe the electron-atom-photon system with (i) a wave-function expansion and (ii) a Hamiltonian that includes the dominant interactions. The wave-function expansion is a quantum superposition of the possible pathways or channels for a given process or reaction. Practical calculations aim at limited, though sufficient, completeness and convergence using different methods developed from atomic collision theory that have been employed in a number of computer codes used to generate vast quantities of atomic data. The most commonly used approximation to calculate impact cross-sections is the close coupling (CC) approximation in which the $R$-matrix method is implemented.

The CC approximation (Percival and Seaton, 1957) has been a standard method for treating low-energy electron-atom interactions. It is based upon the expansion of the total wave function of the system in terms of products of eigenstates of the atomic Hamiltonian and to-be-determined functions describing the motion of the projectile. These are determined from

[^11]the solution of coupled integro-differential equations. The detailed description of the quantum theory of collision is beyond the scope of this thesis, however, when available for our relevant iron energy levels, they have been included in our model atom (see Chapter 4).
In non-LTE, it is of paramount importance to have collisional data for all transitions. In the absence of quantum calculations, especially for multi-electronic systems, they are replaced by classical and semi-classical approximation recipes.

For electron collisional excitation/de-excitation and ionization, the most commonly used semiclassical estimates are those by van Regemorter (1962) and the impact approximation of Seaton (1962a,b) which are explained below.

## Classical approach for excitation/de-excitation transitions: van Regemorter(1962)

van Regemorter (1962) expressed the electron impact excitation cross sections for allowed transitions in terms of the electric-dipole radiative oscillator strength $f_{i j}$ of the corresponding radiative transition, and the effective Gaunt factor $\bar{g}\left(E_{i}\right)$ as a function of the lower level energy. His formula became widely used in the modeling of high temperature plasmas. For an electron impact excitation from level $i$ to an upper level $j$, he expressed the corresponding collision cross section (in $\mathrm{cm}^{2}$ ) as:

$$
\begin{equation*}
\sigma_{i j}^{e}=\frac{8 \pi}{\sqrt{3}} \frac{1}{E_{e}} \frac{f_{i j}}{E_{i j}} \bar{g}\left(E_{i}\right) \pi a_{0}^{2} \tag{2.47}
\end{equation*}
$$

where $E_{e}$ and $E_{i j}$ are expressed in Ry. Using Eqn. 2.43, the van Regemorter collision strength can be expressed as:

$$
\begin{equation*}
\Omega_{i j}=\frac{8 \pi}{\sqrt{3}} \frac{g_{i} f_{i j}}{E_{i j}} \bar{g}\left(E_{i}\right) \tag{2.48}
\end{equation*}
$$

Eqn. 2.47 can be applied only to allowed transitions ${ }^{18}$ for which a radiative oscillator strength value exists. In addition, van Regemorter assumed that $\bar{g}$ can be expressed as a function of the impact electron energy in threshold units $\left(E_{e}\right)$ as $\varepsilon=E_{i} / E_{i j}$. For very high energies for which $\varepsilon \gg 1, \bar{g}$ is given by:

$$
\begin{equation*}
\bar{g}=\frac{\sqrt{3}}{2 \pi} \ln \varepsilon \tag{2.49}
\end{equation*}
$$

For low energies, however, van Regemorter chose $\bar{g}$ such that Eqn. 2.47 gave good agreement with available theoretical and experimental results for H , He and Na. For the region $\varepsilon \leq 3$, which is usually the most important energy region in stellar plasmas, he simply used the value $\bar{g}=0.2$ for positive ions.
Zhang et al. (1991) tested the accuracy of the van Regemorter formula on heavier elements (Ni-like elements), and found out that it is frequently a poor approximation for $\Delta n \geq 1$ transitions, where $\Delta n$ is the difference in principal quantum number corresponding to levels $i$ and $j$. They found it to be a better approximation for the $\Delta n=0$ transitions if a larger $\bar{g}$ was used than the initially recommended one.

Since the publication of van Regemorter, some attempts have been made to infer reasonably accurate Gaunt factors for various classes of transitions (e.g. Crandall (1983); Sobelman et al. (1981)). Fisher et al. (1996) tried fitting the experimental data for 11 different atoms ( $\mathrm{H}, \mathrm{He}, \mathrm{Li}, \mathrm{O}, \mathrm{N}, \mathrm{Na}, \mathrm{Mg}, \mathrm{K}, \mathrm{Rb}, \mathrm{Cs}, \mathrm{Ba}$ ) from different reference sources to derive a relation between

[^12]the effective Gaunt factor and the electron/atom relative energy $x=E_{e} / E_{i j}$. The fits for all the atoms were shown to be $\Delta n$ dependent:
\[

g(x)= $$
\begin{cases}0.33-0.3 x^{-1}+0.08 x^{-2} & \Delta n=0  \tag{2.50}\\ \left(0.276-0.18 x^{-1}\right) \ln x & \Delta n \geq 0\end{cases}
$$
\]

which was found to fit the experimental data with $82 \%$ accuracy.

## Impact parameter method approach for excitation/de-excitation transitions: Seaton(1962a)

A better alternative to van Regemorter's semi-empirical approximation which does not well reproduce the quantum cross-sections for most cases, is Seaton's semi-classical impact parameter approximation for allowed transitions. It starts from the quantum Born approximation (Born, 1926) for excitation of an atomic electron from level $i$ to level $j$ by an impact electron (described by plane-waves, of weak coupling and with no electron exchange with the target atom) of characteristic impact parameter $R_{i}$ (Fig. 2.5). The collisional transition cross-section $\sigma_{i j}$ can be described by:

$$
\begin{equation*}
\sigma_{i j}^{e}=\int_{0}^{\infty} P_{i j}\left(R_{i}\right) 2 \pi R_{i} \mathrm{~d} R_{i} \tag{2.51}
\end{equation*}
$$

where $P_{i j}\left(R_{i}\right)$ is the probability of the transition at an impact parameter $R_{i}$.


Figure 2.5: Closest approach of an electron-atom impact, at which the impact parameter $R$ is calculated.
The Born approximation is valid for large values of $R_{i}$ whereas it overestimates the cross sections at smaller $R_{i}$. Seaton thus introduced a cutoff value $R_{0}$ beyond which the Born approximation may be correctly applied, and he used a semi-classical approach to calculate $P_{i j}$ which at high energies is in good agreement with the quantum Bethe approximation (Seaton, 1955). For weak transition coupling, Eqn. 2.51 can thus be replaced by:

$$
\begin{equation*}
\sigma_{i j}^{0}=\int_{R_{0}}^{\infty} P_{j i}\left(R_{i}\right) 2 \pi R_{i} \mathrm{~d} R_{i} \tag{2.52}
\end{equation*}
$$

whereas for strong transition coupling, Seaton introduced another cutoff parameter $R_{1}$ such that $P_{i j}\left(R_{1}\right)=\frac{1}{2}$, and the cross-section would be written as:

$$
\begin{equation*}
\sigma_{i j}^{1}=\frac{1}{2} \pi R_{1}^{2}+\int_{R_{1}}^{\infty} P_{i j}\left(R_{i}\right) 2 \pi R_{i} \mathrm{~d} R_{i} \tag{2.53}
\end{equation*}
$$

For an impact electron with initial and final energies before and after impact $\epsilon=\frac{1}{2} m v^{2}$ and $\epsilon^{\prime}=\frac{1}{2} m v^{2}$ respectively, Seaton introduced two methods to calculate the cross sections in Eqns.
2.52 and 2.53. The first method is to consider the initial state $i$ to be that with a smaller mean radius $r_{i}$ of the atom (hereafter referred to as case 1), in which the cross section can be written:

$$
\begin{equation*}
\sigma_{i j}=8\left(\frac{\chi_{\mathrm{H}}^{\infty}}{\epsilon}\right)\left(\frac{\chi_{\mathrm{H}}^{\infty}}{E_{i j}} f_{i j}\right) \phi\left(\beta_{0}\right) \pi a_{0}^{2} \tag{2.54}
\end{equation*}
$$

where $E_{i j}=\left|\epsilon-\epsilon^{\prime}\right|$ is the transition energy, $\chi_{\mathrm{H}}^{\infty}=\frac{m e^{4}}{2 \hbar}=13.6 \mathrm{eV}$ is the hydrogen ionization potential and $\phi\left(\beta_{0}\right)=\beta_{0}^{2} K_{0}\left(\beta_{0}\right) K_{1}\left(\beta_{0}\right)$ is calculated by solving the zeroth and first order modified Bessel functions $K_{0}$ and $K_{1}$ respectively, where $\beta_{0}$ is dependent of the cutoff radius $R_{0}$, and which have been tabulated by Seaton.

The second method is by taking the initial state $i$ to be the one with the smaller statistical weight $g_{i}$ (hereafter referred to as case 2). In this case, the cross section can be written as:

$$
\begin{equation*}
\sigma_{i j}=8\left(\frac{\chi_{\mathrm{H}}^{\infty}}{\epsilon}\right)\left(\frac{\chi_{\mathrm{H}}^{\infty}}{E_{i j}} f_{i j}\right)\left\{\frac{1}{2} \zeta\left(\beta_{1}\right)+\phi\left(\beta_{1}\right)\right\} \pi a_{0}^{2} \tag{2.55}
\end{equation*}
$$

where $\zeta\left(\beta_{1}\right)=\beta_{0}^{2}\left\{K_{0}^{2}\left(\beta_{1}\right)+K_{1}^{2}\left(\beta_{1}\right)\right\}$, and $\beta_{i}$ can be calculated as follows:

$$
\begin{equation*}
\beta_{i}=\left(\frac{\epsilon}{\chi_{\mathrm{H}}^{\infty}}\right)^{1 / 2} \frac{E_{i j}}{\left(\epsilon+\epsilon^{\prime}\right)} \frac{R_{i}}{a_{0}} \tag{2.56}
\end{equation*}
$$

where $R_{i}=R_{0}$ for case 1 and $R_{i}=R_{1}$ for case 2 . Neglecting the exchange of energy between the perturber and the target at low $\epsilon$ allows the use the reciprocity condition, from which the inverse process cross-section can be calculated using:

$$
\begin{equation*}
\epsilon g_{i} \sigma_{i j}=\epsilon^{\prime} g_{j} \sigma_{j i} \tag{2.57}
\end{equation*}
$$

The best cross section is taken to be the smaller between the two cases. A drawback of Seaton's impact method for electron impact excitation is the requirement of the knowledge of the radiative oscillator $f_{i j}$ strength of the transition, which can be prone to large experimental errors, and of the cutoff radii $R_{0}$ and $R_{1}$. In addition, the close coupling relation neglects the higher states in the wave-function which leads to various distortion and resonance effects, whose total contribution can be important, in particular for forbidden lines excitation (Bely and van Regemorter, 1970).

For forbidden transitions, Seaton (1962b) suggested the calculation of the excitation crosssection using:

$$
\begin{equation*}
\sigma_{i j}=\frac{h^{2}}{4 \pi m_{e}^{2}} \frac{\Omega_{i j}}{g_{i} v_{e}^{2}} \tag{2.58}
\end{equation*}
$$

where $\Omega_{i j}$ is taken to be equal to 1 for forbidden transitions (Allen, 1973).
Therefore, in the lack of quantum theoretical calculations or experimental determinations, it is more appropriate to use the Seaton impact parameter method to calculate the excitation and de-excitation collisional cross-sections. The van Regemorter approximations, since the latter overestimates the cross-sections at low energies (Fig. 2.6). A recent study by Osorio et al. (2015) showed that the impact parameter method was able to reproduce the Mg IR emission lines, whereas the van Regemorter approximation failed to do so.


Figure 2.6: Collisional rates calculated using the van Regemorter (vR) classical approximation versus those calculated using Seaton semi-classical impact approximation (IP) on a log-log scale (Osorio et al., 2015).

## Impact approximation for ionization transitions: Bely \& van Regemorter (1970)

Bely and van Regemorter (1970) formulated an approach to calculating the electron impact ionization cross-section, referred to as Seaton's dipole impact parameter approximation. As presented in Allen (1973), the cross-section can be calculated as a function of the electron energy $\epsilon$ before impact (in Ry) to the atomic ionization energy $I_{i}^{\mathrm{Ry}}$ of an atomic electron on level $i$ (also in Ry) as:

$$
\begin{equation*}
\sigma_{i c}=1.63 \times 10^{-14} n\left(\frac{1}{I_{i}^{\mathrm{eV}}}\right)\left(\frac{I_{i}^{\mathrm{Ry}}}{\epsilon}\right) F\left(Y, \epsilon / I_{i}^{\mathrm{Ry}}\right) \tag{2.59}
\end{equation*}
$$

where $n$ is the number of optical electrons (i.e. the number of electrons in the outermost shell in the electronic configuration) and $I_{i}^{\mathrm{eV}}$ is the ionization energy of level $i$ in eV . The product $q\left(Y, \epsilon / I_{i}^{\mathrm{Ry}}\right)=\frac{I_{i}^{\mathrm{Ry}}}{\epsilon} F\left(Y, \epsilon / I_{i}^{\mathrm{Ry}}\right)$ is referred to as the reduced cross-section, where $Y$ is the charge of the ionized atom (i.e. $Y=1$ for the ionization of a neutral atom, and $Y=2$ for the ionization of a singly ionized atom, etc..). Experimental determination of $q$ for H are tabulated
in Table 2.1 for different $Y$ and $\frac{I_{i}^{\mathrm{Ry}}}{\epsilon}$ values which are determined from experimental results of Fite and Brackmann (1958). This approach to the ionization cross-section is a generalized form of Thomson (1912) classical two electron collision approach, which neglects any interaction between the ionizing electron and the atomic nucleus which renders Eqn. 2.59 as:

$$
\begin{equation*}
\sigma_{i c}^{\text {classical }}=4 n \pi a_{0}^{2} \frac{1}{I_{i}^{\mathrm{Ry}} \epsilon}\left(1-\frac{I_{i}^{\mathrm{Ry}}}{\epsilon}\right) \tag{2.60}
\end{equation*}
$$

| $\epsilon / I_{i}^{\mathrm{Ry}}$ | 1.0 | 1.2 | 1.5 | 2.0 | 3.0 | 5.0 | 10.0 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| $\mathrm{q}($ classical $)$ | 0.00 | 0.56 | 0.89 | 1.00 | 0.89 | 0.64 | 0.36 |
| $\mathrm{q}\left(1, \epsilon / I_{i}^{\mathrm{Ry}}\right)$ | 0.00 | 0.26 | 0.52 | 0.80 | 0.97 | 0.92 | 0.64 |
| $\mathrm{q}\left(2, \epsilon / I_{i}^{\mathrm{Ry}}\right)$ | 0.00 | 0.44 | 0.78 | 1.01 | 1.09 | 0.94 | 0.64 |
| $\mathrm{q}\left(\infty, \epsilon / I_{i}^{\mathrm{Ry}}\right)$ | 0.00 | 0.62 | 1.03 | 1.28 | 1.28 | 1.00 | 0.64 |

Table 2.1: Reduced cross-section q values for H as a function of ionizing electron energy to ionization energy ratio for the Bely and van Regemorter (1970) approximation, in addition to the Thomson (1912) classical values, from Fite and Brackmann (1958).

The study of inelastic collisions with neutral Hydrogen atoms is the main goal of this PhD dissertation and thus will be discussed in details in Chapter 3.

### 2.3 Stratification of the stellar atmosphere

In order to reproduce stellar spectra, one also needs theoretical or semi-empirical models of the atmospheric layers. In the case of late-type stars, the theoretical modeling of stellar atmospheres is complicated by the presence of turbulent convective motions as well as of magnetic fields in their envelopes (Nordlund and Stein, 2009). Convection can significantly affect both the atmospheric stratification and the emergent spectral energy distribution of these stars.

## One-Dimensional (1D) models:

One dimensional (1D) model atmospheres are commonly used and can be calculated using many public codes such as MARCS (Gustafsson et al., 1975, 2008), ATLAS (Castelli and Kurucz, 2004; Kurucz, 1979), PHOENIX (Hauschildt et al., 1997), and MAFAGS (Grupp, 2004) . These line-blanketed 1D models assume hydrostatic equilibrium, flux constancy, and LTE. The first 1D model atmosphere codes usually assumed a plane-parallel geometry for the atmospheric stratification, which was later improved by allowing for spherical symmetry (Gustafsson et al., 2008; Plez, 1992). That led to lower temperatures in the upper layers, in particular for giant stars, due to the dilution of the radiation field with increasing radius. Line blanketing was included first by means of opacity distribution functions (ODF) (Gustafsson et al., 1975; Strom and Kurucz, 1966) with a few hundred ODF's covering the entire spectrum. These were eventually replaced by opacity sampling (OS) including thousands of wavelength points (Johnson and Krupp, 1976). Nowadays, thousands of ODF's or hundreds of thousands of OS points are used, which result in more accurate models.

The assumption of hydrostatic equilibrium can be written as:

$$
\begin{equation*}
\nabla P_{\mathrm{tot}}=-\rho \frac{G M_{r}}{r^{2}} \tag{2.61}
\end{equation*}
$$

where $\rho$ is the gas density, G is Newton's constant of gravity and $M_{r}$ is the stellar mass inside radius r (one can usually neglects the mass of the atmosphere as compared to the stellar mass, i.e. $M_{r}$ is considered the stellar mass). The contribution to the total pressure is distributed among the gas, radiative and turbulent pressures.

$$
\begin{equation*}
\nabla P_{\text {tot }}=\nabla P_{\text {gas }}+\nabla P_{\text {rad }}+\nabla P_{\text {turb }} \tag{2.62}
\end{equation*}
$$

The radiative pressure is given by Eqn. 2.6, while the turbulent pressure is usually expressed in 1D atmospheres as:

$$
\begin{equation*}
P_{t u r b}=\beta \rho v_{t}^{2} \tag{2.63}
\end{equation*}
$$

where $\beta$ is a parameters depending on the (an)isotropy of the medium and $v_{t}$ is the mean turbulent velocity, which characterizes the motion of the gas in the atmosphere, whether due to convection or other turbulent gas motions. The gas pressure can be written for an ideal gas as:

$$
\begin{equation*}
P_{g}=\frac{\mathcal{R} \rho T}{\mu_{m o l}} \tag{2.64}
\end{equation*}
$$

where $\mathcal{R}$ is the ideal gas constant and $\mu_{m o l}$ is the mean molecular weight of the gas. The net stellar energy flux, for a plane-parallel model, is the sum of both radiative and convective fluxes:

$$
\begin{equation*}
F_{\mathrm{tot}}=F_{\mathrm{rad}}+F_{\mathrm{conv}}=\sigma_{\mathrm{SB}} T_{\mathrm{eff}}^{4} \tag{2.65}
\end{equation*}
$$

For a spherical model, Eqn. 2.65 can be written as:

$$
\begin{equation*}
r^{2} F_{\mathrm{tot}}=\sigma_{\mathrm{SB}} T_{\mathrm{eff}}^{4} R^{2} \tag{2.66}
\end{equation*}
$$

where $r$ is the radius of a spherical layer and $R$ is the stellar radius.
For modeling convective energy transport, 1D atmospheric codes employ the mixing-length theory (Böhm-Vitense, 1958), which is characterized by 1 to 3 free parameters. Henyey et al. (1965) expressed the convective energy flux using the mixing length theory as:

$$
\begin{equation*}
F_{\text {conv }}=\frac{1}{2} \rho c_{\mathrm{p}} T v_{\mathrm{conv}} \alpha_{\mathrm{MLT}} \delta \Delta \tag{2.67}
\end{equation*}
$$

where $c_{\mathrm{p}}$ is the specific heat capacity at constant pressure, T is the temperature, $v_{\text {conv }}$ is the convective velocity and $\alpha_{\text {MLT }}=\frac{l_{m}}{H_{\mathrm{p}}}$ is the free mixing length parameter. $\alpha_{\text {MLT }}$ sets the distance $l_{m}$ in units of the local pressure scale height $H_{\mathrm{p}}=\frac{P}{g \rho}$ over which energy is transported through convection. The factor $\delta \Delta$ is a constant which depends on the adiabatic temperature gradient in the atmosphere, and

$$
\begin{equation*}
v_{\text {conv }}=\alpha_{\mathrm{MLT}} \sqrt{\frac{G M}{r^{2}} H_{\mathrm{p}} \mathcal{Q} \delta \Delta / \nu} \tag{2.68}
\end{equation*}
$$

with $\mathcal{Q}=-\frac{T}{\rho}\left(\frac{\partial \rho}{\partial T}\right)_{\mathrm{p}} . y=0.076$ is the radiative heat loss term, and $\nu=8$ the turbulent viscosity term are free parameters whose values were suggested by Henyey et al. (1965). Hence, in the convective modeling of 1 D atmospheres there is a total of 3 free parameters ( $l_{m}, y$ and $\nu$ ) which need to be calibrated based on observations or their effect on synthetic spectra. Usually $\alpha_{\text {MLT }}$ is calibrated to reproduce selected lines (Barklem et al., 2002; Fuhrmann et al., 1993).


Figure 2.7: Temperature stratification as a function of Rosseland mean opacity of MARCS atmosphere models at $\operatorname{logg}=3$ (cgs) at different $T_{\text {eff }}$ and different metallicities [Me/H] (Gustafsson et al., 2008)

## Three-Dimensional (3D) models:

Constructing more realistic models to reproduce all observed properties accurately, however, requires to abandon the 1 D approximation, since stellar convection is an inherently 3D, timedependent, non-local and turbulent phenomenon. For late-type metal-poor stars, Asplund et al. (1999a,b) showed that the assumption of pure radiative equilibrium in the convectively stable photospheric layers of classical hydrostatic models is generally insufficient: the temperature structure in the upper layers of the photosphere is determined in 1D atmosphere models by radiative cooling and heating, whereas in reality, the radiative heating is balanced by expansion cooling of upwelling gas and spectral from the above granules (Magic et al., 2013a). This requires 3D modeling to be reproduced (Collet et al., 2006). Hydrodynamical models (Nordlund, 1982) revealed that stellar surface convection requires a different modeling approach than the MLT, since instead of homogeneous convective elements, they display highly asymmetrical motions with slow broad up-flows interspersed with fast narrow turbulent down-drafts (Stein and Nordlund, 1998). These inadequacies in the 1D models, can lead to overestimation of the effective temperatures at very low metallicities, which can lead to severe systematic errors in abundance determinations (Asplund, 2005; Collet et al., 2009).

3D simulations are calculated by solving the time-dependent hydrodynamic equations for mass, momentum, and energy conservation, coupled with 3D radiative transfer equations (Magic et al., 2013a,b), from which convective motions and flow patterns emerge which exhibit the surface granulation pattern that is observed. Several 3D magneto-hydrodynamic codes have been developed to model stellar surface convection, such as the STAGGER-code (Nordlund and Galsgaard, 1995) and CO ${ }^{5}$ BOLD (Freytag et al., 2012), which require parallelization techniques, high computational power and large timescales.

To minimize the large amount of data from the full 3D atmospheric models, temporally and spatially averaged models $\langle 3 \mathrm{D}\rangle$ have been calculated (Magic et al., 2013b; Stein and Nordlund, 1998). Fig. 2.8 shows the comparison in temperature stratifications of Rosseland-mean optical depth averaged 3D models $\langle 3 \mathrm{D}\rangle_{\text {Ross }}$ as compared to 1D models with $\alpha_{\text {MLT }}=1.5$ at different atmospheric parameters. It can be noticed that in the continuum forming layers, around $-1.0<\log _{\text {Ross }}<0.5$, the difference between $\langle 3 \mathrm{D}\rangle$ and 1D models are rather small. At lower optical depths, on the other hand, more significant differences can be observed depending on the model, more pronouncedly for lower metallicities, and higher $T_{\text {eff }}$ and $\log g$.


Figure 2.8: $\langle 3 \mathrm{D}\rangle_{\text {Ross }}$ temperature stratification as a function of Rosseland mean optical depth $\tau_{\text {Ross }}$ (solid lines), compared to 1D models with $\alpha_{\mathrm{MLT}}=1.5$ (dashed lines) for different atmospheric parameters (Magic et al., 2013b).

Even though 1D atmospheric models depend on assumptions and free parameters, they have demonstrated high predictive capabilities owing to major improvements in the atomic and molecular data, such as new linelists from VALD ${ }^{19}$, see e.g. VALD \& VALD3 (Kupka et al., 2000; Kurucz, 1993; Piskunov et al., 1995; Ryabchikova et al., 2011). Another advantage of using 1D atmospheric models is the presence of large homogeneous grids of models covering a wide

[^13]range of stellar atmospheric parameters like the MARCS grid ${ }^{20}$ (Gustafsson et al., 2008) and the ATLAS grid ${ }^{21}$. They have proven to be successful in spectroscopic studies when compared with observations and are thus widely applied in astronomy today. Moreover, the radiation fields in 1D models are precisely described by using ODF or OS with $\sim 10^{5}$ frequency points, while only about $\sim 10$ points are used in 3D models.

[^14]
## 3 |he curious case of Hydrogen Collisions

Acommon problem for calculating non-LTE abundance corrections is that they can be subject to errors from uncertainties in the underlying atomic data. Of these uncertainties, inelastic hydrogen collisions remain a very significant source of uncertainty for stellar abundance analysis. This is due to the difficulty of determining accurate cross section data, especially for low-energy atomic collisions either experimentally or theoretically: there exist very few reliable cross-sections. In the Sun, the ratio of neutral hydrogen to electrons densities $n_{\mathrm{H}} / n_{e}$ varies from $10^{4}$ to $10^{6}$ between optical depths at $5000 \AA, \tau_{5000}=1$ and -1 respectively, and it can reach up to $10^{5}$ at lower metallicities (Asplund, 2005; Lambert, 1993).

Most early non-LTE calculations did not include inelastic collisions with hydrogen at all. This assumption was based on the fact that hydrogen contribution to the collisional rates as compared to that of electrons is reduced by the ratio of their corresponding thermal velocities ${ }^{1}$ $\left(v_{\mathrm{H}} / v_{e}=\left(m_{e} / m_{\mathrm{H}}\right)^{1 / 2}=1 / 43\right.$ ). In addition, according to the Massey criterion (Massey, 1949), the hydrogen excitation cross-section is expected to be much less than that of electrons. His argument was also discussed by Anderson (1981), who stated that the characteristic time-scale of a collision is proportional to the ratio of the effective range to the relative velocity between the impact perturber and the atom, i.e. $t_{c} \sim r / v$. From the classical and quantum mechanical points of view, the cross section for excitation and de-excitation is expected to be small unless $1 / t \sim \nu$ (or $t \nu \leq 1$ ), where $\nu=\Delta E / h$ is the frequency corresponding to the transition energy $\Delta E$. Lambert (1993) looked closely at this ratio for both electrons and neutral hydrogen atoms and found that for a typical optical transition of $\Delta E \sim 3 \mathrm{eV}, T=5000 \mathrm{~K}$, and $r \sim 1 \AA$, the product $t \nu \sim 1 / 6$ for electrons and $\sim 7$ for hydrogen. For complex atoms with many high energy lying excitation states (such as $\mathrm{Fe}, \mathrm{Mg}, \mathrm{Ca}, \mathrm{Na}, .$. ) where term to term and fine-structure transition energies can be much less than 1 eV , the product $t \nu<1$ and thus the excitation and de-excitation transitions by hydrogen atoms must be considered. This stresses the importance of including hydrogen collisions in solving the non-LTE problem, as it may dominate the collisional processes especially in cool and metal poor stars, where $n_{\mathrm{H}} / n_{e} \sim 10^{6}$.

In this chapter, I will review the history of classical hydrogen collision treatment in spectroscopic studies and non-LTE abundance analyses in Sect. 3.1. In Sect. 3.2, I will briefly describe the quantum approach to collision cross-section calculations and compare the commonly used classical approaches to recent quantum calculations for some elements which have been treated accordingly. In Sect. 3.3, I will describe the approach to hydrogen collisions used in this work stressing the importance of charge exchange. This will lead us to semi-empirical calibration of hydrogen collision rates in Chapters 6 and 7.

[^15]
### 3.1 Hydrogen collisions: The classical approach

Because of the expectation that neutral hydrogen collision excitation would be negligible as explained above, and because of the almost lack of any reliable calculated or experimental data for H-atom collisions, most early non-LTE studies of cool stars (1960-1970s) neglected the inclusion of neutral H collisions. The first classical approach to H -atom excitation and ionization cross-section calculation was done by Drawin $(1968,1969)$ whose formulation of the problem is discussed below.

### 3.1.1 The Drawin Approximation

The classical recipe proposed by Drawin $(1968,1969)$ was described as a modified Thomson formula for calculating excitation cross-section for like-atoms collisions. Drawin started from Thomson (1912) electron-atom ionization cross section for the process: $\mathbf{e}+\mathbf{A} \longrightarrow \mathbf{2 e}+\mathbf{A}^{-}$ (Eqn. 2.60). Thomson's theory assumes that the bound electron in the target atom is a stationary free classical electron. The Coulomb interaction between the incident electron and the atomic electron is considered by calculating the impact parameter for which the deflection of the incident electron results in an energy transfer between electrons corresponding to the ionization potential. The cross-section can then be calculated easily as all collisions inside this impact parameter will have a larger energy transfer and thus lead to ionization.
Thomson's theory is able to make qualitative predictions regarding the ionization cross-sections and their dependence on the impact energy (Rudge, 1968), however, quantitatively it was found to provide only an order of magnitude precision (Seaton, 1962a). Fig. 3.1 (from Barklem et al. (2011)) compares experimental results for electron collisional ionization crosssections with Thomson's classical formula for the ground-state for some elements ( $\mathrm{H}, \mathrm{O}, \mathrm{Mg}$ and Fe ).

The classical formula is shown to overestimate the cross-sections by a factor of $\sim 5$ at low energies, particularly for O which seems to differ by a factor of $\sim 20$ near the threshold thus showing that the Thomson formula is able to provide only a rough order of magnitude estimate of the cross-sections.

This classical formula of Thomson's was then adapted by Drawin for like-atoms excitation $\mathbf{A}+\mathbf{A}_{i} \longrightarrow \mathbf{A}+\mathbf{A}_{j}$ and ionization $\mathbf{A}+\mathbf{A} \longrightarrow \mathbf{A}+\mathbf{A}^{+}+e^{-}$collisions. He replaced the ionization potential of the atom A, $I_{i}^{\mathrm{A}}$, by the excitation potential from level $i$ to level $j\left(\Delta E_{i j}^{\mathrm{A}}=E_{j}^{\mathrm{A}}-E_{i}^{\mathrm{A}}\right)$. To convert from Eqn. 2.60 to its corresponding $\sigma_{\mathrm{AA}}$ for like-atoms collisions, he formulated a conversion between laboratory and center-of-mass coordinates for energy.
In laboratory coordinates, a collision between two atoms $\mathbf{A}$ and $\mathbf{B}$ includes a projectile $\mathbf{B}$ hitting a stationary target A , with a kinetic energy $E_{\mathrm{B}}^{\mathrm{LAB}}$. In center-of-mass coordinates, the total kinetic energy of the collision is expressed as:

$$
\begin{equation*}
E_{\mathrm{AB}}^{\mathrm{COM}}=\frac{m_{\mathrm{A}}}{m_{\mathrm{A}}+m_{\mathrm{B}}} E_{\mathrm{B}}^{\mathrm{LAB}} \tag{3.1}
\end{equation*}
$$

The excitation of the atomic electron of A requires the condition $E_{\mathrm{AB}}^{\mathrm{COM}} \geq \Delta E_{i j}^{\mathrm{A}}$.
For electron excitation collisions ( $\mathrm{e}^{-}+\mathbf{A}_{\mathbf{i}} \longrightarrow \mathbf{A}_{\mathbf{j}}+\mathbf{e}^{-}$), Drawin introduced the variable:

$$
\begin{equation*}
U_{i j}^{\mathrm{eA}}=\frac{\left(\Delta E_{i j}^{\mathrm{A}}+\Delta E_{e}^{\mathrm{LAB}}\right)}{\Delta E_{i j}^{\mathrm{A}}} \tag{3.2}
\end{equation*}
$$

where $\Delta E_{e}^{\mathrm{LAB}}$ is the electron's projectile energy. At threshold $U_{i j}^{\mathrm{Ae} e}=1$ when $U_{e}^{\mathrm{LAB}}=0$.

Figure 3.1: Comparison of the classical Thomson (1912) ionization collisional cross-sections for H, O, Mg and Fe to experimental results by Shah et al. (1987), Thompson et al. (1995), McCallion et al. (1992) and Shah et al. (1993) respectively. The plot shows the ratio of the experimental values to the classical ones as a function of the incident electron energy $E$ scaled by the ionization potential $I$ (Barklem et al., 2011).


Similarly for like-atoms collisions $\mathbf{A}+\mathbf{A}_{i} \longrightarrow \mathbf{A}+\mathbf{A}_{j}$, Drawin rewrote Eqn. 3.2 as:

$$
\begin{equation*}
W_{i j}^{\mathrm{AA}}=\frac{\Delta E_{i j}^{\mathrm{A}}+\Delta E_{\mathrm{A}}^{\mathrm{LAB}}}{\Delta E_{i j}^{\mathrm{A}}} \tag{3.3}
\end{equation*}
$$

where $E_{\mathrm{A}}^{\mathrm{LAB}}$ is the projectile's kinetic energy above threshold which is attained at $E_{\mathrm{A}}^{\mathrm{LAB}}=$ $2 E_{\mathrm{A}}^{\mathrm{COM}}=2 \Delta E_{i j}^{\mathrm{A}}$. The relation between Eqns. 3.2 and 3.3 stemmed from considering the collision in both cases to occur between the projectile and the atom's "free" electron, and that both types of collisions are equally efficient at equal energies above the threshold in the center-of-mass coordinates, thus allowing for writing:

$$
\begin{equation*}
\frac{m_{e}}{m_{e}+m_{e}} \Delta E_{e}^{\mathrm{LAB}}=\frac{m_{e}}{m_{e}+m_{\mathrm{A}}} \Delta E_{\mathrm{A}}^{\mathrm{LAB}} \tag{3.4}
\end{equation*}
$$

which allows to relate $U_{i j}^{e \mathrm{~A}}$ and $W_{i j}^{\mathrm{AA}}$ as follows:

$$
\begin{equation*}
U_{i j}^{e \mathrm{~A}}=1+\frac{2 m_{e}}{m_{e}+m_{\mathrm{A}}}\left(W_{i j}^{\mathrm{AA}}-1\right) \tag{3.5}
\end{equation*}
$$

Drawin then substituted Eqn. 3.5 above in Eqn. 2.60 to get the collisional cross-section for A+A collisions:

$$
\begin{equation*}
\sigma_{\mathrm{AA}}=4 \pi a_{0}^{2}\left(\frac{I^{\mathrm{H}}}{\Delta E_{i j}^{\mathrm{A}}}\right)^{2} \frac{m_{\mathrm{A}}}{m_{\mathrm{H}}} f_{i j} \frac{2 m_{e}}{m_{e}+m_{\mathrm{A}}} \Phi\left(W_{i j}\right) \tag{3.6}
\end{equation*}
$$

where

$$
\begin{equation*}
\Phi\left(W_{i j}\right)=\frac{W_{i j}-1}{\left[1+\frac{2 m_{e}}{m_{e}+m_{\mathrm{A}}}\left(W_{i j}-1\right)\right]^{2}} \tag{3.7}
\end{equation*}
$$

and

$$
\begin{equation*}
W_{i j}=\frac{\left(E_{\mathrm{A}}^{\mathrm{LAB}}-\Delta E_{i j}^{\mathrm{A}}\right)}{\Delta E_{i j}^{\mathrm{A}}} \tag{3.8}
\end{equation*}
$$

where the oscillator strength $f_{i j}$ was introduced to account for allowed transitions as compared to the forbidden, motivated by an analogy with the Bethe approximation for inelastic collisions with electrons. $m_{\mathrm{A}} / m_{e}$ is a fudge factor introduced to ensure a better fit with measurements of $\mathrm{He}-\mathrm{He}$ and $\mathrm{N}_{2}-\mathrm{N}_{2}$ collisions.
The main physical assumption in Drawin's classical approach is neglecting the nuclei of the perturbing atoms, thus rendering the problem as a two electrons interaction. Even though Drawin found an agreement within a factor of 2 between his formula and experimental values for ionization collisions between light atoms, Fleischmann and Dehmel (1972) found only order of magnitude agreement with more recent experimental rates which become larger for heavier elements.

### 3.1.2 A little bit of history

The H -atom collisional rate can be calculated similarly to that of $e^{-}$-atom collisions starting from Eqn. 2.45 where $N_{e}$ is replaced by $N_{\mathrm{H}}$ and $m_{e}$ by $m_{\mathrm{H}}$, thus allowing for expressing the H collisional rate (per unit volume) for a collisional excitation from level $i$ to level $j$ in terms of the effective collisional strength $\Upsilon_{i j}^{H}$ as

$$
\begin{equation*}
n_{i} C_{i j}^{\mathrm{H}}=2.014 \times 10^{-7} n_{i} N_{\mathrm{H}} \frac{\Upsilon_{i j}^{\mathrm{H}}}{g_{i} \sqrt{T}} e^{-E_{j i} / k_{\mathrm{B}} T} \tag{3.9}
\end{equation*}
$$

where $N_{\mathrm{H}}$ is the H atom density, and

$$
\begin{equation*}
\Upsilon_{i j}^{\mathrm{H}}=4.965 \times 10^{6} g_{i} \sqrt{T}\left\langle\sigma_{i j} \nu\right\rangle . \tag{3.10}
\end{equation*}
$$

$\left\langle\sigma_{i j} \nu\right\rangle$ is the Maxwellian averaged collisional rate. The earliest work to include neutral hydrogen collisions in their non-LTE spectroscopic calculations was Gehren (1975), in his solar study of Na lines, who stated his using Drawin's classical equation for calculating the collisional crosssections without specifying on how the formula was extended from like-atoms to $\mathrm{H}+$ atom collisions. His study however, found that the H atom collisions were relatively unimportant (less than $50 \%$ of the contribution of electrons). Gehren deduced that the influence of atom + H collisions on the kinetic equilibrium was negligible under solar conditions.

Nine years later, Steenbock and Holweger (1984) included H-atom collisions in their Li study. They also started from Drawin's cross-section formula (Eqn. 3.6), substituting $m_{\mathrm{A}}$ by $m_{\mathrm{H}}$ and removing the fudge factor $m_{\mathrm{A}} / m_{e}$. They expressed the Maxwell-averaged cross-section of a particle species A by inelastic collisions with neutral $H$ atom as:

$$
\begin{equation*}
\langle\sigma \nu\rangle=16 \pi a_{0}^{2}\left(\frac{2 k_{\mathrm{B}} T}{\pi \mu}\right)^{1 / 2} Q \frac{m_{\mathrm{A}}}{m_{\mathrm{H}}} \frac{m_{e}}{m_{e}+m_{\mathrm{H}}} \Psi(W) \tag{3.11}
\end{equation*}
$$

where $\mu=\frac{m_{\mathrm{A}} m_{\mathrm{H}}}{m_{\mathrm{A}}}$ is the reduced mass of the A-H system. The variable $Q$ was defined differently for the excitation and ionization cases:

$$
Q=\left\{\begin{array}{ll}
\left(\frac{\chi_{\mathrm{B}}^{\infty}}{\Delta E_{i j}^{\mathrm{A}}}\right)^{2} f_{i j} & \text { with } W=\frac{\Delta E_{i j}^{\mathrm{A}}}{k_{\mathrm{B}} T} \text { for excitation }  \tag{3.12}\\
\left(\frac{\chi_{\mathrm{F}}^{\infty}}{I_{i}^{\mathrm{A}}}\right)^{1 / 2} f_{i} \xi_{i} & \text { with } W=\frac{I_{i}^{\mathrm{A}}}{k_{\mathrm{B}} T}
\end{array} \text { for ionization }, ~ \$\right.
$$

where $\chi_{\mathrm{H}}^{\infty}$ is the hydrogen ionization potential, $I_{i}^{\mathrm{A}}$ is the ionization energy of level $i, f_{i}$ is the effective oscillator strength for ionization, and $\xi_{i}$ is the number of equivalent electrons ${ }^{2}$. The function $\Psi(W)$ was defined as:

$$
\begin{equation*}
\Psi(W)=\left(1+\frac{2}{W}\right) \frac{e^{-W}}{1+\frac{2 m_{e}}{\left(m_{e}+m_{\mathrm{H}}\right) W}} . \tag{3.13}
\end{equation*}
$$

Lambert (1993) then reviewed the two previous approaches to Drawin's approximation for the $\mathrm{H}+$ atom collisional cross-sections. He re-derived an expression for the rate coefficients from Drawin's approach differing from Steenbock and Holweger (1984) by a negligible factor of $m_{\mathrm{A}} /\left(m_{\mathrm{A}}+m_{\mathrm{H}}\right)$ of order unity, and expressed it as:

$$
\begin{equation*}
\langle\sigma \nu\rangle=16 \pi a_{0}^{2}\left(\frac{2 k_{\mathrm{B}} T}{\pi \mu}\right)^{1 / 2} f_{i j}\left(\frac{\chi_{\mathrm{H}}^{\infty}}{\Delta E_{i j}^{\mathrm{A}}}\right)^{2} \frac{m_{e}\left(m_{\mathrm{A}}+m_{\mathrm{H}}\right)}{m_{\mathrm{H}}\left(m_{e}+m_{\mathrm{H}}\right)} \Psi\left(W_{i j}\right), \tag{3.14}
\end{equation*}
$$

with

$$
\begin{equation*}
\Psi\left(W_{i j}\right)=e^{-W_{i j}}\left(1+\frac{2}{W_{i j}}\right) \text { and } W_{i j}=\frac{\Delta E_{i j}^{\mathrm{A}}}{k_{\mathrm{B}} T} . \tag{3.15}
\end{equation*}
$$

### 3.2 Hydrogen collisions: The Quantum scattering approach

According to the first Born approximation "perturbation theory" (Landau and Lifshitz, 1965), valid for high-energy collisions between electrons and atoms, the Coulomb interaction $U$ is considered between the impact electron and the target atom and includes interactions with the atomic nucleus and atomic electrons $U_{\mathrm{e}-\mathrm{nuc}}$ and $U_{\mathrm{e}-\mathrm{e}}$ respectively ( $U=U_{\mathrm{e}-\mathrm{nuc}}+U_{\mathrm{e}-\mathrm{e}}$ ). The direct scattering probability amplitude for the excitation of an atom A from level $i$ to level $j$ is expressed as:

$$
\begin{equation*}
P^{i j}=-\frac{1}{2 \pi}\left\langle\phi_{j}^{\mathrm{A}}(\mathbf{r})\right| \exp (i \mathbf{q} \mathbf{R}) U\left|\phi_{i}^{\mathrm{A}}(\mathbf{r})\right\rangle, \tag{3.16}
\end{equation*}
$$

where $\phi_{i / j}^{\mathrm{A}}(\mathbf{r})$ denote initial/final wave functions, $\mathbf{r}$ represents a set of coordinates of the atomic electrons, $\mathbf{R}$ denotes the impact electron coordinate, $\mathbf{q}=\mathbf{k}_{i}-\mathbf{k}_{j}$ is the momentum transfer during the transition between the two levels and $i$ is the imaginary complex number.

The collisional cross-section is proportional to the square of the scattering probability amplitude and is shown in Bransden and Joachain (2003) to be proportional to the quantity:

$$
\begin{equation*}
\left.\mathcal{F}_{i j}=\frac{2\left(\Delta E_{i j}\right)}{\mathrm{q}^{2}}\left|\left\langle\phi_{j}^{\mathrm{A}}(\mathbf{r})\right| \sum \exp (i \mathbf{q} \mathbf{R}) U\right| \phi_{i}^{\mathrm{A}}(\mathbf{r})\right\rangle\left.\right|_{\mathbf{r}} ^{2}, \tag{3.17}
\end{equation*}
$$

which is called the generalized oscillator strength. In Eqn. 3.17, and according to the first Born approximation, the integration over the impact electron coordinate $\mathbf{R}$ and the orthogonality of the wave functions, has lead to removing the interaction with the nucleus, leaving only the interaction between the incident and atomic electrons. This allows for a bridge between the quantum and the classical Drawin approach which both relate the allowed collisional transitions to their radiative counterparts through the oscillator strength.

The Born approximation, however, is valid only for high-energy electron-atom and electronmolecule collisions. It gives poor results for low-energy collisions, such as inelastic H -atom collisions, which are interesting in the atmospheres of cool stars and are relevant for this thesis

[^16]
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work. In the latter case, the Born-Oppenheimer approach should be used which requires full quantum treatment of the total wave functions of the entire collisional system.

Although the understanding of H -atom collisions has increased in the past 30 years, there are still a lot of experimental difficulties, especially for complex atoms. Fleck et al. (1991) performed an experimental study of the $\mathrm{Na}(3 \mathrm{~s})+\mathbf{H} \longrightarrow \mathbf{N a}(3 \mathrm{p})+\mathrm{H}$ excitation transition. They could not, however, go below the threshold values of 2.1 eV (the relevant temperature regime for stellar atmospheres) due to experimental complications. Fig. 3.2 shows these experimental cross-section results as compared to quantum theoretical calculations (Belyaev et al., 1999) and to those calculated using Lambert's approach of Drawin's approximation. It can be seen that the quantum theoretical calculations fit well to experimental data, while Drawin's approximation overestimates them by many orders of magnitude. In addition, it does not provide cross-sections for forbidden transitions. It can also be markedly seen that the deviation from quantum calculations varies from one transition to another. This is shown in Fig. 3.3, where the quantum scattering rate coefficients, the Drawin approximation rate coefficients and corresponding ratios are shown for $\mathrm{Li}+\mathrm{H}$ and $\mathrm{Na}+\mathrm{H}$ collisions. The Drawin to quantum ratio is specifically shown to overestimate the collisional rates, especially for higher energies which correspond to transitions from low-lying to high-lying energy levels, while the quantum scattering calculations show decreasing rates with increasing transition energies down to negligible values.

Figure 3.2: Calculations for $\mathrm{Na}(3 \mathrm{~s})+\mathrm{H} \longrightarrow \mathrm{Na}(3 \mathrm{p})+\mathrm{H}$ collisional excitation cross-sections as a function of the H collision energy. The solid line represents the quantum scattering calculations (Belyaev et al., 1999), while the circles represent Fleck et al. (1991) experimental data. The dashed line represents the cross-sections calculated using the Drawin approximation which overestimates the experimental data by orders of magnitude (Barklem et al., 2011)


It can be deduced that at low energies, the Drawin approximation does not hold the essential physics behind collisional excitation by H atoms. It is in error by orders of magnitude, well beyond the estimated uncertainties of the quantum calculations (Barklem et al., 2010).

Figure 3.3: $\mathrm{Li}+\mathrm{H}$ (upper left panel) and $\mathrm{Na}+\mathrm{H}$ (upper right panel) quantum scattering H -collision rate coefficients calculation for excitation transitions (Barklem et al., 2003) and Barklem et al. (2010) respectively for different initial energy states. Different symbols denote different transition energies. Lower left and right panels show the corresponding rate coefficients calculated using the Drawin approximation for $\mathrm{Li}+\mathrm{H}$ and $\mathrm{Na}+\mathrm{H}$ respectively. The dotted lines in all panels show the linear fit to the quantum calculations. The smaller panels show the Drawin to quantum ratios which demonstrates the overestimation of the rates as a function of transition energies. Adapted from Barklem et al. (2011).


In the lack of quantum calculations and experimental data for most elements, and in an attempt to correct the Drawin H-collisional rates, a multiplicative fudge scaling factor $\mathbf{S}_{\mathbf{H}}$ has been introduced for the Drawin rates, a method which has been used exhaustively in most non-LTE studies. The $\mathbf{S}_{\mathbf{H}}$ values have been calibrated with different means whether on solar or benchmark star observations.

Several non-LTE studies of iron have included H-Fe collisions by using the Drawin approximation of Steenbock and Holweger (1984) and Lambert (1993). However, many different scaling factors $S_{\mathbf{H}}$ have been used in each study. Thévenin and Idiart (1999) found a best fit upon using a value of $\mathrm{S}_{\mathrm{H}}=1$, and found no important effects whether including the H collisions or not, while finding significant non-LTE effects in their study. Gratton et al. (1999) derived a value of $\mathbf{S}_{\mathbf{H}}=30$ using RR-Lyrae stars, and found very little non-LTE effects, as increasing the

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collisions to large values leads to LTE conditions. It is to be noted that the former two studies used rather incomplete FeI/FeII model atoms which did not include all the necessary levels and lines. In addition, they did not include the high-lying FeI levels which induce important coupling with FeII ground levels (details discussed in Chapter 4). Another study by Gehren et al. (2001) found a best fit when adopting a value of $\mathbf{S}_{\mathbf{H}}=3$. Two more recent studies, which used a rather more complete FeI/II model atoms, are those of Mashonkina et al. (2011) and Bergemann et al. (2012) which included a large number of levels, including the theoretical high-lying levels and lines in their studies, and who both used FeI/FeII excitation balance to determine metallicity dependent values of $\mathbf{S}_{\mathbf{H}}=0.1$ and $\mathbf{S}_{\mathbf{H}}=1$.

Another attempt was to scale the Drawin approximation on an energy basis which was adopted by Zhao and Gehren (2000), who tried to scale $\mathbf{S}_{\mathbf{H}}$, with an exponential factor of the upper level energy $E_{n}$ (applied for Mg ) using the formulation:

$$
\begin{equation*}
\mathbf{S}_{\mathbf{H}}=1000 \times e^{n E_{n} / 2} \tag{3.18}
\end{equation*}
$$

where n is the principal quantum number of the level $n$.
Figure 3.4: $\mathrm{S}_{\mathrm{H}}$ timeline diagram showing the different $\mathrm{S}_{\mathrm{H}}$ values adopted by different references in the literature in the past few years.


Thus different input model atoms and different calibration techniques (as well as different input stellar parameters) deliver different $\mathbf{S}_{\mathbf{H}}$ scaling factors. This calls for a further investigation of the curious case of H -collisions that will be made in Chapters 6 and 7.

### 3.3 Charge Transfer

In addition to the importance of H -atom excitation and ionization collisional processes in the atmospheres of cool stars, it has been shown recently (Barklem et al., 2010, 2012; Belyaev, 2013; Belyaev and Barklem, 2003; Belyaev et al., 2014; Lind et al., 2011; Osorio et al., 2015) that the charge exchange (transfer) processes can be equally important and even dominate over the other collisional processes.

An interpretation of this process is that at certain separations during the collisions between a neutral hydrogen atom and an atomic element A, an AH quasi-molecule is formed momentarily and the optical electron associated with A may tunnel into the H atom, thus leading to the ionization of the element into $\mathbf{A}^{+}$, and producing a negative $\mathbf{H}^{-}$ion. This process is referred to as an ion-pair production.
During an $\mathbf{H}^{-}+\mathbf{A}^{+}$collision, an electron may tunnel towards the atom $\mathbf{A}$. This process corresponds to the inverse of the former one and is referred to as mutual neutralization.

The charge transfer collisional rate (per unit volume) for ion-pair production between an initial level $i$ and a continuum level $c$ can be expressed as:

$$
\begin{equation*}
n_{i} C_{i c}=n_{i} N_{\mathrm{H}}\left\langle\sigma^{\mathrm{ic}} \nu\right\rangle \tag{3.19}
\end{equation*}
$$

whereas the inverse rate for the corresponding mutual neutralization rate can be written as:

$$
\begin{equation*}
n_{c} C_{c i}=n_{c} N_{\mathrm{H}^{-}}\left\langle\sigma^{\mathrm{ci}} \nu\right\rangle \tag{3.20}
\end{equation*}
$$

where $N_{\mathrm{H}^{-}}$is the ionized $\mathrm{H}^{-}$density.
Barklem et al. (2003) first included charge transfer cross-sections into their non-LTE calculations for Li. Their cross-sections were calculated by Belyaev and Barklem (2003) using the quantum scattering method. Their $\mathrm{Li}+\mathrm{H}$ rate coefficients show higher cross-sections for charge exchange than those of excitation from the same initial levels, thus showing that the former are dominant in thermalizing Li, whereas the latter are relatively unimportant.

Similar results have been found in non-LTE studies for late type stars, for $\mathrm{Na}+\mathrm{H}$ (Lind et al., 2011), $\mathrm{Mg}+\mathrm{H}$ (Barklem et al., 2012), Al+H (Belyaev, 2013) and Si+H (Belyaev et al., 2014) where charge-exchange rates dominated for most transitions over those of collisional excitation and ionization.
Fig. 3.5 shows the domination of the ion-pair production transitions (circled symbols) over their corresponding excitation transitions (un-circled symbols) from the same initial levels.

In the absence of an approximation for calculating charge transfer rates, we expanded Lambert's Drawin approximation for $\mathbf{A}+\mathrm{H}$ collisional rate coefficients to those of charge transfer using Eqn. 3.14, replacing $\Delta E_{i j}$ by $\Delta E_{i c}-I_{\mathrm{H}^{-}}$where $I_{\mathrm{H}^{-}}=0.754 \mathrm{eV}$ is the ionization energy of $\mathrm{H}^{-}$. The oscillator strength $f_{i j}$ in Eqn. 3.14 is set to 1 , thus allowing to calculate the rate coefficients for both optically allowed and forbidden transitions. This approach was motivated and justified by the following reasons:

- Steenbock (1985), upon studying the FeI/FeII statistical equilibrium in Pollux and the Sun, set the $Q$-factor in Eqn. 3.12 for excitation transitions with unknown $f$-values equal to 1 .
- A similar approach to removing the $f$ value from the classical approximations, was used by Collet et al. (2005) with the Van Regemorter equation (Eqn. 2.47) for electron collisions by setting a constant $f=10^{-3}$ for all transitions, thus avoiding the problem of forbidden transitions.
- Recent quantum calculations found large H-collisional rates for Mg and other elements for forbidden transitions, which were found to be roughly equal to the allowed transitions (Feautrier et al., 2014).


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Figure 3.5: $\mathrm{Mg}+\mathrm{H}$ rate coefficients calculated via the quantum scattering method as a function of transition energies. Different symbols denote transitions of different initial energy states, while circled symbols denote ion pair production (IPP) transitions from the same initial states (Barklem et al., 2012).


Removing the $f$ dependence allows to compute the rates for all transitions (allowed and forbidden), and for a better comparison with the quantum rates and hence keeping only the $\Delta E$ dependence which can help to reveal the differences in both methods lying in the quantum chemistry of the atom.

Figs. 3.6-3.9 show the charge transfer and de-excitation rate coefficients for H collisions with $\mathrm{Al}, \mathrm{Mg}, \mathrm{Na}$ and Si respectively, calculated via the quantum scattering method (upper panels) and compared to those of the same transitions calculated via Lambert's Drawin's approximation (middle and lower panels) as explained above.

The plots show the dependence of the collisional rate coefficients on the transition energies $\Delta E$ for de-excitation and charge transfer (mutual neutralization) processes respectively. It can be seen that for the four atoms, the charge exchange rate coefficients (filled triangles) calculated using the quantum scattering method exceed the de-excitation rates (empty circles) by up to two orders of magnitude. For de-excitation collisions, a decrease in collisional rates as a function of increasing transition energies $\Delta E$ can be seen, which correspond to transitions between the low-lying levels (ground and first ionized) with those of the higher-lying levels. As for charge exchange, it can be observed that similar behavior exists as a function of $\Delta E$ peaking between $1.2 \& 1.8 \mathrm{eV}$ for all the atoms.

Middle panels show collisional rate coefficients for the same processes corresponding to the same transitions calculated using the Drawin's approximation, that show a decreasing behavior with $\Delta E$ for both de-excitation and charge exchange processes.

The quantum to Drawin ratios (lower panels) clearly show that the Drawin approximation over-estimates all the de-excitation rates by several orders of magnitude. For charge transfer, the ratio is $<1$ for most transitions. In addition, it can be observed that the quantum rates behavior with transition energies is not at all reproduced in the Drawin approximation. The estimated uncertainties in the rate coefficients from the quantum mechanical data are not sufficient to explain the differences with the Drawin approximation (Barklem et al., 2010).

It can thus be generally concluded that charge-exchange processes dominate over the hydrogen collisions for atoms, for which reliable quantum data exist. We can only assume that this is the case for other atoms, including iron, which is at the heart of this work. To test this assumption, we constructed a new iron model atom (see Chapter 4) and adopted different methods for coupling all the levels in our model with H-collisions, including for charge exchange. The details and results of these methods will be presented in Chapters 6 and 7.


Figure 3.6: $\mathrm{Al}+\mathrm{H}$ rate coefficients at $\mathrm{T}=4000 \mathrm{~K}$ (black) and $\mathrm{T}=6000 \mathrm{~K}$ (red) calculated via the quantum scattering method (upper panel) as a function of the transition energies $\Delta E$ from Belyaev (2013) for de-excitation and charge exchange (mutual neutralization). Open circles represent de-excitation rates, while filled triangles represent charge exchange rates. The middle panel shows the corresponding rate coefficients of the same transitions calculated via Lambert (1993) approach to Drawin's approximation (using $f=1$ ). The lower panel shows the ratios of the quantum/Drawin rates. The dotted line corresponds to $\log ($ ratio $)=1$.


Figure 3.7: $\mathrm{Mg}+\mathrm{H}$ rate coefficients at $\mathrm{T}=4000 \mathrm{~K}$ (black) and $\mathrm{T}=6000 \mathrm{~K}$ (red) as a function of the transition energies $\Delta E$ from Belyaev et al. (2012). Panels and symbols represent the same information as in Fig. 3.6.


Figure 3.8: $\mathrm{Na}+\mathrm{H}$ rate coefficients at $\mathrm{T}=4000 \mathrm{~K}$ (black) and $\mathrm{T}=6000 \mathrm{~K}$ (red) as a function of the transition energies $\Delta E$ from Barklem et al. (2010). Panels and symbols represent the same information as in Fig. 3.6.


Figure 3.9: $\mathrm{Si}+\mathrm{H}$ rate coefficients at $\mathrm{T}=4000 \mathrm{~K}$ (black) and $\mathrm{T}=6000 \mathrm{~K}$ (red) as a function of the transition energies $\Delta E$ from Belyaev et al. (2014). Panels and symbols represent the same information as in Fig. 3.6.

## 4 Iron model atom construction

Solving the non-LTE problem of a multi-level atom, as described explicitly in Annex B, requires the build up of the grand matrix which must include all the radiative and collisional rates for all transitions between the energy levels of the atom.
In cool stars ( $\mathrm{T}_{\text {eff }}$ between 3000 K and 7000 K ), lines of neutral iron ( Fe I ) dominate the absorption spectrum (Peterson and Kurucz, 2015) even though iron is almost completely ionized throughout the atmosphere of these stars. Fig. 4.1 shows the ionization fractions for iron as function of the optical depths in the Solar atmosphere and that of the metal-poor sub-giant HD140283. A minority species like Fe I is particularly sensitive to non-LTE effects because any small change in the ionization fraction changes their populations by a large amount. In the non-LTE treatment of iron, it is essential to include all important Fe I and Fe II lines and levels.

The number of levels and discrete radiative transitions in Fe is enormous. Recent calculations of Kurucz ${ }^{1}$ predict $\sim 37000$ theoretical energy levels below and above the first ionization threshold of FeI, as well as 6025000 radiatively permitted transitions between them. Such huge numbers of lines and levels are not treatable by current non-LTE codes. To reduce the amount of computing time, as well as memory requirements, it is important to decrease the size of the rate matrix by including the important levels and lines and combining them into superlevels and superlines respectively as described in the sections below.

In this chapter, the construction of the iron model atom, referred to hereafter as the "Iron model atom", used in the non-LTE calculations with the MULTI2.3 code (Annex B) is described explicitly. The model atom includes the Fe I and Fe II energy levels and the Fe III ground state, and their combination into super levels described in Section 4.1, and their corresponding radiative (Section 4.2) and collisional (Section 4.3) bound-bound and bound-free transitions. In Section 4.5, a comparison of our model with the iron model atoms available in the literature is presented.

### 4.1 Energy levels

The first step in constructing a model atom is to identify the important energy levels. The energies of these states are predicted through quantum mechanics, or are experimentally measured. Four quantum numbers are used to describe the orbitals in which electrons can be found. These are namely:
the principal quantum number $n$
the orbital angular quantum number $l$ whose values can range from 0 to $(n-1)$
We magnetic quantum number $m_{l}$ whose values can range from $(l-1)$ to $(l+1)$

[^17]Figure 4.1: Ionization fraction of Fe I and Fe II in the Sun (left panel) and in the metal poor halo subgiant HD140283 (right panel, $[\mathrm{Fe} / \mathrm{H}]=-2.40, T_{\text {eff }}=5522 \mathrm{~K}, \log g=3.58$ ) as a function of atmospheric optical depth at $5000 \AA \tau_{5000}$.
the electron spin $m_{s}$ which according to Hund's law can have the values of $+1 / 2$ or $-1 / 2$ respectively

These numbers describe the size, shape, and orientation in space of the orbitals of an atom. Orbitals that have the same value of $n$ form a shell which can accommodate $2 n^{2}$ electrons, while orbitals within a shell are divided into sub-shells $l$ which can accommodate $2(2 l+1)$ electrons. These sub-shells are labeled according to their corresponding values of $l$ as shown in table below for the first 10 values of $l$ :

| $l$ | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| label | s | p | d | f | g | h | i | k | 1 | m | n |

In addition, the sub-shells might be further split through the coupling between two close electrons resulting in the formation of a Russel-Saunders LS spectroscopic term coupling denoted by ${ }^{2 \mathbf{S}+1} \mathbf{L}_{\mathbf{J}}$ ( $2 \mathbf{S}+1$ also referred to as multiplicity or degeneracy), where $\mathbf{S}$ is the total electrons spin $\mathrm{S}=\sum_{\mathrm{i}} \mathrm{m}_{\mathrm{si}}$ and L is the total orbital angular momentum of the electrons $\mathbf{L}=\sum_{\mathbf{i}} \mathbf{l}_{\mathbf{i}}$, which can have the same labels as $l$ depending on the values of $\mathbf{L}$, i.e. term labels $\mathbf{S}, \mathbf{P}, \mathbf{D}, \mathbf{F}$.. correspond to $\mathbf{L}=0,1,2,3$.. respectively. On the other hand, farther electrons can also couple via $\mathbf{J J}$ coupling, where $\mathbf{J}=\mathbf{L}+\mathbf{S}$ is the total angular momentum of the electrons. Thus each energy level state is defined by a standard set of notations depending on the positions and coupling of their valence electrons. For example the FeI and FeII ground state electron
configurations, starting by the outermost sub-shells, can be written as:
FeI (groundstate) :[Ar] $3 d^{6} 4 s^{2}-a^{5} \mathrm{D}$
Fe II (groundstate) : [Ar] $3 d^{6} 4 s-a^{6} \mathrm{D}$
where [ Ar ] is the inert gas Argon configuration: ${ }^{18} \mathrm{Ar}: 1 s^{2} 2 s^{2} 2 p^{6} 3 s^{2} 3 p^{6}$. The integers preceding the labels $s, p$ and $d$ correspond to the principal quantum numbers $n$, while the integer superscripts correspond to the number of electrons occupying the respective sub-shells. The terms $a^{5} \mathrm{D}$ and $a^{6} \mathrm{D}$ correspond to the LS coupling spectroscopic terms of the corresponding levels. In addition, each respective energy state is further split into close fine structure splittings corresponding to each value of $\mathbf{J}$.
Finally, the LS and JJ coupling terms may have an odd or even parity determined by the number of electrons occupying the odd orbitals:

- An odd number of electrons in the odd orbitals will give an odd term denoted by a superscript 'o' or '*', such as $z^{7} \mathrm{D}^{*}$.
- An even number of electrons in the odd orbitals will give an even term denoted with no superscript, such as $a^{5} \mathrm{P}$.
The National Institute of Standards and Technology (NIST) ${ }^{2}$ in its $5^{\text {th }}$ version provides several online atomic spectroscopic databases widely used in astrophysics (Ralchenko et al., 2006; Reader et al., 2002). The data include wavelengths, energy levels, and oscillator strengths which are regularly updated for a large number of atoms and molecules.

The iron model atom was built up using all the FeI energy levels extracted from the NIST database ( 846 levels) from the experimental analysis of Nave et al. (1994), up to 7.815 eV . The model also includes the predicted high lying Fe I levels ( 66 levels) from Peterson and Kurucz (2015), up to 8.392 eV . The coupling between these latter high-lying levels and the low-lying levels correspond to important UV transitions, which is important for the determination of abundances for in individual stars from their UV spectra (Peterson, 2011, 2013). The coupling between the high-lying levels themselves corresponds to the important IR transitions which are vital for infrared spectroscopic iron abundances determination in luminous red giants in dust-obscured regions like the bulge, bar, and disk of the Milky Way (Majewski, 2010).
The main NLTE mechanism for Fe I is the over-ionization of low-excitation levels by ultraviolet radiation (Asplund, 2005; Bergemann and Nordlander, 2014). Thus, the role of these highexcitation levels is to compensate, in part, for population losses via collisional coupling to the large continuum reservoir, with subsequent spontaneous transitions down to low-excitation levels (Mashonkina, 2009).

The model atom was completed with all Fe II levels from Nave and Johansson (2013), with 1027 levels up to 19.83 eV , corresponding to 189 spectroscopic terms. Only the ground level of Fe III was included.

### 4.1.1 Superlevels

To reduce the amount of computing time, as well as memory requirements, it is helpful to reduce the number of levels by using the superlevel algorithm, in which the number of individual atomic levels is reduced by combining a set of actual levels into a superlevel.

[^18]A superlevel $I$ consists of a set of actual levels $i \in I$, so that each level is included in exactly one super level, and there is no overlap between two superlevels. The total population density of a super level is necessarily the sum of the population densities of all included levels:

$$
\begin{equation*}
n_{I}=\sum_{i} n_{i} \tag{4.1}
\end{equation*}
$$

Also, all levels of a super level share the same departure coefficient $b_{I}=b_{i}=n_{i} / n_{i}^{\mathrm{LTE}}=$ $n_{I} / n_{I}^{\mathrm{LTE}}$.

However, combining levels into superlevels means that not all actual levels and transitions are treated in full non-LTE. Only the populations of the combined levels are fully calculated via the non-LTE approach, while the populations of the actual levels constituting a super level are then populated according to their statistical weights by redistributing the super level population using the Boltzmann equation. This approach can be justified if levels combined are close in energies and are thus closely coupled via collisions. Hence the closer the combined levels are in energies, the better is the LTE assumption is within a superlevel, and the closer to full non-LTE calculations will the results be.

In our iron model atom, the energy levels for Fe I and Fe II were combined using the code FORMATO (Merle et al., in prep) as follows:

- The fine structure levels of the ground and first ionized states for each of FeI and FeII were included.
- All other fine structure levels were combined into mean levels according to their statistical weights. Thus the excitation potential of each mean level is a weighted mean of the excitation potential of the corresponding fine structure levels:

$$
\begin{equation*}
E_{I}=\frac{\sum_{i=1}^{N} E_{i} g_{i}}{\sum_{i=1}^{N} g_{i}} \tag{4.2}
\end{equation*}
$$

- All mean levels above 5 eV and lying within an energy interval of $0.0124 \mathrm{eV}\left(100 \mathrm{~cm}^{-1}\right)$ were combined into superlevels. The excitation energy of each super level is a weighted mean of the statistical weights and excitation energies of the corresponding mean levels.

The final number of levels in our iron model is 203 Fe I levels, 189 Fe II levels and, 1 Fe III level (Fig. 4.2 and Fig. 4.3), each defined with an excitation energy relative to the neutral ground state, a statistical weight $g=2 \mathbf{J}+1$, a configuration, a spectroscopic term ID, and an ionization stage ( 1 for neutral, 2 for first ionized, etc ..), as shown in Table 4.1 for a few levels in the model.

### 4.2 Radiative transitions

### 4.2.1 Bound-bound transitions

Calculation of the radiative bound-bound rates requires computing the input of Einstein coefficient $B_{i j}$, which can be related to the transitional oscillator strength $f_{i j}$ though Eqn. 2.30. The bound-bound radiative input data in our iron model includes both allowed and forbidden transitions between the available energy levels in the model. The allowed transitions should obey the selection rules:

|  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: |
| $\mathrm{E}\left(\mathrm{cm}^{-1}\right)$ | $g$ | Configuration | term ID | Ion |
|  |  |  |  |  |
| 0.000 | 9.0 | $3 \mathrm{~d}^{6} 4 \mathrm{~s}^{2}$ | $a^{5} \mathrm{D}$ | 1 |
| 6928.268 | 11.0 | $3 \mathrm{~d}^{6}\left({ }^{4} \mathrm{~F}\right) 4 \mathrm{~s}$ | $a^{5} \mathrm{~F}$ | 1 |
| 11976.239 | 9.0 | $3 \mathrm{~d}^{6}\left({ }^{4} \mathrm{~F}\right) 4 \mathrm{~s}$ | $a^{3} \mathrm{~F}$ | 1 |
| $\vdots$ |  |  |  |  |
| 63737.704 | 10.0 | $3 \mathrm{~d}^{6}\left({ }^{5} \mathrm{D}\right) 4 \mathrm{~s}$ | $a^{6} \mathrm{D}$ | 2 |
| 65610.304 | 10.0 | $3 \mathrm{~d}^{7}$ | $a^{4} \mathrm{~F}$ | 2 |
| 71693.023 | 8.0 | $3 \mathrm{~d}^{6}\left({ }^{5} \mathrm{D}\right) 4 \mathrm{~s}$ | $a^{4} \mathrm{D}$ | 2 |
| $\vdots$ |  |  |  |  |
| 194393.104 | 9.0 | $3 \mathrm{~d}^{6}$ | ${ }^{5} \mathrm{D}$ | 3 |

Table 4.1: Excitation energies relative to the neutral ground state, statistical weight $g$, level configuration \& term ID and ionization stage (ion) of the first few levels of FeI and FeII and that of the ground FeIII levels in the FeI/FeII model.

- $\Delta \mathbf{J}=0, \pm 1(\mathbf{J}=0 \leftrightarrow \mathbf{J}=0$ not allowed)
- $\Delta \mathbf{L}=0, \pm 1(\mathbf{L}=0 \leftrightarrow \mathbf{L}=0$ not allowed $)$
- $\Delta \mathbf{S}=0$
- Parity must change

Transitions not obeying one of these rules are referred to as forbidden, while those only violating the $\Delta \mathbf{S}=0$ rule are referred to as semi-forbidden. In our model, the transitions are described by their wavelengths, oscillator strengths $f$, and their radiative and hydrogen collisional broadening coefficients $\gamma^{r}$ from Kurucz (2009) \& $\Gamma_{\mathrm{H}}^{\text {col }}$ from Anstee and O'Mara (1995); Barklem et al. (1998); Barklem and O'Mara (1997) ABO theory calculations when available and using Unsold (1955) approximation otherwise (See Appendix A).

Radiative line transitions can be collected from several available databases, namely that of NIST, Kurucz, the FERRUM project (Johansson et al., 2000) and VALD (versions 1,2, and 3) (Kupka et al., 2000; Kurucz, 1993; Piskunov et al., 1995; Ryabchikova et al., 2011) which is a collection of atomic and molecular transition parameters. These parameters include the oscillator strengths and broadening coefficients of the transitions regularly updated from the most up-to-date references. For our iron model atom, we used the VALD3 interface database to extract all the Fe I and Fe II radiative bound-bound transition accounting to 79594 Fe I lines and 113964 Fe II lines. The UV and IR lines (1568 lines) corresponding to transitions from and to the predicted high lying levels (Peterson and Kurucz, 2015) have also been included in the model, thus increasing the total number of Fe I lines to 81162.

### 4.2.1.1 Superlines

Individual transitions belonging to levels that have been combined to superlevels have also been combined into superlines (super transitions). The radiative rate of each super transition between two super levels $I$ and $J$ is calculated by summing over the rates of all existing transitions between all levels belonging to both super levels. The superline total oscillator

| $\mathrm{E}_{\text {low }}\left(\mathrm{cm}^{-1}\right)$ | $\mathrm{E}_{\text {up }}\left(\mathrm{cm}^{-1}\right)$ | $f$ | $\gamma^{\mathrm{rad}}\left(\mathrm{s}^{-1}\right)$ | $\Gamma^{\mathrm{H}}=\sigma_{\mathrm{H}}^{\mathrm{br}} \cdot \alpha$ | $\lambda_{\text {vac }}(\AA \mathrm{A})$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 0.000 | 19624.0673 | $2.679 \times 10^{-5}$ | $5.36 \times 10^{5}$ | 204.59 | 5113.682 |
| 415.933 | 31566.8014 | $3.925 \times 10^{-4}$ | $3.34 \times 10^{7}$ | 270.26 | 3216.729 |
| 24565.1648 | 37043.8386 | $1.488 \times 10^{-6}$ | $5.70 \times 10^{8}$ | 389.24 | 7741.293 |

Table 4.2: A few transitions from our iron superlevels atom with their lower and upper level energies, their oscillator strength $f$, their radiative broadening coefficient, the hydrogen Van der Waals collisional broadening cross-section $\sigma_{\mathrm{H}}^{\mathrm{br}}$ (the integer part of the number, in Bohr radii squared units) and its velocity parameter $\alpha$ (the decimal part of the number), and their vacuum wavelength.
strength is a weighted average of $g f$-values of individual transitions and can be computed using the relation from Martin et al. (1988):

$$
\begin{equation*}
f_{I J}=\frac{1}{\bar{\nu} \sum_{i} g_{i}} \sum_{i \in I} \sum_{j \in J} g_{i} \nu_{i j} f_{i j} \tag{4.3}
\end{equation*}
$$

where $\bar{\nu}$ is the mean frequency of all the individual transition frequencies $\nu_{i j}$ belonging to the super transition from $I$ to $J$.

Our final iron model includes 9816 FeI transitions and 16745 FeII transitions combined from the individual lines (Fig. 4.4 and Fig. 4.5). An example of a few transitions and their parameters is shown in table 4.2. The line broadening and line profiles are calculated as explained in Appendix A.

### 4.2.2 Bound-free transitions

Calculation of radiative bound-free photoionization and recombination rates requires the input of full cross-section tables as a function of the photon energies. The TOPBASE ${ }^{3}$ (The Opacity Project (OP) collaboration, Cunto et al., 1993) database includes photoionization cross-section tables for a large number of atoms and ions. For Fe I levels, the photoionization cross-section tables calculated by Bautista (1997), and those for Fe II calculated by Nahar and Pradhan (1994) using the ab initio R-matrix close coupling (CC) approximation, were extracted from the NORAD ${ }^{4}$ database (as they were not extractable from the TOPBASE website directly). These tables correspond to calculations for 52 LS Fe I terms (for $n \leq 10$ and $l \leq 9$ ) of spin multiplicities $2 S+1=1,3,5 \& 7$, and for 83 Fe II LS terms of spin multiplicities $2 S+1=2,4,6$ \& 8, coupled through photoionization to the ground Fe II and Fe III levels respectively.

The theoretical threshold ionization energies (expressed in Rydberg energy units) ${ }^{5}$ in the former TOPBASE tables are, however, shifted from those in NIST (Verner et al., 1994), and thus also from our iron model energy levels. Thus, all the photoionization energies from TOPBASE for each level in the model were shifted to match the threshold ionization energies in NIST. In addition, the TOPBASE calculations of the cross-sections (in Mega-barn Mb ) reproduce many

[^19]auto-ionization resonances near the ionization thresholds (Fig. 4.6). These resonances are important for calculating the photoionization rate produced by radiation in spectral lines whose frequency positions coincide with the autoionization resonances. The sharp reasonances in the photoionization tables were smoothed and resampled in our iron model up to a maximum of 200 frequency points, as follows:

- The first 30 frequency point cross-sections corresponding to the photon energies closest to the threshold were all included in the tables.
- The remaining points were smoothed using a box smoothing method (moving average) over windows of 7 frequency points each, and then re-sampled depending on the standard deviation variation relative to the average of the cross-sections in frequency intervals as follows:

1- The cross-sections were divided into intervals of 10 consecutive frequency points each.
2- The average of the cross-sections of each interval was calculated.
3- The standard deviation $\sigma_{\mathrm{sd}}$ relative to this average was also calculated.
4- If $\sigma_{\mathrm{sd}}$ is less than 0.1 Mbarn , only the first and last points of each interval were chosen.
5- If $\sigma_{\text {sd }}$ is greater than 0.1 Mbarn, the intervals were further divided into two equal parts of 5 frequency points each.
6- Steps 2,3 and 4 were repeated on each interval. If $\sigma_{\text {sd }}$ is greater than 0.1 Mbarn , the $1^{\text {st }}, 3^{\text {rd }}$ and $5^{\text {th }}$ points of each interval were chosen.

Figure 4.6: Photoionization cross-section (in Mbarn) as a function of photon energy (in Ry) for the Fe I ground level, showing resonance peaks from TOPBASE data (solid black line). The smoothed resampled cross-sections (see Sect. 4.2.2) are shown (dashed red line), in addition to those calculated using Kramer's $\nu^{-3}$ hydrogenic approximation (Eqn. 2.37, dashed blue line).


The bound-free radiative rate between a superlevel and the continuum is the summation over the bound-free rates of individual levels belonging to the superlevel to that continuum. Since the TOPBASE calculations do not include photoionization cross-section tables for fine structure transitions, the cross-sections of these latter were included as g-weighted average of their corresponding mean level cross-sections at each photon energy:

$$
\begin{equation*}
\sigma_{i}^{f s}=\frac{\sigma_{i}^{m l} g_{f s}}{g_{m l}} \tag{4.4}
\end{equation*}
$$

where $g_{f s}, \sigma_{i}^{f s}, g_{m l}$, and $\sigma_{i}^{m l}$ are the statistical weights and photoionization cross-sections for the fine structure and mean levels respectively.

Cross-section tables from TOPBASE were available for 158 levels of our iron model. For the remaining levels, Kramer's hydrogenic approximation was used. Table 4.3 shows part of the smoothed, re-sampled photoionization table for the Fe I ground state included in our iron model.

|  |  |
| :---: | :---: |
| Ionizing wavelength $(\AA)$ | Photoionization cross-section $\left(\mathrm{cm}^{2}\right)$ |
|  |  |
| 1598.75 | $2.68 \times 10^{-20}$ |
| 1541.63 | $4.06 \times 10^{-18}$ |
| 1520.06 | $9.88 \times 10^{-19}$ |
| 1495.53 | $2.00 \times 10^{-18}$ |
| 1305.84 | $5.33 \times 10^{-19}$ |
| $\vdots$ | $1.33 \times 10^{-19}$ |

Table 4.3: Sample of the photoionization cross-sections (in $\mathrm{cm}^{2}$ ) for the ground Fe I level as a function of the photon ionizing wavelengths (in $\AA$ ) in our iron model. The first value is the cross-section at the threshold wavelength.

### 4.3 Collisional transitions

The calculation of the rates for collisional excitation and de-excitation as per Eqn. 2.41 requires the input of the collisional cross-sections as a function of the collisional perturber's temperature. Levels in our model atom are coupled via collisional with electrons and neutral hydrogen atoms. As has been explained in Chapter 3, the scarcity of the ab initio calculations for the $\mathrm{Fe}+e^{-}$ and $\mathrm{Fe}+\mathrm{H}$ collisional cross-sections calls for the use of different classical or semi-classical approximations for each process as explained below.

### 4.3.1 electron Collisions

For Fe I, quantum electron-impact excitation rates have not yet been calculated for most transitions. Pelan and Berrington (1997) calculated effective excitation collisional strengths for the fine-structure transitions involving the ground term and the first excited term using the

R-matrix method. In our model atom, these results were included for the corresponding transitions, while for all other transitions, the excitation cross-sections were estimated using Seaton (1962a) impact parameter approximation for allowed transitions and that of Seaton (1962b) for forbidden transitions. The cross-sections were then averaged over a Maxwellian velocity distribution to obtain the rate coefficients $\langle\sigma \nu\rangle^{e-}$.

For Fe II, the situation is better, as Zhang and Pradhan (1995), and Bautista and Pradhan (1996) calculated rate coefficients for 10011 excitation transitions among 142 fine structure levels, using the R-matrix method. These calculations were also included in our model atom, and the impact parameter approximation of Seaton (1962a) was used for all other transitions. For bound-free transitions, Bely and van Regemorter (1970) approximation was used to calculate the collisional cross-sections for both FeI and Fe II.

As for radiative rates, the collisional rate for a transition between two superlevels is calculated by summing the collisional rates of the transitions between individual levels belonging to these superlevels.

### 4.3.2 Hydrogen Collisions

For collisions with neutral H atom, being the main aim of this PhD dissertation, various recipes have been adopted which will be detailed in Chapters 6 and 7.

### 4.4 Background Opacities

Background line opacities are important to include in non-LTE calculations (Collet et al., 2005), as a large number of metals contribute to the UV "line haze" typically encountered in the spectra of cool stars.

MULTI2 . 3 allows for the inclusion of background line opacities in addition to its built-in continuous opacities. Thus, opacity sampling tables were extracted using the MARCS code (Gustafsson et al., 2008) including all atomic and molecular lines, except for iron. The opacity sampling tables were calculated as function of the star's metallicity (See Chapter 5).

### 4.5 Comparison with published models

There have been a few different atomic models of iron built for the study of cool stars in recent years, namely that of Collet et al. (2005), Mashonkina et al. (2011) and Bergemann et al. (2012). It is thus interesting to compare these models to ours.

Collet et al. (2005) adopted an updated version of the iron model atom by Thévenin and Idiart (1999). Their model included energy levels extracted from the NIST database with fine structure multiplets ( 334 Fe I, 189 Fe II and 1 Fe III). The $g f$-values of their lines ( 3466 Fe I \& 3440 Fe II) were adopted from Nave et al. (1994) and Kurucz and Bell (1995). Photoionization rates for the levels were included from the calculations of Bautista (1997) (TOPBASE) when available, and using the hydrogenic approximation for the rest. The levels were coupled with electrons \& neutral hydrogen collisions using different recipes as shown in Table 4.4. For the H-collisions, they adopted different values of $0.001 \& 1$ for $\mathrm{S}_{\mathrm{H}}$ using Steenbock and Holweger (1984) approach to Drawin's approximation in order to determine upper and lower limits of
non-LTE abundance corrections respectively.
Mashonkina et al. (2011) built a more complete iron model atom using the superlevel and supertransition algorithm, with all the experimental atomic levels and lines from NIST, in addition to predicted ones from Kurucz (2009) ${ }^{6}$. Ignoring all fine structures, their Fe I levels belong to 233 terms, which where combined into superlevels whenever their energy difference was less than $150 \mathrm{~cm}^{-1}$ for levels below $60000 \mathrm{~cm}^{-1}$, and whenever the difference was less than $210 \mathrm{~cm}^{-1}$ for levels above $60000 \mathrm{~cm}^{-1}$. Photoionization transitions were included using the cross-section tables from Bautista (1997) when available, and using Kramer's hydrogenic approximation when not. When available, quantum calculations for electron bound-bound transitions were adopted in their model from Pelan and Berrington (1997) for Fe I and from Zhang and Pradhan (1995) and Bautista and Pradhan (1996) for Fe II. Otherwise, the van Regemorter approximation was used. For forbidden $e^{-}$transitions, they adopted effective collisional strength values of $\Upsilon^{e}=1$. Mashonkina generalized this assumption from the result of Pelan and Berrington (1997) for the FeI forbidden transition " $a^{5} D-a^{5} F^{\prime \prime}$ at $T=4000 \mathrm{~K}$ ( $\Upsilon^{e}=0.98$ ). For H collisions, they also used Steenbock and Holweger (1984) approximation of Drawin's formula multiplied by $S_{H}=0,0.1$ and 1 , calibrated on benchmark stars as a function of metallicity. For forbidden transitions, the Takeda (1994) approximation was used, which relates the H -collisional rates to their corresponding $e^{-}$- collisional rates using the formulation: $C_{\mathrm{H}}=C_{e^{-}} \sqrt{\left(m_{e} / m_{\mathrm{H}}\right)} N_{\mathrm{H}} / N_{e^{-}}$, where $C_{\mathrm{H}}$ and $C_{e^{-}}$are the H and $e^{-}$- collisional rates respectively, $N_{\mathrm{H}}$ and $N_{e^{-}}$are H and $e^{-}$number densities.

Most recently, Bergemann et al. (2012) built another complete iron model atom, also using the super level algorithm and adopting a large number of levels and radiative lines from the NIST and Kurucz (2009) databases. Fine structure in their model were neglected for all levels except FeI and Fe II ground levels. Their levels were combined into superlevels whenever they had the same parity and lied within an energy difference of $10 \mathrm{~cm}^{-1}$ below $54000 \mathrm{~cm}^{-1}$. Above this value all levels lying within $1000 \mathrm{~cm}^{-1}$ were combined into superlevels. In addition to the photoionization data from Bautista (1997), they claimed to have included more recent data from private communication with him. Their $e^{-}$and H-collisional transitions were calculated using different recipes specified in Table 4.4. They also adopted different $S_{H}$ values ( 0.1 \& 1) by calibrating their lines on different benchmark stars. For forbidden H-collisional transitions, they similarly adopted the Takeda (1994) approximation.

The comparison of the different recipes used in our model as compared to those of Collet et al. (2005), Mashonkina et al. (2011) and Bergemann et al. (2012) are tabulated in Table 4.4, along with all the corresponding references.

[^20]Table 4.4: Atomic data and their references adopted in the FeI/FeII models of Collet et al. (2005) (COLO5), Mashonkina et al. (2011) (MAS11) \& Bergemann et al. (2012) (BER12). References denoted by letters in the table refer to: (a) Nave et al. (1994); (b) Kurucz (2009); (c) Peterson and Kurucz (2015) ; ${ }^{(d)}$ Johansson et al. (2000); (e) Kurucz (1993); (f) Nave and Johansson (2013), (g) VALD3; (h) Bautista (1997); ${ }^{(i)}$ Travis and Matsushima (1968); (j) NORAD (Nahar \& Collaboration); ${ }^{(\mathbf{k})}$ van Regemorter (1962); ${ }^{(1)}$ Seaton (1962a); (m) cox (2000); (n) Steenbock and Holweger (1984); (o) Pelan and Berrington (1997); ${ }^{(\mathrm{p})}$ Zhang and Pradhan (1995); ${ }^{\text {(q) }}$ Bautista and Pradhan (1996); ${ }^{(\mathrm{r})}$ Takeda (1994); ${ }^{(\mathrm{s})}$ Seaton (1962b); ${ }^{(\mathrm{t})}$ Lambert (1993); ${ }^{(\mathrm{u})}$ Allen (1973)

| Model | COL05 | MAS11 | BER12 | Our iron model | notes |
| :---: | :---: | :---: | :---: | :---: | :---: |
| superlevels | no | yes | yes | yes |  |
| Fe I levels | $334{ }^{(1)(a)}$ | 233 terms ${ }^{(2)(a)(b)}$ | 296 terms ${ }^{(3)}$ (a) | 203 terms ${ }^{(a)(c)(4)}$ | ${ }^{(1)}$ up to 6.91 eV above ground FeI; <br> ${ }^{(2)}$ up to 7.89 eV above ground FeI; <br> ${ }^{(3)} 0.03 \mathrm{eV}$ below ionization limit; <br> ${ }^{(4)}$ up to 8.392 above ground FeI |
| Fe II levels | $189{ }^{(5)}$ (d) | 89 terms ${ }^{(6)(e)}$ | 112 terms ${ }^{(7)(d)}$ | 189 terms ${ }^{(8)}$ (f) | ${ }^{(5)}$ up to 16.5 eV above ground FeI; <br> ${ }^{(6)}$ up to 10 eV above ground FeII; <br> (7) 2.72 below ionization limit; <br> ${ }^{\text {(8) }} \mathrm{up}$ to 19.83 eV above ground FeI |
| Fe I radiative bound-bound transitions | $3466{ }^{\text {(a) }}$ | $11958{ }^{(a)(b)}$ | $13888{ }^{\text {(a) }}$ | $9816^{(\mathrm{c})(\mathrm{g})}$ |  |
| Fe II radiative bound-bound transitions | $3440{ }^{\text {(d) }}$ | $1525{ }^{(\mathrm{e})}$ | $2316{ }^{\text {(d) }}$ | $16745^{(\mathrm{g})}$ |  |
| Fe I radiative bound-free transitions | (h) | (h) | (h) (i) | (h) (j) (i) |  |
| Fe II radiative bound-free transitions | (h) | (i) | (h) (i) | (h) (j) (i) |  |
| Fe I $e^{-}$collisional bound-bound transitions (allowed) | (k) (9) | (k) (o) | (k) | (1) (o) | ${ }^{(9)}$ all $f$ values set to $10^{-3}$ |
| Fe II $e^{-}$collisional bound-bound transitions (allowed) | (k) (9) | (k) (p) (q) | (k) | (1) (p) (q) |  |
| FeI $e^{-}$collisional bound-bound transitions (forbidden) |  | $\Gamma=1$ | (u) | (u) |  |
| Fe II $e^{-}$collisional bound-bound transitions (forbidden) |  | $\Gamma=1$ | (u) | (u) |  |
| Fe I H collisional bound-bound transitions (allowed) | (n) (10) | (n) (12) | (n) (12) | (t) (11) | $\begin{aligned} & \left({ }^{(10)} \mathrm{S}_{\mathrm{H}}=0.001 \& 1 ;\right. \\ & (\mathbf{1 1 )} f=1 ; \\ & { }^{(12)} \mathrm{S}_{\mathrm{H}}=0,0.1 \& 1 \\ & \hline \end{aligned}$ |
| Fe II H collisional bound-bound transitions (allowed) | ( n ) (10) | (n) (12) | (n) (12) | (t) (11) |  |
| Fe I H collisional bound-bound transitions (forbidden) |  | (r) | (r) | (t) (11) |  |
| Fe II H collisional bound-bound transitions (forbidden) |  | (r) | (r) | (t) (11) |  |
| Fe I $e^{-}$collisional bound-free transitions | (m) | (s) (13) | (s) | (s) | ${ }^{(13)}$ Gaunt factor $\bar{g}=0.1$ |
| Fe I H collisional bound-free transitions | ( n ) | (n) | ( n ) | (t) |  |
| Fe II $e^{-}$collisional bound-free transitions | (m) | (s) (14) | (s) | (s) | ${ }^{(14)}$ Gaunt factor $\bar{g}=0.2$ |
| Fe II H collisional bound-free transitions | ( n ) | ( $\mathbf{n}$ ) | ( n ) | (t) |  |
| Fe I H collisional charge transfer transitions |  |  |  | (t) (15) | ${ }^{(15)}$ extended in this work to charge transfer process |
| Fe II H collisional charge transfer transitions |  |  |  | (t) (15) |  |

Figure 4.2: Grotrian diagram of FeI levels in our final model atom. The energies of the levels ( y -axis, in eV ) are displayed as a function of their spectroscopic terms (x-axis). Cyan colored solid lines correspond to fine structure levels of the ground and first ionized levels, black solid lines below 5 eV correspond to mean levels, while those above 5 eV correspond to superlevels. Only labels of the levels below 6 eV are included to avoid crowding.

Iron model atom- Fel energy levels


Figure 4.3: Grotrian diagram of FeII levels in our final model atom. The energies of the levels relative to the FeII ground state at 0 eV ( y -axis, in eV ) are displayed as a function of their spectroscopic terms ( x -axis). Colors have the same meaning as those in Fig. 5.2. Only labels of the levels below 12 eV are included to avoid crowding.


Figure 4.4: Grotrian diagram for allowed FeI bound-bound radiative transitions in our final model atom. Gray lines display super transitions between different super levels.


Figure 4.5: Grotrian diagram of allowed FeII bound-bound radiative transitions in our final model atom. Colors have the same meaning as in Fig. 5.2 \& Fig. 5.4.

Iron model atom- Fell radiative transitions


## 5 Benchmark stars as probes of spectroscopic studies

The state of a given star is set by a handful of fundamental parameters such as its mass, age, and its hydrogen, helium \& metal content. These quantities, not directly observable, can be linked to secondary stellar properties comprising generally the effective temperature, luminosity, surface gravity, and the metallicity (or its proxy $[\mathrm{Fe} / \mathrm{H}]$, which denotes the iron content relative to hydrogen) through well-defined relations, in addition to dynamic properties such as its projected rotational velocity $(\nu \sin i)^{1}$

The main aim of the present dissertation work is to reduce the uncertainties in Fe abundance determinations to a limit which places useful constraints on stellar and Galactic evolutionary models. Thus an essential part of the method we apply, is to start from accurate stellar parameters for these stars, which can be provided by different methods discussed in the few sections below. With the good knowledge of these parameters, the spectroscopic determination of the abundances of iron will allow precise calibration of the non-LTE calculations independently of most parameter assumptions.

An example of a good set of cool stars, for which well-known and well-determined parameters exist, is the Gaia-ESO survey FGK-Benchmark stars (Heiter et al., 2015a; Jofré et al., 2014) which present a common set of bright ( $V$ magnitudes ranging between 0 and 8) calibration stars, covering different regions of the HR diagram and spanning a wide range in metallicity, temperature and surface gravities. This makes them an ideal set for testing our method.

In this chapter, a brief description of the methods used to derive the fundamental atmospheric parameters of cool stars will be presented in 5.1, followed by presenting a sample of Benchmark (standard/reference) stars with well-determined parameters in 5.2, upon which our calculations, methods and calibrations were tested (for the method and results see chapters 6 and 7).

### 5.1 Stellar parameters

The input effective temperature $T_{\text {eff }}$ and surface gravity $g$ of the star, in addition to the metallicity $[\mathrm{Fe} / \mathrm{H}]$ and micro-turbulent velocity $\xi_{t}$ (hereafter referred to as atmospheric fundamental parameters, or AFP), are the prerequisites to any detailed abundance or spectral synthesis analysis. In the following sections, some common methods used to determine the AFP of cool stars are briefly explained for $T_{\text {eff }}, \log g$ and $[\mathrm{Fe} / \mathrm{H}]$.

[^21]
### 5.1.1 Effective temperature $T_{\text {eff }}$

### 5.1.1.1 Angular diameter

The effective temperature $T_{\text {eff }}$ of a star is defined to be the temperature of a black body emitting the same total radiative flux $F_{\mathrm{bol}}$, defined by the Stefan-Boltzmann law:

$$
\begin{equation*}
F_{\mathrm{bol}}=\sigma_{\mathrm{SB}} T_{\mathrm{eff}}^{4} \tag{5.1}
\end{equation*}
$$

where $\sigma_{S B}$ is the Stefan-Boltzmann constant. This relation is commonly written in terms of the luminosity of the star $L_{\star}$ as:

$$
\begin{equation*}
L_{\star}=4 \pi R_{\star}^{2} \sigma_{\mathrm{SB}} T_{\mathrm{eff}}^{4} \tag{5.2}
\end{equation*}
$$

where $R_{\star}$ is the radius of the star. It is possible to link $T_{\text {eff }}$ to the angular diameter of the star $\theta_{\mathrm{D} \star}$, a measurable quantity using interferometry, by making use of the concept that the flux at the stellar surface of radius $\mathrm{R}_{\star}$ and that at the Earth, $f_{\text {bol }}{ }^{2}$ at a distance $d$ from the star, satisfy the relation: $F_{\mathrm{bol}} R_{\star}^{2}=f_{\text {bol }} d^{2}$. Plugging this relation into Eqn. 5.2, ignoring interstellar absorption, allows to write $T_{\text {eff }}$ in terms of the measurable quantities $\theta_{D \star}$ and $F_{\text {bol }}$ such as:

$$
\begin{equation*}
T_{\mathrm{eff}}=\left(\frac{f_{\mathrm{bol}}}{\sigma_{\mathrm{SB}}}\right)^{1 / 4}\left(\frac{\theta_{\mathrm{D} \star}}{2}\right)^{1 / 2} \tag{5.3}
\end{equation*}
$$

where $\theta_{\mathrm{D} \star}=2 R_{\star} / d$.
This method, challenging due to the small apparent sizes of stars in the sky, has been improving rapidly due to measurements by CHARA ${ }^{3}$ and other interferometers such as the VLTI ${ }^{4}$ (Kervella and Fouqué, 2008) which have provided angular diameters with unprecedented quality for many giants and dwarf stars (McAlister et al., 2005), in addition to the available $f_{\text {bol }}$ measurements of a large number of these stars from the integration of their observed spectral energy distribution (SED).

### 5.1.1.2 IRFM

The Infra-Red Flux Method (hereafter IRFM) was introduced by Blackwell et al. (1979). The basic idea is to compare the ratio $\mathcal{R}_{\text {obs }}$ of the bolometric flux $f_{\text {bol }}$ to the (IR) flux obtained at Earth $f_{\text {IR }}$ to that ratio obtained at the surface of the star denoted $\mathcal{R}_{\text {theo }}$, which is determined theoretically for a set of input parameters ( $T_{\text {eff }}, \log g$ and $[\mathrm{Fe} / \mathrm{H}]$ ). In this manner, the $T_{\text {eff }}$ input is varied and the method is iterated until $\mathcal{R}_{\text {obs }}=\mathcal{R}_{\text {theo }} . T_{\text {eff }}$ is then calculated using Stefan-Boltzmann Eqn. 5.2:

$$
\begin{equation*}
T_{\mathrm{eff}}=\left(\frac{f_{\mathrm{bol}} F_{\mathrm{IR}}(\text { theo })}{\sigma_{\mathrm{SB}} f_{\mathrm{IR}}}\right)^{1 / 4} \tag{5.4}
\end{equation*}
$$

where $F_{\mathrm{IR}}$ (theo) and $f_{\mathrm{IR}}$ are respectively the (IR) theoretical flux at the surface of the star and that observed at Earth.

This method is argued to be almost model independent (Casagrande et al., 2006) and useful to measure the effective temperature for large sample of stars since for those with $T_{\text {eff }}$ greater than 4500 K, the (IR) SED in the Rayleigh-Jeans tail of the Plank function
(at $\lambda>1.2 \mu \mathrm{~m}$ ) determined via photometry is largely dominated by the continuum and are thus linearly related to $T_{\text {eff }}$ (Casagrande et al., 2010).

The advantage for using the IRFM is the availability of the (IR) photometric data for a very large number of stars provided by the 2MASS ${ }^{5}$ telescope with all-sky coverage. In addition,

[^22]it has been shown that its results have a high internal accuracy, and are independent from non-LTE effects and granulation (Asplund and García Pérez, 2001; Casagrande, 2009). On the other hand, inaccurate reddening and absolute flux calibrations can induce errors as large as 100K (Casagrande et al., 2006).

Casagrande et al. (2010) used this method to compare $\theta_{\mathrm{D}}$ determined from the IRFM to those measured via interferometry (Eqn. 5.3) and found a good agreement for most stars, though a difference of up to $10 \%$ can be found for some.

### 5.1.1.3 Excitation equilibrium

This method is based on the idea that if local thermodynamical equilibrium (LTE) conditions are attained (Sec. 2.1.4.1), then the fraction of ionized to neutral species (specifically iron FeII/FeI) is given by the ionization equilibrium (See Saha equation in Sec. 2.25), and that the FeI and FeII energy level populations are governed by the Boltzmann equation 2.24. Consequently, the abundances derived from a set of lines, should not depend on the ionization stage, or on the excitation energy of the lines. Therefore the $T_{\text {eff }}$ is determined iteratively by the absence of trend in abundances of FeI and FeII lines with their corresponding excitation potentials ${ }^{6}$.

While this method is found to yield good results for a sample of Solar twins with similar properties (Ramírez et al., 2009), it is highly model-dependent and is prone to non-LTE effects (sec. 2.1.4.2) and inhomogeneities which can lead to serious under- or over- estimation of $T_{\text {eff }}$ in some stars especially metal-poor ones.

### 5.1.2 Surface gravity $\log \mathrm{g}$

The surface gravity of a star of radius $R_{\star}$ and mass $M_{\star}$ is:

$$
\begin{equation*}
g=\left(G \frac{M_{\star}}{R_{\star}^{2}}\right) \tag{5.5}
\end{equation*}
$$

most often denoted in logarithmic form as $\log g$. Different methods are used to determine the surface gravities of stars, from which we briefly describe the spectroscopic ionization equilibrium and the asteroseimic methods below.

### 5.1.2.1 Ionization equilibrium

The most commonly used method to determine $\log g$ is the ionization equilibrium of FeI/FeII lines as a function of measured equivalent width (a measurement of the strength of the line). This is based on the fact that increasing gravity increases gas and electron pressures, which cause a change in the ratio of the line absorbers to the continuous opacity, which in turn affects the line strengths (by changing the ionization equilibrium of FeII/FeI). Thus the line strengths are sensitive to $\log g$, and this dependence is used to determine $\log g$ of the model by varying its input values until there is agreement between FeI and FeII abundance with the equivalent widths.

A significant contribution to the uncertainty of this method is due to the correlation between $\log g$ and $T_{\text {eff }}$ in the spectral analysis of the equivalent widths, and in which the abundance

[^23]calculations can also be prone to non-LTE and 3D atmospheric model effects. These uncertainties can result in a difference of $\log g$ up to 0.2 dex (Hekker and Meléndez, 2007; Morel and Miglio, 2012).

### 5.1.2.2 Asteroseismology

In the past decade, asteroseismology has become possible for stars other than the Sun, and has revolutionized our understanding of stellar interiors. The concept is that stars show pulsation variabilities which support standing waves whose frequencies and amplitudes depend on the stellar structure. Two types of modes have been identified: acoustic p-mode waves, in which the restoring force is pressure and buoyancy, $g$-mode waves, where the restoring force is gravity, and whose excitation origin is believed to be turbulent convections.
p-modes are the primary observable modes propagating in the envelopes of solar-like stars which give rise to displacements at the stellar surface, resulting in changes in the brightness which can be detected via photometric methods, or radial velocity shifts in spectral lines that can be detected via spectroscopic methods.

The patterns of the waves at the surface of the star can be described by the spherical wave equation:

$$
\begin{equation*}
\nabla^{2} \psi=\frac{1}{c^{2}} \frac{\mathrm{~d}^{2} \psi}{\mathrm{~d} t^{2}} \tag{5.6}
\end{equation*}
$$

whose eigenvalues are known as the radial order $n$ (the number of nodes seen from the center to the surface radially), the angular degree, $l$, and the azimuthal order, $m$. Modes of low angular degrees, $l$, propagate more deeply into the stellar interior, while modes of higher degrees propagate closer to the stellar surface (see Fig. 5.1). In this manner, each mode samples the conditions at a different depth in the star, and with enough modes, we can invert the problem and determine the stellar sound speed profiles, which in turn depends on pressure, density, and composition (See, for e.g., Christensen-Dalsgaard, 1991).
Moreover, the spacing between adjacent radial orders and the spacing between modes of different angular degrees in a power-frequency spectrum (Fig. 5.2) can be related to the fundamental parameters of the star. The spacing between adjacent radial orders of the same angular degree is termed the large frequency spacing, $\Delta \nu_{n, l}$, and is defined as:

$$
\begin{equation*}
\Delta \nu_{n, l}=\nu_{n, l}-\nu_{n-1, l} \tag{5.7}
\end{equation*}
$$

The small frequency spacing, $\delta \nu_{n, l}$ is that between the pairs of even and odd modes, which is defined as:

$$
\begin{equation*}
\delta \nu_{n, l}=\nu_{n, l}-\nu_{n-1, l+2} \tag{5.8}
\end{equation*}
$$

## Scaling relations with stellar parameters

The average large frequency separation $\Delta \nu_{\star}$ of a star undergoing solar-like oscillations is directly proportional to the square root of its density $\sqrt{\rho}_{\star}$ ) (Kjeldsen and Bedding, 1995), which can be compared to the well known solar value ${ }^{7}$ to determine the mass $M_{\star}$ and radius $R_{\star}$ of the star via:

$$
\begin{align*}
\Delta \nu_{\star} & \propto \sqrt{\rho_{\star}} \\
& \propto\left(\frac{M_{\star}}{R_{\star}^{3}}\right)^{1 / 2}  \tag{5.9}\\
& =\frac{\left(M_{\star} / M_{\odot}\right)^{1 / 2}}{\left(R \star / R_{\odot}\right)^{3 / 2}} \Delta \nu_{\odot}
\end{align*}
$$

[^24]Figure 5.1: Examples of oscillatory surface displacements (i.e. angular components) for a number of modes with different values of $m$ and $l$.

where $M_{\odot}, R_{\odot}$ and $\Delta \nu_{\odot}$ are the solar values for mass, radius and large frequency separation respectively.

In addition, for a given value of effective temperature $T_{\text {eff }}$ of the star, the frequency at maximum power $\nu_{\max }$ of the oscillations is also related to $M_{\star} \& R_{\star}$ (Belkacem et al., 2011; Brown et al., 1991), such that:

$$
\begin{equation*}
\nu_{\max \star} \simeq \frac{M_{\star} / M_{\odot}}{\left(R_{\star} / R_{\odot}\right)^{2}\left(T_{\mathrm{eff}} / T_{\mathrm{eff} \odot}\right)^{1 / 2}} \nu_{\max \odot} \tag{5.10}
\end{equation*}
$$

where $\nu_{\max }=3100 \mu \mathrm{~Hz}$ (Mosser et al., 2013) is the solar maximum power frequency and $T_{\text {eff }}=5777 \mathrm{~K}$ is the solar effective temperature.

Thus the correlation between $\Delta \nu, \nu_{\max }$ and $T_{\text {eff }}$ allows the determination of the mass and radius of the star from which the surface gravity can be calculated.

Two methods are generally used to determine $\log g$ : either directly from $\nu_{\max } \propto g / \sqrt{T_{\text {eff }}}$, where a $0.4 \%$ change in $\log g$ is obtained upon a $1 \%$ change in $\nu_{\max }$ (Hekker et al., 2011), or indirectly by using grid-based modeling, which is based on searching for the "best model" among a large grid of models for a given set of observables ( $\Delta \nu, \nu_{\max }, T_{\text {eff }}$ and metallicity $[\mathrm{Fe} / \mathrm{H}]$ ) (Gai et al., 2011). The advantage of using asteroseismic $\log g$ as input for spectral synthesis models is that it is not prone to non-LTE and 3D effects, and is not correlated with $T_{\text {eff }}$ as is the case

Figure 5.2: Solar power-frequency spectrum showing angular degrees $l=0,1,2,3$ and their respective small and large frequency separations. Taken from BiSON dataset (Asteroseismology of red giant stars, Neil James Tarrant, PhD dissertation, 2010)

in spectroscopic models, where quoted uncertainties of the asteroseismic $\log g$ are often an order of magnitude lower than those quoted in spectroscopic analyses, indicating more precise values (Gai et al., 2011).
Brogaard et al. (2015), tested the accuracy of asteroseismic log $g$ by comparing to those determined from detached eclipsing binaries in open clusters in the Kepler \& CoRoT fields (NGC 6791 , NGC $6819, \ldots$ ) and found an accordance up to 0.01 dex.

Over the past few years the number of stars with detected solar-like oscillations has increased considerably, from a few to over ten thousand thanks to missions like Kepler ${ }^{8}$ and CoRoT ${ }^{9}$ (Convection, Rotation and planetary Transits) (NASA's and CNES ${ }^{10}$-ESA missions respectively).

[^25]
### 5.1.3 Metallicity [Fe/H]

By metals, we denote all chemical elements except hydrogen and helium. The Solar chemical composition comprises $\sim 73 \%$ hydrogen, $\sim 25 \%$ helium and $\sim 2 \%$ metals (Asplund et al., 2009).

A star's metallicity can be indirectly determined from the star's spectral line features. It is generally defined to be equal to the abundance of iron (Fe) compared to its hydrogen (H) abundance, normalized to the solar abundance on a logarithmic scale:

$$
\begin{equation*}
[\mathrm{Fe} / \mathrm{H}]=\log \left(\mathrm{n}_{\mathrm{Fe}} / \mathrm{n}_{\mathrm{H}}\right)-\log \left(\mathrm{n}_{\mathrm{Fe}} / \mathrm{n}_{\mathrm{H}}\right)_{\odot} \tag{5.11}
\end{equation*}
$$

where $n_{F e}$ and $n_{H}$ are the number densities of Fe and H respectively. Iron is chosen as a proxy of the total metal content due to the wealth of iron lines in most stars spectra, thus making them easily measurable as compared to other metals.

## Abundance determination:

The absolute abundance of a chemical element species $A$ is often defined on the following scale:

$$
\begin{equation*}
\log \varepsilon(A)=\log \left(\mathrm{n}_{\mathrm{A}} / \mathrm{n}_{\mathrm{H}}\right)+12 \tag{5.12}
\end{equation*}
$$

One method of determining the abundances is by using a curve of growth (cog) method, which provides a relation between the chemical abundance of an element and the line equivalent width which is defined as:

$$
\begin{equation*}
\mathrm{W}_{\lambda}=\int_{0}^{\infty} \frac{I_{\lambda}-I_{\text {cont }}}{I_{\text {cont }}} \mathrm{d} \lambda \tag{5.13}
\end{equation*}
$$

where $I_{\lambda}$ and $I_{\text {cont }}$ are the respective intensities of the spectral line at a wavelength $\lambda$ and at the continuum, which can also be defined as the width of a rectangle of length $I_{\text {cont }}$ and has the same area as that beneath the corresponding spectral line (Fig. 5.3). Another commonly used abundance determination method is the iterative spectral fitting, which will not be discussed in depth as it was not used in this dissertation.

The curve of growth thus provides a relation between the equivalent width of the spectral line and the number of absorbing atoms $\log A$ of a chemical species. This relation $W_{\lambda} / \lambda$ vs. $\log A$ depends on the strength of the spectral line which is demonstrated in Fig. 5.4. It can generally be divided into 3 parts:

- a linear part which corresponds to weak lines (small $W_{\lambda}$ ): the equivalent width is proportional to $\log A$
- a "plateau" part where the central depth of the line approaches its maximum value due to saturation, and the line strength grows asymptotically towards a constant value.
- a damping part which corresponds to strong lines: the equivalent width is proportional to $\sqrt{\log A}$.

The elemental abundance is then calculated using the ( $\operatorname{cog}$ ) method by computing synthetic equivalent widths using spectral synthesis codes ${ }^{11}$ for different inputs of $\log (\mathrm{A})$, and then the actual abundance is interpolated to the measured equivalent width value of the line.

[^26]Figure 5.3: Equivalent width of a spectral line and its equivalent area.


The effect of microturbulence $\xi_{t}$ :
The observed equivalent widths of spectral lines are found to be greater than predicted by models when calculated using just thermal and damping broadening parameters in the calculations of the synthetic spectral lines (equivalent widths) (see appendix A). This difference is due to the micro-turbulent velocity which is an ad-hoc free parameter which has to be added to the calculations. Its values typically range between 0.5 and $5 \mathrm{~km} / \mathrm{sec}$. The micro-turbulent velocity is determined to be the value of $\xi_{t}$ that makes the strong FeI line abundances independent of $W_{\lambda}$.

### 5.2 Benchmark stars

The determination and calibration of stellar abundances through spectral line synthesis in the light of the present work, requires minimizing the inaccuracies from input data in the calculations. As demonstrated in the previous sections, these calculations are highly affected by the input AFP and their determination methods which alter the atmospheric thermal structure of the models, and can lead to serious inaccuracies in abundance determination and calibration.

This calibration also requires a set of reference stars spanning over a large parameter space to homogenize and validate the method we are proposing and using. For these reasons, the FGK Gaia-ESO Benchmark stars (GBS) proposed by Heiter et al. (2015a), Blanco-Cuaresma et al. (2014) \& Jofré et al. (2014) have been adopted as test benchs of our methods and in our calculations. Most of them will be observed by Gaia ${ }^{12}$ (Perryman et al., 2001; Turon et al., 2005), which has the goal of providing parallaxes and proper motions of exquisite precision for 1 billion stars of our Galaxy. It is complemented by a large set of ground-based spectroscopic and spectrophotometric observations which are led and analyzed by international team collaborations such as the Gaia-ESO survey (Gilmore et al., 2012a,b), RAVE (Steinmetz et al.,

[^27]Figure 5.4: Curve of growth: showing the relation between $\mathrm{W}_{\lambda} / \lambda$ and the abundance (number of absorbing atoms) $\log A$ of the corresponding species (upper panel) for different line strengths (lower panel) from Gray (2008).

2006), APOGEE (Allende Prieto et al., 2008) and GALAH (De Silva et al., 2015).

### 5.2.1 General description and selection criteria

The GBS stars are reference objects for the calibration of all the observed Gaia stars. They are therefore carefully studied from the ground. In addition, they will also serve to calibrate the different methods and input data used in the afore-mentioned complementary spectroscopic ground-based surveys to Gaia.

They have been chosen such that their AFP values cover a wide range of $T_{\text {eff }}, \log g$ and $[\mathrm{Fe} / \mathrm{H}]$ parameter space and thus representing different stellar types and populations. In addition, they were selected to have well-determined angular diameters $\theta_{\mathrm{D}}$ and bolometric fluxes $f_{\text {bol }}$, from which $T_{\text {eff }}$ was calculated, and homogeneous mass determinations from stellar-evolution models from which their $\log g$ were determined, or for which asteroseismic $\log g$ from Kepler and CoRoT existed, thus assuring AFP values as independent from spectroscopic methods as possible.

Another criterion for choosing these stars, is whether they have been subjected to frequent spectroscopic investigation, which allowed for the comparison of their parameters determined via different methods.
Their $V$ magnitudes range from 0 to 8 mag, and their positions are evenly distributed along the celestial equator, with declinations within $\pm 30^{\circ}$.

The list of stars used in this work consisted of 30 stars out of 34 suggested FGK GBS from the Heiter et al. (2015a) paper, for which we had available spectra from the Gaia-ESO collaboration. The spectra were collected using the UVES ${ }^{13}$ spectrograph at the VLT ${ }^{14}$. The sources of the UVES spectra are from the Advanced Data Products collection of the ESO Science Archive Facility, which were reduced by the standard UVES pipeline version 3.2 (Ballester et al., 2000), and from the UVES Paranal Observatory Project UVES-POP library which were reduced with tools written especially for that library (Bagnulo et al., 2003).
Table 5.1 lists their names and IDs, right ascensions ( $\alpha_{\mathrm{RA}}$ ), declinations ( $\delta_{\mathrm{DEC}}$ ) and spectral types extracted from the SIMBAD ${ }^{15}$ database, and their $V$ magnitudes extracted from GCPD ${ }^{16}$ (General Catalog of Photometric Data).

### 5.2.2 $T_{\text {eff }}$ determination

The stars $T_{\text {eff }}$ values were determined using Eqn. 5.3, where $\theta_{\mathrm{D}}$ and $\mathrm{F}_{\text {bol }}$ were extracted from the literature when available, from interferometric measurements and absolute flux measurements respectively (see Heiter et al. (2015a) for more details on the sources).

For $\mu$ Leo and HD107328, the angular diameters were indirectly determined by Cohen et al. (1999), by scaling their (IR) photometry to absolute flux calibrations in the (IR) of reference stars with similar types (using Arcturus for $\mu$ Leo and $\beta$ Gem for HD107283). For HD22879, HD84937, $\epsilon$ For and $\mu$ Ara the surface-brightness relations by Kervella et al. (2004) were used to estimate the angular diameters, in which the interstellar extinction was considered negligible since these stars lie within 40 pc , where interstellar reddening 3D maps show negligible values (Lallement et al., 2014).

Indirect measurements of $f_{\text {bol }}$ were derived using the $V$ magnitudes and the bolometric corrections in the visible $\mathrm{BC}_{V}$ of the stars using the relation:

$$
\begin{equation*}
f_{\mathrm{bol}}=\frac{1}{4 \pi(10 p c)^{2}} L_{0} 10^{-0.4\left(V+B C_{V}\right)} \tag{5.14}
\end{equation*}
$$

where $L_{0}=3.055 \times 10^{28} \mathrm{~W}$ is the zero-point luminosity (Andersen, 1999). The $\mathrm{BC}_{V}$ used were adopted from Alonso et al. (1999) with an uncertainty of 0.05 mag.

[^28]| Star name (ID) | $\alpha_{\text {RA }}($ J2000 | $\delta_{\text {DEC }}$ (J2000) | Spectral Type | $V_{\text {mag }}$ |
| :---: | :---: | :---: | :---: | :---: |
| 18 Sco | 161537.269 | -082209.99 | G2Va | 5.5 |
| 61 Cyg B | 210655.264 | +384431.40 | K7V | 6.0 |
| $\alpha$ Cen A | 143936.494 | -605002.37 | G2V | 0.0 |
| $\alpha$ Cet | 030216.773 | +040523.06 | M1.5IIIa | 2.5 |
| $\alpha$ Tau | 043555.239 | +163033.49 | K5III | 0.9 |
| Arcturus | 141539.672 | +191056.67 | K1.5III | -0.1 |
| $\beta$ Ara | 172517.988 | -553147.59 | K3IB-II | 2.8 |
| $\beta$ Gem | 074518.950 | +280134.32 | KOIIIb | 1.1 |
| $\beta$ Hyi | 002545.070 | -771515.29 | G0V | 2.8 |
| $\beta$ Vir | 115041.718 | +014552.99 | F9V | 3.6 |
| $\delta$ Eri | 034314.901 | -604548.21 | K1III-IV | 3.5 |
| $\epsilon$ Eri | 033255.845 | -092729.73 | K2Vk: | 3.7 |
| $\epsilon$ For | 030137.637 | -280529.60 | K2VFe-1.3CH-08 | 5.9 |
| $\epsilon$ Vir | 130210.598 | +105732.94 | G8III | 2.8 |
| $\eta$ Boo | 135441.079 | +182351.79 | GOIV | 2.8 |
| $\gamma$ Sge | 195845.429 | +192931.73 | MOIII | 3.5 |
| HD 107328 | 122020.981 | +031845.26 | K0IIIb | 5.0 |
| HD 122563 | 140231.845 | +094109.95 | F8IV | 6.2 |
| HD 140283 | 154303.097 | -105600.60 | sdF3 | 7.2 |
| HD 220009 | 232020.583 | +052252.70 | K2III | 5.0 |
| HD 22879 | 034022.064 | -031301.12 | F9V | 6.7 |
| HD 49933 | 065049.832 | -003227.17 | F2V | 5.8 |
| HD 84937 | 094856.098 | +134439.32 | sdF5 | 8.3 |
| $\xi$ Hya | 113300.115 | -315127.44 | G7III | 3.5 |
| $\mu$ Ara | 174408.701 | -51502.59 | G3IV-V | 5.1 |
| $\mu$ Leo | 095245.817 | +260025.03 | K2III | 3.9 |
| Procyon | 073918.119 | +051329.96 | F5IV-V | 0.4 |
| $\psi$ Phe | 015338.741 | -461809.60 | M4III | 4.4 |
| Sun |  |  |  |  |
| $\tau$ Cet | 014404.083 | -155614.93 | G8.5V | 3.5 |

Table 5.1: Gaia Benchmark stars adopted in our study: General information including their names, right ascension $\alpha_{\mathrm{RA}}$, declination $\delta_{\text {DEC }}$ spectral types and visual magnitudes $V$.

### 5.2.3 $\log g$ determination

The $\log g$ values were determined using Eqn. 5.5. The stellar radii were measured using the angular diameters and their distances which were determined from their parallaxes $\pi$. The distances to the stars can be thus calculated using the relation $d=1 / \pi$, where $d$ is measured in parsecs (pc) and $\pi$ in arc seconds (arc-sec).
The parallaxes for the benchmark stars were determined from the HIPPARCOS ${ }^{17}$ measurements (Söderhjelm, 1999; van Leeuwen, 2007; VandenBerg et al., 2014).

The stellar masses were determined using asteroseismic relations (Sec. 5.1.2.2), where the large frequency separation values from Bruntt et al. (2010) \& Kallinger et al. (2010) were adopted. For stars which are part of binary systems, their masses were derived from combined dynamic astrometric and spectroscopic observations ( $\alpha$ Cen A, Pourbaix et al., 2002), from astrometric observations (61 Cyg B, Gorshanov et al., 2006 , $\mu$ Cas, Drummond et al., 1995 and

[^29]Procyon, Girard et al., 2000).
For single stars, and in the case of the absence of asterosismic data, the masses were determined by interpolation in grids of evolutionary tracks using the Padova and the Yonsei-Yale (Yi et al., 2003) stellar evolution models, using $T_{\text {eff }}$, luminosity and [ $\left.\mathrm{Fe} / \mathrm{H}\right]$ constraints. The adopted masses are the averages of the values obtained from both evolutionary model grids. The difference between the latter is that the Yonsei-Yale models take the helium diffusion into account while the Padova models don't.
For most stars, seismic masses agree with those determined from stellar models within $\pm 0.1 \mathrm{M}_{\odot}$.
The $\log g$ determinations of the stars using their masses and radii as explained above, compare well to the seismic $\log g$ calculated using Eqn. 5.10 from the $\nu_{\max }$ measurements of Morel and Miglio (2012), and lie within $\Delta \log g=\log g$ (Heiter et al. )-log $g$ (asteroseismology) $=$ 0.06 dex (15\%). Larger deviations were found for Procyon ( -0.08 dex), $\tau \operatorname{Cet}(+0.08$ dex) and Arcturus ( -0.2 dex ). These deviations are due to large uncertainties in $\nu_{\max }$ measurement for Procyon, and the uncertain evolutionary-models mass for $\tau$ Cet (which was found unreasonable corresponding to its age). Regarding Arcturus, its evolutionary-model mass was found inconsistent with its seismic mass due to uncertain $\Delta \nu$ values resulting from irregularities found in its p-mode oscillations (Retter et al., 2003).

### 5.2.4 [Fe/H] determination

The metallicities of the stars were calculated starting from the non-spectroscopic $T_{\text {eff }}$ and $\log g$ as described above, as inputs to calculating synthetic spectra and equivalent widths for FeI and FeII lines (Jofré et al., 2014). FeI and FeII abundances were calculated for the set of Gaia-ESO survey linelist, version v3 (GES-v3) (Heiter et al., 2015b), by 7 different methods all starting from the same parameters and using the same 1D MARCS model atmospheres (Gustafsson et al., 2008) (see Sect. 2.3 for more details on the models) to provide non-biased and non-model dependent results which are averaged to calculate the metallicity for each star (see below).

The lines were selected as to lie on the linear part of curve of growth (i.e. $\left.\log \left(W_{\lambda} / \lambda\right) \leq-4.8\right)$. This avoided using saturated and strong lines which can be strongly affected by turbulent velocities or damping parameters. The abundances calculated by each method and for each line were then chosen such that the agreement between different methods lies within $2 \sigma$ of the mean abundance. Excitation balance was then checked as a function of excitation potential (EP) and equivalent widths for all the stars. For FeI lines, non-LTE corrections were applied individually to each lines from the calculations of Bergemann et al. (2012). Finally the metallicities were computed by averaging the abundances of these final list of lines and by using an absolute abundance of 7.45 for the Sun (Grevesse et al., 2007).

The list of stars adopted in this work along with their fundamental parameters whose determination methods have been discussed above, including their angular diameters $\theta_{\mathrm{D}}$, bolometric fluxes $f_{\text {bol }}$, masses, parallaxes, $T_{\text {eff }}, \log g,[\mathrm{Fe} / \mathrm{H}]$, and their corresponding uncertainties are listed in Table 5.2.

Table 5.2: Gaia Benchmark stars adopted in our study: fundamental parameters including the adopted angular diameters $\theta_{\mathrm{D}}$, bolometric Fluxes $\mathrm{F}_{\text {bol }}$, $T_{\text {eff }}$ and their uncertainties $\sigma T_{\text {eff }}$, masses M, parallaxes $\pi, \log g$ and their uncertainties $\sigma \log g,[\mathrm{Fe} / \mathrm{H}]$ and their uncertainties $\sigma[\mathrm{Fe} / \mathrm{H}]$ and their microturbulent velocities $\xi_{t}$. The last column shows the method used to determine the stellar mass: Seis. (Asteroseismology), Evol. (Evolutionary tracks), Bin. (Binary system)

| Star name (ID) | $\theta_{\mathrm{D}}$ (mas) | $\mathrm{F}_{\text {bol }}\left(10^{-9} \mathrm{~W} \mathrm{~m}^{-2}\right)$ | $T_{\text {eff }}(\mathrm{K})$ | $\sigma T_{\text {eff }}(\mathrm{K})$ | $\mathrm{M}\left(\mathrm{M}_{\odot}\right)$ | $\pi$ (mas) | $\log g$ | $\sigma \log g$ | [Fe/H] | $\sigma[\mathrm{Fe} / \mathrm{H}]$ | $\xi_{t}\left(\mathrm{Km} \cdot \mathrm{s}^{-1}\right)$ |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 18 Sco | 0.676 | 0.1734 | 5810 | 80 | 1.02 | 71.93 | 4.44 | 0.03 | +0.03 | 0.01 | 1.2 | Seis. |
| 61 Cyg B | 1.581 | 0.2228 | 4044 | 32 | 0.61 | 285.89 | 4.67 | 0.04 | -0.38 | 0.03 | 1.1 | Bin. |
| $\alpha$ Cen A | 8.511 | 27.160 | 5792 | 16 | 1.11 | 747.10 | 4.31 | 0.01 | +0.26 | 0.01 | 1.2 | Seis. |
| $\alpha$ Cet | 12.2 | 10.3 | 3796 | 65 | 1.76 | 13.10 | 0.68 | 0.23 | -0.45 | 0.05 | 1.4 | Bin. |
| $\alpha$ Tau | 20.58 | 33.57 | 3927 | 40 | 0.96 | 48.92 | 1.11 | 0.19 | -0.37 | 0.02 | 1.4 | Evol. |
| Arcturus | 21.050 | 49.8 | 4286 | 35 | 1.03 | 88.83 | 1.64 | 0.09 | -0.52 | 0.01 | 1.3 | Seis. |
| $\beta$ Ara | 5.997 | 3.7179 | 4197 | 50 | 8.21 | 4.54 | 1.05 | 0.15 | -0.05 | 0.04 | 1.5 | Evol. |
| $\beta$ Gem | 7.98 | 11.82 | 4858 | 60 | 2.30 | 96.52 | 2.90 | 0.08 | +0.13 | 0.01 | 1.1 | Seis. |
| $\beta$ Hyi | 2.257 | 2.0191 | 5873 | 45 | 1.15 | 134.07 | 3.98 | 0.02 | -0.04 | 0.01 | 1.3 | Seis. |
| $\beta$ Vir | 1.450 | 0.9590 | 6083 | 41 | 1.34 | 91.50 | 4.10 | 0.02 | +0.24 | 0.01 | 1.4 | Seis. |
| $\delta$ Eri | 2.394 | 1.150 | 4954 | 30 | 1.13 | 110.62 | 3.76 | 0.02 | +0.06 | 0.01 | 1.2 | Seis. |
| $\epsilon$ Eri | 2.126 | 1.0 | 5076 | 30 | 0.80 | 310.95 | 4.61 | 0.03 | -0.09 | 0.01 | 1.1 | Evol. |
| $\epsilon$ For | 0.788 | 0.1425 | 5132 | 78 | 0.91 | 31.05 | 3.52 | 0.08 | -0.60 | 0.01 | 1.2 | Evol. |
| $\epsilon$ Vir | 3.28 | 2.21 | 4983 | 61 | 3.02 | 29.75 | 2.77 | 0.02 | +0.15 | 0.01 | 1.1 | Evol. |
| $\eta$ Boo | 2.189 | 2.21 | 6099 | 28 | 1.64 | 87.77 | 3.79 | 0.02 | +0.32 | 0.01 | 1.4 | Seis. |
| $\gamma$ Sge | 6.060 | 2.57 | 3807 | 49 | 1.11 | 12.61 | 1.05 | 0.32 | -0.17 | 0.04 | 1.4 | Evol. |
| HD 107328 | 1.74 | 0.4122 | 4496 | 59 | 1.41 | 10.60 | 2.09 | 0.13 | -0.33 | 0.01 | 1.2 | Evol. |
| HD 122563 | 0.94 | 0.1303 | 4587 | 60 | 0.86 | 4.22 | 1.61 | 0.07 | -2.64 | 0.01 | 1.3 | Evol. |
| HD 140283 | 0.353 | 0.0386 | 5522 | 105 | 0.68 | 17.18 | 3.58 | 0.11 | -2.36 | 0.02 | 1.3 | Evol. |
| HD 220009 | 2.045 | 0.4409 | 4217 | 60 | 0.83 | 7.55 | 1.43 | 0.12 | -0.74 | 0.01 | 1.3 | Evol. |
| HD 22879 | 0.382 | 0.0577 | 5868 | 89 | 0.75 | 39.13 | 4.27 | 0.04 | -0.86 | 0.01 | 1.2 | Evol. |
| HD 49933 | 0.445 | 0.1279 | 6635 | 91 | 1.17 | 33.68 | 4.20 | 0.03 | -0.41 | 0.01 | 1.9 | Seis. |
| HD 84937 | 0.153 | 0.0127 | 6356 | 97 | 0.75 | 12.24 | 4.06 | 0.04 | -2.03 | 0.02 | 1.5 | Evol. |
| $\xi$ Hya | 2.386 | 1.228 | 5044 | 40 | 2.84 | 25.14 | 2.87 | 0.02 | +0.16 | 0.01 | 1.1 | Seis. |
| $\mu$ Ara | 0.763 | 0.2354 | 5902 | 66 | 1.19 | 64.48 | 4.30 | 0.03 | +0.35 | 0.01 | 1.2 | Seis. |
| $\mu$ Leo | 2.93 | 1.1458 | 4474 | 60 | 1.69 | 26.27 | 2.51 | 0.11 | +0.25 | 0.02 | 1.1 | Evol. |
| Procyon | 5.39 | 17.86 | 6554 | 84 | 1.50 | 284.52 | 4.00 | 0.02 | +0.01 | 0.01 | 1.8 | Seis. |
| $\psi$ Phe | 8.13 | 3.2 | 3472 | 92 | 1.00 | 9.54 | 0.51 | 0.18 | -1.24 | 0.24 | 1.5 | Evol. |
| Sun |  |  | 5777 | 1 |  |  | 4.4380 | 0.0002 | +0.03 | 0.01 | 1.2 |  |
| $\tau$ Cet | 2.015 | 1.162 | 5414 | 21 | 0.71 | 273.96 | 4.49 | 0.02 | -0.49 | 0.01 | 1.1 | Seis. |

## 6 Non-LTE calculations using the Drawin approximation

This chapter presents the results of tests on the role of hydrogen collisions in non-LTE line formation using the Drawin approximation (see Sect. 3.1.1). For that purpose, a silicon model atom was constructed to test our different approximations for the H-collisional rates, as quantum calculation for $\mathrm{H}+\mathrm{Si}$ excitation and charge transfer processes are available from Belyaev et al. (2014). Our aim is thus to scale the Drawin approximation in order to reproduce the $\mathrm{H}+\mathrm{Si}$ quantum rates, and if possible, apply this scaling recipe on iron for which no quantum data have been published yet. This chapter is divided as follows: In Section 6.1, the Si model atom construction is described. In Sections 6.2 and 6.3, the non-LTE calculations for silicon and iron using the Drawin approximation, with various scaling factors $\mathrm{S}_{\mathrm{H}}$ are presented.

### 6.1 Testing our method: Silicon atoms

The silicon model atom was built in a similar manner to the iron model atom described in Chapter 4.

### 6.1.1 Energy levels

The SiI energy levels and the Si II ground level were extracted from the NIST database (Martin and Zalubas, 1983). The total number of SiI fine structure levels used in our model is 296. The same number of levels was used by Shchukina et al. (2012) in their non-LTE, 3D-model atmosphere study of the silicon abundance in the Solar photosphere. Fig. 6.1 shows the grotrian diagram of our Si atom, showing the distribution of the levels as a function of their term IDs and energies.

### 6.1.2 Radiative transitions

Line data for transitions between our model energy levels were extracted from the VALD3 (Ryabchikova et al., 2011) database. The total number of transitions is 8674 , shown in the grotrian diagram of Fig 6.2. The oscillator strengths, the radiative damping coefficients and the wavelengths are from the Kurucz database (Kurucz and Bell, 1995). The Van der Waals hydrogen collisional broadening coefficients were calculated using the ABO theory (see Sec. A.2) by Barklem et al. (2015).

Line profiles were calculated using a Voigt profile function with a maximum of 80 frequency points. In MULTI2.3, the Doppler core and the Lorentzian wings of the line are controlled by two input parameters in the model atom, $\mathrm{Q}_{0}$ and $\mathrm{Q}_{\max }$ defined as:

- $\mathrm{Q}_{0}$ is the transition from Doppler Core to Lorentzian wings, hence it is the distance from the line center (in Doppler widths) at which the transition from Doppler core to Lorentzian wings occurs.
- $\mathrm{Q}_{\text {max }}$ is the distance from the line center (in Doppler widths) to which the line wings are calculated.

Based upon these parameters, the quadrature points ( Q ) of the line profile and their corresponding weights ( $\Delta \mathrm{Q}$ ) are calculated based on the trapezoidal rule depending on the position of the frequency point with respect to the central wavelength. i.e.: for $\mathrm{Q}<\mathrm{Q}_{0}$, the trapezoidal rule is applied on a linear mapping of Q while for $\mathrm{Q}>\mathrm{Q}_{0}$, the trapezoidal rule is applied on a logarithmic (10log) mapping of Q . The input values of $\mathrm{Q}_{0}$ and $\mathrm{Q}_{\text {max }}$ were determined line-by-line based on the values of the damping parameter $a$ (See Sec. A.4).

In addition to the bound-bound transitions, all the levels in the Si model were coupled to the Si II ground level via bound-free transitions. The bound-free photoionization tables were calculated by Nahar (1993) using the close-coupling approximation and the R-matrix method, and are extracted from the NORAD database. They include photoionization cross-sections for 264 SiI LS-coupling terms of multiplicities 1 and 3 , up to $\mathrm{n}=10$ and $\mathrm{l}=8$. The photoionization cross-sections for the mean levels were distributed onto the fine structure levels using their corresponding statistical weights. Due to the large number of points in the tables and the sharp resonance peaks in the data, the cross-sections were smoothed and re-sampled as described for iron in Sec. 4.2.2.
For terms of multiplicity 5 and for JJ-coupling terms for which no photoionization tables exist, Kramer's approximation was used to calculate the cross-sections (Eqn. 2.37).

### 6.1.3 Collisional transitions

All levels in the Si model are coupled via inelastic collisions with electrons and neutral hydrogen atoms.

For allowed electron collisional bound-bound transitions, the Seaton (1962a) impact parameter approximation was used (Eqn. 2.51) to calculate the effective collisional strengths $\Upsilon^{e-}$. For forbidden transitions, Seaton (1962b) approximation as listed in Allen (1973) is used with a collisional strength $\Omega=1$ (Eqn. 2.58).
All the levels were coupled to the Si II ground level through electron collisional ionization using Bely and van Regemorter (1970) dipole impact approximation (Eqn. 2.59).

The neutral $\mathrm{H}+$ Si collisional rates were calculated using the Drawin approximation via the Lambert (1993) derivation (Eqn. 3.14), using an oscillator strength $f=1$, which allows to calculate the collisional rates for both allowed and forbidden transitions.
All the energy levels in the Si model were coupled via H-collisional bound-bound, bound-free and charge transfer transitions as described in Chapter 4. In order to test the effect of hydrogen collisions, different model atoms were created with different $\mathrm{H}+$ Si collisional rates, by applying a scaling factor for the excitation, ionization and charge exchange processes. In the following sections and hereafter, we introduce two different scaling factors such as:
$\star \mathbf{S}_{\mathbf{H}}$ : scaling factor for excitation, de-excitation, and ionization transitions.
$\star \mathrm{S}_{\mathrm{H}}(\mathrm{CE})$ : scaling factor for charge exchange processes: ion-pair production, and mutual neutralization transitions.

| Star | Sun | HD140283 | $\alpha$ Cent A | Procyon | Arcturus | $\mu$ Leo |
| ---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\log \varepsilon(\mathrm{Si})$ | 7.549 | 5.303 | 7.799 | 7.516 | 7.287 | 8.071 |
| $\sigma \log \varepsilon(\mathrm{Si})$ | 0.016 | 0.094 | 0.028 | 0.065 | 0.051 | 0.093 |

Table 6.1: Adopted values for Si abundances in our calculations and their $\sigma$ values.

For comparison, a reference Si model was created using the quantum data of Belyaev et al. (2014) for the $\mathrm{H}+\mathrm{Si}$ collisional rates for the bound-bound and charge transfer processes. The collisional rates of the mean levels were distributed on the fine structure levels according to their statistical weights.

### 6.2 Silicon non-LTE calculations using the Drawin approximation

### 6.2.1 Method

Using the Si atomic data described above, several modified Si model atoms were created by varying the values of $\mathrm{S}_{\mathrm{H}}$ and $\mathrm{S}_{\mathrm{H}}(\mathrm{CE})$ as follows:

- $\mathrm{S}_{\mathrm{H}}$ was varied between 0.0001 and 10 in multiplicative steps of 10 .
- $\mathrm{S}_{\mathrm{H}}$ (CE) was varied between 0.1 and 10 in multiplicative steps of 10 , in addition to the $S_{\mathrm{H}}(C E)=0$ value.

Using MARCS model atmospheres as input, non-LTE calculations were performed for the previously described Si model atoms for all the combinations of $\mathrm{S}_{\mathrm{H}}$ and $\mathrm{S}_{\mathrm{H}}(\mathrm{CE})$ as described above. They are hereafter referred to as the Drawin models. The calculations performed with the reference Si model are hereafter referred to as the quantum model. The calculations were performed for 6 benchmark stars, namely, the Sun, the metal poor halo subgiant HD140283, the metal rich main sequence star $\alpha$ Centauri A, Procyon, and two red giant benchmark stars: Arcturus and $\mu$ Leo. Background line opacity files excluding Si lines were included in the calculations, thus accounting for line blanketing effects. The opacity files were calculated for each star's metallicity and microturbulent velocity. $T_{\text {eff }}$ and $\log g$ are from the GBS values in Table 5.2. The Solar Si abundance value adopted in the calculations is taken from the non-LTE, 3D calculations of Shchukina et al. (2012), while those for the other stars are from Jofré et al. (2015) where line-by-line abundance analyses of Gaia benchmark stars were performed. The abundance values and their corresponding uncertainties are shown in Table 6.1.

### 6.2.2 Results

The calculated non-LTE equivalent widths for the Drawin models ( $\mathrm{EW}_{\text {Drawin }}$ ) were compared to the reference values $\left(\mathrm{EW}_{\mathrm{QM}}\right)$ for different values of $\mathrm{S}_{\mathrm{H}}$ and $\mathrm{S}_{\mathrm{H}}(\mathrm{CE})$ through the computation of a $\chi_{\mathrm{QM}}^{2}$ using chosen equivalent widths corresponding to lines of transition energies lying between 1 eV and $4 \mathrm{eV}(1 \mathrm{eV}<\Delta E<4 \mathrm{eV})$ :

$$
\begin{equation*}
\chi_{\mathrm{QM}}^{2}=\sum_{\mathrm{N}_{\text {lines }}} \frac{\left(\mathrm{EW}_{\text {Drawin }}-\mathrm{EW}_{\mathrm{Quantum}}\right)^{2}}{E W_{\text {Quantum }}} \tag{6.1}
\end{equation*}
$$

Figs. $6.3,6.4,6.5,6.6,6.7$ and 6.8 show the comparison of the calculated equivalent widths for all the models as compared to those of the reference model, for the 6 stars. Table 6.2 shows the obtained $\chi_{Q M}^{2}$ for each corresponding model.

The results obtained for each star are summarized below:

Sun: The best-fit Drawin model is obtained for $S_{H}=0.01$ and $S_{H}(C E)=0.1$. It can be seen from Table 6.2, that as the $S_{H}$ value increases, thus increasing the excitation and de-excitation $\mathrm{H}+\mathrm{Si}$ collisional rates, the Drawin models deviate from the reference calculations.

HD140283: The best-fit Drawin model to reproduce the reference calculations is obtained for $S_{H}=1.0$ and $S_{H}(C E)=0.1$. The $\chi_{Q M}^{2}$ values behavior with $S_{H}$ is, however, opposite to those obtained for the Sun, as the deviation from the reference calculations is increasing with decreasing $\mathrm{S}_{\mathrm{H}}$ (i.e. with decreasing $\mathrm{Si}+\mathrm{H}$ excitation rates).
$\alpha$ Cent A \& Procyon: The best-fit model for both stars is obtained for $\mathrm{S}_{\mathrm{H}}=10$ and $\mathrm{S}_{\mathrm{H}}(\mathrm{CE})=0.1$. The $\chi_{Q M}^{2}$ behavior with $\mathrm{S}_{\mathrm{H}}$ for both is similar to that of HD140283. For these two metal rich stars, high collisional excitation rates are required to reproduce the reference calculations.

Arcturus \& $\mu$ Leo: The best-fit obtained model is for $S_{H}=0.0001$ and $S_{H}(C E)=1$. For both red giant stars, small excitation rates for small values of $S_{H}$ are required for better fitting the reference calculations. For high charge exchange rates at $S_{H}(C E)=10$, larger $\chi_{Q M}^{2}$ values are obtained.

For all the stars, it can be observed that no clear trend is obtained with $S_{H}(C E)$, which is less constrained than $\mathrm{S}_{\mathrm{H}}$.

Figure 6.3: non-LTE calculated equivalent widths using the Drawin Si models vs. the quantum Si model for different scaling factors $S_{H}$ and $S_{H}(C E)$ for the Sun.


Figure 6.4: non-LTE calculated equivalent widths using the Drawin Si models vs. the quantum Si model for different scaling factors $\mathrm{S}_{\mathrm{H}}$ and $\mathrm{S}_{\mathrm{H}}$ (CE) for HD140283.


## 6. Non-LTE calculations using the Drawin approximation

Figure 6.5: non-LTE calculated equivalent widths using the Drawin Si models vs. the quantum Si model for different scaling factors $\mathrm{S}_{\mathrm{H}}$ and $\mathrm{S}_{\mathrm{H}}(\mathrm{CE})$ for the $\alpha$ Cent A .


Figure 6.6: non-LTE calculated equivalent widths using the Drawin Si models vs. the quantum Si model for different scaling factors $\mathrm{S}_{\mathrm{H}}$ and $\mathrm{S}_{\mathrm{H}}(\mathrm{CE})$ for the Procyon.


Figure 6.7: non-LTE calculated equivalent widths using the Drawin Si models vs. the quantum Si model for different scaling factors $\mathrm{S}_{\mathrm{H}}$ and $\mathrm{S}_{\mathrm{H}}(\mathrm{CE})$ for the Arcturus.


Figure 6.8: non-LTE calculated equivalent widths using the Drawin Si models vs. the quantum Si model for different scaling factors $\mathrm{S}_{\mathrm{H}}$ and $\mathrm{S}_{\mathrm{H}}(\mathrm{CE})$ for the $\mu$ Leo.


|  |  |  |  |  | $\mathrm{S}_{\mathrm{H}}$ |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | 0.0001 | 0.001 | 0.01 | 0.1 | 1.0 | 10.0 |
| Sun | $\mathrm{S}_{\mathrm{H}}(\mathrm{CE})$ |  | 0 | 57.099 | 45.776 | 13.237 | 107.358 | 252.183 | 317.127 |
|  |  | 0.1 | 55.986 | 44.733 | 13.080 | 110.062 | 256.387 | 321.084 |
|  |  |  | 48.388 |  | 13.585 | 135.332 | 294.636 | 356.922 |
|  |  |  |  |  |  |  |  |  |
|  |  | 10.0 | 28.972 | 24.723 | 62.607 | 364.666 | 618.549 | 667.761 |
| HD140283 | $\mathrm{S}_{\mathrm{H}}$ (CE) | 0 | 461.176 | 402.107 | 210.132 | 28.148 | 11.202 | 17.052 |
|  |  | 0.1 | 454.951 | 396.229 | 206.158 | 27.314 | 10.816 | 17.519 |
|  |  | 1.0 | 416.261 | 359.931 | 180.655 | 21.909 | 15.181 | 21.758 |
|  |  | 10.0 | 309.631 | 260.832 | 116.140 | 22.805 | 50.366 | 58.479 |
| $\alpha$ Cent A | $\mathrm{S}_{\mathrm{H}}(\mathrm{CE})$ | 0 | 493.696 | 468.430 | 318.271 | 88.562 | 14.430 | 12.405 |
|  |  | 0.1 | 491.336 | 466.030 | 315.833 | 80.484 | 14.434 | 12.049 |
|  |  | 1.0 | 472.496 | 446.885 | 296.302 | 71.530 | 16.282 | 17.002 |
|  |  | 10.0 | 373.565 | 347.512 | 205.985 | 78.745 | 110.670 | 123.594 |
| Procyon | $\mathrm{S}_{\mathrm{H}}(\mathrm{CE})$ | 0 | 667.085 | 651.198 | 519.893 | 176.539 | 26.969 | 21.773 |
|  |  | 0.1 | 660.543 | 649.948 | 518.630 | 175.687 | 26.901 | $\underline{21.570}$ |
|  |  | 1.0 | 658.249 | 639.322 | 507.840 | 168.514 | 26.649 | 23.885 |
|  |  | 10.0 | 585.439 | 567.263 | 434.940 | 128.584 | 46.495 | 62.300 |
| Arcturus | $\mathrm{S}_{\mathrm{H}}(\mathrm{CE})$ | 0 | 11.081 | 12.408 | 13.766 | 17.760 | 46.172 | 35.676 |
|  |  | 0.1 | 11.028 | 12.371 | 13.747 | 17.800 | 46.133 | 35.776 |
|  |  | 1.0 | $\underline{10.885}$ | 12.329 | 13.769 | 18.307 | 46.0759 | 37.581 |
|  |  | 10.0 | 15.145 | 18.840 | 20.7029 | 29.708 | 59.122 | 64.602 |
| $\mu$ Leo | $\mathrm{S}_{\mathrm{H}}(\mathrm{CE})$ | 0 | 4.829 | 5.265 | 5.603 | 7.325 | 20.080 | 17.456 |
|  |  | 0.1 | 4.801 | 5.243 | 5.588 | 7.341 | 20.077 | 17.559 |
|  |  | 1.0 | 4.777 | 5.260 | 5.597 | 7.580 | 20.214 | 18.631 |
|  |  | 10.0 | 11.182 | 11.912 | 11.576 | 14.822 | 30.209 | 36.403 |

Table 6.2: Calculated $\chi_{Q M}^{2}$ values for the Drawin models with different $S_{H}$ and $S_{H}(C E)$ scaling factors, compared to the reference calculations for the Sun, HD140283, $\alpha$ Cent A, Procyon, Arcturus and $\mu$ Leo. The least $\chi_{Q \mathrm{M}}^{2}$ value for each star is underlined.

### 6.2.3 Conclusions

Assuming that the quantum model calculations are the correct ones to reproduce the observed Si line profiles, it has been shown that they could be quite well reproduced using the Drawin models by employing different recipes for the excitation and charge transfer rates through the scaling factors $\mathrm{S}_{\mathrm{H}}$ and $\mathrm{S}_{\mathrm{H}}(\mathrm{CE})$. These recipes are, however, found to be star dependent!

### 6.3 Iron non-LTE calculations using The Drawin approximation

In this section, an attempt is made to better reproduce the observed measured equivalent widths (see Sect. 6.3.1.3 below), and improve the accuracy by which iron abundances are determined.
The possibility of scaling the Drawin approximation for iron with a set of analogous scaling factors $\mathrm{S}_{\mathrm{H}}$ and $\mathrm{S}_{\mathrm{H}}(\mathrm{CE})$ for all of the Gaia benchmark stars is tested.

Iron non-LTE calculations were performed for the Gaia benchmark stars introduced in Chapter 5, using the iron model atom developed in Chapter 4, and were compared to the observed equivalent widths of the stars. The $\mathrm{H}+\mathrm{Fe}$ collisional rates for excitation, ionization and charge transfer were treated using the Drawin approximation. The method and results are presented below.

### 6.3.1 Method

### 6.3.1.1 Model atoms

Modified versions of the iron model atom described in Chapter 4 were constructed by varying the $\mathrm{Fe} \mathrm{I}+\mathrm{H}$ and $\mathrm{Fe} \mathrm{II}+\mathrm{H}$ excitation, ionization and charge exchange rates by varying the scaling fudge factors $\mathrm{S}_{\mathrm{H}}$ and $\mathrm{S}_{\mathrm{H}}(\mathrm{CE})$ as follows:

- $\mathrm{S}_{\mathrm{H}}$ was varied between 0.0001 and 10 in multiplicative steps of 10 .
- $\mathrm{S}_{\mathrm{H}}(\mathrm{CE})$ was varied between 0.1 and 10 in multiplicative steps of 10 for each value of $\mathrm{S}_{\mathrm{H}}$, in addition to the $S_{\mathrm{H}}(\mathrm{CE})=0$ models.


### 6.3.1.2 Model Atmospheres

For each of the GBS stars, 1D MARCS model atmospheres were interpolated to the AFP values of the star (Table 5.2), using the MARCS interpolation routine interpol_marcs.f ${ }^{1}$ written by Thomas Masseron. According to the available models extracted from the MARCS database, spherical models were used for stars with $\log g$ values smaller than 3 cgs , while plane-parallel models were used for $\log g$ values greater than that. For the Sun, a special MARCS model calculated at the exact AFP parameters is used.

Background opacity files were also included in the non-LTE calculations for each star, and were calculated as a function of the star's metallicity and microturbulent velocity.

[^30]
### 6.3.1.3 Linelists and measured equivalent widths

The Fe I and Fe II linelist chosen in the analysis of the non-LTE calculations is a subset of the Gaia-ESO survey "golden" linelist version 4 (v4) (Heiter et al., 2015b).

The observed equivalent widths were measured from the UVES spectra using the code Robospect ${ }^{2}$ (Automated Equivalent Width Measurement) (Waters and Hollek, 2013). The subset linelist was chosen based on the measurements made on the Sun as follows:

- Blended lines were removed.
- Lines with measured equivalent widths $>150 \mathrm{~m} \AA$ and $<10 \mathrm{~m} \AA$ were removed.
- Lines with relative errors on measured equivalent width larger than $3 \%$ were removed.
- Lines whose relative differences with non-LTE calculated equivalent widths $\Delta \mathrm{W}_{\lambda}(\mathrm{rel})>0.3$ were removed, where:

$$
\begin{equation*}
\Delta \mathrm{W}_{\lambda}(\text { rel })=\frac{\mid \mathrm{W}_{\lambda}(\text { non }-\mathrm{LTE})-\mathrm{W}_{\lambda}(\mathrm{obs}) \mid}{\mathrm{W}_{\lambda}(\mathrm{obs})} \tag{6.2}
\end{equation*}
$$

Non-LTE calculations for the Sun were performed for $S_{H}=0.0001$ and $S_{H}(C E)=0.1$ (See Table 6.3 below).

The final subset linelist (hereafter referred to as linelist), includes 160 Fe I and 22 Fe II lines, is listed in Annex D. Equivalent widths were measured for these lines with Robospect for all the GBS stars. All blended lines were again removed for each star.

Non-LTE calculations were performed for each of the modified model atoms described above, thus resulting in 24 calculated models for each star.

### 6.3.2 Results

For convenience, the GBS were grouped into five categories according to their different spectral types:

- metal-poor, including HD122563, HD140283 \& HD 84937.
- FG dwarfs, including $\delta$ Eri, $\epsilon$ For, $\tau$ Cet, 18 Sco, Sun, HD 22879, $\alpha$ Cen A, $\mu$ Ara, $\beta$ Hyi, $\beta$ Vir, $\eta$ Boo , Procyon \& HD 49933.
- FGK giants, including Arcturus, HD 220009, $\mu$ Leo, HD 107328, $\beta$ Gem, $\epsilon$ Vir \& $\xi$ Hya.
- M giants, including $\psi$ Phe, $\alpha$ Cet, $\gamma$ Sge, $\alpha$ Tau $\& \beta$ Ara.
- K dwarfs, including 61 Cyg B \& $\epsilon$ Eri.

The calculated equivalent widths were compared to the observed measured equivalent width using a $\chi^{2}$ test:

$$
\begin{equation*}
\chi^{2}=\frac{1}{\mathrm{~N}_{\mathrm{lines}}} \sum_{\text {lines }}\left(\frac{\mathrm{EW}(\mathrm{calc})-\mathrm{EW}(\mathrm{obs})}{\sigma \mathrm{EW}(\mathrm{obs})}\right)^{2} \tag{6.3}
\end{equation*}
$$

where $\mathrm{N}_{\text {lines }}$ is the total number of lines used in the $\chi^{2}$ test, and $\sigma \mathrm{EW}(\mathrm{obs})$ is the uncertainty on each measured equivalent width (presented in Annex D for each star).

[^31]The scaling factors $\mathrm{S}_{\mathrm{H}}$ and $\mathrm{S}_{\mathrm{H}}(\mathrm{CE})$ at which the smallest $\chi^{2}$ was obtained for the GBS are listed in Table 6.3. The LTE $\chi^{2}$, calculated from the LTE equivalent widths, are included in the table for comparison. The plots of the variation of $\chi^{2}$ as a function of $S_{H}$ and $S_{H}(C E)$ are presented in Figs. 6.9, 6.10, 6.11, 6.12 and 6.13 for the metal-poor, the FG dwarfs, the FGK giants, the M giants and K dwarfs respectively. The LTE $\chi^{2}$ values are also shown on the plots (dotted black lines)

Metal-poor stars: For the three very metal-poor stars, the least $\chi^{2}$ is obtained for small excitation rates (smaller values of $\mathrm{S}_{\mathrm{H}}$ ) and larger values for charge exchange (larger values of $S_{\mathrm{H}}(\mathrm{CE})$ )

FG Dwarfs: For most stars (except $\epsilon$ For, $\tau$ Cet and Procyon), charge exchange rates play an important role for small values of $\mathrm{S}_{\mathrm{H}}(<0.1)$, where very large values of $\chi^{2}$ were obtained upon excluding charge exchange rates at $S_{H}(C E)=0$. For $S_{H} \geq 0.1$, small differences were obtained for different values of $\mathrm{S}_{\mathrm{H}}(\mathrm{CE})$. The least $\chi^{2}$ are obtained for larger excitation rates.

FGK Giants: For the giant stars, the results show that excluding the charge exchange rates from the calculations gave better fits to the observations.

M giants \& K Dwarfs: For the M giants and K dwarfs, the results show that while the best-fit are obtained for $S_{H}(C E)=0$, varying the scaling factors $S_{H}$ and $S_{H}(C E)$ do not play a major effect on $\chi^{2}$ which varies very slightly between the different models, even compared to LTE.

### 6.3.3 Conclusions

The non-LTE calculations for the GBS with different scaling factors have shown that including the charge exchange rates play an important role for metal-poor stars and most FG dwarfs. For the giant stars, however, removing the charge transfer rates is more important for a better fit with the observations. It has to be well noted that while the collisional rates are expected to be an atomic quality, it can be observed that using the Drawin approximation with different scaling factors to calculate the rates, no single set of values for $S_{H}$ and $S_{H}(C E)$ has been found for all the stars upon which the best-fits are obtained. As expected, the non-LTE results do provide better fits with the observations as compared to those of LTE, especially for metal poor stars and FGK giants. This is not the case, however, for the M giants and K dwarfs where no significant differences were found between the different models, even with LTE.

Our results are consistent with previous non-LTE studies of iron, in the sense that no single value of $S_{H}$ is able to reproduce the observations of different types of stars. Even within a given spectral type, no single prescription can be given. This shows that the Drawin approximation should definitely NOT be used!
This failure of the Drawin approximation to reproduce the correct $\mathrm{H}+\mathrm{Fe}$ collisional rates is well expected due to its lack of proper physical assumptions in describing the collisions (see Barklem et al., 2010).

We thus introduce an alternative method for computing the hydrogen collisional rates based on a semi-empirical fitting of existing collisional rates. This is described in the following chapter.

| Star name (ID) | $\mathrm{S}_{\mathrm{H}}$ | $\mathrm{S}_{\mathrm{H}}(\mathrm{CE})$ | Non-LTE $\chi^{2}$ | LTE $\chi^{2}$ |
| :---: | :---: | :---: | :---: | :---: |
| Metal-poor |  |  |  |  |
| HD 122563 | 0.001 | 0.1 | 86.904 | 156.253 |
| HD 140283 | 0.0001 | 1.0 | 65.929 | 266.129 |
| HD 84937 | 0.0001 | 1.0 | 34.177 | 171.124 |
| FG dwarfs |  |  |  |  |
| $\delta$ Eri | 0.0001 | 10.0 | 58.986 | 59.716 |
| $\epsilon$ For | 0.01 | 0.0 | 145.396 | 410.611 |
| $\tau$ Cet | 0.01 | 0.0 | 94.156 | 161.470 |
| 18 Sco | 0.001 | 0.1 | 59.406 | 68.976 |
| Sun | 0.0001 | 0.1 | 40.326 | 65.082 |
| HD 22879 | 0.0001 | 1.0 | 59.048 | 142.106 |
| $\alpha$ Cen A | 0.01 | 10 | 18.929 | 21.041 |
| $\mu$ Ara | 0.0001 | 10.0 | 46.231 | 46.445 |
| $\beta$ Hyi | 1.0 | 0.1 | 139.732 | 146.391 |
| $\beta$ Vir | 0.0001 | 0.1 | 66.936 | 101.372 |
| $\eta$ Boo | 1.0 | 0.1 | 154.691 | 155.076 |
| Procyon | 0.01 | 0.0 | 50.795 | 210.385 |
| HD 49933 | 1.0 | 0.1 | 126.86 | 134.536 |
| FGK giants |  |  |  |  |
| Arcturus | 0.0001 | 0.0 | 66.337 | 122.966 |
| HD 220009 | 0.0001 | 0.0 | 162.848 | 343.342 |
| $\mu$ Leo | 0.001 | 0.0 | 91.011 | 117.479 |
| HD 107328 | 0.1 | 0.0 | 87.007 | 148.616 |
| $\beta$ Gem | 0.001 | 0.0 | 35.949 | 65.209 |
| $\epsilon$ Vir | 0.001 | 0.0 | 104.27 | 347.575 |
| $\xi$ Hya | 0.0001 | 0.0 | 163.191 | 356.553 |
| M giants |  |  |  |  |
| $\psi$ Phe | 0.001 | 0.1 | 28.333 | 28.699 |
| $\alpha$ Cet | 0.0001 | 0.1 | 15.467 | 15.781 |
| $\gamma$ Sge | 0.01 | 0.1 | 53.661 | 53.471 |
| $\alpha$ Tau | 0.0001 | 0.1 | 26.888 | 27.910 |
| $\beta$ Ara | 0.001 | 0.1 | 129.565 | 130.145 |
| K dwarfs |  |  |  |  |
| 61 Cyg B | 0.0001 | 0.1 | 34.831 | 34.853 |
| $\epsilon$ Eri | 0.0001 | 10.0 | 164.23 | 175.01 |
|  |  |  |  |  |
|  |  |  |  |  |
|  |  |  |  |  |

Table 6.3: Gaia Benchmark stars calculated non-LTE smallest $\chi^{2}$ and their corresponding scaling factors. The LTE $\chi^{2}$ is also included for comparison.

Figure 6.9: $\chi_{\text {nLTE }}^{2}$ obtained for different $S_{H}$ and $S_{H}(C E)$ recipes for the metal poor GBS. The dotted lines represents the $\chi_{\mathrm{LTE}}^{2}$.


Figure 6.10: $\chi_{n L T E}^{2}$ obtained for different $S_{H}$ and $S_{H}(C E)$ recipes for the FG dwarf GBS. The dotted lines represents $\chi_{\text {LTE }}^{2}$.

FG Dwarfs $\quad 00 \circ \mathrm{~S}_{\mathrm{H}}(\mathrm{CE})=0 \quad$ ם口 $\quad \mathrm{S}_{\mathrm{H}}(\mathrm{CE})=0.1 \quad \Delta \Delta \Delta \quad \mathrm{~S}_{\mathrm{H}}(\mathrm{CE})=1.0 \quad \times \times \times \quad \mathrm{S}_{\mathrm{H}}(\mathrm{CE})=10.0$


Figure 6.11: $\chi_{\text {nLTE }}^{2}$ obtained for different $S_{H}$ and $S_{H}(C E)$ recipes for the FGK giant GBS. The dotted lines represents $\chi_{\text {LTE }}^{2}$.

$$
\text { FGK Giants } \quad \circ \circ \circ \mathrm{S}_{\mathrm{H}}(\mathrm{CE})=0 \quad \therefore \quad \mathrm{~S}_{\mathrm{H}}(\mathrm{CE})=0.1 \quad \Delta \Delta \Delta \mathrm{~S}_{\mathrm{H}}(\mathrm{CE})=1.0 \quad \times \times \times \quad \mathrm{S}_{\mathrm{H}}(\mathrm{CE})=10.0
$$









Figure 6.12: $\chi_{\text {nLTE }}^{2}$ obtained for different $S_{H}$ and $S_{H}(C E)$ recipes for the $M$ giant GBS. The dotted lines represents $\chi_{\text {LTE }}^{2}$.


Figure 6.13: $\chi_{\text {nLTE }}^{2}$ obtained for different $S_{H}$ and $S_{H}(C E)$ recipes for the $K$ dwarf GBS. The dotted lines represents $\chi_{\text {LTE }}^{2}$.


Figure 6.1: Grotrian diagram of SiI levels. Only labels of the levels below 7 eV are included to avoid crowding.

## Silicon model atom - Energy levels



Figure 6.2: Grotrian diagram for allowed SiI bound-bound radiative transitions. Gray lines display transitions between the different fine structure levels.


## 7 Introducing the quantum fitting method (QFM)

It has been well established so far, in the course of this dissertation and throughout the literature, that the commonly used Drawin approximation, in the lack of quantum calculations for H collisions, is not able to correctly describe the rates for both excitation and charge transfer. Upon comparison with quantum calculations for Na, Mg, Al and Si (Figs. 3.8, 3.7, 3.6 , and 3.9 respectively), it has been shown that not only does the Drawin approximation overestimate the magnitude of the rates by several orders of magnitude for most transitions, it also does not reproduce the correct behavior of the rates with transition energies. While the Drawin approximation adopted in this work depends solely on transition energy, it can be seen that the Drawin collisional rates decrease exponentially with $\Delta E$, while the existing charge transfer quantum rates peak at $\Delta E$ between 1 eV and 2 eV . For Si , it can also be seen that the excitation/de-excitations rates behavior with $\Delta E$ is opposite to that predicted by Drawin's approximation: a peak is observed in the quantum rates for $\Delta E<1 \mathrm{eV}$ (transitions between high lying Si levels).

In the light of these discrepancies, I thus introduce a semi-empirical method to determine the H collision rates for excitation / de-excitation, and charge transfer processes, which is based on fitting the H -collisional rates of $\mathrm{Na}, \mathrm{Mg}, \mathrm{Al}$ and Si . This approach was motivated by the analogous behavior of these rates as a function of energies for all these element.

### 7.1 Fitting the quantum data

### 7.1.1 Charge Transfer rates

Investigation of the charge transfer rates for $\mathrm{Na}, \mathrm{Mg}, \mathrm{Al}$ and Si shows similar behaviors with $\Delta E$. As presented in Figs. 7.1, 7.2, 7.3 and 7.4, where the logarithmic mutual-neutralization (downward charge transfer) rates are plotted as a function of the inverse transition energies, a maximum peak occurs between 0.5 and $1 \mathrm{eV}^{-1}$ for all four elements. In an attempt to fit the quantum data, we divided the rates into two linear parts intersecting at the maximum rate. By ignoring the rates whose value is less than $10^{-4}$ the maximum rate (thus assuring a better fit for dominant values), we were able to describe the rate coefficients $Q=\langle\sigma \nu\rangle$ as a function of $1 / \Delta E$ for all the elements using the following general equations:

$$
\log Q= \begin{cases}a_{1}\left(\frac{1}{\Delta E}-\frac{1}{\Delta E_{0}}\right)+\log Q_{\max } & \text { for } \frac{1}{\Delta E}<\frac{1}{\Delta E_{0}}  \tag{7.1}\\ a_{2}\left(\frac{1}{\Delta E}-\frac{1}{\Delta E_{0}}\right)+\log Q_{\max } & \text { for } \frac{1}{\Delta E}>\frac{1}{\Delta E_{0}}\end{cases}
$$

where $a_{1}$ and $a_{2}$ are respectively the positive and negative slopes of the linear fits, and $Q_{\text {max }}$ is the maximum rate at $\frac{1}{\Delta E_{0}}$. For each element, the mutual-neutralization charge transfer rates,
at $T=6000 \mathrm{~K}$, can be expressed as:

## Na:

$$
\log Q=\left\{\begin{align*}
7.03\left(\frac{1}{\Delta E}-0.72\right)-7.13 & \text { for } \frac{1}{\Delta E}<\frac{1}{\Delta E_{0}}  \tag{7.2}\\
-2.60\left(\frac{1}{\Delta E}-0.72\right)-7.13 & \text { for } \frac{1}{\Delta E}>\frac{1}{\Delta E_{0}}
\end{align*}\right.
$$

## Mg:

$$
\log Q=\left\{\begin{align*}
5.99\left(\frac{1}{\Delta E}-0.63\right)-7.34 & \text { for } \frac{1}{\Delta E}<\frac{1}{\Delta E_{0}}  \tag{7.3}\\
-3.42\left(\frac{1}{\Delta E}-0.63\right)-7.34 & \text { for } \frac{1}{\Delta E}>\frac{1}{\Delta E_{0}}
\end{align*}\right.
$$

Al:

$$
\log Q=\left\{\begin{align*}
3.4\left(\frac{1}{\Delta E}-0.73\right)-7.2 & \text { for } \frac{1}{\Delta E}<\frac{1}{\Delta E_{0}}  \tag{7.4}\\
-4.9\left(\frac{1}{\Delta E}-0.73\right)-7.2 & \text { for } \frac{1}{\Delta E}>\frac{1}{\Delta E_{0}}
\end{align*}\right.
$$

Si:

$$
\log Q=\left\{\begin{array}{rl}
4.39\left(\frac{1}{\Delta E}-0.75\right)-7.44 & \text { for }
\end{array} \frac{1}{\Delta E}<\frac{1}{\Delta E_{0}}, \begin{array}{rl}
-3.52\left(\frac{1}{\Delta E}-0.75\right)-7.44 & \text { for } \tag{7.5}
\end{array} \frac{1}{\Delta E}>\frac{1}{\Delta E_{0}}\right.
$$

Figure 7.1: $\mathrm{Na}+\mathrm{H}$ mutual-neutralization rate fits as a function of $1 / \Delta E$ at $\mathrm{T}=6000 \mathrm{~K}$.


Figure 7.2: $\mathrm{Mg}+\mathrm{H}$ mutual-neutralization rate fits as a function of $1 / \Delta E$ at $\mathrm{T}=6000 \mathrm{~K}$.


Figure 7.3: $\mathrm{Al}+\mathrm{H}$ mutual-neutralization rate fits as a function of $1 / \Delta E$ at $\mathrm{T}=6000 \mathrm{~K}$.


Figure 7.4: $\mathrm{Si}+\mathrm{H}$ mutual-neutralization rate fits as a function of $1 / \Delta E$ at $\mathrm{T}=6000 \mathrm{~K}$.


We see that $\log Q_{\text {max }} \simeq-7.2 \pm 0.3 \mathrm{~cm}^{3} \cdot \mathrm{~s}^{-1}$ and $\frac{1}{\Delta E_{0}} \simeq 0.7 \pm 0.07 \mathrm{eV}^{-1}$ for all four elements.
Temperature dependence plots of the fitting parameters, $a_{1}, a_{2}, \frac{1}{\Delta E_{0}}$ and $\log Q_{\max }$, for all four chemical elements (Figs. 7.5, 7.6, 7.7 and 7.8) show that $a_{1}$ depends roughly linearly on $T, \log Q_{\max }$ depends linearly on $\log T$, while $a_{2}$ and $\frac{1}{\Delta E_{0}}$ do not vary significantly with temperature, except $a_{2}$ for Al. It follows that $a_{1}$ and $\log Q_{\max }$ can be generally written as:

$$
\left\{\begin{array}{l}
a_{1}=a_{11}\left(\frac{T}{10^{4}}\right)+a_{10}  \tag{7.6}\\
Q_{\max }=T^{\alpha} \times 10^{y_{0}}
\end{array}\right.
$$

which for the different elements are found to be:

## Na:

$$
\left\{\begin{array}{l}
a_{1}=-1.50\left(\frac{T}{10^{4}}\right)+7.92  \tag{7.7}\\
Q_{\max }=T^{-0.37} \times 10^{-5.71}
\end{array}\right.
$$

## Mg:

$$
\left\{\begin{array}{l}
a_{1}=-2.12\left(\frac{T}{10^{4}}\right)+7.36  \tag{7.8}\\
Q_{\max }=T^{-0.35} \times 10^{-6.01}
\end{array}\right.
$$

Al:

$$
\left\{\begin{array}{l}
a_{1}=-7.46\left(\frac{T}{10^{4}}\right)+3.74  \tag{7.9}\\
Q_{\max }=T^{-0.56} \times 10^{-5.71}
\end{array}\right.
$$

Si:

$$
\left\{\begin{array}{l}
a_{1}=-1.20\left(\frac{T}{10^{4}}\right)+4.90  \tag{7.10}\\
Q_{\max }=T^{-0.34} \times 10^{-6.19}
\end{array}\right.
$$

where similar values of $\alpha \simeq-0.34 \pm 0.03$ and $y_{0} \simeq-6.0 \pm 0.3$ are obtained for all elements, except for Al where $\alpha=-0.56$. For $T \in[3000,7000]$ (temperature range of interest in cool stellar atmospheres), $a_{1}$ varies within $<20 \%$ while $Q_{\max }$ varies within less than a factor of 5 .

Figure 7.5: $\mathrm{Na}+\mathrm{H}$ charge transfer fitting parameters temperature dependence.


Figure 7.6: $\mathrm{Mg}+\mathrm{H}$ charge transfer fitting parameters temperature dependence.


Figure 7.7: $\mathrm{Al}+\mathrm{H}$ charge transfer fitting parameters temperature dependence.


Figure 7.8: $\mathrm{Si}+\mathrm{H}$ charge transfer fitting parameters temperature dependence.


### 7.1.2 De-excitation rates

The quantum de-excitation rates for all four atoms show larger scatter than charge transfer rates as more transitions are included, and a decreasing behavior with increasing transition energies with large variations in magnitudes between the maximum and minimum rates (up to 10 orders of magnitude). The rates are best fit as a function of $\Delta E$ using a third degree polynomial fit, i.e.:

$$
\begin{equation*}
\log Q=b_{3} \Delta E^{3}+b_{2} \Delta E^{2}+b_{1} \Delta E+b_{0} \tag{7.11}
\end{equation*}
$$

The de-excitation rates and their respective fits are shown in Figs. 7.9, 7.10, 7.11, and 7.12 for $\mathrm{Na}, \mathrm{Mg}, \mathrm{Al}$ and Si respectively.
The rates can be written for the different species, at $\mathrm{T}=6000 \mathrm{~K}$, as follows:
Na:

$$
\begin{equation*}
\log Q=-0.23 \Delta E^{3}+1.74 \Delta E^{2}-5.39 \Delta E-9.84 \tag{7.12}
\end{equation*}
$$

Mg:

$$
\begin{equation*}
\log Q=-0.08 \Delta E^{3}-0.57 \Delta E^{2}-1.38 \Delta E-9.05 \tag{7.13}
\end{equation*}
$$

Al:

$$
\begin{equation*}
\log Q=0.324 \Delta E^{3}-2.72 \Delta E^{2}+2.00 \Delta E-10.87 \tag{7.14}
\end{equation*}
$$

Si:

$$
\begin{equation*}
\log Q=-0.07 \Delta E^{3}-0.68 \Delta E^{2}-1.85 \Delta E-9.45 \tag{7.15}
\end{equation*}
$$

The obtained fitting parameters $b_{3}, b_{2}$ and $b_{1}$ vary from one element to the other, while $b_{0}$ which is the scaling coefficient of $\log Q$ varies between $\simeq-9.0$ and $\simeq-11.0$. For Mg and Si, similar values are obtained for $b_{3} \simeq-0.1, b_{2} \simeq 0.6, b_{1} \simeq-1.5$ and $b_{0} \simeq-9.5$ respectively. In addition, $b_{3}, b_{2}$ and $b_{1}$ are linearly dependent on $\log T$, while $b_{0}$ does not vary much with temperature as is shown in Fig. 7.13 for Si for e.g.

This allows the de-excitation fitting parameters to be written as:

$$
\left\{\begin{array}{l}
b_{3}=b_{31} \log T+b_{30}  \tag{7.16}\\
b_{2}=b_{21} \log T+b_{20} \\
b_{1}=b_{11} \log T+b_{10} \\
b_{0}=\text { constant }
\end{array}\right.
$$

where for Si, they can be written as:

$$
\left\{\begin{array}{l}
b_{3}=-0.08 \log T+0.233  \tag{7.17}\\
b_{2}=0.69 \log T-2.047 \\
b_{1}=-1.356 \log T+3.511 \\
b_{0} \simeq-9.75
\end{array}\right.
$$

Figure 7.9: $\mathrm{Na}+\mathrm{H}$ de-excitation rates fit as a function of $\Delta E$.


Figure 7.10: $\mathrm{Mg}+\mathrm{H}$ de-excitation rates fit as a function of $\Delta E$.


Figure 7.11: $\mathrm{Al}+\mathrm{H}$ de-excitation rates fit as a function of $\Delta E$.


Figure 7.12: $\mathrm{Si}+\mathrm{H}$ de-excitation rates fit as a function of $\Delta E$.


Figure 7.13: $\mathrm{Si}+\mathrm{H}$ de-excitation fitting parameters temperature dependence.


### 7.2 Silicon non-LTE calculations using the quantum fitting method

To test the effects of using the QFM as compared to the real quantum data on the non-LTE calculations, a modified Si model atom (described in Sect. 6.1) was built using the Si quantum fitting parameters described in Eqns. 7.5 and 7.15 for the calculation of the charge transfer and excitation rates, and taking into account the temperature dependence of the parameters from Eqns. 7.10 \& 7.17. The Si model atoms were used to compute non-LTE EW. The tests were performed on three benchmark stars: the Sun, Arcturus and HD140283. Results are shown in Fig. 7.14, where the QFM $\mathrm{EW}_{\text {fit }}$ are compared to the reference $\mathrm{EW}_{\mathrm{QM}}$ (calculated using the real quantum data), for lines whose transition energies are between 1 eV and 4 eV (lines between $2000 \AA \leq \lambda \leq 10000 \AA$ ).
To quantify the differences, we define the average relative difference $\overline{Y_{\text {rel }}}$ between $\mathrm{EW}_{\mathrm{fit}}$ and $\mathrm{EW}_{\mathrm{QM}}$ as:

$$
\begin{equation*}
\overline{Y_{\mathrm{rel}}}=\frac{1}{\mathrm{~N}_{\mathrm{lines}}} \sum_{i=1}^{\text {nlines }} \frac{\mathrm{EW}_{\mathrm{fit}}^{i}-\mathrm{EW}_{\mathrm{QM}}^{i}}{\mathrm{EW}_{\mathrm{QM}}^{i}} \tag{7.18}
\end{equation*}
$$

The non-LTE calculations made using the QFM for $\mathrm{Si}+\mathrm{H}$ collisions are able to well-reproduce those using the quantum data within negligible differences, where $\overline{Y_{\text {rel }}}$ obtained for the three stars was $\leq 3 \%$ ( 0.0384 for the Sun, 0.0056 for Arcturus, and 0.0035 for HD140283).

This also shows that ignoring rates whose magnitudes are 4 orders of magnitude smaller than the maximum rate in the fit as shown in Fig. 7.4, is acceptable and does not propagate onto the computed equivalent widths.


Figure 7.14: Si non-LTE EW calculated using the $\mathrm{QMF}\left(\mathrm{EW}_{\mathrm{fit}}\right)$ vs. real quantum rates $\left(\mathrm{EW}_{\mathrm{QM}}\right)$ for the Sun, Arcturus, and HD140283.

### 7.2.1 Testing the effects of the QFM parameters

To test the effects of varying the different fitting parameters on the calculated EW, modified Si model atoms were used where the Si fitting parameters for charge transfer and de-excitation were varied around their nominal values from Eqns. 7.5 \& 7.15 (hereafter denoted reference fit). Each parameter was respectively decreased and increased from its reference value as shown in Table 7.1. $a_{11}$ and $\alpha$ are kept to their reference values of -1.2 and -0.35 respectively, to avoid larger number of fitting parameters. Changing one parameter at a time, non-LTE Si calculations were performed for each model for the Sun and the metal poor star HD140283. Calculated $\mathrm{EW}_{\text {mod }}$ for each model, are compared to those obtained by the reference fit (Figs. 7.16, 7.17, 7.18 and 7.19).

To quantify the difference, the relative difference standard deviation $\sigma Y_{\text {rel }}=\sqrt{\text { var } Y_{\text {rel }}}$ was calculated for each model from the variance, where:

$$
\begin{equation*}
\operatorname{var} Y_{\mathrm{rel}}=\frac{1}{\mathrm{~N}_{\mathrm{lines}}-1} \sum_{i=1}^{\text {nlines }}\left(\frac{\mathrm{EW}_{\mathrm{mod}}^{i}-\mathrm{EW}_{\mathrm{ref}}^{i}}{\mathrm{EW}_{\mathrm{ref}}^{i}}\right)^{2} \tag{7.19}
\end{equation*}
$$

is the relative difference variance. Table 7.1 shows $\sigma Y_{\text {rel }}$ obtained for each model for the two stars.

It is shown that varying the charge transfer fitting parameters $a_{10}, a_{2}$, and $\frac{1}{\Delta E_{0}}$ within $\pm 50 \%$ of their reference values, results in a small percentage of variation in the computed $\mathrm{EW}_{\text {mod }}$ ( $Y_{\text {rel }}<0.1$, i.e. $<10 \%$ ) and a small scatter (dotted lines show $\sigma Y<0.01$ for $a_{1}$ and $a_{2}$, and $\sigma Y_{\text {rel }}<0.03$ for $\left.\frac{1}{\Delta E_{0}}\right)$, for the two stars.
Varying $y_{0}$ within $\pm 1$ order of magnitude from its reference value, shows slightly larger scatter ( $\sigma Y_{\text {rel }}<0.05$ ) than other parameters with relative differences $Y_{\text {rel }}<0.1$. This shows that $y_{0}$ plays an expected important role in shifting the computed $\mathrm{EW}_{\text {mod }}$, as it scales and shifts the
rates by orders of magnitudes from their nominal values.
Varying the de-excitation fitting parameters within $\pm 50 \%$ and $b_{0}$ within $\pm 1$ order of magnitude from their respective reference values, results in a relative difference up to 0.1 (i.e. 10\%), with a scatter $\sigma Y<0.05$ for all models and both stars (See Table 7.1 for detailed numbers).
The results thus show that a variation in the fit within $\pm 50 \%$ from its reference value, as presented in Fig. 7.15 for the variation of $a_{1}$ and $a_{2}$ (dark and light gray shaded areas respectively), propagates onto a relative difference of $<10 \%$ and a scatter of $\sigma Y<5 \%$ in the computed $\mathrm{EW}_{\text {mod }}$. This means that the acceptable range of variation around the optimal values is quite broad.


Figure 7.15: $\mathrm{Si}+\mathrm{H}$ mutual neutralization rates fits as a function of $1 / \Delta E$ at $\mathrm{T}=6000 \mathrm{~K}$, also showing the range of variation of $a_{1}$ between [2,6] (dark gray shaded area) and $a_{2}$ between [-6,-2] (light gray shaded area).

Sun


Figure 7.16: $\mathrm{Si}+\mathrm{H}$ charge transfer fitting parameter variation effects on the calculated non-LTE EW as compared to the reference fit for the Sun. Solid and dotted lines show the relative difference average $\overline{Y_{\text {rel }}}$, and its standard deviation $\sigma Y$ for each corresponding model.

HD140283


Figure 7.17: $\mathrm{Si}+\mathrm{H}$ charge transfer fitting parameter variation effects on the calculated non-LTE EW as compared to the reference fit for HD140283. Solid and dotted lines represent the same thing as in Fig. 7.16.

Sun





Figure 7.18: $\mathrm{Si}+\mathrm{H}$ de-excitation fitting parameter variation effects on the calculated non-LTE EW as compared to the reference fit for the Sun. Solid and dotted lines represent the same thing as in Fig. 7.16.

HD140283


Figure 7.19: $\mathrm{Si}+\mathrm{H}$ de-excitation fitting parameter variation effects on the calculated non-LTE EW as compared to the reference fit for HD140283. Solid and dotted lines represent the same thing as in Fig. 7.16.

| fitting parameter | reference value | value | $\sigma Y_{\text {rel }}$ |  | value | $\sigma Y_{\text {rel }}$ |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  |  | Sun | HD140283 |  | Sun | HD140283 |
| Mutual-neutralization rate parameters |  |  |  |  |  |  |  |
| $a_{1}$ | 4.9 | 2 | $7.98 \times 10^{-3}$ | $1.94 \times 10^{-2}$ | 7 | $1.09 \times 10^{-3}$ | $4.26 \times 10^{-2}$ |
| $a_{2}$ | -3.52 | -2 | $1.88 \times 10^{-3}$ | $1.62 \times 10^{-2}$ | -6 | $2.16 \times 10^{-3}$ | $1.23 \times 10^{-2}$ |
| $\frac{1}{\Delta E_{0}}$ | 0.75 | 0.5 | $1.02 \times 10^{-2}$ | $1.78 \times 10^{-2}$ | 1.00 | $1.29 \times 10^{-2}$ | $1.75 \times 10^{-2}$ |
| $y_{0}$ | -6.0 | -5.0 | $4.41 \times 10^{-2}$ | $1.55 \times 10^{-2}$ | -7.0 | $4.79 \times 10^{-2}$ | $3.51 \times 10^{-2}$ |
| De-excitation rate parameters |  |  |  |  |  |  |  |
| $b_{31}$ | -0.08 | -0.001 | $3.57 \times 10^{-2}$ | $8.72 \times 10^{-2}$ | -0.5 | $2.62 \times 10^{-3}$ | $9.85 \times 10^{-2}$ |
| $b_{30}$ | 0.233 | 0.1 | $9.41 \times 10^{-3}$ | $9.375 \times 10^{-2}$ | 0.5 | $3.57 \times 10^{-2}$ | $8.72 \times 10^{-2}$ |
| $b_{21}$ | 0.69 | 0.2 | $4.01 \times 10^{-2}$ | $9.87 \times 10^{-2}$ | 0.9 | $9.92 \times 10^{-2}$ | $8.72 \times 10^{-2}$ |
| $b_{20}$ | -2.047 | -1.0 | $9.75 \times 10^{-2}$ | $8.73 \times 10^{-2}$ | -3.0 | $2.71 \times 10^{-2}$ | $9.70 \times 10^{-2}$ |
| $b_{11}$ | -1.35 | -0.5 | $1.88 \times 10^{-2}$ | $8.62 \times 10^{-2}$ | -2.0 | $7.59 \times 10^{-2}$ | $9.95 \times 10^{-2}$ |
| $b_{10}$ | 3.5 | 2.0 | $5.73 \times 10^{-2}$ | $9.50 \times 10^{-2}$ | 5.0 | $1.87 \times 10^{-2}$ | $8.64 \times 10^{-2}$ |
| $b_{0}$ | -9.75 | -8.0 | $9.88 \times 10^{-2}$ | $8.52 \times 10^{-2}$ | -11.0 | $9.52 \times 10^{-2}$ | $9.80 \times 10^{-2}$ |

Table 7.1: $\mathrm{Si}+\mathrm{H}$ rates fitting parameters variations from the reference values for which non-LTE calculations were performed.

### 7.3 Iron non-LTE calculations using the QFM

The similarity in the behavior of the mutual neutralization and de-excitation quantum rates as a function of transition energies for the different chemical species, and the similar values obtained for the fitting parameters, especially for charge transfer rates, has motivated us to apply the QFM recipe to iron, instead of using Drawin approximation. The aim in this section, is therefore to calibrate the iron fitting parameters using the benchmark stars (Chapter 5).

### 7.3.1 Method

We implement collisional rates in our iron model atom using Eqns. 7.1 and 7.11 to calculate Fe $\mathrm{I}+\mathrm{H}$ charge transfer rates and Fe I + H excitation rates respectively. For the Fe I + H ionization rates and Fe II + H rates, Lambert's version of the Drawin approximation was used since no quantum data for the other chemical species have been calculated for these processes, and thus the QFM can only be applied for the charge transfer and bound-bound transitions for neutral iron. It can be stated though, that using the Drawin approximation to calculate the Fe II + H collisional rates should be acceptable since it is well established in all previous iron non-LTE studies, that Fe II species, being the dominant in cool stars, are not subject to nonLTE effects (Bergemann et al., 2012; Lind et al., 2011; Mashonkina et al., 2011; Thévenin and Idiart, 1999). On the other hand, using the Drawin approximation to calculate Fe I+H ionization rates, for the lack of an alternative, can be acceptable under the assumption that ionization collisions are higher-energy collisions than excitations, that can be well described by the Born approximation, which is the basis of the Drawin approximation (Barklem et al., 2010).

### 7.3.2 Charge transfer fitting

The best fitting parameters for Fe I+H charge transfer rates are determined starting with the fitting parameters for Si , and calculating a grid of non-LTE models defined by varying the fitting parameters $a_{11}, a_{2}, \frac{1}{\Delta E_{0}}$ and $y_{0}$ between the values shown in Table 7.2, while keeping the de-excitation rates constant. The different models were tested on 3 types of benchmark stars: a dwarf (Sun), a giant (Arcturus) and a metal-poor star (HD140283). Hence, a total of 72
models were calculated for each star. The calculated $\mathrm{EW}_{\text {mod }}$ of each model were compared to the measured $\mathrm{EW}_{\text {obs }}$ using the $\chi^{2}$ defined in Eqn. 6.3. The results for the different models are shown in Figs. 7.20, 7.21 and 7.22 for the Sun, Arcturus and HD140283 respectively. Missing symbols for Arcturus and HD140283 correspond to models where no numerical convergence could be obtained.

| parameter | values range | step |
| :---: | :--- | :--- |
| $a_{10}$ | $[2.0,6.0]$ | $\Delta=2.0$ |
| $a_{2}$ | $[-6.0,-2.0]$ | $\Delta=2.0$ |
| $\frac{1}{\Delta E_{0}}$ | $[0.5,1.0]$ | $\Delta=0.25$ |
| $y_{0}$ | $[-11.0,-3.0]$ | $\Delta=1$ |

Table 7.2: Fe $\mathrm{I}+\mathrm{H}$ charge transfer rates fitting parameters range of values, for which non-LTE calculations were performed.

For the 3 stars (Figs. 7.20, 7.21 and 7.22), a clear flat minimum is obtained around $y_{0} \simeq-9.0$ which is independent of other parameters, within the range of variation.
For the Sun, $a_{2}$ does not play an important role: negligible $\chi^{2}$ differences are obtained for all the models. For Arcturus and HD140283, $\chi^{2}$ decreases slightly with increasing $a_{2}$.
Increasing $a_{11}$ and $\frac{1}{\Delta E_{0}}$ also induces a decrease in $\chi^{2}$ for all values of $y_{0}$. While increasing values of $a_{11}, a_{2}$ and $\frac{1}{\Delta E_{0}}$ give general decreasing $\chi^{2}$ values, it can be seen that $y_{0}$ plays the most important role in the $\chi^{2}$ variation. We find a single set of best fitting parameters for Fe I +H charge transfer fits for all 3 stars: $a_{10}=6.0, a_{2}=-6.0, \frac{1}{\Delta E_{0}}=0.75$ and $y_{0}=-9.0$.


Figure 7.20: $\chi^{2}$ variation as a function of Fe I +H charge transfer fitting parameters for the Sun.

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Figure 7.21: $\chi^{2}$ variation as a function of $\mathrm{Fe} \mathrm{I}+\mathrm{H}$ charge transfer fitting parameters for Arcturus.


Figure 7.22: $\chi^{2}$ variation as a function of Fe I +H charge transfer fitting parameters for HD140283.

### 7.3.3 De-excitation fitting

To find the best fitting parameters for the de-excitation rates, the fitting parameters from Eqn. 7.15 are varied for the values shown in Table 7.3. The charge transfer rates were kept constant at the best fitting values discussed in Sect. 7.3.2. The calculated EW ${ }_{\text {calc }}$ were compared to the measured $\mathrm{EW}_{\text {obs }}$ for the Sun, Arcturus and HD140283 using the $\chi^{2}$ in Eqn. 6.3. The fitting parameter $b_{0}$ is found to play the most important role in varying the calculated $\mathrm{EW}_{\text {calc }}$. Table 7.4 shows the $\chi^{2}$ values obtained for different values of $b_{0}$ for the three stars. It can be seen that for $b_{0}=-12 \& b_{0}=-6, \mathrm{EW}_{\text {calc }}$ are driven away from their corresponding $\mathrm{EW}_{\text {obs }}$ with $\chi^{2}$ increasing to large values. The best fit obtained for the 3 types of stars is at $b_{31}=-0.1$, $b_{30}=0.2, b_{21}=0.7, b_{20}=-2.0, b_{11}=-1.5, b_{10}=3.5$ and $b_{0}=-9.0$.

| parameter | values range | step |
| :---: | :--- | :--- |
| $b_{31}$ | $[-0.30,-0.10]$ | $\Delta=0.10$ |
| $b_{30}$ | $[0.1,0.3]$ | $\Delta=0.1$ |
| $b_{21}$ | $[0.5,0.9]$ | $\Delta=0.2$ |
| $b_{20}$ | $[-3.0,-1.0]$ | $\Delta=1.0$ |
| $b_{11}$ | $[-2.0,-1.0]$ | $\Delta=0.5$ |
| $b_{10}$ | $[2.5,4.5]$ | $\Delta=1.0$ |
| $b_{0}$ | $[-12.0,-6.0]$ | $\Delta=1.0$ |

Table 7.3: Fe I+H de-excitation rates fitting parameters range of values for which non-LTE calculations were performed.

| Star | $y_{0}$ | $b_{0}$ | $\chi^{2}$ |
| :---: | :---: | :---: | :---: |
| HD140283 | -9.0 | -6.0 | 241.158 |
|  | -9.0 | -9.0 | 61.481 |
|  | -9.0 | -12.0 | 258.817 |
| Arcturus | -9.0 | -6.0 | 110.171 |
|  | -9.0 | -9.0 | 64.452 |
|  | -9.0 | -12.0 | 160.835 |
| Sun | -9.0 | -6.0 | 60.940 |
|  | -9.0 | -9.0 | 40.571 |
|  | -9.0 | -12.0 | 86.432 |

Table 7.4: $\chi^{2}$ obtained for different $b_{0}$ fitting parameters used in the Fe I +H calculations.

### 7.4 Iron abundance determinations for GBS

Using the best fit model, for the best Fe I + H fitting parameters described in Sect. 7.3.2 \& 7.3.3 (hereafter denoted our final iron model atom), non-LTE iron abundances were determined for the Gaia benchmark stars. The abundances are calculated using MARCS model atmospheres, and are normalized to the Solar Fe abundance $\varepsilon(\mathrm{Fe})_{\odot}=7.45$ from Asplund et al. (2000).

The $\chi_{\text {NLTE }}^{2}$ and $\chi_{\text {LTE }}^{2}$ were calculated using Eqn. 6.3 for all the stars. Fe I and Fe II average iron abundances were derived from individual Fe I and Fe II lines. The [Fe I/H] and [Fe II/H] abundances and their corresponding standard deviation together with the non-LTE and LTE metallicities $\left([\mathrm{Fe} / \mathrm{H}]\right.$ and $[\mathrm{Fe} / \mathrm{H}]_{\text {LTE }}$ respectively), calculated by averaging abundances from all Fe I and Fe II lines, and their standard deviations are shown in Table 7.5. The non-LTE effect defined by the difference between non-LTE and LTE total metallicity, $\Delta[\mathrm{Fe} / \mathrm{H}]=[\mathrm{Fe} / \mathrm{H}]$ $-[\mathrm{Fe} / \mathrm{H}]_{\mathrm{LTE}}$, was calculated for each star as well. The number of Fe I and Fe II lines used in the abundance analyses of the stars are also included. The results are categorized into the different stellar types defined in Sect. 6.3.2. No numerical convergence was obtained for most M giants (to be investigated in future work), which were thus removed from the GBS list.

### 7.4.1 Results and analysis

The non-LTE Fe I and Fe II abundances for the different types of stars are plotted as a function of excitation potential and measured observed equivalent widths in Fig. 7.23 for the metal poor stars, Figs. 7.25, 7.26 and 7.27 for the FG dwarfs, Figs. 7.28 \& 7.29 for the FGK giants and Fig. 7.30 for the K dwarfs.

## Metal poor stars

The non-LTE iron abundances for the metal poor stars HD122563, HD140283 and HD84937 show excellent agreement between Fe I and Fe II lines, in addition to very small dispersion in the FeI lines abundances. Fig. 7.24 represents the corresponding LTE abundances for the same stars. The comparison between the LTE and non-LTE abundances shows that the difference between Fe I and Fe II abundances is $\leq 0.05$ in non-LTE for all three stars ( 0.019 dex for HD122563, 0.028 dex for HD140283 and 0.052 dex for HD84937), while it is $>0.12$ dex in LTE ( 0.198 dex for HD122563, 0.154 dex for HD140283 and 0.124 dex for HD84937).

It has to be noted that Fe II lines also show small dispersion and are not affected by non-LTE, as already noted in previous non-LTE studies (Bergemann et al., 2012; Mashonkina et al., 2011; Thévenin and Idiart, 1999).

## FG dwarfs

The dispersion of Fe I non-LTE and LTE line abundances is small ( $\sigma<0.1$ dex) in all stars. The results also show good agreement between FeI and Fe II lines, with differences between Fe I and Fe II abundances less than 0.1 dex for most stars, except $\epsilon$ For ( 0.154 dex) and $\alpha$ Cen A ( 0.012 dex). All stars in this category display small non-LTE effects ( $\leq 0.05$ dex), except $\epsilon$ For and HD49933 with slightly larger non-LTE corrections ( 0.061 and 0.072 dex respectively). Although no significant differences are found between LTE and non-LTE abundances for these stars, the $\chi_{N L T E}^{2}$ are smaller than $\chi_{L T E}^{2}$ for most stars. Again FeII lines are not affected by non-LTE.

Table 7.5: Non-LTE iron abundance calculations using the final iron model for the Gaia benchmark stars. The columns correspond to the calculated $\chi_{\text {NLTE }}^{2}$ and $\chi_{\text {LTE }}^{2}$, the Fe I average abundances and their standard deviations, the FeII average abundances and their standard deviations, the non-LTE and LTE total iron abundances and their standard deviations, the non-LTE effects, in addition to the number of Fe I and Fe II lines used in the analyses respectively.

| Star name (ID) | $\chi_{\text {NLTE }}^{2}$ | $\chi_{\text {LTE }}^{2}$ | [FeI/H] | $\sigma[\mathrm{FeI} / \mathrm{H}]$ | [FeII/H] | $\sigma$ [FeII/H] | $[\mathrm{Fe} / \mathrm{H}]_{\text {NLTE }}$ | $\sigma[\mathrm{Fe} / \mathrm{H}]_{\text {NLTE }}$ | $[\mathrm{Fe} / \mathrm{H}]_{\text {LTE }}$ | $\sigma[\mathrm{Fe} / \mathrm{H}]_{\text {LTE }}$ | $\Delta[\mathrm{Fe} / \mathrm{H}]$ | N Fe I | N Fe II |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Metal-poor |  |  |  |  |  |  |  |  |  |  |  |  |  |
| HD 122563 | 58.15 | 261.861 | -2.611 | 0.022 | -2.592 | 0.018 | -2.610 | 0.022 | -2.773 | 0.130 | 0.163 | 110 | 10 |
| HD 140283 | 60.66 | 248.545 | -2.347 | 0.047 | -2.378 | 0.035 | -2.348 | 0.041 | -2.522 | 0.087 | 0.174 | 63 | 3 |
| HD 84937 | 29.48 | 352.243 | -2.025 | 0.068 | -2.077 | 0.035 | -2.028 | 0.067 | -2.191 | 0.093 | 0.163 | 68 | 4 |
| FG dwarfs |  |  |  |  |  |  |  |  |  |  |  |  |  |
| $\delta$ Eri | 62.16 | 79.10 | 0.100 | 0.096 | 0.013 | 0.096 | 0.093 | 0.098 | 0.071 | 0.098 | 0.022 | 165 | 14 |
| $\epsilon$ For | 68.49 | 74.98 | -0.577 | 0.065 | -0.731 | 0.074 | -0.593 | 0.080 | -0.654 | 0.072 | 0.061 | 150 | 17 |
| $\tau$ Cet | 79.68 | 84.76 | -0.524 | 0.081 | -0.552 | 0.057 | -0.525 | 0.077 | -0.559 | 0.080 | 0.034 | 175 | 12 |
| 18 Sco | 98.36 | 124.97 | 0.033 | 0.066 | 0.028 | 0.080 | 0.033 | 0.067 | -0.009 | 0.076 | 0.042 | 174 | 18 |
| Sun | 40.64 | 65.00 | -0.010 | 0.071 | -0.051 | 0.086 | -0.015 | 0.073 | -0.062 | 0.074 | 0.047 | 154 | 16 |
| HD 22879 | 61.75 | 144.31 | -0.853 | 0.054 | -0.888 | 0.072 | -0.857 | 0.057 | -0.918 | 0.058 | 0.061 | 130 | 17 |
| $\alpha$ Cen A | 30.06 | 31.36 | 0.347 | 0.069 | 0.235 | 0.079 | 0.333 | 0.079 | 0.308 | 0.081 | 0.025 | 183 | 22 |
| $\mu$ Ara | 46.63 | 45.87 | 0.388 | 0.079 | 0.319 | 0.095 | 0.381 | 0.083 | 0.352 | 0.085 | 0.029 | 180 | 19 |
| $\beta$ Hyi | 112.89 | 147.25 | 0.017 | 0.066 | -0.018 | 0.083 | 0.014 | 0.068 | -0.038 | 0.083 | 0.052 | 180 | 18 |
| $\beta$ Vir | 77.57 | 145.28 | 0.203 | 0.079 | 0.227 | 0.089 | 0.206 | 0.081 | 0.165 | 0.072 | 0.041 | 217 | 27 |
| $\eta$ Boo | 85.97 | 81.78 | 0.406 | 0.086 | 0.437 | 0.114 | 0.408 | 0.089 | 0.366 | 0.101 | 0.041 | 171 | 17 |
| Procyon | 62.43 | 84.17 | 0.013 | 0.033 | 0.030 | 0.046 | 0.015 | 0.035 | -0.027 | 0.046 | 0.042 | 136 | 20 |
| HD 49933 | 101.59 | 109.37 | -0.363 | 0.092 | -0.370 | 0.081 | -0.363 | 0.091 | -0.435 | 0.091 | 0.072 | 125 | 14 |
| FGK giants |  |  |  |  |  |  |  |  |  |  |  |  |  |
| Arcturus | 35.17 | 48.36 | -0.482 | 0.076 | -0.558 | 0.126 | -0.490 | 0.085 | -0.535 | 0.092 | 0.045 | 148 | 17 |
| HD 220009 | 92.25 | 110.21 | -0.680 | 0.093 | -0.866 | 0.076 | -0.693 | 0.102 | -0.787 | 0.126 | 0.094 | 177 | 13 |
| $\mu$ Leo | 38.55 | 47.97 | 0.245 | 0.192 | 0.192 | 0.164 | 0.241 | 0.121 | 0.229 | 0.124 | 0.012 | 160 | 14 |
| HD 107328 | 63.60 | 121.98 | -0.242 | 0.053 | -0.389 | 0.085 | -0.259 | 0.074 | -0.328 | 0.082 | 0.069 | 96 | 13 |
| $\beta$ Gem | 18.13 | 21.66 | 0.082 | 0.094 | 0.036 | 0.096 | 0.079 | 0.094 | 0.035 | 0.106 | 0.044 | 150 | 12 |
| $\epsilon$ Vir | 75.86 | 88.68 | 0.204 | 0.077 | 0.159 | 0.115 | 0.198 | 0.084 | 0.122 | 0.093 | 0.076 | 128 | 21 |
| $\xi$ Hya | 104.08 | 213.84 | 0.116 | 0.098 | 0.044 | 0.107 | 0.108 | 0.102 | -0.001 | 0.137 | 0.109 | 133 | 17 |
| K dwarfs |  |  |  |  |  |  |  |  |  |  |  |  |  |
| $61 \text { Cyg B }$ | 33.28 | 33.31 | -0.426 | 0.110 |  |  | -0.426 | 0.109 | -0.427 | 0.109 | 0.001 | 107 | 0 |
| $\epsilon$ Eri | 79.03 | 91.92 | -0.108 | 0.077 | -0.085 | 0.077 | -0.107 | 0.077 | -0.102 | 0.078 | -0.005 | 153 | 10 |

Metal-poor stars


Figure 7.23: Non-LTE iron abundance determination for the metal-poor stars using our final iron model. Total line abundance average $[\mathrm{Fe} / \mathrm{H}]$ is presented by the dotted lines. Solid lines represent the abundance fits as a function of EW.

## Metal-poor stars



Figure 7.24: LTE iron abundance determination for the metal-poor stars.

FG Dwarfs


Figure 7.25: Non-LTE iron abundance determination for the FG dwarfs stars $\delta$ Eri, $\epsilon$ For, $\tau$ Cet, 18 Sco and the Sun using our final iron model.

## FG Dwarfs



Figure 7.26: Non-LTE iron abundance determination for the FG dwarfs stars HD22879, $\alpha$ Cent A, $\mu$ Ara, $\beta$ Hyi and the $\beta$ Vir using our final iron model.

FG Dwarfs


Figure 7.27: Non-LTE iron abundance determination for the FG dwarfs stars $\eta$ Boo, Procyon and HD49933 using our final iron model.

## FGK Giants

The stars in this category also show small scatter in FeI lines ( $\leq 0.1$ dex) and good agreement between FeI and FeII, i.e. $\leq 0.07$ dex for most stars except HD220009 ( 0.186 dex) and HD107328 (0.147) which show larger differences. The possible explanations for these larger differences for the two stars is that the AFP for HD220009 calculated by Heiter et al. (2015a) and Jofré et al. (2014), were found to be inconsistent with the previous literature studies, which they explained as due to erroneous calibrations of $T_{\text {eff }}$, and thus rendering its parameters less reliable than others. In addition, the fundamental $\log g$ used in this work for HD107328 was found to be $30 \%$ smaller than the spectroscopic one by Heiter et al. (2015a). The values obtained for these two stars are however, lower than the non-LTE ionization imbalance of 0.2 dex found by Jofré et al. (2014) for the FGK giants. Also a slightly smaller scatter is found in non-LTE than in LTE for all the stars, whereas smaller $\chi_{N L T E}^{2}$ are found than the $\chi_{L T E}^{2}$ for all stars.

## K dwarfs

The two stars in this category show larger FeI dispersion for 61 Cyg B ( $\sigma[\mathrm{FeI} / \mathrm{H}]=0.11 \mathrm{dex}$ ) than stars in other categories. While no FeII lines could be measured for 61 Cyg B (due to blends with molecular bands). The agreement is good between Fe I and Fe II for $\epsilon$ Eri and the Fe I dispersion is small ( $\sigma[\mathrm{FeI} / \mathrm{H}]=0.077 \mathrm{dex}$ ).

## FGK Giants



Figure 7.28: Non-LTE iron abundance determination for the FGK giant stars Arcturus, HD220009, $\mu$ Leo and HD107328 using our final iron model.

## FGK Giants



Figure 7.29: Non-LTE iron abundance determination for the FGK giant stars $\beta$ Gem, $\epsilon$ Vir and $\xi$ Hya using our final iron model.


Figure 7.30: Non-LTE iron abundance determination for the $K$ dwarfs stars 61 Cyg B and $\epsilon$ Eri using our final iron model.

### 7.4.1.1 3D effects

The dispersion in FeI line abundances obtained in the Giants and K dwarfs may be due to 3D effects, which are not taken care of in 1D models. In order to test for this effect, we calculated an average $\langle 3 \mathrm{D}\rangle$ non-LTE corrections for the Sun using the published $\langle 3 \mathrm{D}\rangle$ Solar model from the Stagger 3D model grid ${ }^{1}$ (Magic et al., 2013b). We used the $\tau_{\text {Rosseland }}$ averaged model as recommended by Magic et al. (2013b). The results of the calculations are shown in Fig. 7.31. While the 1D, non-LTE calculations gave a dispersion of 0.071 dex for Fe I and 0.086 for Fe II lines, the $\langle 3 \mathrm{D}\rangle$ model gives a smaller dispersion of 0.069 and 0.070 dex for Fe I and Fe II respectively. In addition, while the difference obtained between [FeI/H] and [FeII/H] is 0.05 in the 1D model, a difference of 0.008 is obtained using the $\langle 3 \mathrm{D}\rangle$ model. The absolute Solar iron abundance obtained with the $\langle 3 \mathrm{D}\rangle$ model is 7.456 dex, which is equal to that obtained from the full 3D hydrodynamical model for the Sun and the meteoritic value (Asplund et al., 2000). The abundance obtained with the 1D model is 7.435 in non-LTE, and 7.398 in LTE.

[^32]

Figure 7.31: $\langle 3 \mathrm{D}\rangle$, non-LTE iron abundance determination for the Sun with our final iron model.

### 7.4.2 Comparison with the literature abundances

We compared our non-LTE Fe I and Fe II abundances with the results of 1D and $\langle 3 \mathrm{D}\rangle$ calculations by Bergemann et al. (2012) (hereafter BER12), and 1D calculations by Mashonkina et al. (2011) (hereafter MAS11) for 5 stars in common: the Sun, Procyon, HD84937, HD140283 and HD122563. They used $S_{H}=1$ with the Drawin recipe, and did not include any charge transfer collisional rates. Details of the atomic models used in these studies can be found in Sect. 4.5. The results of the determined abundances by the different studies are listed in Table 7.6.

MAS11 determined Solar 1D abundances of 7.54 and 7.56 for Fe I and Fe II respectively. Smaller values of 7.44 and 7.41 were found by BER12, and this work. Our $\langle 3 \mathrm{D}\rangle$ Solar abundances agree very well with BER12, with no difference obtained between Fe I and Fe II as compared to a 0.02 dex difference by BER12.

For Procyon, a 0.1 dex abundance difference is found between Fe I and Fe II by MAS11, which agrees well with the 1D BER12 determinations within uncertainties (though a smaller difference of 0.03 dex was found by BER12). Larger values, though, are determined in this work with a difference of 0.02 dex, which are in better agreement with the $\langle 3 \mathrm{D}\rangle$ results of BER12. It has to be noted that while the input $T_{\text {eff }}$ in the three studies agree within uncertainties, the $\log g$ used in this work is slightly larger by 0.04 dex.

1D abundance determinations for HD84937 agree well between the three studies within uncertainties, with the results in this work closer to the $\langle 3 \mathrm{D}\rangle$ values by BER12. For HD140283, our abundances are only compared to BER12 (no calculations for this star by MAS11) which agree well, though smaller dispersions are obtained by us ( $\sigma \leq 0.05$ ). Again, our results for this star agree well with $\langle 3 \mathrm{D}\rangle$ determinations of BER12, although a 0.12 cgs difference in $\log g$ is present between both studies.
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| Object |  | $T_{\text {eff }}$ | $\log g$ | 1D |  | 〈3D |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  |  |  | Fe I | Fe II | Fe I | Fe II |
| Sun | MAS11 | 5777 | 4.44 | $7.54 \pm 0.09$ | $7.56 \pm 0.05$ |  |  |
|  | BER12 | 5777 | 4.44 | $7.44 \pm 0.05$ | $7.44 \pm 0.04$ | $7.45 \pm 0.04$ | $7.47 \pm 0.04$ |
|  | This work | 5777 | 4.44 | $7.44 \pm 0.07$ | $7.41 \pm 0.08$ | $7.46 \pm 0.07$ | $7.46 \pm 0.07$ |
| Procyon | MAS11 | $6510 \pm 49$ | $3.96 \pm 0.02$ | $7.32 \pm 0.07$ | $7.42 \pm 0.05$ | $7.43 \pm 0.04$ | $7.43 \pm 0.04$ |
|  | BER12 | $6543 \pm 84$ | $3.94 \pm 0.02$ | $7.37 \pm 0.04$ | $7.40 \pm 0.04$ |  |  |
|  | This work | $6554 \pm 84$ | $4.00 \pm 0.02$ | $7.46 \pm 0.03$ | $7.48 \pm 0.04$ |  |  |
| HD84937 | MAS11 | $6350 \pm 37$ | $4.09 \pm 0.05$ | $5.32 \pm 0.07$ | $5.37 \pm 0.04$ | $5.45 \pm 0.06$ | $5.38 \pm 0.03$ |
|  | BER12 | $6408 \pm 66$ | $4.13 \pm 0.09$ | $5.39 \pm 0.07$ | $5.33 \pm 0.04$ |  |  |
|  | This work | $6356 \pm 97$ | $4.06 \pm 0.04$ | $5.42 \pm 0.06$ | $5.38 \pm 0.04$ |  |  |
| HD140283 | BER12 | $5777 \pm 80$ | $3.70 \pm 0.08$ | $5.07 \pm 0.09$ | $5.01 \pm 0.04$ | $5.05 \pm 0.05$ | $5.09 \pm 0.04$ |
|  | This work | $5522 \pm 102$ | $3.58 \pm 0.11$ | $5.10 \pm 0.05$ | $5.07 \pm 0.04$ |  |  |
| HD122563 | MAS11 | $4600 \pm 61$ | $1.60 \pm 0.07$ | $4.98 \pm 0.10$ | $4.89 \pm 0.07$ | $4.85 \pm 0.08$ | $5.01 \pm 0.05$ |
|  | BER12 | $4665 \pm 61$ | $1.64 \pm 0.16$ | $4.87 \pm 0.12$ | $4.95 \pm 0.05$ |  |  |
|  | This work | $4587 \pm 60$ | $1.61 \pm 0.07$ | $4.84 \pm 0.02$ | $4.86 \pm 0.02$ |  |  |

Table 7.6: This work's non-LTE Fe I and Fe II abundance results compared to those of Mashonkina et al. (2011) (MAS11) and Bergemann et al. (2012) (BER12) for the Sun, Procyon, HD84937, HD140283 and HD122563

An interesting case of comparison is the well studied very metal-poor star HD122563 ([Fe/H]< 2.50 dex). Our FeI abundance ( $4.84 \pm 0.02$ dex) is lower than those obtained by MAS11 and BER12 ( $4.98 \pm 0.10$ dex and $4.87 \pm 0.12$ dex respectively), and is in excellent agreement with the $\langle 3 \mathrm{D}\rangle$ value ( $4.85 \pm 0.08 \mathrm{dex}$ ). In addition, while a 0.1 dex difference was found between Fe I and Fe II by both MAS11 and BER12, an excellent agreement with a 0.02 dex difference is obtained in this work.

### 7.5 Comparison with preliminary quantum calculations

We have very recently obtained Fe I+H quantum calculations from private communication with Paul Barklem. The plots of the charge transfer rates (Fig. 7.32) as a function of $\frac{1}{\Delta E}$ shows the same behavior as those obtained for $\mathrm{Mg}, \mathrm{Na}, \mathrm{Al}$ and Si , with a peak observed between 0.5 and $1 \mathrm{eV}^{-1}$. The fits of these rates at $T=6000 \mathrm{~K}$ also shown on the figure and compared to those we obtained: an excellent agreement is found!.

The de-excitation rates as a function of $\Delta E$ at 6000 K are plotted in Fig. 7.33. The rates show a decreasing trend with transition energies. The fits to the data are shown in blue solid line, while those obtained with our QFM method are shown with a red dotted line. The fits agree well for $\Delta E<4 \mathrm{eV}$, i.e. for rates $>10^{-15} \mathrm{~cm}^{3} \cdot \mathrm{~s}^{-1}$.

Although the data from Paul Barklem are preliminary, and further comparisons are to be made in future work with calculations with the actual quantum data, they validate our method and show that our proposed QFM is able to reproduce the quantum data. This could be extended to other atoms where no quantum data have yet been published.

Figure 7.32: FeI+H charge transfer rates calculated by Paul Barklem (private communication) and their fits as a function of $1 / \Delta E$ Our best fits obtained using the QFM are also shown (black dotted lines).


Figure 7.33: Fe I + H de-excitation rates (private communication P. Barklem) and their fits as a function of $\Delta E$. The data fits with a third degree polynomial are shown in blue solid line, while best fits obtained in this work using the QFM are also shown (red dotted line).


## 8 Conclusions and Perspectives

The work in this dissertation shed the light on the role of hydrogen collisions in non-LTE iron modeling in cool stellar atmospheres, which is usually modeled with the semi-classical Drawin approximation.
In the first part of this work, the commonly used Drawin approximation to calculate the hydrogen collisional rates was put to test:

The Drawin approximation was extended and used to calculate charge transfer collisional rates, in addition to excitation and ionization rates. It was shown that Drawin approximation over estimates, and predicts the rates with a completely different behavior with transition energies. A silicon test model atom was developed and utilized to compare non-LTE calculations using the Drawin approximation rates to those using the quantum data. The results showed that different sets of multiplicative scaling factors for different stars are required to reproduce the reference calculations made with the quantum data.

The Drawin approximation was then tested on iron, using a newly developed, rather complete, model atom. Non-LTE calculations using the Drawin approximation were compared to observed equivalent widths for 30 Gaia-ESO benchmark stars of different spectral types with well determined atmospheric parameters. The results have shown once again that no single set of scaling factors for excitation and charge transfer could be used for all the stars to produce a best fit of the observations. Even within same spectral type categories no single recipe could be found.

In the light of these results, we deduce that the Drawin approximation is unreliable and should not be used to calculate collisional rates.

In the second part, we introduce a new method to calculate hydrogen collisional rates, which we call the Quantum Fitting Method (QFM), which is based on fitting the existing quantum calculations of a few elements, namely, $\mathrm{Na}, \mathrm{Mg}, \mathrm{Al}$ and Si . We show that a general fitting recipe for charge transfer rates can be used for all four elements. A different recipe is adopted for de-excitation rates as well.

The fitting recipes are first tested on Si , where non-LTE calculations using the QFM are shown to reproduce the equivalent width calculations using the real quantum data within a scatter of $<1 \%$. Our calculations also demonstrate that a variation in the fitting parameters within $\pm 50 \%$ from their reference values, only alters the results of the calculations within $< \pm 10 \%$.

The QFM was then extended to iron, for which no quantum data existed. The general form of the excitation and charge transfer collisional rate fits obtained for other elements were conserved and used. The fitting parameters for each of charge transfer and excitation rates were varied at once, thus creating a multidimensional grid of parameters for which non-LTE calculations were computed. A best fit minimum was found at the same set of parameters for
three stars of different stellar types.
The best fit model was used to determine 1D, non-LTE and LTE Fe I and Fe II abundances for the benchmark stars. The non-LTE iron abundances demonstrated much smaller scatter than the LTE, especially for metal-poor stars and FGK giants. An excellent agreement was also found between Fe I and Fe II abundances, within $\leq 0.05$ dex. Larger non-LTE effects were determined for metal-poor stars, as expected. 3D effects were tested on the Sun using an average $\langle 3 \mathrm{D}\rangle$ Solar model, and an excellent agreement was found between Fe I and Fe II lines $(\log \varepsilon(\mathrm{Fe} \mathrm{I})=$ $\log \varepsilon(\mathrm{Fe}$ II $)=7.46 \mathrm{dex})$, with a dispersion of $\sigma<0.01$. These values are in agreement with the full 3D results and the meteoritic values by Asplund et al. (2000). Our results also agree well with the most recent iron abundance calculations from the literature (Bergemann et al., 2012; Mashonkina et al., 2011), with less scatter obtained in this work.

We thus deduce that our proposed QFM method is able to reproduce the observations with high accuracy. Luckily, we were able to compare our method to recent preliminary iron quantum collisional rates (private communication from Paul Barklem). Our determined best fits show very good agreement with the fits of quantum data. This strengthens the validity of our method and suggests it could be extended to other elements when no quantum calculations exist.

In future work, we aim to implement the iron quantum data into our model atom and compare the calculations to this work's results.

As we find slightly more consistent results using a $\langle 3 \mathrm{D}\rangle$ model for the Sun, we plan to extend the $\langle 3 \mathrm{D}\rangle$ calculations to the whole sample of stars.

As part of the GES-CoRoT collaboration, which is an ongoing international collaboration whose objective is to derive the best stellar parameters using the seismic constraints (surface gravity) from the CoRoT satellite, combined with high resolution spectroscopic data, we plan to determine non-LTE corrections on the fundamental atmospheric parameters of a sample of 700 stars with high resolution spectra (obtained with UVES and GIRAFFE).

Another future interest is to utilize our QFM in non-LTE calculations for other elements prone to non-LTE effects in cool stars, e.g. B I, OI, S I, KI, Sc I, Ti I, Co I, SrI, ... (See e.g. review by Bergemann and Nordlander, 2014).

A priority of ours is to provide a line-by-line non-LTE corrections grid for a large parameter space, that would be accessible through the world wide web.


Figure 8.1: Abundance determination journey through essential steps of spectroscopic modeling (Bengt Gustafsson, 2009).

## A Spectral line formation and Broadening Coefficients

Observed spectral lines are not delta-like functions (infinitely narrow) in the continuum, but are rather broadened due to several mechanisms. In what follows I will explain the microscopic processes responsible for broadening spectral emission and absorption lines.

## A. 1 Natural (radiative) broadening

Due to the Heisenberg uncertainty principle, an electron in an atom lying at an energy level of energy $E$ above the ground state, and of a lifetime $\Delta t$ on that state has an uncertainty in energy:

$$
\begin{equation*}
\Delta E \Delta t \sim \hbar \tag{A.1}
\end{equation*}
$$

hence a photon emitted in a transition from this level to another level will have a range of possible frequencies

$$
\begin{equation*}
\Delta \nu \sim \frac{\Delta E}{h} \sim \frac{1}{2 \pi \Delta t} \tag{A.2}
\end{equation*}
$$

The sum of all spontaneous (natural) decay rates (in $\mathrm{s}^{-1}$ ) of an electron in an atomic energy state $j$ to all possible lower energy states $i$ is:

$$
\begin{equation*}
\gamma_{i}^{\mathrm{rad}}=\sum_{i} A_{j i} \tag{A.3}
\end{equation*}
$$

then the line emission profile (can be considered the same for absorption under detailed balancing) due to natural broadening (damping) is called a Lorentzian or natural line profile (for derivation see Bransden and Joachain (2003)) and is of the form:

$$
\begin{equation*}
\phi^{\mathrm{rad}}\left(\nu-\nu_{0}\right)=\frac{\gamma^{\mathrm{rad}} / 4 \pi^{2}}{\left(\nu-\nu_{0}\right)^{2}+\left(\gamma^{\mathrm{rad}} / 4 \pi\right)^{2}} \tag{A.4}
\end{equation*}
$$

where $\nu_{0}$ is the central frequency around which the line is broadened. The classical value for $\gamma^{\text {rad }}$ for a damped harmonic oscillator is:

$$
\begin{equation*}
\gamma_{\text {rad }}=\frac{8 \pi e^{2} \nu_{0}^{2}}{3 m_{e} c^{3}}=2.47 \times 10^{-22} \nu_{0}^{2} \tag{A.5}
\end{equation*}
$$

## A. 2 Collisional (pressure) broadening

The presence of collisional perturbers in the neighborhood of atoms, mainly electrons and neutral hydrogen atoms for late-type cool stars, whose charges affect the radiating atom through Coulomb's interactions and therefore affects the frequency of the photons of the bound-bound
transitions, by further decreasing the lifetime of the energy states than the radiative broadening and thus further broadening the spectral lines. HI atoms in particular have large polarization due to bad shielding of the proton by the single electron in the atom. They are thus important spectral line broadeners in cool atmospheres.

The commonly classical description of collisional broadening is to distinguish between the different interactions based on the different closest seperation distances $r^{\mathrm{p}}$ between the absorbing atom and the corresponding pertuber. Hence starting from Heisenberg's uncertainty principle again, one can write:

$$
\begin{equation*}
\Delta \nu=\frac{\Delta E}{h} \equiv \frac{C_{n}}{r_{n}^{\mathrm{p}}} \tag{A.6}
\end{equation*}
$$

where $C_{n}$ is the interaction constant and the index $n$ defines the type of possible interactions. In this thesis we will consider the relevant broadening interaction contributions in late-type cool stars, namely from electrons and neutral hydrogen atoms.

## Stark effect ( $\mathrm{n}=4$ )

This defines the collisional broadening due to interaction of atoms with free electrons. The spatial dependence of this type of broadening is $r^{-4}$ in which the electrons at large speeds cause a momentary disruption of the radiation emitted by the atom. Similar to the natural broadening, electron Stark effect contributes to the Lorentzian line profile by $\Gamma_{e}^{\mathrm{col}}$. Electron broadening dominates in atmospheres of hot stars where electron density is high (Griem, 1974).

## Van der Waals broadening ( $\mathrm{n}=6$ )

Neutral hydrogen atoms dominate in cools stars (See Appendix B for details) which make them the dominant broadeners of spectral lines there. The classical approach to calculating the hydrogen broadening coefficient $\Gamma_{\mathrm{H}}^{\text {col }}$ (commonly called the Van der Waals damping coefficient, also denoted $\gamma_{6}$ ) was described by Unsold (1955), where he formulated the latter coefficient as:

$$
\begin{equation*}
\gamma_{6}=\log \Gamma_{\mathrm{H}}^{\mathrm{col}} \approx 6.33+0.4 \log \overline{r^{2}}+\log P_{g}-0.7 \log T \tag{A.7}
\end{equation*}
$$

where $\overline{r^{2}}$ is the mean square radius (in atomic units) between the upper and lower levels of the atom, extended from the hydrogenic approximation by ? to non-hydrogenic atoms of ionization stage Z as:

$$
\begin{equation*}
\overline{r^{2}}=\frac{n^{* 2}}{2 Z^{2}}\left(5 n^{* 2}+1-3 l(l+1)\right) \tag{A.8}
\end{equation*}
$$

where 1 is the angular quantum number of the corresponding level and $n^{*}$ is its effective principal quantum number given by:

$$
\begin{equation*}
n^{* 2}=R \frac{Z^{2}}{E_{\infty}-E_{n}} \tag{A.9}
\end{equation*}
$$

with $\mathrm{R}=13.6 \mathrm{eV}$ is the Rydberg constant and $E_{\infty}-E_{n}$ is the ionization energy from the corresponding level. For non-hydrogenic lines, the observed line profiles from cool stars seem to suffer more damping than the values estimated from Unsöld's approximation, and thus it is common to apply an enhancement fudge factor to the Van der Waals damping coefficient which ranges between 2 to 5 depending on the atom and ionization stage.

Anstee, Barklem and O'Mara (ABO) theory The ABO theory (Anstee and O'Mara, 1995; Barklem et al., 1998; Barklem and O'Mara, 1997) has been originally developed by Anstee and O'Mara (1995) as a universal theory for the hydrogen broadening of atomic and ionic lines which is more intricate than the $r^{-6}$ dependence formulated by Unsöld. The ABO theory
presented results of the variation of the hydrogen broadening cross-sections $\sigma_{H}^{\text {br }}$ as a function of collisional speed of hydrogen atoms $v$, and found to be a power law dependent on a velocity parameter $\alpha$ such as:

$$
\begin{equation*}
\sigma_{\mathrm{H}}^{\mathrm{br}} \propto v^{-\alpha} \tag{A.10}
\end{equation*}
$$

The damping coefficient can then be calculated using:

$$
\begin{equation*}
\gamma_{6}=2\left(\frac{4}{\pi}\right)^{\alpha / 2} \Gamma \frac{4-\alpha}{2} \bar{v} \sigma_{\mathrm{H}}^{\mathrm{br}} n_{\mathrm{H}} \tag{A.11}
\end{equation*}
$$

where $\Gamma$ is Euler's Gamma function, $\bar{v}=\left(8 k_{\mathrm{B}} T / \pi \mu\right)^{1 / 2}$, and $\mu$ is the reduced mass of the two atoms in contact and $v_{0}=10^{4} \mathrm{~m} / \mathrm{s}$ the relative collisional speed.

The ABO theory has been implemented in most spectral synthesis codes used nowadays (LTE \& non-LTE) which will provide $\sigma_{\mathrm{H}}^{\mathrm{br}}$ and $\alpha$ for large grids of lines calculated for different elements and their ions useful in many astrophysical approximations. This allowed for much better improvement of spectral lines synthesis which resulted in better fits with the observed lines, that allowed for more reliable derivations of stellar parameters.

## A. 3 Thermal broadening

Individual atoms in a stellar atmospheric gas of temperature $T$ have random motions away or toward the observer (or observation instrument), leading to red- or blue-wards Doppler frequency shifting. Considering a Maxwell velocity distribution of an atom of mass $m$, the line of sight mean kinetic energy can be written as $\frac{1}{2} m\left\langle V^{2}\right\rangle=\frac{3}{2} k_{\mathrm{B}} T$, where the thermal light of sight velocity (Doppler velocity) is $v_{D} \equiv \sqrt{\frac{2 k_{\mathrm{B}} T}{m}}$. In addition, small-scale mass motions characterized with a mean micro-turbulent velocity $\xi$ also produce Doppler shifts analogous to the ones produces by thermal motions and thus should also be added to the broadening coefficient.
Hence Doppler width shift in frequency can be written as:

$$
\begin{equation*}
\Delta \nu_{\mathrm{D}}=\nu_{0} \frac{v_{D}}{c}=\frac{\nu_{0}}{c} \sqrt{\frac{2 k_{\mathrm{B}} T}{m}+\xi^{2}} \tag{A.12}
\end{equation*}
$$

and the thermally broadened cross-section calculated from the integrating over the absorption coefficient of the atoms moving at velocity $v$ at Maxwell velocity distribution

$$
\begin{equation*}
\sigma_{\nu}^{\operatorname{th}} \propto \frac{1}{\Delta \nu_{\mathrm{D}}} e^{-\left(\frac{\nu-\nu_{0}}{\Delta \nu_{\mathrm{D}}}\right)^{2}} \tag{A.13}
\end{equation*}
$$

Thermal broadening causes a Gaussian (or Doppler) shaped profile.

## A. 4 Line profile

The final line profile is a convolution of the profiles for all the broadening processes, i.e. of a Lorentzian profile (from radiative and collisional broadening) and a Gaussian profile (from thermal broadening) $f_{\mathrm{V}}(\nu)=f_{\mathrm{L}}(\nu) \otimes f_{\mathrm{D}}(\nu)$ which results in a Voigt profile.

$$
\begin{equation*}
\phi^{V}(\nu)=\frac{\sqrt{\pi}}{\Delta \nu_{\mathrm{D}}} H(a, x) \tag{A.14}
\end{equation*}
$$

where $\mathrm{H}(\mathrm{a}, \mathrm{x})$ is called the Hjerting function (Hjerting, 1938),

$$
\begin{equation*}
H(a, x)=\frac{a}{\pi} \int_{-\infty}^{+\infty} \frac{e^{-y^{2}}}{(x-y)^{2}+a^{2}} \mathrm{~d} y \tag{A.15}
\end{equation*}
$$

with $a$ the damping parameter, determined by:

$$
a=\frac{\gamma^{\text {tot }}}{4 \pi} \frac{1}{\Delta \nu_{\mathrm{D}}} \text { and } x=\frac{\nu-\nu_{0}}{\Delta \nu_{\mathrm{D}}}
$$

where $\gamma^{\text {tot }}=\gamma^{\text {rad }}+\gamma_{4}+\gamma_{6}$ is the total broadening coefficient.


Figure A.1: Hjerting function line profile variation as a function of its parameters $a$ and $x$.
As is shown in Fig. (A.1), for small values of $a$ the line profile is close to that of a Gaussian, and the wings grow with increasing $a$.

## B <br> Numerical Solution to the multi-level non-LTE problems (MULTI2.3)

The non-linear coupling between the radiative transfer equation (Eqn. 3.15) and the statistical equilibrium rate equation (Eqn. 3.36) and the complexity introduced by many different atomic processes asks for a non-analytical numerical solution to the non-LTE problem.

## B. 1 Approximate Lambda Iteration (ALI)

In this thesis, I used the fortran77 numerical code MULTI2.3 (Carlsson, 1986, 1992) to solve for the non-LTE equations, which uses the Approximate Lambda Iteration (ALI) method and the Newton-Raphson iterative scheme to solve for non-LTE populations. The coupling of eqns (3.15), (3.36) and that of the particle conservation equation $\sum_{j=1}^{N} n_{j}=n_{\text {tot }}$ can be written as:

$$
\begin{equation*}
\Lambda[\mathrm{n}]=\mathrm{b} \tag{B.1}
\end{equation*}
$$

where $\Lambda$ is called the Lambda operator containing the radiative and collisional rates (A matrix of dimensions $\left(N_{\text {lev }} \times N_{\text {depth }}\right)^{2}$ where $N_{\text {lev }}$ is the number of levels in the considered atom and $N_{\text {depth }}$ is the number of optical depth points in the considered model atmosphere), and $\mathbf{n}$ is a 1 D array containing the populations of each level at each atmospheric depth point.

Supposing that an estimate of the population numbers $\mathbf{n}^{(i)}$ for a certain iteration $i$ produces an error $\mathbf{e}^{(i)}$, equation (B.1) can then be expressed as:

$$
\begin{equation*}
\boldsymbol{\Lambda}\left[\mathbf{n}^{(i)}\right]=\mathbf{b}+\mathbf{e}^{(i)} \tag{B.2}
\end{equation*}
$$

and if a correction $\delta^{(i)} \mathbf{n}$ is needed to obtain the required solution $\mathbf{n}$, this gives:

$$
\begin{equation*}
\boldsymbol{\Lambda}\left[\mathbf{n}^{(i)}+\delta^{(i)} \mathbf{n}\right]=\mathbf{b}+\mathbf{e}^{(i)} \tag{B.3}
\end{equation*}
$$

An approximate lambda operator $\Lambda^{*}$ can be defined such that:

$$
\begin{equation*}
\boldsymbol{\Lambda}^{*(i)}\left[\delta^{(i)} \mathbf{n}\right] \approx \boldsymbol{\Lambda}\left[\mathbf{n}^{(i)}+\delta^{(i)} \mathbf{n}\right]-\boldsymbol{\Lambda}\left[\mathbf{n}^{(i)}\right] \tag{B.4}
\end{equation*}
$$

Subtracting eqns. (B.2) from (B.3) we obtain

$$
\begin{equation*}
\Lambda^{*(i)}\left[\delta^{(i)} \mathbf{n}\right] \approx-\mathbf{e}^{(i)} \tag{B.5}
\end{equation*}
$$

Si Thus an iterative procedure can be constructed from the equations above to determine the populations at each iteration until convergence is obtained:

$$
\left\{\begin{array}{l}
\mathbf{e}^{(i)}=\boldsymbol{\Lambda}\left[\mathbf{n}^{(i)}\right]-\mathbf{b}  \tag{B.6}\\
\delta \mathbf{n}^{(i)}=\boldsymbol{\Lambda}^{*(i)-\mathbf{1}}\left[-\mathbf{e}^{(i)}\right] \\
\mathbf{n}^{i+1}=\mathbf{n}^{i}+\delta \mathbf{n}^{(i)}
\end{array}\right.
$$

The construction of the approximate Lambda operator $\Lambda^{*(i)}$ is of fundamental importance, which should be chosen to contain all the important interactions and to be useful, in the terms that it could be easily assembled and inverted within possible computational effort.

In MULTI2.3, $\Lambda^{*}$ is constructed by making use of Scharmer's operator (Scharmer, 1981) to represent the radiative interactions and corresponding to the coefficient matrix (denoted the Grand Matrix) of a set of linear equations in the code which determine the relative corrections of $\delta \mathbf{n}^{(i)} / \mathbf{n}^{(i)}$ at each iteration. Different elements of the Grand Matrix demonstrate different physical properties:

- Each row in the Grand Matrix corresponds to the statistical equilibrium equation for one atomic level at one depth point in the atmosphere.
- The grand matrix itself then consists of smaller matrices each of size $N_{\text {lev }} \times N_{\text {lev }}$, where each corresponds to the influence from changes of the population numbers at one depth in the atmosphere on the population numbers at another depth.
- Each element in each small matrix corresponds to the influence from changing the population number of one specific atomic level on the population number of another level.
- Diagonal element matrices correspond to the local interactions while all non-diagonal blocks correspond to the non-local interactions through the radiative transfer in the lines.


## B. 2 Starting Approximation

The use of the iterative correction method which depends on its previous approximation at each iteration, requires a good starting approximation which can have notable effect on the actual, the divergence or the slow convergence of the solution. The standard procedure is to start from LTE populations and then perform one or two Lambda iterations Auer et al. (1972). In MULTI2.3, I have started from zero radiation field and continued by solving the statistical equilibrium equations until convergence is obtained. In the case of divergence of the latter, I started from LTE populations and performed several Lambda iterations until convergence was obtained. A slower convergence is observed for when starting from LTE population as compared to when starting from zero populations (see Fig. B.1).

## B. 3 Properties of multi2.3

The code MULTI2.3 is a useful program to use for solving non-LTE radiative transfer problems in 1D, plane parallel, semi-infinite atmospheres of cool stars for its many interesting properties:

- A local approximate lambda operator option is implemented (Rybicki and Hummer, 1991), which is much less memory demanding thus makes it possible to solve problems with very large model atoms (more than 100 levels)
- The model atom of the considered element can contain many atomic levels and several ionization stages which can be treated in details simultaneously, thus making it ideal for the non-LTE study of FeI/II atom.
- The bound-bound lines are assumed to be formed with complete redistribution over the profile function which is assumed to be a Voigt profile.
- The code is relatively efficient. The CPU time scales almost linearly with the number of frequencies points and angles making it useful for solving problems including velocity fields.
- The code, written in FORTRAN77, is highly portable and well commented, thus facilitating changes and additions.
- It is possible to go through the formal solution with a new set of atomic levels and transitions in which the converged populations are redistributed to the new levels, done proportionally to their statistical weights. This is ideal for the use of superlevels and superlines (described in sections 4.1.1 \& 4.2.1.1 respectively) in the case of complex large atoms such as FeI/FeII.


Figure B.1: Convergence of the populations of an atomic level four in a five level CaII atom plus continuum calculations for different iteration numbers. The lines show the log of the ratio of the populations to that of the global final populations at that level, $\log \left(n_{4}^{i t} / n_{4}^{\infty}\right)$ as a function of depth points (depth point 1 is at the top of the atmosphere) for iteration numbers it $=1-5$. Dashed lines represent relative populations at different iterations when starting from LTE populations, while the solid lines for when starting from zero populations and solving the statistical equilibrium equations (Carlsson, 1986).

## C | Physical Constants \& Conversion of units

Below, I present the values of the physical constants utilized in this thesis, the conversion of units commonly used, and the Solar fundamental parameters values. Values adopted in sections C. 1 and C. 2 are from the 2014 values of the CODATA measurements of the Physical Measurement Laboratory of the National Institute of Standards and Technology (NIST) ${ }^{1}$, while the Solar parameters are adopted from the "Sun fact sheet" ${ }^{2}$ by Williams, D.R. (2013).

## C. 1 Physical constants

Newtonian constant of Gravitation $G$
Planck constant $h$
speed of light (vacuum) $c$
elementary charge $e^{-}$
electron mass $m_{e}$
proton mass $m_{p}$
Bohr radius $a_{0}$
Rydberg constant $R_{\infty}$
Boltzmann constant $k_{\mathrm{B}}$
Stefan-Boltzmann constant $\sigma_{\mathrm{SB}}$

$$
\begin{array}{ll}
= & 6.67408 \times 10^{-11} \mathrm{~m}^{3} \cdot \mathrm{~kg}^{-1} \cdot \mathrm{~s}^{-1} \\
= & 6.626070040 \times 10^{-34} \mathrm{~J} \cdot \mathrm{~s} \\
= & 299792458 \mathrm{~m} \cdot \mathrm{~s}^{-1} \\
= & 1.6021766208 \times 10^{-19} \mathrm{C} \\
= & 9.10938356 \times 10^{-31} \mathrm{~kg} \\
= & 1.672621898 \times 10^{-27} \mathrm{~kg} \\
= & 0.52917721067 \times 10^{-10} \mathrm{~m} \\
= & 10973731.568508 \mathrm{~m}^{-1} \\
= & 1.38064852 \times 10^{-23} \mathrm{~J} \cdot \mathrm{~K}^{-1} \\
= & 5.670367 \times 10^{-8} \mathrm{~W} \cdot \mathrm{~m}^{-2} \cdot \mathrm{~K}^{-4}
\end{array}
$$

## C. 2 Conversion of units

1 electron Volts (eV)
1 electron Volts (eV)
1 Rydberg energy unit (Ry)
1 Rydberg energy unit (Ry)
1 Mega-barn (Mb)
1 parsec (pc)
1 dyne
1 light year (ly)
$=\quad 1.60210 \times 10^{-19}$ Joules $(\mathrm{J})$
$=\quad 8065.73 \mathrm{~cm}^{-1}$
$=\quad 13.60569172 \mathrm{eV}$
$=109737.31568 \mathrm{~cm}^{-1}$
$=1 \times 10^{-16} \mathrm{~cm}^{2}$
$=3.08567758 \times 10^{16} \mathrm{~m}$
$=\quad 1 \mathrm{~g} \cdot \mathrm{~cm} \cdot \mathrm{~s}^{-2}$
$=\quad 9.46053 \times 10^{15} \mathrm{~m}$

[^33]
## C. 3 Solar fundamental parameters

| Equatorial Solar Radius $\mathrm{R}_{\odot}$ | $=$ | $6.9599 \times 10^{8} \mathrm{~m}$ |
| :--- | :--- | :--- |
| Solar mass M $_{\odot}$ | $=$ | $1.989 \times 10^{30} \mathrm{~kg}$ |
| Solar luminosity $\mathrm{L}_{\odot}$ | $=$ | $3.846 \times 10^{26} \mathrm{~W}$ |

## D Linelist, EW and iron abundances



|  |  |  |  |  |  | Sun |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  |  |  |  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m}$ ¢ $)$ |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m}$ A） |  |  | $\varepsilon_{\mathrm{Fe}}(\mathrm{dex})$ |  |
| element | $\lambda$（air） | EP（eV） | $\log g f$ | $\Gamma^{\mathrm{H}}=\sigma_{\mathrm{H}}^{\mathrm{br}} \cdot \alpha$ | $\gamma_{\text {rad }}$ | EW | $\sigma$ EW | 1D，nLTE | 1D，LTE | 〈3D〉，nLTE | 1D，nLTE | 〈3D ${ }^{\text {，nLTE }}$ |
| Fe I | 5651.469 | 4.473 | －1．900 | 898.278 | $1.86 \mathrm{E}+08$ | 15.66 | 0.37 | 13.997 | 15.116 | 13.602 | 7.511 | 7.526 |
| Fe I | 5652.317 | 4.260 | －1．850 | 754.210 | $1.02 \mathrm{E}+08$ | 23.53 | 0.29 | 21.873 | 23.469 | 21.267 | 7.480 | 7.498 |
| Fe I | 5679.023 | 4.652 | －0．820 | 1106.291 | $1.62 \mathrm{E}+08$ | 55.18 | 0.36 | 56.258 | 59.785 | 56.105 | 7.427 | 7.431 |
| Fe I | 5680.240 | 4.186 | －2．480 | －7．770 | $4.90 \mathrm{E}+07$ | 8.59 | 0.80 | 7.503 | 8.155 | 7.306 | 7.493 | 7.506 |
| Fe I | 5691.497 | 4.301 | －1．450 | 746.231 | $2.34 \mathrm{E}+08$ | 37.01 | 0.88 | 37.543 | 39.982 | 36.624 | 7.446 | 7.466 |
| Fe I | 5717.833 | 4.284 | －0．990 | 758.209 | $1.51 \mathrm{E}+08$ | 57.6 | 2.82 | 62.341 | 65.347 | 61.891 | 7.349 | 7.362 |
| Fe I | 5731.762 | 4.256 | －1．200 | 727.232 | $2.40 \mathrm{E}+08$ | 55.38 | 1.80 | 52.633 | 55.287 | 51.704 | 7.501 | 7.518 |
| Fe I | 5741.848 | 4.256 | －1．672 | 725.232 | $2.95 \mathrm{E}+08$ | 30.62 | 0.54 | 29.359 | 31.366 | 28.539 | 7.474 | 7.494 |
| Fe I | 5760.344 | 3.642 | －2．390 | 386.250 | $7.76 \mathrm{E}+07$ | 21.69 | 1.56 | 23.955 | 25.758 | 23.237 | 7.363 | 7.380 |
| Fe I | 5848.126 | 4.608 | －1．056 | －7．520 | $2.14 \mathrm{E}+08$ | 38.96 | 0.66 | 43.193 | 46.048 | 42.508 | 7.342 | 7.357 |
| Fe I | 5849.683 | 3.695 | －2．890 | 379.305 | $6.03 \mathrm{E}+07$ | 6.61 | 0.45 | 6.925 | 7.560 | 6.752 | 7.434 | 7.446 |
| Fe I | 5855.076 | 4.608 | －1．478 | 962.279 | $2.14 \mathrm{E}+08$ | 20.85 | 0.35 | 24.201 | 26.051 | 23.530 | 7.339 | 7.355 |
| Fe I | 5858.778 | 4.220 | －2．160 | 786.278 | $3.02 \mathrm{E}+08$ | 12.05 | 0.12 | 13.513 | 14.624 | 13.128 | 7.425 | 7.440 |
| Fe I | 5861.108 | 4.283 | －2．304 | 854.279 | $2.40 \mathrm{E}+08$ | 6.98 | 0.16 | 9.019 | 9.782 | 8.769 | 7.481 | 7.495 |
| Fe I | 5873.212 | 4.256 | －2．040 | 712.228 | $2.40 \mathrm{E}+08$ | 16.78 | 0.42 | 16.277 | 17.559 | 15.824 | 7.483 | 7.498 |
| Fe I | 5881.280 | 4.608 | －1．740 | 950.279 | $2.14 \mathrm{E}+08$ | 14.77 | 0.72 | 15.121 | 16.365 | 14.669 | 7.434 | 7.451 |
| Fe I | 5909.972 | 3.211 | －2．587 | 716.243 | $1.62 \mathrm{E}+08$ | 30.49 | 0.92 | 34.123 | 36.456 | 32.930 | 7.475 | 7.503 |
| Fe I | 5927.789 | 4.652 | －0．990 | 984.281 | $2.09 \mathrm{E}+08$ | 40.96 | 0.49 | 46.237 | 49.451 | 45.535 | 7.332 | 7.346 |
| Fe I | 5987.065 | 4.796 | －0．429 | －7．420 | $2.00 \mathrm{E}+08$ | 73.56 | 2.03 | 73.824 | 78.872 | 74.750 | 7.448 | 7.434 |
| Fe I | 6034.035 | 4.313 | －2．312 | 710.223 | $1.95 \mathrm{E}+08$ | 7.44 | 0.31 | 8.563 | 9.308 | 8.315 | 7.404 | 7.418 |
| Fe I | 6093.643 | 4.608 | －1．400 | 866.274 | $2.14 \mathrm{E}+08$ | 29.58 | 1.33 | 27.674 | 29.789 | 26.908 | 7.521 | 7.540 |
| Fe I | 6096.664 | 3.984 | －1．830 | 963.250 | $5.62 \mathrm{E}+07$ | 36.54 | 0.96 | 35.822 | 38.149 | 34.809 | 7.482 | 7.504 |
| Fe I | 6127.906 | 4.143 | －1．399 | 290.250 | $1.00 \mathrm{E}+08$ | 46.87 | 1.05 | 50.155 | 53.074 | 48.963 | 7.443 | 7.466 |
| Fe I | 6151.617 | 2.176 | －3．295 | 277.263 | $1.95 \mathrm{E}+08$ | 48.14 | 0.78 | 48.761 | 51.873 | 46.162 | 7.440 | 7.498 |
| Fe I | 6157.728 | 4.076 | －1．160 | －7．790 | $7.76 \mathrm{E}+07$ | 60.59 | 1.65 | 67.274 | 70.518 | 66.406 | 7.304 | 7.323 |
| Fe I | 6165.360 | 4.143 | －1．473 | 380.250 | $1.00 \mathrm{E}+08$ | 44.51 | 0.32 | 46.108 | 48.947 | 44.903 | 7.410 | 7.434 |
| Fe I | 6170.506 | 4.796 | －0．440 | 1057.288 | $2.00 \mathrm{E}+08$ | 75.93 | 6.79 | 72.969 | 77.544 | 73.505 | 7.496 | 7.485 |
| Fe I | 6173.334 | 2.223 | －2．880 | 281.266 | $2.04 \mathrm{E}+08$ | 66.38 | 1.29 | 66.428 | 69.924 | 63.025 | 7.460 | 7.539 |
| Fe I | 6180.203 | 2.728 | －2．591 | 335.259 | $1.62 \mathrm{E}+08$ | 53.63 | 4.97 | 56.992 | 60.055 | 54.165 | 7.409 | 7.470 |
| Fe I | 6187.989 | 3.943 | －1．620 | 903.244 | $5.62 \mathrm{E}+07$ | 47.2 | 0.98 | 48.133 | 49.115 | 49.435 | 7.411 | 7.436 |
| Fe I | 6200.312 | 2.609 | －2．433 | 350.235 | $1.20 \mathrm{E}+08$ | 70.01 | 1.76 | 70.332 | 73.723 | 67.105 | 7.462 | 7.533 |
| Fe I | 6226.734 | 3.884 | －2．120 | 845.244 | $6.76 \mathrm{E}+07$ | 27.7 | 0.52 | 26.751 | 28.734 | 25.938 | 7.467 | 7.488 |
| Fe I | 6229.226 | 2.845 | －2．805 | 350.250 | $1.58 \mathrm{E}+08$ | 36.12 | 2.39 | 40.734 | 43.426 | 38.822 | 7.366 | 7.405 |
| Fe I | 6270.224 | 2.858 | －2．470 | 350.249 | $1.58 \mathrm{E}+08$ | 52.28 | 2.08 | 56.839 | 59.894 | 54.120 | 7.360 | 7.416 |
| Fe I | 6271.278 | 3.332 | －2．703 | 720.247 | $1.66 \mathrm{E}+08$ | 22.87 | 0.60 | 24.413 | 26.335 | 23.580 | 7.386 | 7.406 |
| Fe I | 6293.924 | 4.835 | －1．717 | －7．420 | $2.00 \mathrm{E}+08$ | 11.79 | 0.17 | 10.585 | 11.543 | 10.202 | 7.542 | 7.561 |
| Fe I | 6297.792 | 2.223 | －2．737 | 278.264 | $1.95 \mathrm{E}+08$ | 72.6 | 0.86 | 74.222 | 78.046 | 70.556 | 7.421 | 7.501 |
| Fe I | 6311.500 | 2.832 | －3．141 | 344.250 | $1.58 \mathrm{E}+08$ | 26.57 | 4.32 | 26.141 | 28.261 | 25.077 | 7.466 | 7.495 |
| Fe I | 6380.743 | 4.186 | －1．375 | 380.250 | $7.59 \mathrm{E}+07$ | 50.03 | 0.55 | 49.506 | 52.554 | 48.230 | 7.491 | 7.516 |
| Fe I | 6436.406 | 4.186 | －2．580 | －7．810 | $3.02 \mathrm{E}+07$ | 8.74 | 0.29 | 6.368 | 6.975 | 6.190 | 7.495 | 7.509 |
| Fe I | 6469.192 | 4.835 | －0．730 | 982.286 | $2.51 \mathrm{E}+08$ | 55.84 | 5.13 | 52.155 | 55.900 | 51.378 | 7.557 | 7.567 |
| Fe I | 6481.870 | 2.279 | －2．981 | 308.243 | $1.95 \mathrm{E}+08$ | 61.08 | 2.91 | 60.234 | 63.740 | 56.894 | 7.475 | 7.551 |
| Fe I | 6569.214 | 4.733 | －0．380 | 835.271 | $2.57 \mathrm{E}+08$ | 79.59 | 4.17 | 80.894 | 85.241 | 81.377 | 7.422 | 7.417 |
| Fe I | 6574.227 | 0.990 | －5．004 | 227.254 | $1.66 \mathrm{E}+04$ | 26.41 | 0.17 | 24.832 | 27.622 | 23.783 | 7.501 | 7.532 |
| Fe I | 6581.209 | 1.485 | －4．679 | 254.245 | $1.78 \mathrm{E}+07$ | 17.51 | 0.27 | 18.627 | 20.697 | 17.935 | 7.343 | 7.362 |
| Fe I | 6591.313 | 4.593 | －2．081 | 276.262 | $1.66 \mathrm{E}+08$ | 7.61 | 0.13 | 8.401 | 9.181 | 8.132 | 7.374 | 7.390 |
| Fe I | 6593.870 | 2.433 | －2．420 | 321.247 | $1.02 \mathrm{E}+08$ | 80.04 | 0.22 | 80.939 | 85.020 | 77.169 | 7.434 | 7.513 |
| Fe I | 6597.559 | 4.796 | －0．970 | 893.276 | $2.51 \mathrm{E}+08$ | 40.31 | 0.19 | 40.946 | 43.886 | 39.950 | 7.439 | 7.458 |
| Fe I | 6608.025 | 2.279 | －3．930 | 306.242 | $2.00 \mathrm{E}+08$ | 15.97 | 0.23 | 17.558 | 19.295 | 16.915 | 7.362 | 7.381 |
| Fe I | 6609.110 | 2.559 | －2．691 | 335.245 | $9.77 \mathrm{E}+07$ | 63.49 | 5.94 | 61.122 | 64.543 | 57.812 | 7.514 | 7.591 |
| Fe I | 6625.021 | 1.011 | －5．336 | －7．830 | $1.15 \mathrm{E}+04$ | 14.05 | 1.34 | 13.221 | 14.922 | 12.798 | 7.531 | 7.550 |
| Fe I | 6627.544 | 4.549 | －1．590 | 754.209 | $2.14 \mathrm{E}+08$ | 26.56 | 0.48 | 22.461 | 24.230 | 21.743 | 7.556 | 7.577 |
| Fe I | 6703.566 | 2.759 | －3．060 | 320.264 | $1.20 \mathrm{E}+08$ | 35.58 | 0.76 | 33.668 | 36.202 | 32.034 | 7.494 | 7.536 |
| Fe I | 6710.318 | 1.485 | －4．764 | 252.246 | $1.86 \mathrm{E}+07$ | 16.67 | 0.69 | 16.131 | 17.983 | 15.556 | 7.475 | 7.496 |
| Fe I | 6716.236 | 4.580 | －1．836 | 274.260 | $6.61 \mathrm{E}+07$ | 14.96 | 1.23 | 11.578 | 12.626 | 11.201 | 7.553 | 7.571 |
| Fe I | 6739.521 | 1.557 | －4．794 | 256.244 | $1.74 \mathrm{E}+07$ | 11.78 | 0.34 | 13.327 | 14.891 | 12.885 | 7.354 | 7.370 |
| Fe I | 6745.956 | 4.076 | －2．500 | －7．820 | $3.09 \mathrm{E}+07$ | 8.57 | 1.52 | 9.603 | 10.495 | 9.319 | 7.395 | 7.409 |
| Fe I | 6750.151 | 2.424 | －2．618 | 335.241 | $4.90 \mathrm{E}+06$ | 71.84 | 1.07 | 71.564 | 75.331 | 67.831 | 7.448 | 7.531 |
| Fe I | 6752.707 | 4.638 | －1．204 | 778.274 | $2.63 \mathrm{E}+08$ | 34.53 | 1.04 | 35.569 | 38.123 | 34.507 | 7.435 | 7.458 |
| Fe I | 6786.858 | 4.191 | －1．970 | 962.248 | $2.51 \mathrm{E}+08$ | 24.59 | 6.36 | 21.121 | 21.842 | 21.805 | 7.486 | 7.506 |
| Fe I | 6810.262 | 4.607 | －0．986 | 873.275 | $2.63 \mathrm{E}+08$ | 46.55 | 1.04 | 49.358 | 52.564 | 48.150 | 7.401 | 7.424 |
| Fe II | 4993.350 | 2.807 | －3．684 | 172.220 | $3.09 \mathrm{E}+08$ | 35.3 | 1.15 | 41.347 | 41.019 | 36.689 | 7.307 | 7.415 |
| Fe II | 5100.654 | 2.807 | －4．197 | 173.221 | $3.47 \mathrm{E}+08$ | 18.4 | 0.48 | 20.671 | 20.507 | 17.705 | 7.378 | 7.473 |
| Fe II | 5132.661 | 2.807 | －4．094 | 172.219 | $3.47 \mathrm{E}+08$ | 19.2 | 0.59 | 24.368 | 24.175 | 21.028 | 7.298 | 7.392 |
| Fe II | 5256.931 | 2.891 | －4．182 | 174.210 | $3.47 \mathrm{E}+08$ | 15.9 | 0.42 | 18.672 | 18.524 | 15.925 | 7.355 | 7.449 |
| Fe II | 5264.802 | 3.230 | －3．130 | 186.300 | $3.63 \mathrm{E}+08$ | 43.8 | 0.44 | 48.492 | 48.155 | 43.280 | 7.342 | 7.462 |
| Fe II | 5284.103 | 2.891 | －3．195 | 174.209 | $3.47 \mathrm{E}+08$ | 59.5 | 1.62 | 60.230 | 59.811 | 54.614 | 7.433 | 7.565 |
| Fe II | 5325.552 | 3.221 | －3．160 | 179.252 | $2.95 \mathrm{E}+08$ | 41.2 | 0.54 | 47.577 | 47.246 | 42.418 | 7.303 | 7.420 |
| Fe II | 5414.069 | 3.221 | －3．580 | 185.303 | $3.63 \mathrm{E}+08$ | 23.9 | 0.41 | 29.452 | 29.218 | 25.481 | 7.302 | 7.405 |
| Fe II | 6149.245 | 3.889 | －2．841 | 186.269 | $3.16 \mathrm{E}+08$ | 33.9 | 0.51 | 34.319 | 34.080 | 29.842 | 7.439 | 7.554 |
| Fe II | 6238.385 | 3.889 | －2．600 | 186.271 | $3.16 \mathrm{E}+08$ | 43.1 | 0.82 | 44.894 | 44.582 | 39.734 | 7.408 | 7.531 |
| Fe II | 6239.942 | 3.889 | －3．573 | 186.271 | $3.16 \mathrm{E}+08$ | 11.4 | 0.29 | 10.749 | 10.674 | 8.799 | 7.481 | 7.584 |
| Fe II | 6369.459 | 2.891 | －4．110 | 169.204 | $2.95 \mathrm{E}+08$ | 17.0 | 0.31 | 21.747 | 21.574 | 18.906 | 7.300 | 7.385 |
| Fe II | 6456.379 | 3.903 | －2．185 | 185.276 | $3.16 \mathrm{E}+08$ | 59.2 | 0.38 | 64.144 | 63.761 | 57.909 | 7.345 | 7.478 |
| Fe II | 6516.076 | 2.891 | －3．310 | 169.203 | $2.95 \mathrm{E}+08$ | 56.3 | 1.19 | 56.997 | 56.601 | 51.335 | 7.435 | 7.563 |


| HD122563 |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m}$ ) |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m} \AA)$ |  | $\varepsilon_{\mathrm{Fe}}$ (dex) |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 4789.6509 | 16.800 | 1.1300 | 12.034 | 21.48 | 4.821 | 4.698 |
| Fe | 4872.1377 | 69.600 | 0.8500 | 61.694 | 77.99 | 4.878 | . 636 |
| Fe I | 4882.1431 | 7.000 | 0.4700 | 5.396 | 9.82 | 4.835 | 4.665 |
| Fe I | 4891.4922 | 92.300 | 1.1500 | 86.383 | 101.15 | 4.877 | . 624 |
| Fe I | 4903.3101 | 52.700 | 0.5800 | 46.477 | 62.13 | 4.852 | 4.633 |
| Fe I | 4924.7695 | 31.500 | 0.3900 | 21.712 | 32.50 | 4.825 | . 797 |
| Fe I | 4938.8140 | 44.600 | 0.5600 | 38.634 | 53.80 | 4.844 | 4.647 |
| Fe I | 4950.1055 | 6.300 | 0.5900 | 5.329 | 9.72 | 4.831 | 4.606 |
| Fe I | 4957.2979 | 82.800 | 1.3000 | 73.649 | 87.67 | 4.901 | 4.710 |
| Fe I | 4966.0884 | 33.300 | 0.4200 | 25.428 | 39.54 | 4.833 | 4.709 |
| Fe I | 4967.8970 | 6.100 | 0.4800 | 5.763 | 11.27 | 4.819 | 4.455 |
| Fe I | 4985.2529 | 15.600 | 0.4400 | 11.967 | 22.03 | 4.829 | 4.630 |
| Fe I | 4985.5469 | 31.100 | 0.5200 | 27.814 | 41.20 | 4.830 | 4.614 |
| Fe I | 5001.8633 | 30.800 | 0.5600 | 27.876 | 46.00 | 4.830 | 4.456 |
| Fe I | 5002.7920 | 8.400 | 0.3800 | 6.067 | 10.95 | 4.833 | 4.704 |
| Fe I | 5014.9424 | 22.000 | 0.5900 | 18.627 | 32.85 | 4.831 | 4.538 |
| Fe I | 5022.2354 | 13.800 | 0.3000 | 12.198 | 22.50 | 4.826 | 4.509 |
| Fe I | 5028.1260 | 9.000 | 0.5000 | 8.942 | 16.55 | 4.811 | 4.429 |
| Fe I | 5044.2109 | 9.600 | 0.3500 | 7.754 | 13.07 | 4.835 | 4.678 |
| Fe I | 5049.8198 | 74.100 | 0.7500 | 64.330 | 77.41 | 4.904 | . 748 |
| Fe I | 5068.7656 | 41.900 | 0.8200 | 36.853 | 52.20 | 4.839 | 4.623 |
| Fe I | 5079.2227 | 43.800 | 0.5800 | 33.027 | 46.25 | 4.847 | 4.778 |
| Fe I | 5090.7729 | 8.200 | 0.4000 | 5.411 | 10.73 | 4.831 | 4.702 |
| Fe I | 5133.6880 | 31.300 | 0.7000 | 28.161 | 46.70 | 4.832 | 4.446 |
| Fe I | 5150.8394 | 76.100 | 0.7900 | 60.815 | 76.01 | 4.889 | 4.811 |
| Fe I | 5151.9106 | 64.300 | 0.6300 | 43.117 | 59.22 | 4.839 | 4.866 |
| Fe I | 5162.2725 | 26.200 | 0.5500 | 16.164 | 29.60 | 4.799 | 4.755 |
| Fe I | 5195.4717 | 13.200 | 0.4100 | 12.427 | 22.97 | 4.819 | 4.444 |
| Fe I | 5198.7109 | 37.200 | 0.5300 | 29.090 | 41.85 | 4.842 | 4.744 |
| Fe I | 5215.1802 | 27.800 | 0.3600 | 25.638 | 41.08 | 4.825 | 4.504 |
| Fe I | 5217.3892 | 23.200 | 0.6300 | 20.737 | 33.55 | 4.827 | 4.570 |
| Fe I | 5229.8447 | 23.600 | 0.5900 | 20.532 | 34.56 | 4.828 | 4.554 |
| Fe I | 5232.9399 | 92.600 | 0.9500 | 87.507 | 101.28 | 4.867 | 4.636 |
| Fe | 5242.4907 | 12.100 | 0.4300 | 9.002 | 16.82 | 4.827 | 4.656 |
| Fe I | 5253.4619 | 9.200 | 0.2900 | 6.361 | 11.73 | 4.830 | 4.714 |
| Fe I | 5263.3062 | 27.200 | 0.4400 | 25.270 | 40.30 | 4.824 | 4.510 |
| Fe I | 5273.1636 | 22.600 | 0.4600 | 19.118 | 32.18 | 4.829 | 4.590 |
| Fe I | 5281.7896 | 43.900 | 0.4400 | 41.602 | 57.94 | 4.827 | 4.526 |
| Fe I | 5307.3608 | 33.200 | 0.7100 | 28.839 | 41.43 | 4.837 | 4.670 |
| Fe I | 5324.1787 | 71.800 | 0.8200 | 65.971 | 83.82 | 4.864 | 4.554 |
| Fe I | 5339.9292 | 39.700 | 0.4800 | 36.511 | 53.85 | 4.832 | 4.522 |
| Fe I | 5364.8711 | 19.400 | 0.6000 | 13.335 | 25.11 | 4.823 | 4.682 |
| Fe I | 5365.3989 | 10.000 | 0.4500 | 9.386 | 17.70 | 4.818 | 4.461 |
| Fe I | 5367.4658 | 23.900 | 0.3500 | 20.673 | 36.91 | 4.832 | 4.480 |
| Fe I | 5369.9614 | 27.300 | 0.4100 | 25.798 | 44.47 | 4.823 | 4.355 |
| Fe I | 5383.3687 | 37.700 | 0.7100 | 32.958 | 54.11 | 4.842 | 4.438 |
| Fe I | 5393.1670 | 38.100 | 0.5300 | 34.608 | 51.12 | 4.833 | 4.553 |
| Fe I | 5400.5010 | 10.000 | 0.3900 | 7.307 | 14.64 | 4.831 | 4.626 |
| Fe I | 5410.9097 | 19.800 | 0.3900 | 17.020 | 31.40 | 4.831 | 4.490 |
| Fe I | 5415.1987 | 32.000 | 0.6200 | 29.161 | 49.34 | 4.831 | 4.382 |
| Fe I | 5445.0420 | 14.200 | 0.5100 | 9.390 | 18.52 | 4.820 | 4.691 |
| Fe I | 5463.2754 | 12.000 | 0.4600 | 10.054 | 19.67 | 4.830 | 4.520 |
| Fe I | 5476.5640 | 12.600 | 0.6300 | 10.356 | 20.46 | 4.827 | 4.527 |
| Fe I | 5567.3911 | 6.600 | 0.4000 | 5.073 | 8.71 | 4.843 | 4.700 |
| Fe I | 5569.6182 | 37.700 | 0.7900 | 32.505 | 51.10 | 4.838 | 4.543 |
| Fe I | 5572.8423 | 50.000 | 0.4600 | 44.752 | 64.76 | 4.846 | 4.506 |
| Fe I | 5586.7554 | 59.000 | 0.9800 | 55.838 | 75.867 | 4.837 | 4.435 |
| Fe I | 5615.6440 | 71.400 | 0.9100 | 66.769 | 85.821 | 4.852 | 4.497 |
| Fe I | 5658.8164 | 26.900 | 0.6500 | 24.155 | 39.213 | 4.827 | 4.535 |
| Fe I | 5662.5161 | 7.300 | 0.3700 | 6.491 | 13.523 | 4.824 | 4.445 |
| Fe I | 5701.5444 | 14.600 | 0.4700 | 13.083 | 20.933 | 4.828 | 4.626 |
| Fe I | 6065.4819 | 47.300 | 0.3700 | 37.824 | 52.171 | 4.856 | 4.742 |
| Fe I | 6136.6147 | 67.400 | 0.5800 | 55.458 | 69.846 | 4.892 | 4.772 |
| Fe I | 6136.9937 | 10.500 | 0.3500 | 7.325 | 12.168 | 4.843 | 4.758 |
| Fe I | 6137.6914 | 57.800 | 0.6100 | 46.269 | 60.960 | 4.873 | 4.766 |
| Fe I | 6173.3345 | 11.300 | 0.3700 | 7.969 | 13.216 | 4.842 | 4.754 |
| Fe I | 6191.5576 | 64.100 | 0.8600 | 56.317 | 70.750 | 4.873 | 4.698 |
| Fe I | 6200.3125 | 10.500 | 0.3700 | 7.513 | 12.439 | 4.843 | 4.749 |
| Fe I | 6213.4292 | 22.500 | 0.3000 | 17.848 | 27.757 | 4.839 | 4.712 |
| Fe I | 6219.2803 | 28.400 | 0.3700 | 20.694 | 31.594 | 4.838 | 4.763 |
| Fe I | 6230.7222 | 68.200 | 0.7100 | 55.223 | 69.814 | 4.895 | 4.786 |
| Fel | 6232.6401 | 8.200 | 0.4500 | 5.168 | 10.483 | 4.823 | 4.714 |
| Fe I | 6246.3179 | 17.800 | 0.4100 | 15.594 | 28.047 | 4.826 | 4.521 |
| Fe I | 6252.5547 | 54.500 | 0.4700 | 43.118 | 57.644 | 4.869 | 4.767 |
| Fe I | 6254.2578 | 25.000 | 0.3300 | 17.015 | 26.544 | 4.832 | 4.787 |
| Fe I | 6265.1323 | 25.300 | 0.4200 | 17.609 | 27.386 | 4.835 | 4.779 |
| Fe I | 6297.7925 | 15.400 | 1.1500 | 10.911 | 17.713 | 4.839 | 4.758 |
| Fe I | 6301.5000 | 18.200 | 0.3900 | 14.939 | 27.665 | 4.828 | 4.557 |
| Fe I | 6322.6851 | 12.300 | 0.3800 | 8.108 | 13.357 | 4.838 | 4.783 |

HD122563

| $\mathrm{EW}_{\text {obs }}$ (m $\left.\AA\right)$ |  |  |  |  |  |  |  |  | EW $_{\text {calc }}(\mathrm{m} \AA)$ |  | $\varepsilon_{\text {Fe }}(\mathrm{dex})$ |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |  |  |  |  |  |
| Fe I | 6335.3301 | 38.900 | 0.4000 | 32.017 | 45.739 | 4.847 | 4.708 |  |  |  |  |  |
| Fe I | 6393.6006 | 60.500 | 0.6700 | 55.222 | 69.990 | 4.855 | 4.646 |  |  |  |  |  |
| Fe I | 6400.0005 | 37.700 | 0.4400 | 35.195 | 54.736 | 4.827 | 4.441 |  |  |  |  |  |
| Fe I | 6400.3169 | 16.500 | 0.3600 | 10.415 | 20.145 | 4.801 | 4.729 |  |  |  |  |  |
| Fe I | 6408.0176 | 11.700 | 0.5700 | 7.916 | 15.583 | 4.823 | 4.686 |  |  |  |  |  |
| Fe I | 6411.6479 | 21.900 | 0.3500 | 19.126 | 33.851 | 4.827 | 4.510 |  |  |  |  |  |
| Fe I | 6421.3501 | 45.300 | 0.3800 | 35.420 | 49.538 | 4.855 | 4.753 |  |  |  |  |  |
| Fe I | 6430.8452 | 55.300 | 0.4800 | 42.672 | 57.509 | 4.869 | 4.781 |  |  |  |  |  |
| Fe I | 6494.9805 | 80.300 | 0.8400 | 67.353 | 81.938 | 4.921 | 4.783 |  |  |  |  |  |
| Fe I | 6546.2383 | 32.500 | 0.3900 | 29.516 | 43.026 | 4.832 | 4.616 |  |  |  |  |  |
| Fe I | 6592.9126 | 38.200 | 0.4700 | 34.707 | 48.883 | 4.835 | 4.624 |  |  |  |  |  |
| Fe I | 6593.8696 | 18.800 | 0.5000 | 12.660 | 20.288 | 4.836 | 4.783 |  |  |  |  |  |
| Fe I | 6750.1514 | 12.900 | 0.3900 | 8.729 | 14.428 | 4.841 | 4.771 |  |  |  |  |  |
| Fe II | 4993.3501 | 7.500 | 0.3600 | 5.153 | 5.057 | 4.864 | 4.863 |  |  |  |  |  |
| Fe II | 5197.5674 | 39.000 | 0.4100 | 39.011 | 38.548 | 4.809 | 4.815 |  |  |  |  |  |
| Fe II | 5234.6226 | 42.700 | 0.4900 | 34.641 | 34.230 | 4.870 | 4.870 |  |  |  |  |  |
| Fe II | 5264.8022 | 7.800 | 0.4000 | 5.868 | 5.764 | 4.859 | 4.860 |  |  |  |  |  |
| Fe II | 5284.1030 | 18.800 | 0.5200 | 11.974 | 11.774 | 4.848 | 4.845 |  |  |  |  |  |
| Fe II | 5325.5522 | 7.300 | 0.3100 | 5.663 | 5.563 | 4.857 | 4.859 |  |  |  |  |  |
| Fe II | 5362.8613 | 26.200 | 0.5000 | 19.547 | 19.239 | 4.857 | 4.856 |  |  |  |  |  |
| Fe II | 5425.2485 | 7.400 | 0.6000 | 5.313 | 5.219 | 4.864 | 4.864 |  |  |  |  |  |
| Fe II | 6247.5571 | 8.300 | 0.3900 | 5.193 | 5.101 | 4.870 | 4.869 |  |  |  |  |  |


| HD140283 |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m} \AA)$ |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m}$ ) |  | $\varepsilon_{\mathrm{Fe}}$ (dex) |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 4872.1377 | 28.600 | 0.69 | 29.760 | 40.216 | 5.066 | 4.843 |
| Fe I | 4891.4922 | 54.300 | 0.90 | 52.212 | 64.143 | 5.127 | 4.890 |
| Fe I | 4903.3101 | 18.500 | 0.34 | 17.706 | 24.973 | 5.112 | 4.915 |
| Fe I | 4938.8140 | 12.900 | 0.24 | 13.116 | 18.791 | 5.082 | 4.888 |
| Fe I | 4939.6865 | 9.900 | 0.21 | 8.240 | 11.908 | 5.171 | 4.998 |
| Fe I | 4957.2979 | 40.200 | 0.73 | 39.098 | 49.806 | 5.110 | 4.897 |
| Fe I | 4966.0884 | 10.500 | 0.19 | 9.314 | 13.901 | 5.143 | 4.949 |
| Fe I | 4985.2529 | 6.200 | 0.11 | 5.526 | 8.528 | 5.138 | 4.938 |
| Fe I | 4985.5469 | 7.400 | 0.15 | 8.157 | 11.908 | 5.048 | 4.859 |
| Fe I | 4994.1294 | 14.800 | 0.27 | 12.906 | 18.203 | 5.154 | 4.978 |
| Fe I | 5001.8633 | 14.300 | 0.20 | 14.657 | 21.975 | 5.078 | 4.858 |
| Fe I | 5014.9424 | 9.000 | 0.12 | 9.213 | 14.066 | 5.080 | 4.866 |
| Fe I | 5022.2354 | 6.000 | 0.10 | 5.800 | 8.964 | 5.104 | 4.898 |
| Fe I | 5049.8198 | 24.500 | 0.34 | 24.283 | 31.618 | 5.095 | 4.922 |
| Fe I | 5068.7656 | 11.400 | 0.25 | 12.484 | 18.093 | 5.049 | 4.849 |
| Fe I | 5083.3384 | 16.500 | 0.26 | 15.233 | 20.953 | 5.128 | 4.957 |
| Fe I | 5107.4473 | 12.400 | 0.26 | 10.600 | 15.143 | 5.160 | 4.986 |
| Fe I | 5107.6406 | 14.100 | 0.26 | 14.921 | 20.136 | 5.062 | 4.894 |
| Fe I | 5133.6880 | 15.300 | 0.20 | 16.823 | 25.072 | 5.043 | 4.812 |
| Fe I | 5150.8394 | 10.800 | 0.18 | 12.489 | 17.640 | 5.025 | 4.833 |
| Fe I | 5151.9106 | 7.000 | 0.12 | 6.438 | 9.223 | 5.125 | 4.957 |
| Fe I | 5171.5962 | 44.000 | 0.60 | 43.086 | 51.050 | 5.109 | 4.935 |
| Fe I | 5194.9414 | 25.700 | 0.36 | 26.706 | 34.064 | 5.067 | 4.896 |
| Fe I | 5198.7109 | 6.800 | 0.16 | 6.120 | 8.706 | 5.136 | 4.972 |
| Fe I | 5215.1802 | 8.300 | 0.10 | 9.154 | 14.040 | 5.048 | 4.828 |
| Fe I | 5216.2739 | 21.300 | 0.25 | 22.386 | 29.186 | 5.062 | 4.892 |
| Fe I | 5217.3892 | 6.500 | 0.13 | 6.708 | 10.241 | 5.077 | 4.871 |
| Fe I | 5229.8447 | 7.800 | 0.30 | 7.051 | 11.034 | 5.132 | 4.922 |
| Fe I | 5232.9399 | 50.800 | 0.63 | 51.509 | 62.816 | 5.078 | 4.847 |
| Fe I | 5263.3062 | 8.300 | 0.16 | 8.877 | 13.594 | 5.061 | 4.845 |
| Fe I | 5281.7896 | 14.200 | 0.22 | 15.439 | 22.311 | 5.051 | 4.840 |
| Fe I | 5324.1787 | 35.100 | 0.29 | 35.677 | 48.082 | 5.079 | 4.830 |
| Fe I | 5339.9292 | 13.300 | 0.14 | 14.401 | 21.430 | 5.053 | 4.831 |
| Fe I | 5364.8711 | 9.300 | 0.13 | 7.987 | 12.441 | 5.157 | 4.946 |
| Fe I | 5367.4658 | 12.100 | 0.18 | 12.872 | 19.773 | 5.061 | 4.831 |
| Fe I | 5393.1670 | 12.100 | 0.14 | 13.000 | 19.345 | 5.057 | 4.840 |
| Fe I | 5410.9097 | 10.100 | 0.14 | 10.565 | 16.431 | 5.070 | 4.841 |
| Fe I | 5463.2754 | 5.600 | 0.17 | 5.827 | 9.279 | 5.073 | 4.851 |
| Fe I | 5501.4648 | 15.400 | 0.16 | 12.911 | 18.083 | 5.172 | 5.003 |
| Fe I | 5506.7788 | 22.600 | 0.26 | 19.119 | 26.119 | 5.176 | 5.000 |
| Fe I | 5569.6182 | 13.500 | 0.14 | 13.306 | 20.598 | 5.097 | 4.862 |
| Fe I | 5572.8423 | 20.600 | 0.25 | 20.707 | 30.768 | 5.087 | 4.843 |
| Fe I | 5576.0889 | 6.700 | 0.14 | 5.968 | 9.657 | 5.137 | 4.914 |
| Fe I | 5615.6440 | 35.600 | 0.33 | 36.833 | 50.318 | 5.067 | 4.797 |
| Fe I | 5658.8164 | 8.500 | 0.21 | 8.689 | 13.555 | 5.081 | 4.858 |
| Fe I | 6065.4819 | 11.800 | 0.18 | 10.240 | 14.443 | 5.155 | 4.986 |
| Fe I | 6136.6147 | 19.200 | 0.14 | 17.746 | 23.884 | 5.131 | 4.961 |
| Fe I | 6137.6914 | 15.500 | 0.15 | 13.785 | 19.014 | 5.147 | 4.978 |
| Fe I | 6230.7222 | 19.100 | 0.23 | 18.288 | 24.614 | 5.113 | 4.939 |
| Fe I | 6246.3179 | 5.800 | 0.15 | 5.601 | 9.273 | 5.104 | 4.866 |
| Fe I | 6252.5547 | 11.200 | 0.20 | 11.257 | 15.613 | 5.088 | 4.917 |
| Fe I | 6318.0181 | 8.400 | 0.17 | 8.255 | 11.676 | 5.098 | 4.927 |
| Fe I | 6335.3301 | 6.300 | 0.20 | 6.511 | 9.275 | 5.076 | 4.905 |
| Fe I | 6393.6006 | 15.200 | 0.17 | 17.145 | 23.138 | 5.030 | 4.852 |
| Fe I | 6400.0005 | 15.100 | 0.25 | 15.057 | 23.712 | 5.091 | 4.836 |
| Fe I | 6411.6479 | 8.300 | 0.28 | 7.253 | 12.048 | 5.145 | 4.907 |
| Fe I | 6421.3501 | 9.700 | 0.16 | 7.786 | 11.044 | 5.189 | 5.025 |
| Fe I | 6430.8452 | 11.200 | 0.21 | 9.802 | 13.709 | 5.152 | 4.986 |
| Fe I | 6494.9805 | 24.300 | 1.12 | 24.668 | 32.162 | 5.081 | 4.903 |
| Fe I | 6546.2383 | 7.200 | 0.22 | 7.635 | 11.001 | 5.064 | 4.882 |
| Fe I | 6592.9126 | 8.300 | 0.23 | 9.358 | 13.274 | 5.037 | 4.854 |
| Fe II | 5234.6226 | 14.500 | 0.18 | 14.928 | 14.810 | 5.074 | 5.079 |
| Fe II | 5316.6089 | 25.900 | 0.60 | 28.472 | 28.302 | 5.028 | 5.032 |
| Fe II | 5362.8613 | 7.600 | 0.11 | 7.227 | 7.170 | 5.114 | 5.118 |


| HD84937 |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m} \AA)$ |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m}$ ) |  | $\varepsilon_{\mathrm{Fe}}$ (dex) |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 4872.1377 | 24.900 | 0.89 | 28.151 | 37.736 | 5.347 | 5.149 |
| Fe I | 4891.4922 | 51.600 | 1.16 | 50.917 | 62.398 | 5.432 | 5.207 |
| Fe I | 4903.3101 | 17.400 | 0.27 | 16.351 | 22.647 | 5.451 | 5.270 |
| Fe I | 4920.5024 | 62.600 | 1.17 | 60.877 | 72.129 | 5.449 | 5.228 |
| Fe I | 4938.8140 | 11.400 | 0.33 | 11.979 | 16.801 | 5.397 | 5.219 |
| Fe I | 4957.2979 | 36.500 | 1.33 | 37.361 | 47.412 | 5.404 | 5.204 |
| Fe I | 4966.0884 | 11.800 | 0.55 | 9.175 | 13.259 | 5.534 | 5.360 |
| Fe I | 4985.2529 | 6.300 | 0.21 | 6.094 | 8.988 | 5.435 | 5.249 |
| Fe I | 4985.5469 | 6.500 | 0.26 | 7.358 | 10.452 | 5.366 | 5.193 |
| Fe I | 4994.1294 | 8.400 | 0.30 | 8.558 | 11.739 | 5.412 | 5.254 |
| Fe I | 5001.8633 | 15.100 | 0.30 | 15.888 | 22.860 | 5.395 | 5.195 |
| Fe I | 5014.9424 | 9.600 | 0.27 | 10.154 | 14.823 | 5.394 | 5.200 |
| Fe I | 5022.2354 | 6.100 | 0.21 | 6.461 | 9.529 | 5.395 | 5.207 |
| Fe I | 5049.8198 | 20.600 | 0.51 | 20.654 | 26.963 | 5.419 | 5.257 |
| Fe I | 5068.7656 | 11.000 | 0.36 | 11.494 | 16.280 | 5.400 | 5.218 |
| Fe I | 5079.2227 | 6.800 | 0.22 | 5.802 | 8.070 | 5.490 | 5.338 |
| Fe I | 5083.3384 | 10.500 | 0.21 | 10.218 | 13.827 | 5.433 | 5.279 |
| Fe I | 5127.3594 | 5.400 | 0.25 | 5.121 | 7.152 | 5.443 | 5.287 |
| Fe I | 5133.6880 | 19.200 | 0.41 | 18.959 | 27.123 | 5.427 | 5.217 |
| Fe I | 5150.8394 | 6.500 | 0.29 | 8.317 | 11.472 | 5.313 | 5.149 |
| Fe I | 5162.2725 | 14.600 | 0.33 | 10.046 | 14.861 | 5.595 | 5.411 |
| Fe I | 5171.5962 | 33.800 | 0.63 | 36.058 | 43.707 | 5.374 | 5.213 |
| Fe I | 5194.9414 | 19.100 | 0.43 | 20.618 | 26.673 | 5.379 | 5.221 |
| Fe I | 5195.4717 | 7.000 | 0.31 | 7.589 | 11.210 | 5.384 | 5.193 |
| Fe I | 5215.1802 | 7.400 | 0.26 | 8.882 | 13.217 | 5.340 | 5.140 |
| Fe I | 5216.2739 | 14.000 | 0.30 | 17.038 | 22.389 | 5.321 | 5.165 |
| Fe I | 5217.3892 | 6.400 | 0.21 | 6.421 | 9.499 | 5.419 | 5.231 |
| Fe I | 5229.8447 | 8.900 | 0.18 | 6.858 | 10.375 | 5.533 | 5.344 |
| Fe I | 5232.9399 | 49.400 | 0.80 | 50.387 | 61.149 | 5.403 | 5.191 |
| Fe I | 5263.3062 | 8.600 | 0.29 | 8.597 | 12.774 | 5.420 | 5.224 |
| Fe I | 5273.1636 | 7.200 | 0.31 | 6.251 | 9.414 | 5.481 | 5.290 |
| Fe I | 5281.7896 | 12.700 | 0.26 | 14.487 | 20.520 | 5.358 | 5.167 |
| Fe I | 5324.1787 | 34.200 | 0.52 | 35.157 | 46.876 | 5.401 | 5.173 |
| Fe I | 5339.9292 | 12.700 | 0.32 | 14.007 | 20.329 | 5.374 | 5.172 |
| Fe I | 5364.8711 | 12.800 | 0.33 | 9.531 | 14.162 | 5.558 | 5.368 |
| Fe I | 5367.4658 | 16.200 | 0.36 | 15.110 | 22.155 | 5.455 | 5.246 |
| Fe I | 5369.9614 | 18.400 | 0.24 | 18.882 | 27.565 | 5.406 | 5.186 |
| Fe I | 5383.3687 | 21.100 | 0.28 | 24.381 | 35.081 | 5.337 | 5.112 |
| Fe I | 5393.1670 | 11.100 | 0.27 | 12.559 | 18.228 | 5.363 | 5.165 |
| Fe I | 5397.1279 | 51.600 | 0.94 | 49.334 | 56.511 | 5.462 | 5.313 |
| Fe I | 5410.9097 | 13.500 | 0.30 | 12.568 | 18.675 | 5.455 | 5.247 |
| Fe I | 5415.1987 | 21.700 | 0.33 | 21.943 | 31.894 | 5.414 | 5.183 |
| Fe I | 5424.0679 | 24.400 | 0.34 | 19.705 | 28.851 | 5.539 | 5.314 |
| Fe I | 5434.5234 | 39.400 | 0.81 | 38.526 | 46.194 | 5.437 | 5.277 |
| Fe I | 5445.0420 | 9.200 | 0.21 | 6.311 | 9.606 | 5.585 | 5.399 |
| Fe I | 5463.2754 | 8.500 | 0.24 | 6.984 | 10.582 | 5.507 | 5.312 |
| Fe I | 5476.5640 | 6.100 | 0.35 | 5.818 | 8.965 | 5.440 | 5.237 |
| Fe I | 5569.6182 | 13.600 | 0.24 | 13.246 | 19.919 | 5.432 | 5.216 |
| Fe I | 5572.8423 | 19.100 | 0.31 | 20.606 | 29.951 | 5.380 | 5.155 |
| Fe I | 5586.7554 | 27.600 | 0.33 | 28.449 | 39.845 | 5.402 | 5.166 |
| Fe I | 5615.6440 | 36.500 | 0.48 | 36.706 | 49.536 | 5.416 | 5.169 |
| Fe I | 5658.8164 | 8.700 | 0.13 | 8.577 | 12.956 | 5.426 | 5.222 |
| Fe I | 6065.4819 | 9.400 | 0.22 | 8.710 | 12.097 | 5.455 | 5.293 |
| Fe I | 6136.6147 | 11.900 | 0.86 | 15.022 | 20.110 | 5.306 | 5.145 |
| Fe I | 6137.6914 | 11.200 | 0.30 | 11.775 | 16.064 | 5.396 | 5.232 |
| Fe I | 6191.5576 | 12.100 | 0.24 | 15.229 | 20.332 | 5.307 | 5.146 |
| Fe I | 6252.5547 | 8.300 | 0.35 | 9.242 | 12.660 | 5.371 | 5.210 |
| Fe I | 6393.6006 | 11.800 | 0.40 | 14.397 | 19.325 | 5.323 | 5.161 |
| Fe I | 6430.8452 | 8.700 | 0.34 | 7.680 | 10.608 | 5.477 | 5.322 |
| Fe I | 6494.9805 | 19.700 | 0.64 | 21.126 | 27.580 | 5.382 | 5.217 |
| Fe II | 4923.9214 | 70.000 | 1.46 | 73.108 | 72.962 | 5.348 | 5.352 |
| Fe II | 5018.4355 | 76.400 | 1.93 | 80.312 | 80.232 | 5.330 | 5.332 |
| Fe II | 5234.6226 | 18.400 | 0.32 | 18.677 | 18.584 | 5.412 | 5.414 |
| Fe II | 5316.6089 | 33.200 | 0.82 | 33.994 | 33.859 | 5.402 | 5.405 |


| $\delta$ Eri |  |  |  |  |  |  |  | $\delta$ Eri |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m}$ ) |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m} \AA)$ |  | $\varepsilon_{\mathrm{Fe}}$ (dex) |  |  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m}$ ) |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m}$ ) |  | $\varepsilon_{\mathrm{Fe}}$ (dex) |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE | el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 4794.3540 | 38.500 | 1.14 | 32.624 | 34.233 | 7.653 | 7.613 | Fe I | 5859.5864 | 94.600 | 1.86 | 102.821 | 105.349 | 7.382 | 7.343 |
| Fe I | 4799.4058 | 61.200 | 1.22 | 54.013 | 55.569 | 7.693 | 7.652 | Fe I | 5873.2124 | 38.200 | 0.53 | 31.944 | 33.344 | 7.654 | 7.620 |
| Fe I | 4802.8799 | 82.100 | 2.41 | 79.223 | 80.840 | 7.578 | 7.540 | Fe I | 5879.4868 | 16.100 | 1.24 | 14.387 | 15.176 | 7.574 | 7.544 |
| Fe I | 4809.9385 | 41.500 | 1.59 | 35.942 | 37.323 | 7.646 | 7.611 | Fe I | 5881.2798 | 29.300 | 0.53 | 28.121 | 29.477 | 7.540 | 7.506 |
| Fe I | 4874.3530 | 42.500 | 3.21 | 38.961 | 40.458 | 7.599 | 7.561 | Fe I | 5883.8164 | 91.500 | 1.36 | 88.418 | 90.222 | 7.566 | 7.533 |
| Fe I | 4875.8770 | 85.000 | 2.35 | 82.352 | 83.862 | 7.567 | 7.534 | Fe I | 5898.2153 | 25.500 | 0.59 | 23.270 | 24.546 | 7.571 | 7.536 |
| Fe I | 4882.1431 | 103.300 | 1.90 | 103.754 | 105.334 | 7.502 | 7.476 | Fe I | 5905.6714 | 73.000 | 1.40 | 77.824 | 80.563 | 7.418 | 7.367 |
| Fe I | 4885.4302 | 92.300 | 2.48 | 97.827 | 99.317 | 7.407 | 7.379 | Fe I | 5909.9722 | 64.500 | 0.78 | 57.946 | 60.048 | 7.667 | 7.614 |
| Fe I | 4892.8589 | 74.100 | 1.74 | 67.277 | 69.215 | 7.658 | 7.616 | Fe I | 5927.7886 | 57.500 | 1.29 | 61.429 | 63.856 | 7.428 | 7.380 |
| Fe I | 4905.1328 | 59.800 | 1.00 | 58.354 | 59.912 | 7.546 | 7.507 | Fe I | 5929.6763 | 55.600 | 1.24 | 50.531 | 52.418 | 7.623 | 7.580 |
| Fe I | 4907.7319 | 87.200 | 2.34 | 88.531 | 89.971 | 7.483 | 7.455 | Fe I | 5952.7178 | 86.800 | 2.09 | 82.089 | 83.936 | 7.600 | 7.565 |
| Fe I | 4917.2300 | 85.300 | 1.59 | 79.097 | 81.125 | 7.636 | 7.594 | Fe I | 5969.5620 | 10.900 | 0.37 | 8.086 | 8.566 | 7.660 | 7.631 |
| Fe I | 4918.0127 | 74.400 | 1.43 | 68.250 | 70.216 | 7.642 | 7.600 | Fe I | 5976.7769 | 92.300 | 1.28 | 90.864 | 92.435 | 7.536 | 7.508 |
| Fe I | 4950.1055 | 103.600 | 2.13 | 103.789 | 105.477 | 7.507 | 7.479 | Fe I | 5984.8149 | 100.100 | 1.04 | 109.203 | 113.047 | 7.381 | 7.329 |
| Fe I | 4961.9136 | 52.400 | 1.76 | 52.147 | 53.704 | 7.516 | 7.478 | Fe I | 5987.0649 | 84.900 | 0.82 | 86.849 | 90.846 | 7.476 | 7.411 |
| Fe I | 4962.5718 | 73.000 | 1.51 | 74.767 | 76.606 | 7.473 | 7.435 | Fe I | 6003.0112 | 108.200 | 1.79 | 105.589 | 107.197 | 7.551 | 7.526 |
| Fe I | 4969.9175 | 96.000 | 1.63 | 101.992 | 104.500 | 7.413 | 7.374 | Fe I | 6007.9595 | 80.000 | 1.06 | 80.373 | 82.859 | 7.503 | 7.455 |
| Fe I | 4986.2227 | 65.300 | 1.61 | 67.270 | 69.137 | 7.467 | 7.428 | Fe I | 6008.5557 | 113.900 | 2.18 | 115.477 | 117.117 | 7.488 | 7.464 |
| Fe I | 4999.1123 | 51.400 | 1.67 | 50.012 | 51.665 | 7.544 | 7.504 | Fe I | 6015.2437 | 21.200 | 0.42 | 25.493 | 27.236 | 7.391 | 7.349 |
| Fe I | 5002.7920 | 106.600 | 1.44 | 107.965 | 109.721 | 7.488 | 7.460 | Fe I | 6024.0576 | 123.200 | 1.45 | 132.149 | 135.122 | 7.406 | 7.372 |
| Fe I | 5022.2354 | 124.600 | 2.29 | 139.486 | 141.898 | 7.330 | 7.302 | Fe I | 6027.0508 | 84.400 | 1.53 | 88.924 | 91.204 | 7.426 | 7.385 |
| Fe I | 5023.1860 | 54.600 | 1.68 | 53.406 | 55.171 | 7.538 | 7.497 | Fe I | 6034.0352 | 19.100 | 0.34 | 19.116 | 20.122 | 7.509 | 7.479 |
| Fe I | 5023.4976 | 49.800 | 1.07 | 44.170 | 45.772 | 7.641 | 7.602 | Fe I | 6056.0044 | 90.300 | 1.41 | 98.789 | 102.160 | 7.377 | 7.326 |
| Fe I | 5025.3027 | 27.600 | 1.36 | 30.656 | 31.967 | 7.432 | 7.401 | Fe I | 6078.4912 | 95.600 | 1.59 | 94.859 | 98.504 | 7.522 | 7.465 |
| Fe I | 5029.6177 | 77.400 | 3.73 | 71.943 | 73.637 | 7.648 | 7.604 | Fe I | 6079.0078 | 65.000 | 0.97 | 60.132 | 62.248 | 7.612 | 7.567 |
| Fe I | 5048.4355 | 95.600 | 4.13 | 90.930 | 92.597 | 7.604 | 7.571 | Fe I | 6093.6431 | 48.600 | 0.72 | 43.302 | 45.200 | 7.630 | 7.585 |
| Fe I | 5054.6426 | 61.500 | 2.42 | 60.029 | 61.631 | 7.552 | 7.506 | Fe I | 6096.6641 | 61.800 | 0.89 | 55.813 | 57.480 | 7.642 | 7.605 |
| Fe I | 5067.1494 | 90.700 | 1.65 | 83.920 | 85.808 | 7.642 | 7.605 | Fe I | 6098.2441 | 32.400 | 0.56 | 25.522 | 26.781 | 7.685 | 7.649 |
| Fe I | 5143.7227 | 51.200 | 1.96 | 54.537 | 56.574 | 7.421 | 7.371 | Fe I | 6120.2466 | 30.800 | 0.42 | 23.304 | 25.581 | 7.699 | 7.637 |
| Fe I | 5236.2021 | 51.300 | 1.09 | 56.845 | 58.603 | 7.378 | 7.339 | Fe I | 6127.9063 | 70.400 | 1.33 | 67.783 | 69.879 | 7.566 | 7.521 |
| Fe I | 5242.4907 | 118.700 | 2.32 | 122.347 | 124.717 | 7.459 | 7.426 | Fe I | 6151.6172 | 81.300 | 1.98 | 76.019 | 79.352 | 7.642 | 7.557 |
| Fe I | 5243.7764 | 84.900 | 3.74 | 77.506 | 79.412 | 7.662 | 7.623 | Fe I | 6157.7280 | 83.700 | 0.98 | 84.440 | 86.694 | 7.496 | 7.452 |
| Fe I | 5253.0210 | 39.200 | 1.67 | 41.222 | 43.164 | 7.460 | 7.415 | Fe I | 6165.3599 | 65.600 | 0.99 | 64.006 | 66.122 | 7.545 | 7.499 |
| Fe I | 5285.1274 | 43.700 | 1.28 | 39.044 | 40.629 | 7.618 | 7.580 | Fe I | 6180.2026 | 87.900 | 1.18 | 80.480 | 83.485 | 7.685 | 7.611 |
| Fe I | 5288.5249 | 81.000 | 1.09 | 82.138 | 83.986 | 7.485 | 7.445 | Fe I | 6187.3979 | 15.700 | 0.66 | 12.848 | 13.756 | 7.620 | 7.583 |
| Fe I | 5293.9590 | 45.900 | 2.73 | 46.814 | 48.462 | 7.488 | 7.449 | Fe I | 6187.9893 | 72.900 | 0.77 | 69.003 | 70.772 | 7.592 | 7.555 |
| Fe I | 5294.5474 | 27.500 | 1.57 | 28.187 | 29.515 | 7.492 | 7.459 | Fe I | 6199.5063 | 17.400 | 0.45 | 13.411 | 14.405 | 7.655 | 7.615 |
| Fe I | 5295.3120 | 37.800 | 2.20 | 43.165 | 44.870 | 7.386 | 7.351 | Fe I | 6219.2803 | 123.600 | 2.06 | 122.495 | 127.732 | 7.527 | 7.447 |
| Fe I | 5307.3608 | 123.000 | 2.15 | 114.325 | 118.226 | 7.687 | 7.606 | Fe I | 6221.6719 | 10.400 | 0.42 | 7.978 | 8.944 | 7.643 | 7.586 |
| Fe I | 5315.0698 | 54.000 | 1.36 | 47.105 | 48.763 | 7.668 | 7.628 | Fe I | 6226.7344 | 51.300 | 0.82 | 46.983 | 48.738 | 7.607 | 7.567 |
| Fe I | 5320.0356 | 42.600 | 1.04 | 37.041 | 38.544 | 7.645 | 7.607 | Fe I | 6229.2261 | 68.300 | 0.90 | 65.234 | 67.670 | 7.587 | 7.525 |
| Fe I | 5321.1079 | 63.000 | 0.78 | 66.930 | 69.000 | 7.426 | 7.384 | Fe I | 6232.6401 | 110.600 | 2.20 | 111.283 | 113.438 | 7.500 | 7.467 |
| Fe I | 5322.0405 | 93.200 | 1.74 | 87.414 | 90.304 | 7.649 | 7.578 | Fe I | 6240.6460 | 81.500 | 1.88 | 75.770 | 79.009 | 7.661 | 7.573 |
| Fe I | 5373.7085 | 80.200 | 1.10 | 87.046 | 89.553 | 7.386 | 7.342 | Fe I | 6253.8286 | 36.100 | 1.07 | 42.212 | 44.063 | 7.373 | 7.336 |
| Fe I | 5379.5737 | 85.300 | 1.87 | 81.253 | 83.166 | 7.600 | 7.557 | Fe I | 6265.1323 | 121.900 | 1.94 | 115.919 | 121.127 | 7.609 | 7.522 |
| Fe I | 5401.2666 | 44.900 | 0.95 | 37.187 | 38.696 | 7.691 | 7.653 | Fe I | 6270.2236 | 81.200 | 1.33 | 79.495 | 82.293 | 7.551 | 7.485 |
| Fe I | 5412.7837 | 35.500 | 0.95 | 36.657 | 38.184 | 7.482 | 7.448 | Fe I | 6271.2778 | 50.000 | 1.32 | 47.475 | 49.505 | 7.569 | 7.521 |
| Fe I | 5417.0332 | 50.800 | 1.44 | 43.834 | 45.518 | 7.669 | 7.629 | Fe I | 6290.5430 | 16.600 | 0.19 | 15.332 | 16.451 | 7.555 | 7.515 |
| Fe I | 5441.3389 | 45.100 | 0.91 | 46.397 | 48.030 | 7.480 | 7.443 | Fe I | 6293.9243 | 25.600 | 0.31 | 20.144 | 21.294 | 7.665 | 7.629 |
| Fe I | 5460.8726 | 24.700 | 0.64 | 26.439 | 27.831 | 7.463 | 7.427 | Fe I | 6297.7925 | 107.300 | 1.42 | 101.484 | 105.933 | 7.624 | 7.536 |
| Fe I | 5466.3960 | 97.300 | 0.80 | 99.370 | 101.502 | 7.477 | 7.442 | Fe I | 6311.4995 | 58.000 | 0.64 | 51.843 | 54.116 | 7.661 | 7.603 |
| Fe I | 5466.9873 | 59.300 | 0.44 | 53.255 | 54.959 | 7.665 | 7.620 | Fe I | 6315.8110 | 64.500 | 0.71 | 59.600 | 61.634 | 7.621 | 7.574 |
| Fe I | 5487.1450 | 56.100 | 1.87 | 50.974 | 52.768 | 7.626 | 7.585 | Fe I | 6338.8760 | 58.800 | 0.56 | 55.491 | 57.924 | 7.581 | 7.528 |
| Fe I | 5539.2798 | 40.100 | 0.54 | 36.657 | 38.224 | 7.594 | 7.555 | Fe I | 6380.7432 | 72.900 | 0.87 | 67.012 | 69.227 | 7.636 | 7.588 |
| Fe I | 5543.9355 | 83.100 | 1.05 | 77.526 | 79.270 | 7.631 | 7.594 | Fe I | 6408.0176 | 119.300 | 2.14 | 130.152 | 132.673 | 7.371 | 7.340 |
| Fe I | 5546.5059 | 70.700 | 1.34 | 63.529 | 65.426 | 7.670 | 7.626 | Fe I | 6411.1055 | 15.200 | 0.89 | 17.103 | 18.060 | 7.442 | 7.410 |
| Fe I | 5573.1021 | 61.800 | 1.23 | 66.428 | 68.201 | 7.407 | 7.368 | Fe I | 6421.3501 | 155.900 | 4.37 | 146.453 | 151.765 | 7.633 | 7.563 |
| Fe I | 5577.0249 | 18.700 | 0.89 | 18.223 | 19.616 | 7.526 | 7.481 | Fe I | 6495.7412 | 59.800 | 1.32 | 60.274 | 62.982 | 7.500 | 7.447 |
| Fe I | 5584.7646 | 66.400 | 2.87 | 62.316 | 64.177 | 7.611 | 7.564 | Fe I | 6496.4658 | 80.900 | 0.96 | 79.867 | 82.678 | 7.529 | 7.478 |
| Fe I | 5594.6553 | 85.400 | 3.13 | 86.735 | 89.418 | 7.486 | 7.440 | Fe I | 6518.3657 | 85.900 | 1.40 | 84.831 | 88.090 | 7.533 | 7.464 |
| Fe I | 5595.0601 | 15.200 | 0.40 | 11.209 | 12.079 | 7.675 | 7.634 | Fe I | 6533.9282 | 56.500 | 0.43 | 47.938 | 49.883 | 7.700 | 7.654 |
| Fe I | 5624.0220 | 52.300 | 1.98 | 49.966 | 51.725 | 7.563 | 7.523 | Fe I | 6569.2139 | 92.900 | 0.93 | 95.349 | 98.096 | 7.471 | 7.428 |
| Fe I | 5636.6958 | 43.100 | 1.26 | 39.069 | 40.697 | 7.607 | 7.567 | Fe I | 6581.2090 | 59.500 | 0.56 | 51.965 | 55.223 | 7.695 | 7.611 |
| Fe I | 5638.2622 | 95.900 | 2.38 | 95.697 | 97.253 | 7.514 | 7.485 | Fe I | 6591.3130 | 19.200 | 0.49 | 17.410 | 18.423 | 7.569 | 7.535 |
| Fe I | 5650.7056 | 44.600 | 1.68 | 44.051 | 47.469 | 7.523 | 7.450 | Fe I | 6597.5591 | 60.200 | 0.63 | 55.728 | 57.990 | 7.603 | 7.556 |
| Fe I | 5653.8652 | 44.200 | 2.79 | 42.714 | 44.355 | 7.544 | 7.506 | Fe I | 6608.0249 | 49.200 | 0.72 | 45.497 | 48.043 | 7.597 | 7.536 |
| Fe I | 5680.2402 | 15.500 | 0.35 | 17.512 | 18.453 | 7.440 | 7.410 | Fe I | 6633.7485 | 84.300 | 1.09 | 77.528 | 79.843 | 7.638 | 7.594 |
| Fe I | 5691.4971 | 56.400 | 0.56 | 54.032 | 55.876 | 7.567 | 7.522 | Fe I | 6653.8511 | 23.300 | 0.27 | 30.089 | 31.507 | 7.338 | 7.308 |
| Fe I | 5696.0894 | 31.600 | 0.68 | 31.417 | 32.897 | 7.515 | 7.479 | Fe I | 6667.4180 | 23.400 | 0.23 | 23.509 | 25.170 | 7.507 | 7.463 |
| Fe I | 5701.5444 | 111.300 | 1.23 | 109.831 | 113.462 | 7.535 | 7.473 | Fe I | 6699.1411 | 18.400 | 0.24 | 16.409 | 17.382 | 7.578 | 7.544 |
| Fe I | 5717.8325 | 81.900 | 1.45 | 77.020 | 78.914 | 7.615 | 7.575 | Fe I | 6703.5659 | 67.100 | 0.83 | 59.972 | 62.601 | 7.686 | 7.616 |
| Fe I | 5720.8862 | 40.000 | 1.46 | 35.365 | 36.915 | 7.618 | 7.581 | Fe I | 6710.3179 | 53.800 | 0.87 | 48.664 | 51.881 | 7.633 | 7.554 |
| Fe I | 5742.9600 | 18.700 | 0.30 | 19.971 | 21.000 | 7.470 | 7.439 | Fe I | 6713.0459 | 44.000 | 0.33 | 39.562 | 41.210 | 7.614 | 7.575 |
| Fe I | 5754.4023 | 38.800 | 1.54 | 35.328 | 36.915 | 7.594 | 7.555 | Fe I | 6725.3560 | 35.700 | 0.28 | 37.855 | 39.473 | 7.461 | 7.426 |
| Fe I | 5759.2622 | 14.800 | 0.62 | 11.360 | 12.021 | 7.652 | 7.622 | Fe I | 6732.0649 | 15.100 | 0.51 | 19.162 | 20.256 | 7.370 | 7.339 |
| Fe I | 5760.3438 | 44.100 | 1.31 | 44.454 | 46.210 | 7.501 | 7.460 | Fe I | 6739.5205 | 43.200 | 0.52 | 43.724 | 46.714 | 7.498 | 7.432 |
| Fe I | 5849.6831 | 19.200 | 1.06 | 18.158 | 19.174 | 7.544 | 7.511 | Fe I | 6745.9556 | 17.200 | 0.23 | 21.855 | 23.078 | 7.365 | 7.333 |
| Fe I | 5853.1484 | 29.700 | 1.36 | 28.110 | 30.258 | 7.550 | 7.496 | Fe I | 6746.9536 | 16.400 | 0.16 | 16.040 | 17.247 | 7.523 | 7.481 |
| Fe I | 5855.0757 | 35.700 | 1.48 | 39.579 | 41.314 | 7.420 | 7.384 | Fe I | 6750.1514 | 104.800 | 1.15 | 96.362 | 100.587 | 7.696 | 7.600 |
| Fe I | 5858.7778 | 32.500 | 0.71 | 27.516 | 28.813 | 7.637 | 7.602 | Fe I | 6752.7065 | 55.800 | 0.64 | 50.645 | 52.536 | 7.627 | 7.584 |


| $\delta$ Eri |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m} \AA)$ |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m}$ A $)$ |  | $\varepsilon_{\mathrm{Fe}}$ (dex) |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 6786.8584 | 45.800 | 0.18 | 39.691 | 41.345 | 7.644 | 7.606 |
| Fe I | 6804.2710 | 28.500 | 0.33 | 26.595 | 28.024 | 7.561 | 7.522 |
| Fe I | 6810.2622 | 67.600 | 0.70 | 64.655 | 66.861 | 7.571 | 7.525 |
| Fe II | 4993.3501 | 33.600 | 2.00 | 39.756 | 39.168 | 7.337 | 7.351 |
| Fe II | 5234.6226 | 77.800 | 1.05 | 84.402 | 83.155 | 7.364 | 7.390 |
| Fe II | 5256.9321 | 16.500 | 0.85 | 19.801 | 19.489 | 7.388 | 7.398 |
| Fe II | 5264.8022 | 43.100 | 0.64 | 43.559 | 42.915 | 7.497 | 7.515 |
| Fe II | 5325.5522 | 43.100 | 0.49 | 42.730 | 42.099 | 7.520 | 7.538 |
| Fe II | 5414.0698 | 24.000 | 1.02 | 27.746 | 27.336 | 7.390 | 7.402 |
| Fe II | 5534.8379 | 47.200 | 2.18 | 53.063 | 52.176 | 7.357 | 7.377 |
| Fe II | 6084.1016 | 20.500 | 0.28 | 18.665 | 18.335 | 7.576 | 7.590 |
| Fe II | 6113.3193 | 11.600 | 0.57 | 10.130 | 9.961 | 7.588 | 7.598 |
| Fe II | 6149.2461 | 29.900 | 0.34 | 28.311 | 27.893 | 7.560 | 7.574 |
| Fe II | 6238.3857 | 38.300 | 0.53 | 36.476 | 35.902 | 7.562 | 7.580 |
| Fe II | 6247.5571 | 43.300 | 0.40 | 42.476 | 41.766 | 7.532 | 7.553 |
| Fe II | 6369.4590 | 16.300 | 0.37 | 21.228 | 20.771 | 7.332 | 7.345 |
| Fe II | 6456.3794 | 50.900 | 0.43 | 51.878 | 50.961 | 7.485 | 7.508 |

## $\epsilon$ For

|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m} \AA)$ |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m} \AA)$ |  | $\varepsilon_{\mathrm{Fe}}$ (dex) |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 4787.8267 | 41.200 | 0.83 | 39.084 | 42.253 | 6.897 | 6.827 |
| Fe I | 4793.9614 | 9.100 | 0.29 | 8.850 | 10.000 | 6.864 | 6.803 |
| Fe I | 4794.3540 | 13.400 | 0.24 | 12.308 | 13.986 | 6.895 | 6.827 |
| Fe I | 4799.4058 | 31.400 | 0.40 | 28.791 | 31.500 | 6.912 | 6.848 |
| Fe I | 4802.8799 | 55.200 | 1.38 | 55.937 | 59.318 | 6.833 | 6.755 |
| Fe I | 4808.1479 | 26.800 | 0.43 | 23.225 | 25.663 | 6.943 | 6.879 |
| Fe I | 4809.9385 | 14.600 | 0.48 | 14.188 | 15.835 | 6.865 | 6.806 |
| Fe I | 4869.4634 | 19.800 | 0.76 | 17.842 | 19.824 | 6.911 | 6.849 |
| Fe I | 4874.3530 | 18.200 | 1.42 | 16.477 | 18.431 | 6.906 | 6.843 |
| Fe I | 4875.8770 | 56.000 | 0.97 | 56.041 | 59.303 | 6.849 | 6.779 |
| Fe I | 4877.6045 | 21.400 | 0.89 | 16.972 | 18.963 | 6.984 | 6.921 |
| Fe I | 4892.8589 | 42.900 | 0.63 | 38.964 | 42.491 | 6.934 | 6.859 |
| Fe I | 4896.4385 | 28.500 | 0.55 | 27.772 | 30.418 | 6.868 | 6.804 |
| Fe I | 4907.7319 | 55.800 | 1.15 | 60.775 | 64.041 | 6.744 | 6.675 |
| Fe I | 4917.2300 | 52.800 | 0.67 | 50.387 | 54.238 | 6.901 | 6.820 |
| Fe I | 4918.0127 | 42.300 | 0.66 | 39.781 | 43.334 | 6.904 | 6.828 |
| Fe I | 4962.5718 | 45.600 | 0.57 | 46.496 | 49.996 | 6.831 | 6.759 |
| Fe I | 4986.2227 | 37.300 | 0.57 | 39.157 | 42.562 | 6.810 | 6.739 |
| Fe I | 4999.1123 | 21.800 | 0.62 | 24.834 | 27.380 | 6.767 | 6.704 |
| Fe I | 5023.1860 | 27.200 | 0.80 | 26.489 | 29.302 | 6.868 | 6.799 |
| Fe I | 5023.4976 | 22.900 | 0.66 | 19.072 | 21.191 | 6.959 | 6.897 |
| Fe I | 5025.3027 | 8.900 | 0.63 | 10.788 | 12.135 | 6.754 | 6.694 |
| Fe I | 5029.6177 | 44.600 | 1.02 | 48.412 | 51.833 | 6.765 | 6.691 |
| Fe I | 5031.9141 | 17.800 | 0.33 | 20.328 | 22.612 | 6.773 | 6.710 |
| Fe I | 5036.9214 | 24.900 | 1.13 | 21.304 | 23.724 | 6.947 | 6.881 |
| Fe I | 5067.1494 | 59.000 | 0.61 | 54.573 | 58.304 | 6.943 | 6.865 |
| Fe I | 5088.1533 | 28.900 | 0.50 | 25.019 | 27.524 | 6.946 | 6.883 |
| Fe I | 5115.7769 | 17.100 | 0.65 | 14.002 | 15.680 | 6.959 | 6.898 |
| Fe I | 5129.6309 | 36.500 | 1.20 | 36.009 | 39.183 | 6.861 | 6.793 |
| Fe I | 5243.7764 | 49.900 | 0.64 | 48.964 | 52.649 | 6.870 | 6.793 |
| Fe I | 5253.0210 | 20.200 | 0.31 | 17.899 | 20.294 | 6.920 | 6.847 |
| Fe I | 5267.2695 | 19.800 | 0.59 | 19.657 | 21.865 | 6.854 | 6.791 |
| Fe I | 5285.1274 | 17.000 | 0.32 | 15.500 | 17.357 | 6.901 | 6.838 |
| Fe I | 5293.9590 | 19.900 | 0.45 | 22.034 | 24.482 | 6.788 | 6.722 |
| Fe I | 5294.5474 | 9.800 | 0.29 | 9.745 | 11.011 | 6.853 | 6.791 |
| Fe I | 5295.3120 | 17.900 | 0.52 | 18.297 | 20.421 | 6.837 | 6.774 |
| Fe I | 5320.0356 | 16.000 | 0.19 | 14.891 | 16.713 | 6.889 | 6.826 |
| Fe I | 5361.6250 | 31.300 | 0.66 | 28.026 | 31.037 | 6.927 | 6.856 |
| Fe I | 5373.7085 | 50.100 | 0.54 | 54.777 | 59.218 | 6.755 | 6.670 |
| Fe I | 5379.5737 | 52.500 | 0.91 | 55.554 | 59.226 | 6.783 | 6.705 |
| Fe I | 5401.2666 | 17.300 | 0.44 | 14.577 | 16.305 | 6.944 | 6.883 |
| Fe I | 5412.7837 | 12.700 | 0.26 | 14.059 | 15.779 | 6.796 | 6.734 |
| Fe I | 5417.0332 | 22.800 | 0.30 | 18.699 | 20.916 | 6.967 | 6.902 |
| Fe I | 5436.2949 | 27.700 | 0.20 | 25.000 | 27.685 | 6.918 | 6.850 |
| Fe I | 5441.3389 | 20.800 | 0.17 | 20.856 | 23.173 | 6.848 | 6.784 |
| Fe I | 5452.0884 | 10.000 | 0.28 | 9.043 | 10.241 | 6.900 | 6.838 |
| Fe I | 5460.8726 | 8.700 | 0.23 | 9.028 | 10.294 | 6.832 | 6.766 |
| Fe I | 5466.3960 | 64.400 | 0.59 | 64.756 | 69.036 | 6.843 | 6.759 |
| Fe I | 5466.9873 | 27.000 | 0.26 | 28.481 | 31.401 | 6.813 | 6.744 |
| Fe I | 5470.0928 | 15.800 | 0.21 | 13.894 | 15.646 | 6.919 | 6.855 |
| Fe I | 5472.7085 | 35.500 | 0.22 | 30.302 | 33.372 | 6.970 | 6.898 |
| Fe I | 5473.1626 | 11.100 | 0.29 | 12.520 | 14.083 | 6.788 | 6.726 |
| Fe I | 5473.9004 | 65.300 | 0.55 | 69.199 | 72.995 | 6.768 | 6.685 |
| Fe I | 5481.2432 | 50.800 | 0.65 | 47.696 | 51.508 | 6.916 | 6.835 |
| Fe I | 5483.0986 | 36.000 | 0.46 | 37.732 | 41.102 | 6.811 | 6.738 |
| Fe I | 5487.1450 | 24.400 | 0.40 | 24.167 | 26.852 | 6.856 | 6.788 |
| Fe I | 5494.4624 | 18.700 | 0.54 | 14.403 | 16.147 | 6.995 | 6.933 |


| $\epsilon$ For |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m} \AA)$ |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m} \AA)$ |  | $\varepsilon_{\mathrm{Fe}}$ (dex) |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 5522.4463 | 32.800 | 0.19 | 32.349 | 35.509 | 6.861 | 6.788 |
| Fe I | 5539.2798 | 13.900 | 0.31 | 14.566 | 16.385 | 6.825 | 6.760 |
| Fe I | 5543.9355 | 50.800 | 0.32 | 50.813 | 54.638 | 6.850 | 6.767 |
| Fe I | 5546.5059 | 38.300 | 0.22 | 35.718 | 39.036 | 6.907 | 6.834 |
| Fe I | 5546.9907 | 19.900 | 0.33 | 18.208 | 20.321 | 6.902 | 6.838 |
| Fe I | 5554.8945 | 66.600 | 0.65 | 74.392 | 79.991 | 6.708 | 6.607 |
| Fe I | 5560.2114 | 39.100 | 0.21 | 38.243 | 41.841 | 6.868 | 6.792 |
| Fe I | 5567.3911 | 64.400 | 1.58 | 61.816 | 65.902 | 6.912 | 6.815 |
| Fe I | 5577.0249 | 6.200 | 0.30 | 5.256 | 6.184 | 6.929 | 6.851 |
| Fe I | 5584.7646 | 32.200 | 0.85 | 36.924 | 40.310 | 6.742 | 6.672 |
| Fe I | 5594.6553 | 51.300 | 1.39 | 53.845 | 58.400 | 6.799 | 6.712 |
| Fe I | 5618.6323 | 41.900 | 0.54 | 41.233 | 44.818 | 6.865 | 6.787 |
| Fe I | 5636.6958 | 17.800 | 0.47 | 16.150 | 18.146 | 6.905 | 6.839 |
| Fe I | 5638.2622 | 66.100 | 0.96 | 66.151 | 70.001 | 6.849 | 6.767 |
| Fe I | 5652.3174 | 13.200 | 0.90 | 15.636 | 17.529 | 6.758 | 6.695 |
| Fe I | 5653.8652 | 22.600 | 0.65 | 18.108 | 20.232 | 6.981 | 6.916 |
| Fe I | 5655.1763 | 29.400 | 0.25 | 28.577 | 33.345 | 6.871 | 6.762 |
| Fe I | 5679.0229 | 43.700 | 0.51 | 40.011 | 44.211 | 6.928 | 6.840 |
| Fe I | 5691.4971 | 32.700 | 1.01 | 28.133 | 31.190 | 6.959 | 6.885 |
| Fe I | 5717.8325 | 50.600 | 1.09 | 49.968 | 53.903 | 6.864 | 6.779 |
| Fe I | 5731.7617 | 46.100 | 0.29 | 41.711 | 45.240 | 6.945 | 6.869 |
| Fe I | 5741.8477 | 21.800 | 0.31 | 21.612 | 24.067 | 6.855 | 6.788 |
| Fe I | 5742.9600 | 5.900 | 0.26 | 6.159 | 6.991 | 6.830 | 6.769 |
| Fe I | 5754.4023 | 11.500 | 0.61 | 13.704 | 15.467 | 6.758 | 6.693 |
| Fe I | 5760.3438 | 19.500 | 0.44 | 20.061 | 22.440 | 6.833 | 6.766 |
| Fe I | 5838.3716 | 18.300 | 0.60 | 14.720 | 16.521 | 6.970 | 6.907 |
| Fe I | 5848.1265 | 28.100 | 0.35 | 30.866 | 34.372 | 6.783 | 6.705 |
| Fe I | 5849.6831 | 6.100 | 0.27 | 5.529 | 6.312 | 6.897 | 6.834 |
| Fe I | 5853.1484 | 11.700 | 0.31 | 9.684 | 11.433 | 6.946 | 6.862 |
| Fe I | 5855.0757 | 15.900 | 0.28 | 15.755 | 17.742 | 6.855 | 6.789 |
| Fe I | 5859.5864 | 61.900 | 1.15 | 66.185 | 71.090 | 6.768 | 6.675 |
| Fe I | 5873.2124 | 9.300 | 0.39 | 11.253 | 12.687 | 6.755 | 6.693 |
| Fe I | 5883.8164 | 57.300 | 0.75 | 56.906 | 60.797 | 6.858 | 6.781 |
| Fe I | 5905.6714 | 44.600 | 0.69 | 46.179 | 51.027 | 6.817 | 6.721 |
| Fe I | 5909.9722 | 29.900 | 0.26 | 31.603 | 34.920 | 6.810 | 6.737 |
| Fe I | 5927.7886 | 32.100 | 0.40 | 32.102 | 35.908 | 6.850 | 6.766 |
| Fe I | 5934.6543 | 72.200 | 0.98 | 69.017 | 72.803 | 6.911 | 6.838 |
| Fe I | 5952.7178 | 50.700 | 0.93 | 51.501 | 55.318 | 6.834 | 6.758 |
| Fe I | 5976.7769 | 60.700 | 0.60 | 58.965 | 62.729 | 6.884 | 6.810 |
| Fe I | 5984.8149 | 64.500 | 0.71 | 68.329 | 74.432 | 6.779 | 6.671 |
| Fe I | 5987.0649 | 51.300 | 0.58 | 51.942 | 57.713 | 6.837 | 6.728 |
| Fe I | 6003.0112 | 72.300 | 0.87 | 70.316 | 74.095 | 6.888 | 6.815 |
| Fe I | 6007.9595 | 48.400 | 0.53 | 50.267 | 54.817 | 6.811 | 6.719 |
| Fe I | 6020.1685 | 74.600 | 1.12 | 71.841 | 77.165 | 6.900 | 6.804 |
| Fe I | 6027.0508 | 55.800 | 0.83 | 58.230 | 62.479 | 6.801 | 6.716 |
| Fe I | 6056.0044 | 59.100 | 0.70 | 61.505 | 67.072 | 6.804 | 6.701 |
| Fe I | 6078.4912 | 59.200 | 0.52 | 57.970 | 63.773 | 6.874 | 6.765 |
| Fe I | 6079.0078 | 34.200 | 0.25 | 31.101 | 34.557 | 6.920 | 6.842 |
| Fe I | 6082.7100 | 39.700 | 0.48 | 36.780 | 40.821 | 6.915 | 6.826 |
| Fe I | 6093.6431 | 20.200 | 0.25 | 18.265 | 20.592 | 6.909 | 6.839 |
| Fe I | 6096.6641 | 29.600 | 0.37 | 28.023 | 30.930 | 6.887 | 6.819 |
| Fe I | 6098.2441 | 10.000 | 0.21 | 8.386 | 9.519 | 6.937 | 6.875 |
| Fe I | 6127.9063 | 40.300 | 0.44 | 39.361 | 43.112 | 6.870 | 6.791 |
| Fe I | 6136.9937 | 71.600 | 1.54 | 67.464 | 72.698 | 6.946 | 6.826 |
| Fe I | 6151.6172 | 53.300 | 1.22 | 52.785 | 57.500 | 6.862 | 6.760 |
| Fe I | 6157.7280 | 52.800 | 0.62 | 54.673 | 58.915 | 6.811 | 6.726 |
| Fe I | 6165.3599 | 36.800 | 0.44 | 35.894 | 39.487 | 6.870 | 6.793 |
| Fe I | 6173.3345 | 71.700 | 1.03 | 68.738 | 73.991 | 6.921 | 6.798 |
| Fe I | 6180.2026 | 57.700 | 0.86 | 56.762 | 61.166 | 6.871 | 6.775 |
| Fe I | 6187.9893 | 38.600 | 0.37 | 39.974 | 43.450 | 6.821 | 6.750 |
| Fe I | 6200.3125 | 74.000 | 0.94 | 69.811 | 74.664 | 6.948 | 6.835 |
| Fe I | 6226.7344 | 22.800 | 0.26 | 21.029 | 23.470 | 6.899 | 6.832 |
| Fe I | 6229.2261 | 38.000 | 0.42 | 40.561 | 44.475 | 6.793 | 6.712 |
| Fe I | 6232.6401 | 73.700 | 0.93 | 75.847 | 80.007 | 6.809 | 6.728 |
| Fe I | 6240.6460 | 54.400 | 0.64 | 53.271 | 57.966 | 6.876 | 6.773 |
| Fe I | 6271.2778 | 22.800 | 0.66 | 21.896 | 24.575 | 6.875 | 6.803 |
| Fe I | 6311.4995 | 30.800 | 0.24 | 26.432 | 29.599 | 6.955 | 6.878 |
| Fe I | 6315.8110 | 36.300 | 0.43 | 32.184 | 35.562 | 6.942 | 6.866 |
| Fe I | 6338.8760 | 28.400 | 0.23 | 26.963 | 30.467 | 6.885 | 6.801 |
| Fe I | 6355.0283 | 67.800 | 1.09 | 62.624 | 67.193 | 6.968 | 6.863 |
| Fe I | 6380.7432 | 41.700 | 0.23 | 38.427 | 42.320 | 6.920 | 6.837 |
| Fe I | 6469.1919 | 40.100 | 0.31 | 35.250 | 39.607 | 6.955 | 6.860 |
| Fe I | 6496.4658 | 49.700 | 0.80 | 47.168 | 52.119 | 6.901 | 6.803 |
| Fe I | 6533.9282 | 25.400 | 0.20 | 21.762 | 24.507 | 6.947 | 6.873 |
| Fe I | 6569.2139 | 63.200 | 0.49 | 59.084 | 64.222 | 6.928 | 6.831 |
| Fe I | 6574.2266 | 41.900 | 0.41 | 36.611 | 41.937 | 6.964 | 6.849 |
| Fe I | 6581.2090 | 28.500 | 0.55 | 25.974 | 29.993 | 6.912 | 6.815 |
| Fe I | 6593.8696 | 83.000 | 0.95 | 80.525 | 86.586 | 6.906 | 6.774 |
| Fe I | 6597.5591 | 30.600 | 0.21 | 27.043 | 30.351 | 6.935 | 6.856 |
| Fe I | 6608.0249 | 20.200 | 0.25 | 20.469 | 23.420 | 6.842 | 6.761 |


| $\epsilon$ For |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m} \AA)$ |  | $\mathrm{EW}_{\text {calc }}\left(\mathrm{m}\right.$ ( ${ }^{\text {a }}$ |  | $\varepsilon_{\mathrm{Fe}}$ (dex) |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 6609.1099 | 65.200 | 0.36 | 61.594 | 66.588 | 6.933 | 6.820 |
| Fe I | 6625.0215 | 27.000 | 0.69 | 21.481 | 25.331 | 6.992 | 6.890 |
| Fe I | 6627.5439 | 17.900 | 0.28 | 14.869 | 16.801 | 6.953 | 6.886 |
| Fe I | 6633.7485 | 51.100 | 0.57 | 46.776 | 51.177 | 6.938 | 6.848 |
| Fe I | 6653.8511 | 10.900 | 0.70 | 10.378 | 11.753 | 6.875 | 6.811 |
| Fe I | 6703.5659 | 37.100 | 0.16 | 34.253 | 38.059 | 6.914 | 6.829 |
| Fe I | 6710.3179 | 22.400 | 0.18 | 22.865 | 26.587 | 6.837 | 6.744 |
| Fe I | 6713.0459 | 16.000 | 0.27 | 16.196 | 18.321 | 6.843 | 6.773 |
| Fe I | 6750.1514 | 74.100 | 0.64 | 72.065 | 77.656 | 6.898 | 6.772 |
| Fe I | 6752.7065 | 24.600 | 0.61 | 24.368 | 27.349 | 6.856 | 6.780 |
| Fe I | 6786.8584 | 17.600 | 0.17 | 15.585 | 17.551 | 6.917 | 6.852 |
| Fe I | 6804.2710 | 8.400 | 0.32 | 8.969 | 10.262 | 6.818 | 6.750 |
| Fe II | 4893.8125 | 8.800 | 0.63 | 7.822 | 7.691 | 6.909 | 6.918 |
| Fe II | 4993.3501 | 25.600 | 0.77 | 29.791 | 29.351 | 6.735 | 6.746 |
| Fe II | 5256.9321 | 8.800 | 0.20 | 11.606 | 11.412 | 6.705 | 6.713 |
| Fe II | 5264.8022 | 29.300 | 0.28 | 33.826 | 33.359 | 6.730 | 6.741 |
| Fe II | 5284.1030 | 41.500 | 0.84 | 46.060 | 45.379 | 6.739 | 6.754 |
| Fe II | 5325.5522 | 25.300 | 0.32 | 33.000 | 32.544 | 6.642 | 6.652 |
| Fe II | 5414.0698 | 13.000 | 0.26 | 18.257 | 17.969 | 6.650 | 6.659 |
| Fe II | 5425.2485 | 23.000 | 0.25 | 31.534 | 31.068 | 6.614 | 6.625 |
| Fe II | 5525.1172 | 5.600 | 0.51 | 8.211 | 8.082 | 6.660 | 6.668 |
| Fe II | 5534.8379 | 38.200 | 0.26 | 43.903 | 43.297 | 6.709 | 6.723 |
| Fe II | 6084.1016 | 9.900 | 0.21 | 11.111 | 10.904 | 6.788 | 6.798 |
| Fe II | 6149.2461 | 17.600 | 0.28 | 19.199 | 18.915 | 6.793 | 6.803 |
| Fe II | 6238.3857 | 23.500 | 0.56 | 27.035 | 26.635 | 6.745 | 6.755 |
| Fe II | 6247.5571 | 30.800 | 0.32 | 33.001 | 32.513 | 6.791 | 6.803 |
| Fe II | 6456.3794 | 37.800 | 0.29 | 42.470 | 41.842 | 6.734 | 6.748 |
| Fe II | 6516.0767 | 33.300 | 0.56 | 41.715 | 40.937 | 6.647 | 6.663 |


| $\tau$ Cet |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m} \AA)$ |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m}$ ¢ $)$ |  | $\varepsilon_{\mathrm{Fe}}$ (dex) |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 4787.8267 | 32.200 | 0.49 | 31.918 | 33.179 | 6.967 | 6.926 |
| Fe I | 4788.7568 | 57.900 | 1.11 | 57.426 | 58.898 | 6.971 | 6.916 |
| Fe I | 4793.9614 | 7.900 | 0.31 | 6.698 | 7.110 | 7.041 | 7.010 |
| Fe I | 4794.3540 | 10.400 | 0.45 | 8.731 | 9.298 | 7.050 | 7.015 |
| Fe I | 4799.4058 | 26.400 | 0.27 | 24.406 | 25.529 | 7.013 | 6.977 |
| Fe I | 4802.8799 | 50.000 | 1.17 | 49.699 | 51.183 | 6.967 | 6.914 |
| Fe I | 4808.1479 | 18.900 | 0.72 | 18.474 | 19.405 | 6.974 | 6.939 |
| Fe I | 4809.9385 | 10.700 | 0.45 | 11.562 | 12.196 | 6.919 | 6.889 |
| Fe I | 4875.8770 | 50.700 | 0.97 | 50.859 | 52.378 | 6.957 | 6.912 |
| Fe I | 4882.1431 | 66.500 | 1.10 | 70.740 | 72.405 | 6.886 | 6.843 |
| Fe I | 4885.4302 | 62.300 | 1.02 | 66.734 | 68.445 | 6.874 | 6.823 |
| Fe I | 4892.8589 | 40.600 | 0.53 | 36.923 | 38.502 | 7.036 | 6.994 |
| Fe I | 4896.4385 | 23.400 | 0.46 | 23.732 | 24.798 | 6.951 | 6.914 |
| Fe I | 4905.1328 | 21.200 | 0.34 | 28.815 | 30.047 | 6.758 | 6.726 |
| Fe I | 4907.7319 | 51.900 | 0.89 | 56.749 | 58.324 | 6.865 | 6.823 |
| Fe I | 4917.2300 | 51.100 | 0.55 | 49.252 | 51.091 | 6.995 | 6.950 |
| Fe I | 4918.0127 | 42.200 | 0.63 | 37.845 | 39.463 | 7.048 | 7.006 |
| Fe I | 4950.1055 | 66.200 | 0.68 | 70.489 | 72.222 | 6.885 | 6.841 |
| Fe I | 4962.5718 | 41.800 | 0.42 | 44.434 | 46.046 | 6.907 | 6.866 |
| Fe I | 4969.9175 | 64.900 | 0.62 | 70.862 | 73.205 | 6.863 | 6.815 |
| Fe I | 4979.5859 | 11.500 | 0.29 | 9.165 | 9.698 | 7.076 | 7.046 |
| Fe I | 4986.2227 | 33.400 | 0.41 | 36.900 | 38.438 | 6.884 | 6.846 |
| Fe I | 4993.6797 | 37.600 | 0.81 | 33.312 | 34.736 | 7.053 | 7.014 |
| Fe I | 4999.1123 | 19.500 | 0.57 | 22.022 | 23.084 | 6.884 | 6.850 |
| Fe I | 5002.7920 | 70.200 | 0.68 | 73.943 | 75.684 | 6.897 | 6.853 |
| Fe I | 5023.1860 | 24.400 | 0.59 | 24.429 | 25.661 | 6.959 | 6.924 |
| Fe I | 5023.4976 | 19.200 | 0.59 | 17.314 | 18.225 | 7.019 | 6.987 |
| Fe I | 5029.6177 | 39.000 | 1.05 | 41.555 | 43.018 | 6.899 | 6.852 |
| Fe I | 5031.9141 | 15.500 | 0.42 | 18.717 | 19.723 | 6.855 | 6.824 |
| Fe I | 5036.9214 | 20.400 | 0.44 | 16.415 | 17.315 | 7.091 | 7.055 |
| Fe I | 5044.2109 | 67.800 | 0.74 | 66.368 | 68.000 | 6.989 | 6.933 |
| Fe I | 5054.6426 | 28.700 | 0.62 | 30.866 | 32.085 | 6.898 | 6.853 |
| Fe I | 5067.1494 | 57.300 | 0.81 | 53.913 | 55.753 | 7.023 | 6.976 |
| Fe I | 5072.6719 | 51.900 | 0.82 | 61.993 | 63.976 | 6.781 | 6.737 |
| Fe I | 5088.1533 | 25.300 | 0.55 | 22.379 | 23.458 | 7.038 | 7.004 |
| Fe I | 5129.6309 | 30.400 | 0.89 | 33.127 | 34.543 | 6.900 | 6.865 |
| Fe I | 5235.3867 | 63.400 | 1.15 | 63.254 | 65.210 | 6.963 | 6.907 |
| Fe I | 5242.4907 | 75.300 | 0.98 | 86.731 | 88.773 | 6.781 | 6.732 |
| Fe I | 5243.7764 | 47.700 | 0.69 | 47.395 | 49.165 | 6.966 | 6.921 |
| Fe I | 5253.0210 | 14.200 | 0.27 | 12.630 | 13.450 | 7.025 | 6.987 |
| Fe I | 5285.1274 | 15.000 | 0.32 | 14.184 | 14.994 | 6.990 | 6.958 |
| Fe I | 5288.5249 | 44.700 | 0.61 | 51.417 | 53.062 | 6.816 | 6.768 |
| Fe I | 5293.9590 | 16.500 | 0.49 | 19.286 | 20.301 | 6.867 | 6.833 |
| Fe I | 5295.3120 | 15.300 | 0.50 | 16.790 | 17.711 | 6.909 | 6.877 |


| $\tau$ Cet |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m}$ ) |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m} \AA)$ |  | $\varepsilon_{\mathrm{Fe}}(\mathrm{dex})$ |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 5315.0698 | 19.500 | 0.24 | 19.403 | 20.424 | 6.963 | 6.930 |
| Fe I | 5320.0356 | 12.500 | 0.23 | 12.164 | 12.858 | 6.975 | 6.941 |
| Fe I | 5322.0405 | 54.700 | 0.59 | 53.117 | 54.816 | 7.002 | 6.925 |
| Fe I | 5326.1426 | 27.100 | 0.26 | 29.416 | 30.706 | 6.898 | 6.857 |
| Fe I | 5361.6250 | 27.900 | 1.16 | 26.343 | 27.700 | 6.998 | 6.960 |
| Fe I | 5373.7085 | 50.000 | 0.49 | 56.626 | 58.863 | 6.844 | 6.798 |
| Fe I | 5379.5737 | 47.600 | 1.05 | 50.429 | 52.042 | 6.899 | 6.849 |
| Fe I | 5398.2793 | 57.400 | 0.48 | 63.125 | 65.482 | 6.864 | 6.815 |
| Fe I | 5401.2666 | 13.800 | 0.24 | 13.051 | 13.781 | 6.990 | 6.959 |
| Fe I | 5409.1333 | 39.500 | 0.60 | 34.270 | 35.810 | 7.070 | 7.029 |
| Fe I | 5417.0332 | 19.700 | 0.37 | 17.161 | 18.121 | 7.039 | 7.005 |
| Fe I | 5436.2949 | 25.300 | 0.23 | 23.106 | 24.297 | 7.017 | 6.982 |
| Fe I | 5441.3389 | 18.200 | 0.27 | 18.872 | 19.865 | 6.939 | 6.906 |
| Fe I | 5466.3960 | 64.700 | 0.60 | 67.026 | 69.313 | 6.922 | 6.873 |
| Fe I | 5466.9873 | 22.200 | 0.28 | 23.484 | 24.616 | 6.922 | 6.883 |
| Fe I | 5470.0928 | 14.500 | 0.25 | 12.681 | 13.433 | 7.031 | 6.999 |
| Fe I | 5472.7085 | 30.400 | 0.20 | 27.093 | 28.399 | 7.044 | 7.003 |
| Fe I | 5473.1626 | 9.300 | 0.30 | 10.967 | 11.605 | 6.876 | 6.844 |
| Fe I | 5473.9004 | 66.700 | 0.80 | 67.419 | 69.361 | 6.947 | 6.892 |
| Fe I | 5481.2432 | 46.900 | 0.32 | 43.974 | 45.664 | 7.022 | 6.973 |
| Fe I | 5483.0986 | 32.000 | 0.42 | 33.863 | 35.311 | 6.915 | 6.872 |
| Fe I | 5487.1450 | 21.700 | 0.25 | 22.415 | 23.595 | 6.940 | 6.904 |
| Fe I | 5494.4624 | 15.100 | 0.27 | 12.385 | 13.092 | 7.068 | 7.035 |
| Fe I | 5522.4463 | 29.600 | 0.26 | 28.982 | 30.316 | 6.976 | 6.934 |
| Fe I | 5539.2798 | 10.100 | 0.19 | 11.953 | 12.662 | 6.872 | 6.839 |
| Fe I | 5543.1470 | 48.000 | 0.97 | 43.476 | 44.960 | 7.079 | 7.014 |
| Fe I | 5543.9355 | 48.600 | 0.40 | 47.360 | 49.129 | 6.987 | 6.935 |
| Fe I | 5546.5059 | 37.200 | 0.21 | 33.698 | 35.212 | 7.036 | 6.995 |
| Fe I | 5546.9907 | 17.000 | 0.33 | 16.014 | 16.892 | 6.994 | 6.960 |
| Fe I | 5554.8945 | 71.400 | 1.46 | 83.768 | 86.896 | 6.788 | 6.737 |
| Fe I | 5560.2114 | 37.500 | 0.28 | 36.766 | 38.418 | 6.975 | 6.933 |
| Fe I | 5567.3911 | 53.800 | 1.08 | 50.049 | 51.704 | 7.057 | 6.985 |
| Fe I | 5584.7646 | 24.700 | 0.24 | 31.246 | 32.616 | 6.790 | 6.752 |
| Fe I | 5594.6553 | 52.200 | 1.13 | 55.760 | 58.083 | 6.898 | 6.851 |
| Fe I | 5600.2241 | 23.800 | 0.43 | 28.159 | 29.517 | 6.844 | 6.805 |
| Fe I | 5618.6323 | 37.000 | 0.16 | 37.416 | 38.975 | 6.950 | 6.903 |
| Fe I | 5619.5952 | 22.100 | 0.21 | 17.569 | 18.513 | 7.094 | 7.060 |
| Fe I | 5636.6958 | 11.200 | 0.21 | 13.278 | 14.051 | 6.869 | 6.835 |
| Fe I | 5638.2622 | 62.800 | 0.48 | 64.107 | 66.022 | 6.935 | 6.880 |
| Fe I | 5641.4341 | 48.500 | 0.28 | 43.667 | 45.392 | 7.065 | 7.013 |
| Fe I | 5650.7056 | 21.100 | 0.42 | 18.646 | 20.071 | 7.031 | 6.986 |
| Fe I | 5651.4688 | 9.300 | 0.23 | 8.244 | 8.742 | 7.020 | 6.989 |
| Fe I | 5652.3174 | 15.100 | 0.20 | 13.785 | 14.572 | 7.011 | 6.977 |
| Fe I | 5655.1763 | 35.300 | 1.03 | 30.121 | 32.319 | 7.070 | 7.016 |
| Fe I | 5661.3447 | 13.000 | 0.14 | 15.670 | 16.547 | 6.856 | 6.823 |
| Fe I | 5679.0229 | 43.800 | 0.30 | 40.608 | 42.655 | 7.021 | 6.975 |
| Fe I | 5691.4971 | 26.700 | 0.26 | 25.388 | 26.696 | 6.995 | 6.953 |
| Fe I | 5701.5444 | 75.800 | 0.77 | 70.351 | 72.527 | 7.076 | 6.999 |
| Fe I | 5717.8325 | 47.200 | 0.53 | 46.822 | 48.621 | 6.968 | 6.915 |
| Fe I | 5741.8477 | 21.000 | 0.22 | 19.167 | 20.197 | 7.016 | 6.980 |
| Fe I | 5760.3438 | 14.500 | 0.31 | 16.600 | 17.529 | 6.883 | 6.848 |
| Fe I | 5838.3716 | 13.400 | 0.45 | 12.685 | 13.423 | 6.989 | 6.957 |
| Fe I | 5848.1265 | 24.900 | 0.25 | 29.262 | 30.835 | 6.849 | 6.809 |
| Fe I | 5853.1484 | 7.600 | 0.24 | 6.135 | 6.668 | 7.065 | 7.022 |
| Fe I | 5855.0757 | 13.500 | 0.17 | 14.745 | 15.620 | 6.913 | 6.879 |
| Fe I | 5858.7778 | 9.000 | 0.32 | 8.260 | 8.769 | 7.003 | 6.972 |
| Fe I | 5859.5864 | 59.300 | 0.66 | 70.752 | 73.394 | 6.779 | 6.728 |
| Fe I | 5861.1084 | 5.900 | 0.16 | 5.347 | 5.688 | 7.007 | 6.977 |
| Fe I | 5873.2124 | 10.400 | 0.19 | 10.030 | 10.636 | 6.978 | 6.948 |
| Fe I | 5883.8164 | 54.400 | 0.60 | 55.538 | 57.433 | 6.940 | 6.894 |
| Fe I | 6098.2441 | 9.000 | 0.19 | 7.669 | 8.159 | 7.039 | 7.007 |
| Fe I | 6127.9063 | 35.700 | 0.49 | 36.570 | 38.253 | 6.941 | 6.897 |
| Fe I | 6151.6172 | 44.100 | 0.94 | 40.176 | 41.981 | 7.063 | 6.992 |
| Fe I | 6157.7280 | 49.100 | 0.53 | 52.346 | 54.357 | 6.897 | 6.847 |
| Fe I | 6165.3599 | 32.800 | 0.30 | 33.048 | 34.642 | 6.954 | 6.912 |
| Fe I | 6180.2026 | 48.400 | 0.34 | 45.689 | 47.444 | 7.028 | 6.960 |
| Fe I | 6187.9893 | 34.400 | 0.24 | 36.641 | 38.208 | 6.912 | 6.872 |
| Fe I | 6213.4292 | 76.600 | 1.01 | 74.567 | 77.352 | 7.002 | 6.915 |
| Fe I | 6219.2803 | 83.900 | 1.02 | 78.114 | 81.031 | 7.075 | 6.985 |
| Fe I | 6226.7344 | 18.600 | 0.15 | 18.231 | 19.251 | 6.972 | 6.937 |
| Fe I | 6229.2261 | 29.100 | 0.25 | 31.796 | 33.294 | 6.888 | 6.840 |
| Fe I | 6232.6401 | 74.100 | 1.23 | 74.664 | 76.736 | 6.951 | 6.900 |
| Fe I | 6240.6460 | 42.900 | 0.61 | 40.750 | 42.581 | 7.017 | 6.947 |
| Fe I | 6271.2778 | 16.500 | 0.21 | 17.727 | 18.759 | 6.918 | 6.882 |
| Fe I | 6338.8760 | 27.500 | 0.24 | 26.809 | 28.460 | 6.977 | 6.934 |
| Fe I | 6364.3638 | 17.100 | 0.37 | 13.866 | 14.798 | 7.073 | 7.036 |
| Fe I | 6380.7432 | 38.800 | 0.27 | 35.827 | 37.555 | 7.024 | 6.978 |


| $\tau$ Cet |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m} \AA)$ |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m}$ ( $)$ |  | $\varepsilon_{\mathrm{Fe}}$ (dex) |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 6408.0176 | 83.300 | 0.83 | 90.338 | 92.654 | 6.861 | 6.813 |
| Fe I | 6469.1919 | 38.400 | 0.38 | 36.066 | 38.165 | 7.007 | 6.958 |
| Fe I | 6496.4658 | 48.100 | 0.90 | 49.258 | 51.742 | 6.939 | 6.886 |
| Fe I | 6518.3657 | 49.300 | 0.53 | 48.706 | 50.577 | 6.974 | 6.907 |
| Fe I | 6533.9282 | 22.900 | 0.17 | 20.339 | 21.546 | 7.033 | 6.993 |
| Fe I | 6569.2139 | 63.800 | 1.22 | 62.412 | 65.080 | 6.983 | 6.928 |
| Fe I | 6574.2266 | 27.800 | 0.22 | 24.008 | 25.843 | 7.068 | 7.003 |
| Fe I | 6581.2090 | 16.000 | 0.25 | 17.245 | 18.583 | 6.915 | 6.865 |
| Fe I | 6597.5591 | 28.200 | 0.24 | 26.623 | 28.172 | 6.998 | 6.957 |
| Fe I | 6608.0249 | 14.700 | 0.24 | 14.541 | 15.569 | 6.966 | 6.923 |
| Fe I | 6625.0215 | 14.300 | 0.18 | 13.394 | 14.606 | 6.997 | 6.944 |
| Fe I | 6627.5439 | 15.500 | 0.58 | 13.597 | 14.434 | 7.032 | 6.997 |
| Fe I | 6633.7485 | 49.500 | 0.36 | 45.782 | 47.889 | 7.033 | 6.980 |
| Fe I | 6703.5659 | 28.800 | 0.24 | 26.288 | 27.730 | 7.029 | 6.979 |
| Fe I | 6710.3179 | 13.100 | 0.14 | 15.044 | 16.264 | 6.881 | 6.833 |
| Fe I | 6752.7065 | 21.700 | 0.43 | 22.841 | 24.170 | 6.927 | 6.886 |
| Fe I | 6786.8584 | 16.100 | 0.32 | 13.891 | 14.731 | 7.039 | 7.006 |
| Fe I | 6804.2710 | 8.900 | 0.37 | 8.222 | 8.775 | 7.000 | 6.965 |
| Fe II | 4993.3501 | 18.900 | 0.68 | 18.679 | 18.494 | 6.968 | 6.968 |
| Fe II | 5234.6226 | 55.700 | 0.45 | 59.952 | 59.535 | 6.861 | 6.847 |
| Fe II | 5264.8022 | 22.700 | 0.33 | 22.691 | 22.489 | 6.960 | 6.958 |
| Fe II | 5284.1030 | 35.200 | 1.46 | 32.062 | 31.776 | 7.049 | 7.041 |
| Fe II | 5325.5522 | 20.300 | 0.33 | 22.024 | 21.828 | 6.902 | 6.900 |
| Fe II | 5425.2485 | 16.800 | 0.37 | 20.843 | 20.657 | 6.815 | 6.816 |
| Fe II | 5534.8379 | 31.500 | 0.75 | 31.149 | 30.871 | 6.970 | 6.965 |
| Fe II | 6084.1016 | 6.600 | 0.23 | 6.512 | 6.435 | 6.967 | 6.971 |
| Fe II | 6149.2461 | 13.400 | 0.20 | 12.743 | 12.629 | 6.990 | 6.991 |
| Fe II | 6238.3857 | 16.200 | 0.42 | 18.779 | 18.611 | 6.861 | 6.861 |
| Fe II | 6247.5571 | 25.600 | 0.15 | 23.633 | 23.422 | 7.023 | 7.020 |
| Fe II | 6456.3794 | 32.500 | 0.19 | 31.777 | 31.494 | 6.981 | 6.976 |
| Fe II | 6516.0767 | 26.700 | 0.39 | 28.424 | 28.087 | 6.909 | 6.908 |
| Fe II | 5898.2153 | 7.800 | 0.23 | 6.851 | 7.312 | 7.022 | 6.990 |
| Fe II | 5905.6714 | 43.400 | 0.37 | 47.554 | 49.952 | 6.882 | 6.833 |
| Fe II | 5909.9722 | 23.100 | 0.26 | 25.776 | 27.076 | 6.886 | 6.848 |
| Fe II | 5927.7886 | 28.600 | 0.29 | 31.634 | 33.404 | 6.891 | 6.849 |
| Fe II | 5930.1797 | 75.200 | 1.28 | 79.205 | 82.334 | 6.903 | 6.850 |
| Fe II | 5934.6543 | 66.000 | 0.56 | 69.558 | 71.562 | 6.902 | 6.856 |
| Fe II | 5940.9912 | 12.000 | 0.15 | 11.259 | 11.927 | 6.994 | 6.961 |
| Fe II | 5952.7178 | 47.300 | 0.57 | 49.485 | 51.333 | 6.919 | 6.874 |
| Fe II | 5976.7769 | 55.500 | 0.63 | 57.432 | 59.331 | 6.925 | 6.880 |
| Fe II | 5984.8149 | 67.400 | 0.61 | 77.166 | 80.549 | 6.821 | 6.767 |
| Fe II | 5987.0649 | 53.000 | 0.59 | 56.644 | 59.625 | 6.900 | 6.846 |
| Fe II | 6003.0112 | 72.800 | 0.75 | 70.578 | 72.536 | 6.996 | 6.949 |
| Fe II | 6007.9595 | 47.100 | 0.56 | 49.852 | 52.038 | 6.906 | 6.852 |
| Fe II | 6020.1685 | 75.800 | 0.95 | 78.597 | 81.532 | 6.920 | 6.866 |
| Fe II | 6024.0576 | 92.500 | 1.37 | 95.073 | 98.216 | 6.928 | 6.877 |
| Fe II | 6027.0508 | 53.500 | 0.78 | 56.528 | 58.578 | 6.903 | 6.854 |
| Fe II | 6056.0044 | 59.400 | 0.69 | 67.436 | 70.392 | 6.835 | 6.783 |
| Fe II | 6078.4912 | 62.000 | 0.75 | 63.914 | 66.996 | 6.930 | 6.876 |
| Fe II | 6079.0078 | 31.200 | 0.26 | 30.308 | 31.937 | 6.980 | 6.939 |
| Fe II | 6082.7100 | 30.000 | 0.45 | 26.960 | 28.439 | 7.044 | 6.990 |
| Fe II | 6093.6431 | 18.600 | 0.19 | 17.167 | 18.205 | 7.006 | 6.970 |
| Fe II | 6096.6641 | 25.100 | 0.16 | 25.023 | 26.285 | 6.962 | 6.926 |

## 18 Sco

|  |  | $\mathrm{EW}_{\text {obs }}$ (m $\left.\AA\right)$ |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m} \AA)$ |  | $\varepsilon_{\mathrm{Fe}}(\mathrm{dex})$ |  |
| :--- | :--- | :---: | :---: | :---: | :---: | :---: | :---: |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 4793.9614 | 9.000 | 0.25 | 10.113 | 10.957 | 7.421 | 7.380 |
| Fe I | 4794.3540 | 13.400 | 0.22 | 11.904 | 12.967 | 7.542 | 7.497 |
| Fe I | 4799.4058 | 37.700 | 0.66 | 35.638 | 37.672 | 7.525 | 7.481 |
| Fe I | 4802.8799 | 62.400 | 1.49 | 64.148 | 66.613 | 7.441 | 7.388 |
| Fe I | 4808.1479 | 28.000 | 0.69 | 26.966 | 28.748 | 7.506 | 7.462 |
| Fe I | 4809.9385 | 17.800 | 0.94 | 18.260 | 19.571 | 7.465 | 7.425 |
| Fe I | 4869.4634 | 21.700 | 1.23 | 22.155 | 23.670 | 7.467 | 7.424 |
| Fe I | 4875.8770 | 58.100 | 1.60 | 63.680 | 66.058 | 7.369 | 7.324 |
| Fe I | 4892.8589 | 54.800 | 0.87 | 52.175 | 54.863 | 7.531 | 7.479 |
| Fe I | 4896.4385 | 39.000 | 0.95 | 35.724 | 37.723 | 7.553 | 7.508 |
| Fe I | 4907.7319 | 64.200 | 1.08 | 70.085 | 72.552 | 7.367 | 7.321 |
| Fe I | 4917.2300 | 67.400 | 0.82 | 65.018 | 68.010 | 7.525 | 7.469 |
| Fe I | 4918.0127 | 57.100 | 0.96 | 53.249 | 55.993 | 7.554 | 7.501 |
| Fe I | 4950.1055 | 78.300 | 0.87 | 83.807 | 86.399 | 7.383 | 7.338 |
| Fe I | 4962.5718 | 55.900 | 0.61 | 60.085 | 62.850 | 7.400 | 7.350 |
| Fe I | 4986.2227 | 48.300 | 0.75 | 52.194 | 54.883 | 7.404 | 7.354 |
| Fe I | 4999.1123 | 32.300 | 0.70 | 34.446 | 36.528 | 7.431 | 7.385 |
| Fe I | 5002.7920 | 81.900 | 0.62 | 87.224 | 89.829 | 7.389 | 7.345 |
| Fe I | 5023.1860 | 36.500 | 0.98 | 37.845 | 40.133 | 7.452 | 7.405 |


| 18 Sco |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m} \AA)$ |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m}$ ) |  | $\varepsilon_{\mathrm{Fe}}$ (dex) |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 5023.4976 | 29.000 | 0.40 | 28.555 | 30.442 | 7.490 | 7.447 |
| Fe I | 5025.3027 | 15.500 | 0.66 | 16.935 | 18.190 | 7.431 | 7.391 |
| Fe I | 5029.6177 | 49.000 | 0.98 | 54.794 | 57.256 | 7.354 | 7.304 |
| Fe I | 5031.9141 | 25.300 | 0.59 | 30.692 | 32.721 | 7.352 | 7.310 |
| Fe I | 5036.9214 | 24.800 | 0.44 | 23.619 | 25.342 | 7.511 | 7.466 |
| Fe I | 5048.4355 | 73.800 | 3.77 | 76.689 | 79.388 | 7.423 | 7.369 |
| Fe I | 5067.1494 | 71.000 | 0.84 | 70.089 | 73.009 | 7.497 | 7.444 |
| Fe I | 5088.1533 | 36.900 | 0.48 | 34.835 | 36.901 | 7.525 | 7.480 |
| Fe I | 5104.4375 | 35.100 | 1.68 | 33.495 | 35.633 | 7.515 | 7.469 |
| Fe I | 5129.6309 | 46.000 | 0.32 | 47.050 | 49.526 | 7.460 | 7.413 |
| Fe I | 5151.9106 | 96.500 | 1.94 | 94.521 | 98.768 | 7.527 | 7.428 |
| Fe I | 5180.0557 | 49.400 | 0.37 | 47.258 | 50.221 | 7.521 | 7.465 |
| Fe I | 5197.9360 | 31.100 | 1.49 | 35.267 | 37.518 | 7.388 | 7.343 |
| Fe I | 5243.7764 | 61.700 | 0.81 | 63.609 | 66.537 | 7.444 | 7.390 |
| Fe I | 5247.0503 | 67.700 | 1.41 | 65.270 | 69.362 | 7.546 | 7.437 |
| Fe I | 5250.6455 | 101.200 | 1.16 | 102.581 | 106.744 | 7.456 | 7.385 |
| Fe I | 5253.0210 | 17.000 | 0.63 | 16.744 | 18.240 | 7.489 | 7.440 |
| Fe I | 5267.2695 | 29.500 | 1.49 | 29.650 | 31.644 | 7.477 | 7.432 |
| Fe I | 5285.1274 | 27.700 | 0.35 | 24.432 | 26.186 | 7.560 | 7.516 |
| Fe I | 5293.9590 | 28.300 | 0.51 | 30.784 | 32.784 | 7.420 | 7.375 |
| Fe I | 5294.5474 | 12.300 | 0.67 | 13.015 | 14.070 | 7.450 | 7.409 |
| Fe I | 5295.3120 | 27.100 | 0.86 | 28.152 | 30.109 | 7.455 | 7.410 |
| Fe I | 5307.3608 | 88.400 | 1.14 | 87.905 | 91.759 | 7.492 | 7.401 |
| Fe I | 5320.0356 | 19.800 | 0.23 | 19.386 | 20.845 | 7.493 | 7.449 |
| Fe I | 5322.0405 | 63.900 | 0.65 | 65.432 | 68.372 | 7.443 | 7.376 |
| Fe I | 5326.1426 | 38.800 | 0.47 | 41.805 | 44.145 | 7.413 | 7.363 |
| Fe I | 5401.2666 | 24.000 | 0.38 | 22.402 | 24.011 | 7.523 | 7.480 |
| Fe I | 5409.1333 | 56.000 | 0.39 | 49.946 | 52.686 | 7.596 | 7.542 |
| Fe I | 5412.7837 | 18.500 | 0.23 | 22.351 | 23.982 | 7.369 | 7.327 |
| Fe I | 5417.0332 | 33.100 | 0.47 | 28.714 | 30.710 | 7.578 | 7.532 |
| Fe I | 5436.2949 | 40.300 | 0.25 | 36.619 | 38.915 | 7.556 | 7.508 |
| Fe I | 5441.3389 | 30.800 | 0.18 | 30.753 | 32.786 | 7.481 | 7.436 |
| Fe I | 5452.0884 | 13.400 | 0.39 | 12.112 | 13.122 | 7.533 | 7.491 |
| Fe I | 5466.3960 | 78.900 | 0.71 | 84.959 | 88.499 | 7.383 | 7.328 |
| Fe I | 5466.9873 | 35.800 | 0.23 | 34.556 | 36.723 | 7.508 | 7.459 |
| Fe I | 5470.0928 | 25.700 | 0.38 | 22.217 | 23.864 | 7.570 | 7.526 |
| Fe I | 5472.7085 | 43.200 | 0.31 | 40.982 | 43.367 | 7.528 | 7.476 |
| Fe I | 5473.1626 | 17.500 | 0.43 | 18.905 | 20.328 | 7.436 | 7.394 |
| Fe I | 5473.9004 | 81.300 | 1.20 | 84.920 | 87.818 | 7.415 | 7.362 |
| Fe I | 5481.2432 | 65.300 | 0.40 | 59.914 | 62.803 | 7.586 | 7.528 |
| Fe I | 5483.0986 | 46.700 | 0.54 | 48.879 | 51.452 | 7.434 | 7.382 |
| Fe I | 5487.1450 | 36.200 | 0.52 | 35.833 | 38.120 | 7.488 | 7.440 |
| Fe I | 5522.4463 | 43.100 | 0.33 | 43.280 | 45.751 | 7.476 | 7.424 |
| Fe I | 5536.5801 | 8.100 | 0.26 | 9.455 | 10.333 | 7.403 | 7.358 |
| Fe I | 5539.2798 | 17.300 | 0.20 | 19.048 | 20.526 | 7.424 | 7.381 |
| Fe I | 5543.9355 | 62.700 | 0.43 | 63.873 | 66.743 | 7.456 | 7.400 |
| Fe I | 5546.5059 | 52.200 | 0.65 | 49.253 | 51.955 | 7.538 | 7.485 |
| Fe I | 5546.9907 | 26.000 | 0.56 | 26.512 | 28.355 | 7.467 | 7.422 |
| Fe I | 5549.9487 | 8.800 | 0.34 | 8.787 | 9.551 | 7.481 | 7.439 |
| Fe I | 5552.6919 | 6.700 | 0.29 | 6.020 | 6.637 | 7.531 | 7.485 |
| Fe I | 5560.2114 | 52.900 | 0.19 | 53.046 | 55.956 | 7.477 | 7.423 |
| Fe I | 5567.3911 | 67.000 | 1.47 | 62.721 | 65.608 | 7.580 | 7.512 |
| Fe I | 5577.0249 | 9.500 | 0.39 | 10.666 | 11.760 | 7.421 | 7.373 |
| Fe I | 5594.6553 | 69.600 | 2.20 | 73.750 | 77.632 | 7.410 | 7.349 |
| Fe I | 5600.2241 | 37.800 | 0.49 | 42.477 | 44.997 | 7.379 | 7.328 |
| Fe I | 5618.6323 | 51.600 | 0.38 | 53.005 | 55.736 | 7.450 | 7.395 |
| Fe I | 5636.6958 | 19.900 | 0.32 | 20.969 | 22.572 | 7.449 | 7.404 |
| Fe I | 5641.4341 | 65.100 | 0.54 | 60.066 | 62.896 | 7.582 | 7.524 |
| Fe I | 5651.4688 | 16.700 | 0.56 | 15.159 | 16.353 | 7.533 | 7.492 |
| Fe I | 5652.3174 | 24.600 | 0.35 | 23.379 | 25.058 | 7.512 | 7.468 |
| Fe I | 5655.1763 | 53.600 | 1.16 | 47.434 | 52.011 | 7.597 | 7.508 |
| Fe I | 5661.3447 | 22.600 | 0.27 | 26.197 | 28.048 | 7.385 | 7.340 |
| Fe I | 5679.0229 | 60.200 | 0.49 | 58.046 | 61.685 | 7.519 | 7.454 |
| Fe I | 5691.4971 | 42.600 | 1.09 | 39.171 | 41.671 | 7.554 | 7.499 |
| Fe I | 5698.0200 | 14.900 | 0.30 | 18.639 | 20.129 | 7.354 | 7.311 |
| Fe I | 5701.5444 | 82.500 | 0.53 | 84.232 | 87.742 | 7.443 | 7.373 |
| Fe I | 5717.8325 | 62.300 | 1.04 | 63.577 | 66.573 | 7.454 | 7.396 |
| Fe I | 5731.7617 | 59.200 | 0.44 | 54.021 | 56.685 | 7.586 | 7.531 |
| Fe I | 5741.8477 | 33.200 | 0.30 | 31.006 | 33.055 | 7.531 | 7.483 |
| Fe I | 5754.4023 | 15.100 | 0.59 | 17.996 | 19.434 | 7.381 | 7.338 |
| Fe I | 5760.3438 | 22.800 | 0.40 | 25.647 | 27.548 | 7.404 | 7.358 |
| Fe I | 5838.3716 | 21.800 | 0.28 | 20.868 | 22.463 | 7.506 | 7.462 |
| Fe I | 5848.1265 | 42.800 | 0.30 | 44.939 | 47.858 | 7.436 | 7.379 |
| Fe I | 5849.6831 | 8.900 | 0.25 | 7.626 | 8.316 | 7.556 | 7.514 |
| Fe I | 5855.0757 | 24.500 | 0.31 | 25.808 | 27.751 | 7.447 | 7.401 |
| Fe I | 5858.7778 | 16.000 | 0.29 | 14.660 | 15.849 | 7.528 | 7.485 |
| Fe I | 5861.1084 | 9.900 | 0.18 | 9.858 | 10.680 | 7.482 | 7.442 |
| Fe I | 5873.2124 | 19.500 | 0.24 | 17.637 | 19.005 | 7.536 | 7.494 |


| 18 Sco |  |  |  |  |  |  |  | 18 Sco |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m}$ ) |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m}$ ) |  | $\varepsilon_{\mathrm{Fe}}$ (dex) |  |  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m} \AA)$ |  | $\mathrm{EW}_{\text {calc }}\left(\mathrm{m}\right.$ ( ${ }^{\text {a }}$ |  | $\varepsilon_{\mathrm{Fe}}$ (dex) |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE | el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 5879.4868 | 9.000 | 0.38 | 7.332 | 7.961 | 7.580 | 7.540 | Fe II | 5256.9321 | 19.000 | 0.56 | 19.188 | 19.074 | 7.474 | 7.478 |
| Fe I | 5880.0273 | 14.000 | 0.20 | 14.767 | 15.964 | 7.451 | 7.410 | Fe II | 5264.8022 | 48.000 | 0.42 | 48.293 | 48.053 | 7.473 | 7.479 |
| Fe I | 5881.2798 | 16.300 | 0.49 | 16.341 | 17.666 | 7.479 | 7.435 | Fe II | 5284.1030 | 63.900 | 1.89 | 59.728 | 59.431 | 7.577 | 7.585 |
| Fe I | 5883.8164 | 69.200 | 0.89 | 71.398 | 74.450 | 7.442 | 7.390 | Fe II | 5325.5522 | 46.000 | 0.42 | 47.415 | 47.179 | 7.446 | 7.452 |
| Fe I | 5909.9722 | 39.700 | 0.34 | 36.090 | 38.475 | 7.557 | 7.506 | Fe II | 5414.0698 | 26.800 | 0.30 | 29.803 | 29.655 | 7.400 | 7.404 |
| Fe I | 5927.7886 | 45.500 | 0.61 | 48.055 | 51.286 | 7.431 | 7.373 | Fe II | 5425.2485 | 41.000 | 0.44 | 45.798 | 45.570 | 7.366 | 7.371 |
| Fe I | 5934.6543 | 79.800 | 0.83 | 85.945 | 89.062 | 7.382 | 7.333 | Fe II | 5525.1172 | 11.800 | 0.29 | 15.220 | 15.129 | 7.338 | 7.341 |
| Fe I | 5940.9912 | 20.500 | 0.44 | 19.330 | 20.830 | 7.515 | 7.470 | Fe II | 5534.8379 | 59.900 | 1.28 | 59.808 | 59.510 | 7.482 | 7.489 |
| Fe I | 5952.7178 | 65.700 | 1.55 | 65.204 | 68.205 | 7.489 | 7.436 | Fe II | 6084.1016 | 21.900 | 0.23 | 19.947 | 19.828 | 7.540 | 7.543 |
| Fe I | 5956.6938 | 54.800 | 1.24 | 49.974 | 53.735 | 7.591 | 7.503 | Fe II | 6149.2461 | 38.500 | 0.43 | 34.449 | 34.278 | 7.579 | 7.584 |
| Fe I | 5976.7769 | 70.700 | 1.08 | 73.484 | 76.466 | 7.432 | 7.381 | Fe II | 6238.3857 | 45.300 | 0.52 | 44.758 | 44.535 | 7.493 | 7.498 |
| Fe I | 5984.8149 | 85.400 | 0.83 | 97.179 | 102.726 | 7.316 | 7.247 | Fe II | 6247.5571 | 55.900 | 0.69 | 52.040 | 51.781 | 7.567 | 7.573 |
| Fe I | 5987.0649 | 71.800 | 0.68 | 75.725 | 80.903 | 7.417 | 7.341 | Fe II | 6456.3794 | 64.900 | 0.55 | 63.568 | 63.252 | 7.509 | 7.516 |
| Fe I | 6003.0112 | 86.700 | 0.98 | 86.880 | 89.938 | 7.477 | 7.429 | Fe II | 6516.0767 | 60.500 | 0.80 | 56.720 | 56.382 | 7.563 | 7.571 |
| Fe I | 6007.9595 | 64.700 | 0.66 | 68.290 | 72.036 | 7.414 | 7.349 |  |  |  |  |  |  |  |  |
| Fe I | 6008.5557 | 90.500 | 0.97 | 95.763 | 98.929 | 7.402 | 7.355 |  |  |  |  |  |  |  |  |
| Fe I | 6024.0576 | 109.500 | 2.03 | 116.169 | 121.009 | 7.400 | 7.343 | HD22879 |  |  |  |  |  |  |  |
| Fe I | 6034.0352 | 8.300 | 0.26 | 9.383 | 10.188 | 7.420 | 7.379 |  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m}$ A $)$ |  |  |  |  |  |
| Fe I | 6056.0044 | 76.600 | 0.84 | 87.058 | 92.027 | 7.322 | 7.254 |  |  |  |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m}$ A $)$ |  | $\varepsilon_{\mathrm{Fe}}(\mathrm{dex})$ |  |
| Fe I | 6078.4912 | 80.100 | 1.10 | 83.598 | 88.745 | 7.427 | 7.354 | el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 6079.0078 | 49.100 | 0.64 | 46.624 | 49.600 | 7.527 | 7.471 | Fe I | 4788.7568 | 30.700 | 0.26 | 28.456 | 31.202 | 6.644 | 6.578 |
| Fe I | 6082.7100 | 36.900 | 0.49 | 34.728 | 37.382 | 7.529 | 7.469 | Fe I | 4789.6509 | 51.300 | 0.61 | 54.423 | 58.206 | 6.527 | 6.448 |
| Fe I | 6093.6431 | 32.900 | 0.31 | 29.361 | 31.537 | 7.559 | 7.510 | Fe I | 4799.4058 | 7.500 | 0.22 | 7.192 | 8.163 | 6.610 | 6.549 |
| Fe I | 6096.6641 | 40.300 | 0.32 | 37.770 | 40.138 | 7.532 | 7.483 | Fe I | 4802.8799 | 22.300 | 0.55 | 22.784 | 25.287 | 6.577 | 6.510 |
| Fe I | 6098.2441 | 17.100 | 0.22 | 14.366 | 15.548 | 7.575 | 7.532 | Fe I | 4875.8770 | 17.100 | 0.51 | 20.266 | 22.518 | 6.495 | 6.433 |
| Fe I | 6127.9063 | 51.500 | 0.63 | 51.892 | 54.854 | 7.472 | 7.416 | Fe I | 4882.1431 | 30.000 | 0.51 | 34.317 | 37.464 | 6.496 | 6.429 |
| Fe I | 6136.9937 | 72.200 | 1.75 | 65.835 | 69.373 | 7.625 | 7.541 | Fe I | 4885.4302 | 32.800 | 0.46 | 35.980 | 39.322 | 6.519 | 6.446 |
| Fe I | 6151.6172 | 52.400 | 1.04 | 50.500 | 53.666 | 7.522 | 7.453 | Fe I | 4892.8589 | 14.400 | 0.19 | 13.017 | 14.742 | 6.643 | 6.577 |
| Fe I | 6157.7280 | 64.300 | 0.72 | 68.797 | 72.114 | 7.397 | 7.339 | Fe I | 4896.4385 | 5.900 | 0.24 | 7.333 | 8.323 | 6.488 | 6.425 |
| Fe I | 6165.3599 | 47.200 | 0.54 | 47.892 | 50.733 | 7.466 | 7.412 | Fe I | 4907.7319 | 20.500 | 0.18 | 24.268 | 26.845 | 6.490 | 6.426 |
| Fe I | 6170.5059 | 81.300 | 1.01 | 74.815 | 79.506 | 7.584 | 7.508 | Fe I | 4917.2300 | 23.800 | 0.28 | 20.072 | 22.527 | 6.691 | 6.624 |
| Fe I | 6173.3345 | 70.000 | 0.93 | 67.467 | 71.018 | 7.539 | 7.457 | Fe I | 4950.1055 | 30.400 | 0.19 | 34.060 | 37.224 | 6.510 | 6.443 |
| Fe I | 6180.2026 | 59.200 | 0.66 | 58.363 | 61.435 | 7.499 | 7.432 | Fe I | 4962.5718 | 17.500 | 0.24 | 17.247 | 19.357 | 6.598 | 6.533 |
| Fe I | 6187.9893 | 50.100 | 0.44 | 51.322 | 54.080 | 7.457 | 7.405 | Fe I | 4969.9175 | 35.000 | 0.24 | 34.407 | 38.061 | 6.603 | 6.526 |
| Fe I | 6200.3125 | 76.200 | 0.81 | 71.296 | 74.734 | 7.590 | 7.512 | Fe I | 4985.2529 | 56.900 | 0.62 | 58.477 | 62.676 | 6.558 | 6.471 |
| Fe I | 6219.2803 | 91.600 | 1.11 | 91.616 | 96.134 | 7.480 | 7.392 | Fe I | 4986.2227 | 12.100 | 0.15 | 13.117 | 14.838 | 6.549 | 6.483 |
| Fe I | 6226.7344 | 31.000 | 0.21 | 28.574 | 30.626 | 7.536 | 7.488 | Fe I | 4993.6797 | 11.300 | 0.30 | 11.384 | 12.907 | 6.586 | 6.521 |
| Fe I | 6229.2261 | 40.300 | 0.31 | 42.586 | 45.304 | 7.429 | 7.373 | Fe I | 5002.7920 | 34.300 | 0.36 | 36.562 | 39.828 | 6.542 | 6.474 |
| Fe I | 6232.6401 | 86.700 | 1.24 | 90.553 | 93.837 | 7.418 | 7.365 | Fe I | 5022.2354 | 56.000 | 0.50 | 59.829 | 64.194 | 6.513 | 6.423 |
| Fe I | 6240.6460 | 51.100 | 0.67 | 51.358 | 54.520 | 7.474 | 7.406 | Fe I | 5023.1860 | 6.900 | 0.42 | 7.569 | 8.650 | 6.546 | 6.481 |
| Fe I | 6265.1323 | 87.500 | 1.13 | 86.575 | 90.940 | 7.500 | 7.411 | Fe I | 5028.1260 | 41.200 | 0.41 | 47.620 | 51.315 | 6.458 | 6.382 |
| Fe I | 6271.2778 | 25.000 | 0.56 | 26.233 | 28.238 | 7.449 | 7.401 | Fe I | 5044.2109 | 32.300 | 0.29 | 33.853 | 36.757 | 6.555 | 6.491 |
| Fe I | 6293.9243 | 14.100 | 0.56 | 11.500 | 12.527 | 7.586 | 7.541 | Fe I | 5067.1494 | 27.500 | 0.26 | 23.287 | 26.019 | 6.694 | 6.626 |
| Fe I | 6297.7925 | 77.800 | 1.06 | 75.163 | 79.036 | 7.539 | 7.454 | Fe I | 5088.1533 | 7.900 | 0.20 | 6.771 | 7.703 | 6.663 | 6.602 |
| Fe I | 6311.4995 | 30.800 | 0.24 | 28.044 | 30.252 | 7.546 | 7.493 | Fe I | 5090.7729 | 44.500 | 0.29 | 46.235 | 50.641 | 6.557 | 6.473 |
| Fe I | 6315.8110 | 43.600 | 0.46 | 42.945 | 45.638 | 7.493 | 7.439 | Fe I | 5104.4375 | 6.800 | 0.46 | 6.298 | 7.206 | 6.626 | 6.562 |
| Fe I | 6322.6851 | 78.100 | 0.73 | 72.912 | 76.428 | 7.595 | 7.516 | Fe I | 5127.3594 | 63.900 | 0.77 | 60.646 | 63.704 | 6.674 | 6.595 |
| Fe I | 6338.8760 | 44.800 | 0.33 | 42.840 | 46.015 | 7.518 | 7.457 | Fe I | 5129.6309 | 10.600 | 0.35 | 10.575 | 11.990 | 6.591 | 6.528 |
| Fe I | 6380.7432 | 53.900 | 0.38 | 51.259 | 54.357 | 7.531 | 7.471 | Fe I | 5151.9106 | 59.700 | 0.93 | 56.423 | 59.455 | 6.672 | 6.596 |
| Fe I | 6421.3501 | 113.100 | 2.42 | 112.114 | 117.274 | 7.497 | 7.411 | Fe I | 5159.0576 | 27.300 | 0.25 | 27.004 | 30.206 | 6.597 | 6.523 |
| Fe I | 6469.1919 | 59.800 | 0.44 | 53.970 | 57.784 | 7.585 | 7.515 | Fe I | 5180.0557 | 12.700 | 0.23 | 10.599 | 12.141 | 6.681 | 6.613 |
| Fe I | 6481.8696 | 65.900 | 0.72 | 61.596 | 65.181 | 7.577 | 7.495 | Fe I | 5198.7109 | 57.300 | 0.88 | 57.741 | 60.973 | 6.580 | 6.509 |
| Fe I | 6495.7412 | 42.600 | 0.87 | 47.835 | 51.325 | 7.380 | 7.321 | Fe I | 5225.5259 | 34.500 | 0.38 | 31.989 | 35.269 | 6.649 | 6.572 |
| Fe I | 6496.4658 | 69.400 | 1.86 | 68.399 | 72.610 | 7.497 | 7.427 | Fe I | 5235.3867 | 33.600 | 0.64 | 33.213 | 36.699 | 6.599 | 6.521 |
| Fe I | 6518.3657 | 62.200 | 1.09 | 62.150 | 65.421 | 7.481 | 7.414 | Fe I | 5242.4907 | 48.200 | 0.28 | 48.720 | 52.557 | 6.579 | 6.500 |
| Fe I | 6533.9282 | 38.100 | 0.40 | 33.642 | 36.097 | 7.575 | 7.521 | Fe I | 5243.7764 | 19.700 | 0.19 | 19.335 | 21.749 | 6.601 | 6.532 |
| Fe I | 6569.2139 | 83.100 | 2.72 | 82.756 | 87.112 | 7.485 | 7.420 | Fe I | 5247.0503 | 27.700 | 0.30 | 26.347 | 29.372 | 6.624 | 6.549 |
| Fe I | 6574.2266 | 30.500 | 0.14 | 27.130 | 30.111 | 7.561 | 7.489 | Fe I | 5307.3608 | 47.800 | 0.44 | 49.104 | 52.238 | 6.559 | 6.486 |
| Fe I | 6581.2090 | 18.400 | 0.27 | 20.530 | 22.786 | 7.415 | 7.354 | Fe I | 5361.6250 | 8.500 | 0.21 | 8.474 | 9.718 | 6.591 | 6.524 |
| Fe I | 6593.8696 | 84.400 | 0.76 | 81.791 | 86.005 | 7.536 | 7.447 | Fe I | 5373.7085 | 21.900 | 0.17 | 24.468 | 27.554 | 6.524 | 6.449 |
| Fe I | 6597.5591 | 45.000 | 0.18 | 42.783 | 45.806 | 7.523 | 7.465 | Fe I | 5379.5737 | 20.400 | 0.20 | 22.026 | 24.610 | 6.544 | 6.475 |
| Fe I | 6608.0249 | 18.700 | 0.20 | 19.256 | 21.137 | 7.463 | 7.408 | Fe I | 5389.4790 | 39.300 | 0.14 | 40.571 | 44.929 | 6.565 | 6.480 |
| Fe I | 6625.0215 | 16.200 | 0.16 | 14.815 | 16.702 | 7.529 | 7.463 | Fe I | 5398.2793 | 28.900 | 0.19 | 28.864 | 32.395 | 6.591 | 6.512 |
| Fe I | 6633.7485 | 67.500 | 0.81 | 64.023 | 67.606 | 7.543 | 7.478 | Fe I | 5400.5010 | 55.400 | 1.14 | 55.802 | 60.919 | 6.583 | 6.491 |
| Fe I | 6667.7104 | 9.400 | 0.19 | 8.492 | 9.281 | 7.531 | 7.486 | Fe I | 5409.1333 | 14.700 | 0.20 | 12.054 | 13.729 | 6.692 | 6.626 |
| Fe I | 6699.1411 | 8.600 | 0.18 | 8.552 | 9.346 | 7.483 | 7.439 | Fe I | 5417.0332 | 5.400 | 0.23 | 5.019 | 5.782 | 6.624 | 6.558 |
| Fe I | 6703.5659 | 38.300 | 0.22 | 35.673 | 38.317 | 7.538 | 7.480 | Fe I | 5436.2949 | 8.400 | 0.20 | 7.189 | 8.244 | 6.664 | 6.599 |
| Fe I | 6710.3179 | 16.000 | 0.31 | 17.878 | 19.909 | 7.417 | 7.357 | Fe I | 5441.3389 | 5.200 | 0.29 | 5.590 | 6.411 | 6.557 | 6.491 |
| Fe I | 6713.0459 | 29.700 | 1.32 | 26.177 | 28.178 | 7.566 | 7.516 | Fe I | 5445.0420 | 61.800 | 0.66 | 63.098 | 68.585 | 6.568 | 6.473 |
| Fe I | 6716.2363 | 15.600 | 0.34 | 12.571 | 13.694 | 7.595 | 7.550 | Fe I | 5466.3960 | 33.900 | 0.18 | 32.055 | 35.736 | 6.630 | 6.551 |
| Fe I | 6750.1514 | 74.700 | 0.52 | 72.556 | 76.375 | 7.528 | 7.444 | Fe I | 5472.7085 | 8.400 | 0.27 | 9.060 | 10.378 | 6.553 | 6.484 |
| Fe I | 6752.7065 | 37.000 | 0.34 | 37.230 | 39.861 | 7.475 | 7.420 | Fe I | 5473.9004 | 34.300 | 0.21 | 36.400 | 40.132 | 6.544 | 6.463 |
| Fe I | 6804.2710 | 15.500 | 0.28 | 15.378 | 16.733 | 7.484 | 7.438 | Fe I | 5483.0986 | 10.700 | 0.25 | 12.375 | 14.078 | 6.516 | 6.448 |
| Fe I | 6810.2622 | 48.700 | 0.52 | 51.062 | 54.321 | 7.434 | 7.374 | Fe I | 5522.4463 | 8.800 | 0.30 | 9.961 | 11.397 | 6.529 | 6.460 |
| Fe II | 4993.3501 | 36.800 | 1.05 | 41.429 | 41.223 | 7.368 | 7.372 | Fe I | 5543.9355 | 20.500 | 0.23 | 20.960 | 23.630 | 6.577 | 6.503 |
| Fe II | 5000.7305 | 10.300 | 0.26 | 8.179 | 8.122 | 7.596 | 7.599 | Fe I | 5546.5059 | 14.200 | 0.18 | 11.903 | 13.557 | 6.681 | 6.615 |
| Fe II | 5100.6548 | 20.000 | 0.21 | 21.198 | 21.072 | 7.443 | 7.447 | Fe I | 5554.8945 | 36.700 | 0.66 | 41.720 | 46.459 | 6.492 | 6.405 |
| Fe II | 5132.6611 | 21.600 | 0.30 | 24.870 | 24.722 | 7.386 | 7.389 | Fe I | 5560.2114 | 14.800 | 0.36 | 13.347 | 15.236 | 6.644 | 6.574 |


| HD22879 |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m} \AA)$ |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m}$ ) |  | $\varepsilon_{\mathrm{Fe}}(\mathrm{dex})$ |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 5587.5742 | 7.600 | 0.23 | 6.175 | 7.098 | 6.687 | 6.623 |
| Fe I | 5618.6323 | 12.900 | 0.2 | 14.595 | 16.58 | 6.525 | 6.454 |
| Fe I | 5619.5952 | 5.800 | 0.17 | 5.185 | 5.960 | 6.642 | 6.577 |
| Fe I | 5638.2622 | 31.500 | 0.23 | 33.772 | 37.441 | 6.539 | 6.458 |
| Fe I | 5641.4341 | 18.400 | 0.33 | 18.451 | 20.896 | 6.588 | 6.515 |
| Fe I | 5655.1763 | 13.000 | 0.38 | 10.696 | 12.525 | 6.690 | 6.609 |
| Fe I | 5691.4971 | 8.700 | 0.18 | 393 | 669 | 6.6 | 37 |
| Fe I | 5701.5444 | 40.300 | 0.28 | 0.901 | 4.02 | 6.577 | 6.508 |
| Fe I | 5705.4644 | 9.200 | 0.29 | 10.187 | 11.69 | 6.540 | 6.469 |
| Fe I | 5717.8325 | 20.500 | 0.34 | 20.659 | 23.317 | 6.585 | 6.511 |
| Fe I | 5731.7617 | 16.700 | 0.25 | 14.976 | 17.018 | 6.649 | 6.579 |
| Fe I | 5741.8477 | 6.000 | 0.32 | 5.819 | 6.704 | 6.604 | 6.537 |
| Fe I | 5883.8164 | 23.300 | 0.23 | 23.074 | 25.926 | 6.596 | 6.524 |
| Fe I | 5905.6714 | 18.300 | 0.24 | 9.267 | 22.121 | 6.561 | 6.481 |
| Fe I | 5909.9722 | 7.700 | 0.31 | 7.335 | 8.345 | 6.613 | 6.55 |
| Fe I | 5927.7886 | 11.200 | 0.20 | 10.976 | 12.718 | 6.600 | 6.525 |
| Fe I | 5930.1797 | 44.200 | 1.12 | 39.182 | 43.877 | 6.687 | 6.596 |
| FeI | 5956.6938 | 14.800 | 0.26 | 13.758 | 15.634 | 6.629 | 6.560 |
| FeI | 5976.7769 | 22.200 | . 23 | 24.471 | 27.434 | . 532 | 6.459 |
| Fe I | 5984.8149 | 35.400 | 0.42 | 37.212 | 41.953 | 6.553 | 6.462 |
| Fe I | 5987.0649 | 23.300 | 0.30 | 24.084 | 27.588 | 6.570 | 6.486 |
| FeI | 6003.0112 | 35.300 | 0.33 | 33.412 | 37.001 | 6.629 | 6.555 |
| FeI | 6008.5557 | 38.800 | 0.36 | 39.214 | 43.140 | 6.582 | 6.504 |
| FeI | 6027.0508 | 25.100 | 0.23 | 25.228 | 28.378 | 6.587 | 6.510 |
| FeI | 6056.0044 | 29.300 | 0.28 | 31.330 | 5.481 | 6.545 | 6.459 |
| FeI | 6065.4819 | 74.000 | 0.98 | 70.249 | 73.791 | 6.669 | 6.594 |
| FeI | 6078.4912 | 30.400 | 0.23 | 28.736 | 32.692 | 6.627 | 6.541 |
| FeI | 6079.0078 | 10.600 | 0.45 | 10.447 | 12.091 | 6.597 | 6.523 |
| FeI | 6093.6431 | 6.000 | 0.18 | 5.169 | 6.017 | 6.659 | 6.589 |
| FeI | 6096.6641 | 7.800 | 0.17 | 7.509 | 8.621 | 6.608 | 6.541 |
| FeI | 6127.9063 | 13.500 | 0.24 | 13.056 | 14.955 | 6.60 | 6.535 |
| Fe I | 6136.9937 | 25.700 | 0.33 | 24.481 | 27.051 | 6.622 | 6.556 |
| Fe I | 6151.6172 | 13.800 | 0.30 | 13.925 | 15.646 | 6.585 | 6.522 |
| FeI | 6157.7280 | 21.900 | 0.24 | 22.560 | 25.520 | 6.572 | 6.496 |
| Fe I | 6165.3599 | 11.600 | 0.18 | 11.322 | 13.014 | 6.602 | 6.530 |
| Fe I | 6170.5059 | 27.800 | 18 | 23.833 | 27.207 | 6.68 | 6.604 |
| Fe I | 6173.3345 | 28.000 | 0.32 | 6.264 | 8.95 | . 633 | 6.56 |
| FeI | 6200.3125 | 30.800 | 0.34 | 29.083 | 31.85 | 6.631 | 6.565 |
| FeI | 6213.4292 | 43.700 | 0.57 | 44.171 | 47.496 | 6.580 | 6.508 |
| FeI | 6219.2803 | 50.200 | 0.55 | 47.511 | 50.868 | 6.649 | 6.575 |
| Fe I | 6229.2261 | 9.400 | 0.40 | 10.024 | 11.352 | 6.558 | 6.494 |
| Fe I | 6232.6401 | 35.600 | 0.17 | 37.497 | 41.342 | 6.551 | 6.472 |
| Fe I | 6240.6460 | 12.400 | 0.19 | 14.525 | 16.284 | 6.507 | 6.444 |
| Fe I | 6252.5547 | 75.200 | 0.90 | 71.598 | 75.366 | 6.668 | 6.586 |
| Fe I | 6265.1323 | 45.700 | 0.57 | 43.166 | 46.465 | 6.646 | 6.573 |
| Fe I | 6280.6172 | 22.500 | 0.51 | 20.697 | 23.255 | 6.641 | 6.569 |
| Fe I | 6297.7925 | 33.700 | 0.27 | 32.626 | 35.618 | 6.615 | 6.546 |
| Fe I | 6311.4995 | 5.400 | 0.23 | 5.166 | 5.884 | 6.611 | 6.549 |
| FeI | 6322.6851 | 31.400 | 0.27 | 30.322 | 33.139 | 6.615 | 6.550 |
| Fe I | 6335.3301 | 58.300 | 0.61 | 59.542 | 63.141 | 6.563 | 6.484 |
| FeI | 6344.1479 | 18.000 | 0.79 | 17.699 | 19.731 | 6.600 | 6.536 |
| Fe I | 6355.0283 | 24.100 | 0.29 | 23.686 | 26.230 | 6.601 | 6.535 |
| Fe I | 6380.7432 | 15.000 | 0.22 | 12.753 | 14.692 | 6.674 | 6.601 |
| Fe I | 6400.3169 | 22.300 | 0.56 | 21.528 | 24.162 | 6.611 | 6.540 |
| Fe I | 6408.0176 | 46.300 | 0.30 | 47.950 | 52.290 | 6.559 | 6.476 |
| Fe I | 6421.3501 | 66.900 | 0.77 | 63.252 | 66.863 | 6.672 | 6.591 |
| FeI | 6430.8452 | 70.300 | 0.69 | 68.586 | 72.501 | 6.627 | 6.543 |
| Fe I | 6469.1919 | 13.500 | 0.34 | 13.360 | 15.481 | 6.595 | 6.517 |
| Fe I | 6475.6240 | 14.300 | 0.15 | 13.664 | 15.336 | 6.614 | 6.552 |
| Fe I | 6481.8696 | 22.200 | 0.15 | 20.950 | 23.304 | 6.625 | 6.560 |
| Fe I | 6496.4658 | 21.100 | 0.32 | 20.628 | 23.710 | 6.603 | 6.520 |
| Fe I | 6533.9282 | 6.200 | 0.16 | 6.371 | 7.443 | 6.577 | 6.502 |
| Fe I | 6593.8696 | 39.900 | 0.22 | 38.162 | 41.346 | 6.629 | 6.558 |
| Fe I | 6597.5591 | 9.200 | 0.17 | 9.028 | 10.485 | 6.599 | 6.525 |
| Fe I | 6609.1099 | 22.900 | 0.28 | 21.592 | 23.938 | 6.626 | 6.562 |
| Fel | 6633.7485 | 23.100 | 0.46 | 19.160 | 22.023 | 6.699 | 6.619 |
| Fe I | 6703.5659 | 8.100 | 0.29 | 7.419 | 8.412 | 6.632 | 6.571 |
| Fel | 6750.1514 | 32.200 | 0.23 | 29.984 | 32.913 | 6.642 | 6.573 |
| Fe II | 4993.3501 | 15.200 | 0.33 | 16.898 | 16.831 | 6.529 | 6.531 |
| Fe II | 5100.6548 | 5.200 | 0.26 | 6.300 | 6.269 | 6.498 | 6.500 |
| Fe II | 5132.6611 | 5.700 | 0.22 | 7.811 | 7.772 | 6.437 | 6.440 |
| Fe II | 5234.6226 | 59.600 | 0.60 | 60.708 | 60.526 | 6.563 | 6.568 |
| Fe II | 5264.8022 | 20.900 | 0.27 | 22.030 | 21.942 | 6.556 | 6.558 |
| Fe II | 5284.1030 | 31.200 | 0.30 | 31.719 | 31.593 | 6.577 | 6.580 |
| Fe II | 5325.5522 | 18.000 | 0.11 | 21.350 | 21.265 | 6.483 | 6.486 |
| Fe II | 5362.8613 | 47.000 | 0.73 | 45.395 | 45.259 | 6.629 | 6.632 |
| Fe II | 5414.069 | 8.300 | 0.20 | 153 | 102 | 6.487 | 6.49 |


| HD22879 |  |  |  |  |  |  |  |
| :--- | :--- | :--- | :--- | :---: | :---: | :---: | :---: |
|  |  | EW $_{\text {obs }}(\mathrm{m} \AA)$ | EW $_{\text {calc }}$ (mÅ) |  | $\varepsilon_{\text {Fe }}($ dex $)$ |  |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe II | 5425.2485 | 16.300 | 0.15 | 20.131 | 20.051 | 6.463 | 6.465 |
| Fe II | 55344.8379 | 31.800 | 0.28 | 31.643 | 31.517 | 6.594 | 6.597 |
| Fe II | 6149.2461 | 14.200 | 0.15 | 12.890 | 12.839 | 6.644 | 6.647 |
| Fe II | 6238.3857 | 17.600 | 0.23 | 19.601 | 19.523 | 6.523 | 6.525 |
| Fe II | 6247.5751 | 27.800 | 0.32 | 25.078 | 24.978 | 6.666 | 6.669 |
| Fe II | 6456.3794 | 37.600 | 0.47 | 34.362 | 34.225 | 6.671 | 6.675 |
| Fe II | 6516.0767 | 28.200 | 0.30 | 28.551 | 28.437 | 6.581 | 6.584 |


| $\alpha$ Cen A |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m} \AA)$ |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m} \AA$ ) |  | $\varepsilon_{\mathrm{Fe}}(\mathrm{dex})$ |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 4787.8267 | 51.700 | 2.62 | 47.462 | 49.595 | 7.873 | 7.821 |
| Fe I | 4789.6509 | 102.000 | 2.77 | 110.343 | 113.172 | 7.642 | 7.600 |
| Fe I | 4799.4058 | 45.600 | 1.86 | 42.002 | 44.120 | 7.856 | 7.805 |
| Fe I | 4802.8799 | 72.300 | 2.00 | 67.367 | 69.666 | 7.891 | 7.834 |
| Fe I | 4809.9385 | 26.300 | 1.75 | 24.080 | 25.672 | 7.830 | 7.787 |
| Fe I | 4874.3530 | 23.000 | 2.49 | 23.992 | 25.660 | 7.742 | 7.697 |
| Fe I | 4875.8770 | 66.600 | 2.83 | 66.966 | 69.180 | 7.762 | 7.712 |
| Fe I | 4877.6045 | 26.600 | 1.90 | 24.266 | 25.981 | 7.833 | 7.786 |
| Fe I | 4882.1431 | 81.800 | 2.16 | 85.798 | 87.998 | 7.694 | 7.651 |
| Fe I | 4885.4302 | 83.100 | 1.60 | 85.191 | 87.375 | 7.728 | 7.684 |
| Fe I | 4892.8589 | 61.500 | 1.61 | 58.281 | 60.900 | 7.839 | 7.783 |
| Fe I | 4905.1328 | 46.600 | 1.16 | 48.228 | 50.448 | 7.731 | 7.680 |
| Fe I | 4907.7319 | 77.100 | 0.78 | 73.046 | 75.228 | 7.856 | 7.810 |
| Fe I | 4950.1055 | 91.200 | 2.77 | 85.766 | 88.055 | 7.872 | 7.829 |
| Fe I | 4962.5718 | 64.300 | 1.42 | 65.260 | 67.908 | 7.750 | 7.695 |
| Fe I | 4985.2529 | 114.700 | 2.45 | 118.264 | 121.048 | 7.721 | 7.682 |
| Fe I | 4986.2227 | 59.800 | 1.47 | 58.285 | 60.840 | 7.803 | 7.748 |
| Fe I | 4992.7852 | 12.800 | 1.24 | 13.093 | 14.078 | 7.758 | 7.719 |
| Fe I | 4999.1123 | 43.100 | 1.49 | 41.491 | 43.675 | 7.809 | 7.757 |
| Fe I | 5002.7920 | 94.700 | 1.55 | 88.978 | 91.259 | 7.874 | 7.832 |
| Fe I | 5022.2354 | 116.600 | 2.27 | 121.648 | 124.639 | 7.703 | 7.662 |
| Fe I | 5023.1860 | 41.900 | 1.76 | 45.151 | 47.527 | 7.696 | 7.646 |
| Fe I | 5023.4976 | 38.900 | 1.07 | 36.113 | 38.255 | 7.834 | 7.785 |
| Fe I | 5025.3027 | 21.900 | 1.94 | 23.333 | 24.902 | 7.729 | 7.687 |
| Fe I | 5029.6177 | 60.500 | 1.69 | 58.899 | 61.226 | 7.810 | 7.752 |
| Fe I | 5031.9141 | 37.700 | 0.89 | 38.379 | 40.656 | 7.75 | 7.704 |
| Fe I | 5036.9214 | 29.900 | 1.31 | 29.376 | 31.318 | 7.783 | 7.735 |
| Fe I | 5048.4355 | 84.500 | 4.21 | 79.777 | 82.160 | 7.870 | 7.820 |
| Fe | 5054.6426 | 50.600 | 39 | 49.300 | 51.515 | 7.805 | 7.746 |
| Fe I | 5072.6719 | 79.800 | 1.66 | 82.352 | 85.162 | 7.723 | 7.671 |
| Fe I | 5104.4375 | 45.800 | 3.23 | 40.984 | 43.232 | 7.879 | 7.826 |
| Fe I | 5180.0557 | 56.000 | 1.19 | 54.184 | 57.277 | 7.809 | 7.744 |
| Fe I | 5197.9360 | 40.400 | 1.66 | 42.796 | 45.143 | 7.716 | 7.666 |
| Fe I | 5236.2021 | 45.600 | 1.26 | 48.255 | 50.688 | 7.707 | 7.653 |
| Fe I | 5242.4907 | 99.700 | 2.24 | 103.500 | 106.372 | 7.708 | 7.662 |
| Fe I | 5253.0210 | 24.400 | 1.13 | 21.096 | 22.906 | 7.864 | 7.811 |
| Fe I | 5267.2695 | 37.000 | 1.75 | 37.277 | 39.488 | 7.764 | 7.714 |
| Fe I | 5288.5249 | 69.300 | 1.25 | 69.668 | 72.195 | 7.762 | 7.705 |
| Fe I | 5293.9590 | 37.400 | 0.97 | 37.953 | 40.119 | 7.757 | 7.706 |
| Fe I | 5294.5474 | 19.500 | 1.20 | 17.936 | 19.307 | 7.820 | 7.776 |
| Fe I | 5295.3120 | 37.700 | 1.25 | 35.823 | 38.029 | 7.814 | 7.763 |
| Fe I | 5320.0356 | 24.500 | 0.82 | 25.442 | 27.211 | 7.744 | 7.698 |
| Fe I | 5326.1426 | 52.100 | 1.76 | 47.527 | 49.871 | 7.884 | 7.824 |
| Fe I | 5373.7085 | 75.000 | 1.28 | 78.911 | 82.457 | 7.698 | 7.636 |
| Fe I | 5379.5737 | 73.800 | 1.60 | 68.823 | 71.393 | 7.884 | 7.824 |
| Fe I | 5386.3330 | 42.700 | 0.90 | 42.770 | 45.068 | 7.768 | 7.717 |
| Fe I | 5398.2793 | 83.300 | 0.89 | 85.414 | 88.880 | 7.733 | 7.675 |
| Fe I | 5401.2666 | 27.700 | 1.31 | 29.561 | 31.481 | 7.722 | 7.676 |
| Fe I | 5406.7749 | 39.600 | 1.12 | 36.428 | 38.589 | 7.843 | 7.793 |
| Fe I | 5412.7837 | 25.700 | 0.85 | 29.695 | 31.658 | 7.668 | 7.623 |
| Fe I | 5441.3389 | 40.600 | 1.23 | 38.345 | 40.577 | 7.822 | 7.771 |
| Fe I | 5452.0884 | 17.800 | 0.90 | 16.779 | 18.100 | 7.805 | 7.760 |
| Fe I | 5466.3960 | 87.500 | 1.01 | 89.551 | 92.607 | 7.736 | 7.685 |
| Fe I | 5473.1626 | 27.800 | 0.92 | 25.509 | 27.253 | 7.830 | 7.784 |
| Fe I | 5473.9004 | 95.200 | 2.20 | 88.403 | 90.763 | 7.896 | 7.853 |
| Fe I | 5483.0986 | 56.400 | 0.91 | 55.059 | 57.533 | 7.801 | 7.744 |
| Fel | 5487.1450 | 48.800 | 1.12 | 43.517 | 45.952 | 7.887 | 7.832 |
| Fel | 5491.8315 | 16.000 | 1.03 | 14.193 | 15.311 | 7.837 | 7.795 |
| Fe I | 5522.4463 | 54.600 | 1.17 | 49.865 | 52.269 | 7.881 | 7.824 |
| Fe I | 5524.2495 | 6.900 | 0.91 | 6.118 | 6.636 | 7.828 | 7.789 |
| Fe I | 5525.5435 | 68.600 | 0.91 | 65.850 | 68.451 | 7.832 | 7.773 |
| Fe I | 5536.5801 | 10.400 | 1.01 | 12.812 | 13.987 | 7.659 | 7.613 |
| Fe I | 5539.2798 | 25.100 | 0.76 | 25.061 | 26.861 | 7.771 | 7.723 |
| Fel | 5543.9355 | 73.000 | 0.75 | 68.674 | 71.239 | 7.865 | 7.808 |
| Fe I | 5546.5059 | 61.400 | 0.88 | 55.772 | 58.461 | 7.894 | 7.8 |


| $\alpha$ Cen A |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m} \AA)$ |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m} \AA)$ |  | $\varepsilon_{\mathrm{Fe}}$ (dex) |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 5546.9907 | 38.200 | 0.88 | 33.806 | 35.849 | 7.875 | 7.825 |
| Fe I | 5554.8945 | 104.400 | 1.98 | 107.073 | 111.767 | 7.733 | 7.671 |
| Fe I | 5560.2114 | 60.200 | 1.21 | 59.578 | 62.385 | 7.783 | 7.725 |
| Fe I | 5577.0249 | 15.800 | 0.85 | 15.998 | 17.619 | 7.763 | 7.708 |
| Fe I | 5584.7646 | 51.500 | 1.24 | 49.668 | 52.172 | 7.814 | 7.754 |
| Fe I | 5618.6323 | 63.400 | 0.98 | 58.677 | 61.186 | 7.880 | 7.821 |
| Fe I | 5636.6958 | 27.900 | 0.80 | 27.204 | 29.126 | 7.788 | 7.739 |
| Fe I | 5638.2622 | 85.700 | 1.69 | 85.718 | 88.097 | 7.770 | 7.724 |
| Fe I | 5650.7056 | 47.100 | 0.94 | 41.369 | 45.361 | 7.896 | 7.805 |
| Fe I | 5651.4688 | 23.600 | 1.12 | 21.326 | 22.882 | 7.835 | 7.790 |
| Fe I | 5652.3174 | 34.000 | 0.97 | 30.485 | 32.431 | 7.857 | 7.808 |
| Fe I | 5679.0229 | 71.000 | 1.15 | 64.528 | 68.139 | 7.898 | 7.824 |
| Fe I | 5680.2402 | 14.700 | 0.88 | 12.116 | 13.113 | 7.874 | 7.832 |
| Fe I | 5717.8325 | 74.200 | 1.87 | 68.556 | 71.264 | 7.893 | 7.833 |
| Fe I | 5741.8477 | 41.500 | 1.00 | 38.331 | 40.519 | 7.845 | 7.793 |
| Fe I | 5742.9600 | 17.400 | 1.26 | 14.019 | 15.139 | 7.892 | 7.848 |
| Fe I | 5754.4023 | 26.800 | 1.20 | 23.862 | 25.631 | 7.849 | 7.801 |
| Fe I | 5760.3438 | 27.600 | 0.77 | 32.230 | 34.360 | 7.652 | 7.604 |
| Fe I | 5838.3716 | 32.200 | 1.11 | 27.542 | 29.425 | 7.883 | 7.836 |
| Fe I | 5848.1265 | 54.900 | 1.31 | 52.111 | 55.086 | 7.832 | 7.766 |
| Fe I | 5855.0757 | 29.200 | 0.67 | 33.638 | 35.938 | 7.662 | 7.614 |
| Fe I | 5858.7778 | 20.900 | 0.90 | 20.417 | 21.954 | 7.785 | 7.739 |
| Fe I | 5861.1084 | 14.600 | 0.60 | 14.359 | 15.490 | 7.779 | 7.737 |
| Fe I | 5873.2124 | 27.000 | 0.80 | 24.214 | 25.925 | 7.842 | 7.797 |
| Fe I | 5880.0273 | 18.300 | 0.53 | 20.944 | 22.520 | 7.688 | 7.644 |
| Fe I | 5881.2798 | 20.600 | 0.66 | 22.930 | 24.629 | 7.702 | 7.658 |
| Fe I | 5883.8164 | 78.600 | 1.66 | 75.877 | 78.629 | 7.822 | 7.769 |
| Fe I | 5898.2153 | 23.500 | 0.64 | 19.208 | 20.788 | 7.894 | 7.846 |
| Fe I | 5902.4731 | 18.800 | 0.81 | 24.093 | 25.934 | 7.612 | 7.567 |
| Fe I | 5905.6714 | 72.200 | 0.79 | 71.645 | 75.416 | 7.780 | 7.710 |
| Fe I | 5909.9722 | 46.300 | 0.83 | 42.194 | 44.697 | 7.865 | 7.806 |
| Fe I | 5927.7886 | 55.900 | 0.61 | 55.471 | 58.762 | 7.779 | 7.713 |
| Fe I | 5934.6543 | 89.300 | 1.31 | 89.675 | 92.258 | 7.764 | 7.720 |
| Fe I | 5940.9912 | 28.600 | 0.55 | 25.869 | 27.697 | 7.842 | 7.793 |
| Fe I | 5976.7769 | 80.300 | 0.86 | 77.917 | 80.493 | 7.815 | 7.766 |
| Fe I | 5984.8149 | 93.600 | 1.26 | 102.352 | 107.626 | 7.645 | 7.574 |
| Fe I | 5987.0649 | 82.400 | 1.47 | 81.481 | 86.682 | 7.786 | 7.700 |
| Fe I | 6003.0112 | 97.200 | 1.31 | 90.489 | 93.000 | 7.882 | 7.840 |
| Fe I | 6007.9595 | 76.800 | 1.03 | 74.102 | 77.594 | 7.822 | 7.755 |
| Fe I | 6008.5557 | 100.800 | 1.47 | 99.039 | 101.683 | 7.797 | 7.756 |
| Fe I | 6015.2437 | 9.800 | 1.08 | 10.315 | 11.436 | 7.744 | 7.691 |
| Fe I | 6024.0576 | 122.700 | 1.94 | 121.511 | 125.788 | 7.784 | 7.734 |
| Fe I | 6027.0508 | 76.900 | 1.27 | 77.616 | 80.682 | 7.756 | 7.698 |
| Fe I | 6034.0352 | 11.400 | 0.83 | 13.805 | 14.924 | 7.668 | 7.627 |
| Fe I | 6056.0044 | 86.600 | 1.21 | 92.440 | 97.203 | 7.678 | 7.607 |
| Fe I | 6078.4912 | 91.400 | 2.04 | 89.249 | 94.344 | 7.804 | 7.725 |
| Fe I | 6079.0078 | 60.500 | 1.20 | 54.258 | 57.174 | 7.899 | 7.837 |
| Fe I | 6093.6431 | 40.400 | 0.95 | 37.351 | 39.820 | 7.839 | 7.783 |
| Fe I | 6096.6641 | 47.900 | 0.85 | 44.997 | 47.415 | 7.833 | 7.780 |
| Fe I | 6098.2441 | 24.000 | 1.00 | 20.401 | 21.984 | 7.873 | 7.826 |
| Fe I | 6120.2466 | 6.400 | 0.63 | 5.803 | 6.655 | 7.817 | 7.751 |
| Fe I | 6127.9063 | 62.200 | 1.22 | 58.108 | 61.038 | 7.858 | 7.794 |
| Fe I | 6157.7280 | 75.900 | 1.29 | 73.517 | 76.580 | 7.818 | 7.757 |
| Fe I | 6165.3599 | 56.900 | 1.11 | 54.439 | 57.304 | 7.824 | 7.761 |
| Fe I | 6187.3979 | 5.100 | 0.74 | 5.588 | 6.181 | 7.726 | 7.678 |
| Fe I | 6187.9893 | 62.200 | 1.04 | 57.529 | 60.114 | 7.869 | 7.813 |
| Fe I | 6199.5063 | 6.300 | 0.64 | 5.337 | 5.923 | 7.849 | 7.799 |
| Fe I | 6226.7344 | 39.900 | 1.05 | 35.745 | 38.027 | 7.864 | 7.811 |
| Fe I | 6229.2261 | 50.600 | 0.89 | 47.694 | 50.523 | 7.840 | 7.772 |
| Fe I | 6232.6401 | 94.000 | 1.37 | 93.517 | 96.409 | 7.778 | 7.729 |
| Fe I | 6253.8286 | 31.400 | 1.13 | 37.119 | 39.615 | 7.637 | 7.587 |
| Fe I | 6270.2236 | 64.300 | 0.84 | 61.762 | 64.876 | 7.833 | 7.756 |
| Fe I | 6271.2778 | 34.100 | 1.35 | 32.609 | 34.913 | 7.806 | 7.751 |
| Fe I | 6293.9243 | 17.700 | 0.58 | 16.969 | 18.405 | 7.795 | 7.747 |
| Fe I | 6315.8110 | 51.900 | 0.62 | 49.741 | 52.469 | 7.818 | 7.758 |
| Fe I | 6338.8760 | 54.900 | 1.06 | 50.817 | 54.061 | 7.855 | 7.787 |
| Fe I | 6408.0176 | 109.100 | 2.17 | 109.494 | 112.532 | 7.764 | 7.721 |
| Fe I | 6495.7412 | 52.300 | 0.82 | 55.747 | 59.368 | 7.700 | 7.632 |
| Fe I | 6496.4658 | 75.000 | 1.14 | 74.866 | 78.889 | 7.772 | 7.701 |
| Fe I | 6569.2139 | 89.000 | 1.11 | 89.100 | 93.103 | 7.768 | 7.706 |
| Fe I | 6581.2090 | 25.500 | 0.97 | 24.553 | 27.160 | 7.795 | 7.728 |
| Fe I | 6591.3130 | 13.600 | 1.02 | 13.634 | 14.836 | 7.769 | 7.722 |
| Fe I | 6597.5591 | 55.600 | 0.86 | 50.981 | 54.063 | 7.865 | 7.801 |
| Fe I | 6608.0249 | 25.700 | 0.75 | 23.970 | 26.225 | 7.817 | 7.756 |
| Fe I | 6625.0215 | 21.900 | 1.12 | 17.802 | 20.070 | 7.894 | 7.822 |
| Fe I | 6667.4180 | 12.000 | 1.04 | 9.989 | 11.074 | 7.865 | 7.812 |
| Fe I | 6667.7104 | 15.100 | 1.03 | 12.708 | 13.828 | 7.865 | 7.818 |


| $\alpha$ Cen A |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m}$ ) |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m} \AA$ ) |  | $\varepsilon_{\mathrm{Fe}}$ (dex) |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 6699.1411 | 12.100 | 0.99 | 12.794 | 13.937 | 7.740 | 7.694 |
| Fe I | 6703.5659 | 45.700 | 0.92 | 41.274 | 44.143 | 7.874 | 7.805 |
| Fe I | 6710.3179 | 20.800 | 0.50 | 21.656 | 24.089 | 7.745 | 7.678 |
| Fe I | 6739.5205 | 16.600 | 0.71 | 18.316 | 20.442 | 7.712 | 7.649 |
| Fe I | 6752.7065 | 42.300 | 1.42 | 45.032 | 47.703 | 7.708 | 7.650 |
| Fe I | 6786.8584 | 35.500 | 1.01 | 30.831 | 32.939 | 7.877 | 7.827 |
| Fe II | 4893.8125 | 23.300 | 1.29 | 22.036 | 21.948 | 7.808 | 7.811 |
| Fe II | 4993.3501 | 46.500 | 1.66 | 51.989 | 51.833 | 7.625 | 7.629 |
| Fe II | 5000.7305 | 15.100 | 1.07 | 14.766 | 14.707 | 7.783 | 7.785 |
| Fe II | 5100.6548 | 26.400 | 0.92 | 32.052 | 31.924 | 7.615 | 7.618 |
| Fe II | 5132.6611 | 27.800 | 1.65 | 36.078 | 35.934 | 7.550 | 7.553 |
| Fe II | 5234.6226 | 99.600 | 2.18 | 103.804 | 103.597 | 7.692 | 7.696 |
| Fe II | 5256.9321 | 25.700 | 1.72 | 29.798 | 29.679 | 7.655 | 7.658 |
| Fe II | 5264.8022 | 54.200 | 0.87 | 58.815 | 58.639 | 7.650 | 7.654 |
| Fe II | 5325.5522 | 55.800 | 1.04 | 58.049 | 57.875 | 7.712 | 7.716 |
| Fe II | 5414.0698 | 33.400 | 0.82 | 41.449 | 41.284 | 7.560 | 7.563 |
| Fe II | 5425.2485 | 49.600 | 0.87 | 56.620 | 56.451 | 7.590 | 7.594 |
| Fe II | 5525.1172 | 22.500 | 1.26 | 25.104 | 25.004 | 7.692 | 7.694 |
| Fe II | 5534.8379 | 69.500 | 2.20 | 69.725 | 69.516 | 7.764 | 7.770 |
| Fe II | 6084.1016 | 30.700 | 0.83 | 30.934 | 30.811 | 7.764 | 7.767 |
| Fe II | 6113.3193 | 15.800 | 0.89 | 18.241 | 18.150 | 7.682 | 7.685 |
| Fe II | 6149.2461 | 47.100 | 1.05 | 46.686 | 46.500 | 7.781 | 7.785 |
| Fe II | 6238.3857 | 53.400 | 0.82 | 56.740 | 56.570 | 7.687 | 7.691 |
| Fe II | 6239.9429 | 18.800 | 0.66 | 19.729 | 19.650 | 7.738 | 7.741 |
| Fe II | 6247.5571 | 62.300 | 0.65 | 63.704 | 63.513 | 7.736 | 7.741 |
| Fe II | 6369.4590 | 24.300 | 0.71 | 33.478 | 33.311 | 7.524 | 7.527 |
| Fe II | 6456.3794 | 73.400 | 0.82 | 74.987 | 74.763 | 7.734 | 7.739 |
| Fe II | 6516.0767 | 65.800 | 1.46 | 67.274 | 67.006 | 7.735 | 7.741 |


| $\mu$ Ara |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m}$ ) |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m} \AA)$ |  | $\varepsilon_{\mathrm{Fe}}$ (dex) |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 4787.8267 | 59.100 | 0.85 | 51.888 | 53.603 | 7.973 | 7.931 |
| Fe I | 4788.7568 | 82.200 | 1.46 | 77.713 | 79.461 | 7.906 | 7.865 |
| Fe I | 4793.9614 | 15.600 | 0.28 | 15.973 | 16.974 | 7.787 | 7.752 |
| Fe I | 4794.3540 | 22.100 | 0.27 | 18.165 | 19.407 | 7.918 | 7.879 |
| Fe I | 4799.4058 | 49.600 | 1.09 | 45.998 | 47.716 | 7.884 | 7.843 |
| Fe I | 4802.8799 | 73.800 | 1.86 | 72.067 | 73.764 | 7.841 | 7.801 |
| Fe I | 4808.1479 | 40.300 | 0.90 | 36.901 | 38.519 | 7.880 | 7.841 |
| Fe I | 4809.9385 | 28.500 | 1.34 | 27.146 | 28.485 | 7.835 | 7.800 |
| Fe I | 4869.4634 | 33.600 | 1.59 | 31.599 | 33.053 | 7.851 | 7.814 |
| Fe I | 4875.8770 | 69.400 | 2.10 | 71.749 | 73.363 | 7.749 | 7.714 |
| Fe I | 4882.1431 | 86.800 | 1.73 | 91.030 | 92.510 | 7.722 | 7.694 |
| Fe I | 4885.4302 | 85.300 | 1.66 | 90.358 | 91.827 | 7.702 | 7.672 |
| Fe I | 4892.8589 | 66.500 | 1.14 | 62.595 | 64.598 | 7.881 | 7.839 |
| Fe I | 4905.1328 | 47.400 | 0.57 | 52.350 | 54.081 | 7.688 | 7.651 |
| Fe I | 4907.7319 | 76.000 | 1.52 | 77.997 | 79.508 | 7.759 | 7.727 |
| Fe I | 4917.2300 | 79.800 | 1.07 | 74.235 | 76.373 | 7.911 | 7.868 |
| Fe I | 4918.0127 | 68.600 | 1.34 | 63.642 | 65.678 | 7.903 | 7.860 |
| Fe I | 4950.1055 | 91.800 | 1.88 | 91.078 | 92.653 | 7.813 | 7.784 |
| Fe I | 4962.5718 | 67.300 | 1.20 | 69.801 | 71.812 | 7.749 | 7.708 |
| Fe I | 4986.2227 | 59.600 | 1.30 | 62.633 | 64.637 | 7.737 | 7.696 |
| Fe I | 4999.1123 | 47.700 | 1.12 | 45.330 | 47.072 | 7.855 | 7.814 |
| Fe I | 5002.7920 | 95.600 | 1.05 | 94.423 | 96.056 | 7.821 | 7.792 |
| Fe I | 5023.1860 | 48.200 | 1.58 | 49.082 | 50.915 | 7.781 | 7.742 |
| Fe I | 5023.4976 | 41.100 | 0.71 | 39.685 | 41.382 | 7.832 | 7.794 |
| Fe I | 5025.3027 | 24.000 | 1.12 | 26.119 | 27.436 | 7.744 | 7.712 |
| Fe I | 5028.1260 | 99.400 | 1.71 | 106.025 | 107.859 | 7.690 | 7.658 |
| Fe I | 5029.6177 | 62.300 | 1.68 | 63.548 | 65.379 | 7.770 | 7.727 |
| Fe I | 5031.9141 | 38.100 | 1.27 | 42.041 | 43.884 | 7.714 | 7.677 |
| Fe I | 5036.9214 | 33.100 | 1.20 | 33.129 | 34.799 | 7.799 | 7.760 |
| Fe I | 5054.6426 | 53.100 | 1.44 | 53.634 | 55.407 | 7.786 | 7.742 |
| Fe I | 5067.1494 | 81.600 | 1.31 | 79.179 | 81.126 | 7.847 | 7.809 |
| Fe I | 5088.1533 | 53.300 | 1.21 | 45.965 | 47.682 | 7.963 | 7.923 |
| Fe I | 5180.0557 | 60.800 | 0.66 | 58.392 | 60.825 | 7.850 | 7.799 |
| Fe I | 5197.9360 | 43.000 | 1.92 | 46.702 | 48.597 | 7.720 | 7.681 |
| Fe I | 5236.2021 | 46.900 | 0.53 | 52.417 | 54.318 | 7.676 | 7.636 |
| Fe I | 5243.7764 | 72.800 | 1.29 | 73.297 | 75.254 | 7.790 | 7.751 |
| Fe I | 5253.0210 | 26.100 | 1.05 | 24.493 | 26.140 | 7.843 | 7.799 |
| Fe I | 5267.2695 | 41.400 | 1.94 | 40.927 | 42.721 | 7.811 | 7.771 |
| Fe I | 5285.1274 | 40.600 | 0.54 | 35.313 | 36.977 | 7.918 | 7.879 |
| Fe I | 5288.5249 | 69.900 | 0.91 | 74.618 | 76.531 | 7.697 | 7.655 |
| Fe I | 5293.9590 | 40.800 | 1.06 | 41.739 | 43.523 | 7.778 | 7.738 |
| Fe I | 5294.5474 | 20.600 | 0.87 | 20.479 | 21.671 | 7.804 | 7.769 |
| Fe I | 5295.3120 | 38.300 | 1.39 | 39.395 | 41.165 | 7.776 | 7.737 |


| $\mu$ Ara |  |  |  |  |  |  |  | $\mu$ Ara |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $\mathrm{EW}_{\text {obs }}$ (mA) |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m} \AA)$ |  | $\varepsilon_{\mathrm{Fe}}$ (dex) |  |  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m} \AA)$ |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m} \AA)$ |  | $\varepsilon_{\mathrm{Fe}}$ (dex) |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE | el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 5320.0356 | 30.800 | 0.35 | 28.691 | 30.169 | 7.853 | 7.815 | Fe I | 6007.9595 | 77.800 | 1.17 | 79.276 | 81.728 | 7.773 | 7.727 |
| Fe I | 5322.0405 | 76.900 | 0.90 | 72.664 | 75.222 | 7.909 | 7.842 | Fe I | 6008.5557 | 103.800 | 1.75 | 105.138 | 106.631 | 7.780 | 7.757 |
| Fe I | 5326.1426 | 53.500 | 0.52 | 51.908 | 53.791 | 7.838 | 7.793 | Fe I | 6027.0508 | 79.900 | 1.31 | 82.999 | 85.215 | 7.742 | 7.701 |
| Fe I | 5379.5737 | 73.000 | 1.36 | 73.793 | 75.763 | 7.783 | 7.739 | Fe I | 6034.0352 | 13.100 | 0.43 | 15.735 | 16.686 | 7.701 | 7.670 |
| Fe I | 5401.2666 | 34.000 | 0.88 | 32.827 | 34.374 | 7.828 | 7.791 | Fe I | 6056.0044 | 90.800 | 1.37 | 98.038 | 101.489 | 7.691 | 7.640 |
| Fe I | 5406.7749 | 47.000 | 0.74 | 40.074 | 41.787 | 7.951 | 7.912 | Fe I | 6078.4912 | 94.200 | 1.41 | 94.757 | 98.500 | 7.792 | 7.736 |
| Fe I | 5409.1333 | 69.400 | 0.50 | 60.953 | 63.033 | 7.975 | 7.931 | Fe I | 6079.0078 | 62.100 | 0.76 | 58.673 | 60.864 | 7.868 | 7.824 |
| Fe I | 5412.7837 | 30.100 | 0.60 | 32.940 | 34.565 | 7.733 | 7.697 | Fe I | 6082.7100 | 51.600 | 0.98 | 44.583 | 47.078 | 7.963 | 7.902 |
| Fe I | 5417.0332 | 46.000 | 0.67 | 40.096 | 41.854 | 7.929 | 7.888 | Fe I | 6093.6431 | 44.700 | 0.79 | 41.059 | 43.039 | 7.879 | 7.835 |
| Fe I | 5436.2949 | 52.400 | 0.43 | 48.202 | 50.054 | 7.890 | 7.850 | Fe I | 6096.6641 | 53.200 | 0.74 | 49.327 | 51.169 | 7.881 | 7.842 |
| Fe I | 5441.3389 | 43.500 | 0.48 | 42.110 | 43.865 | 7.831 | 7.792 | Fe I | 6098.2441 | 25.600 | 0.56 | 22.943 | 24.253 | 7.872 | 7.835 |
| Fe I | 5460.8726 | 13.600 | 0.64 | 16.466 | 17.573 | 7.694 | 7.659 | Fe I | 6127.9063 | 65.000 | 0.93 | 62.843 | 65.055 | 7.845 | 7.799 |
| Fe I | 5466.9873 | 49.600 | 0.41 | 45.061 | 46.939 | 7.907 | 7.862 | Fe I | 6151.6172 | 63.800 | 1.61 | 59.676 | 62.553 | 7.899 | 7.829 |
| Fe I | 5470.0928 | 36.800 | 0.34 | 32.820 | 34.439 | 7.891 | 7.853 | Fe I | 6157.7280 | 77.900 | 1.03 | 78.810 | 81.080 | 7.783 | 7.739 |
| Fe I | 5472.7085 | 59.200 | 0.68 | 51.938 | 53.766 | 7.965 | 7.923 | Fe I | 6165.3599 | 59.900 | 0.81 | 59.056 | 61.261 | 7.818 | 7.772 |
| Fe I | 5473.1626 | 27.600 | 0.77 | 28.556 | 29.996 | 7.776 | 7.741 | Fe I | 6180.2026 | 75.600 | 0.84 | 67.310 | 70.042 | 7.998 | 7.928 |
| Fe I | 5473.9004 | 94.000 | 1.57 | 93.920 | 95.350 | 7.801 | 7.775 | Fe I | 6187.3979 | 7.600 | 0.26 | 6.646 | 7.200 | 7.865 | 7.826 |
| Fe I | 5483.0986 | 58.000 | 0.79 | 59.576 | 61.419 | 7.765 | 7.725 | Fe I | 6187.9893 | 64.600 | 0.65 | 62.361 | 64.290 | 7.846 | 7.806 |
| Fe I | 5487.1450 | 48.600 | 0.87 | 47.468 | 49.343 | 7.824 | 7.784 | Fe I | 6199.5063 | 7.000 | 0.20 | 6.388 | 6.943 | 7.844 | 7.804 |
| Fe I | 5491.8315 | 18.500 | 0.57 | 16.165 | 17.124 | 7.878 | 7.845 | Fe I | 6219.2803 | 106.300 | 1.75 | 99.114 | 103.244 | 7.943 | 7.859 |
| Fe I | 5494.4624 | 38.200 | 0.79 | 30.625 | 32.135 | 7.980 | 7.941 | Fe I | 6226.7344 | 43.300 | 0.50 | 39.698 | 41.525 | 7.878 | 7.838 |
| Fe I | 5522.4463 | 54.300 | 0.76 | 54.150 | 55.940 | 7.803 | 7.763 | Fe I | 6229.2261 | 55.600 | 0.55 | 52.677 | 55.101 | 7.868 | 7.811 |
| Fe I | 5539.2798 | 28.300 | 0.30 | 28.297 | 29.818 | 7.800 | 7.763 | Fe I | 6232.6401 | 100.000 | 1.15 | 99.745 | 101.677 | 7.804 | 7.773 |
| Fe I | 5543.9355 | 74.300 | 0.56 | 73.592 | 75.402 | 7.815 | 7.777 | Fe I | 6240.6460 | 64.500 | 1.03 | 60.329 | 63.172 | 7.903 | 7.831 |
| Fe I | 5546.5059 | 63.700 | 1.04 | 60.161 | 62.214 | 7.875 | 7.831 | Fe I | 6265.1323 | 101.900 | 1.50 | 94.129 | 98.153 | 7.963 | 7.875 |
| Fe I | 5546.9907 | 40.500 | 0.79 | 37.411 | 39.051 | 7.871 | 7.833 | Fe I | 6271.2778 | 37.000 | 0.79 | 36.629 | 38.597 | 7.808 | 7.765 |
| Fe I | 5549.9487 | 14.300 | 0.48 | 14.407 | 15.327 | 7.796 | 7.762 | Fe I | 6290.5430 | 9.000 | 0.34 | 7.494 | 8.146 | 7.891 | 7.849 |
| Fe I | 5552.6919 | 10.600 | 0.43 | 10.699 | 11.517 | 7.795 | 7.757 | Fe I | 6293.9243 | 22.200 | 0.29 | 19.109 | 20.307 | 7.891 | 7.854 |
| Fe I | 5554.8945 | 107.600 | 2.28 | 112.860 | 116.231 | 7.730 | 7.686 | Fe I | 6297.7925 | 91.400 | 1.27 | 83.060 | 86.701 | 7.990 | 7.903 |
| Fe I | 5560.2114 | 63.800 | 0.57 | 64.099 | 66.150 | 7.794 | 7.753 | Fe I | 6311.4995 | 44.500 | 0.47 | 38.181 | 40.360 | 7.943 | 7.891 |
| Fe I | 5577.0249 | 16.000 | 0.59 | 18.015 | 19.392 | 7.732 | 7.691 | Fe I | 6315.8110 | 58.000 | 0.74 | 54.255 | 56.398 | 7.880 | 7.834 |
| Fe I | 5594.6553 | 79.900 | 2.28 | 84.174 | 86.957 | 7.726 | 7.679 | Fe I | 6338.8760 | 58.000 | 0.83 | 55.076 | 57.611 | 7.859 | 7.808 |
| Fe I | 5600.2241 | 52.000 | 0.63 | 53.497 | 55.380 | 7.766 | 7.725 | Fe I | 6380.7432 | 68.200 | 0.55 | 62.412 | 64.743 | 7.919 | 7.870 |
| Fe I | 5618.6323 | 63.000 | 0.55 | 63.290 | 65.180 | 7.794 | 7.751 | Fe I | 6408.0176 | 109.800 | 2.26 | 116.307 | 118.318 | 7.709 | 7.680 |
| Fe I | 5619.5952 | 48.600 | 0.47 | 40.539 | 42.316 | 7.976 | 7.934 | Fe I | 6469.1919 | 73.800 | 0.79 | 65.980 | 68.873 | 7.947 | 7.892 |
| Fe I | 5636.6958 | 28.800 | 0.54 | 30.617 | 32.228 | 7.755 | 7.717 | Fe I | 6495.7412 | 60.400 | 2.31 | 60.238 | 63.076 | 7.803 | 7.750 |
| Fe I | 5641.4341 | 79.200 | 0.85 | 70.132 | 71.930 | 7.993 | 7.956 | Fe I | 6496.4658 | 80.300 | 1.00 | 80.022 | 82.924 | 7.805 | 7.755 |
| Fe I | 5650.7056 | 49.300 | 0.32 | 45.171 | 48.467 | 7.887 | 7.816 | Fe I | 6518.3657 | 73.700 | 1.15 | 71.406 | 74.381 | 7.852 | 7.785 |
| Fe I | 5651.4688 | 25.700 | 0.75 | 23.938 | 25.224 | 7.847 | 7.812 | Fe I | 6533.9282 | 52.200 | 0.49 | 45.627 | 47.727 | 7.939 | 7.893 |
| Fe I | 5652.3174 | 36.300 | 0.52 | 33.872 | 35.431 | 7.857 | 7.820 | Fe I | 6569.2139 | 95.600 | 2.61 | 94.942 | 97.677 | 7.810 | 7.769 |
| Fe I | 5655.1763 | 67.100 | 1.53 | 59.621 | 64.109 | 7.950 | 7.855 | Fe I | 6574.2266 | 43.400 | 0.49 | 36.178 | 39.239 | 7.960 | 7.889 |
| Fe I | 5661.3447 | 33.800 | 0.32 | 37.059 | 38.724 | 7.724 | 7.687 | Fe I | 6581.2090 | 32.300 | 0.57 | 28.901 | 31.346 | 7.881 | 7.822 |
| Fe I | 5679.0229 | 70.900 | 0.49 | 69.145 | 71.876 | 7.833 | 7.782 | Fe I | 6591.3130 | 14.300 | 0.61 | 15.506 | 16.531 | 7.755 | 7.719 |
| Fe I | 5680.2402 | 16.700 | 0.15 | 13.853 | 14.706 | 7.904 | 7.871 | Fe I | 6597.5591 | 57.000 | 0.46 | 55.343 | 57.709 | 7.833 | 7.786 |
| Fe I | 5691.4971 | 53.900 | 0.95 | 50.325 | 52.313 | 7.881 | 7.836 | Fe I | 6608.0249 | 29.300 | 0.27 | 27.844 | 29.908 | 7.836 | 7.786 |
| Fe I | 5698.0200 | 23.800 | 0.47 | 27.819 | 29.345 | 7.695 | 7.659 | Fe I | 6625.0215 | 26.300 | 0.19 | 21.507 | 23.712 | 7.928 | 7.866 |
| Fe I | 5701.5444 | 96.100 | 0.90 | 91.713 | 94.745 | 7.892 | 7.828 | Fe I | 6627.5439 | 41.900 | 0.29 | 35.024 | 36.713 | 7.955 | 7.915 |
| Fe I | 5717.8325 | 76.600 | 1.67 | 73.519 | 75.482 | 7.864 | 7.824 | Fe I | 6633.7485 | 82.600 | 0.81 | 75.809 | 78.154 | 7.924 | 7.881 |
| Fe I | 5731.7617 | 71.300 | 0.69 | 64.490 | 66.212 | 7.949 | 7.912 | Fe I | 6667.7104 | 15.900 | 0.33 | 14.479 | 15.436 | 7.852 | 7.817 |
| Fe I | 5741.8477 | 46.000 | 0.37 | 42.172 | 43.883 | 7.887 | 7.848 | Fe I | 6699.1411 | 14.600 | 0.19 | 14.574 | 15.537 | 7.801 | 7.766 |
| Fe I | 5742.9600 | 20.100 | 0.40 | 15.986 | 16.952 | 7.934 | 7.900 | Fe I | 6703.5659 | 51.400 | 0.45 | 46.142 | 48.622 | 7.919 | 7.861 |
| Fe I | 5754.4023 | 25.900 | 1.02 | 27.020 | 28.532 | 7.771 | 7.733 | Fe I | 6710.3179 | 28.600 | 0.52 | 25.674 | 27.967 | 7.874 | 7.815 |
| Fe I | 5759.2622 | 11.800 | 0.38 | 10.003 | 10.653 | 7.885 | 7.853 | Fe I | 6713.7427 | 32.400 | 0.21 | 25.100 | 26.589 | 7.978 | 7.937 |
| Fe I | 5760.3438 | 33.800 | 0.74 | 36.010 | 37.786 | 7.748 | 7.709 | Fe I | 6716.2363 | 26.000 | 0.53 | 20.470 | 21.753 | 7.954 | 7.915 |
| Fe I | 5838.3716 | 33.700 | 0.50 | 30.882 | 32.439 | 7.866 | 7.829 | Fe I | 6746.9536 | 8.300 | 0.26 | 7.942 | 8.642 | 7.822 | 7.780 |
| Fe I | 5848.1265 | 58.700 | 0.66 | 56.434 | 58.724 | 7.849 | 7.799 | Fe I | 6752.7065 | 48.800 | 0.88 | 49.252 | 51.251 | 7.790 | 7.747 |
| Fe I | 5849.6831 | 12.500 | 0.35 | 12.666 | 13.518 | 7.793 | 7.758 | Fe I | 6786.8584 | 39.900 | 0.56 | 34.442 | 36.141 | 7.918 | 7.880 |
| Fe I | 5853.1484 | 15.200 | 0.49 | 11.196 | 12.303 | 7.962 | 7.912 | Fe I | 6804.2710 | 24.400 | 0.41 | 24.317 | 25.787 | 7.802 | 7.763 |
| Fe I | 5855.0757 | 36.500 | 0.46 | 37.107 | 38.937 | 7.786 | 7.747 | Fe I | 6810.2622 | 64.200 | 0.71 | 63.218 | 65.579 | 7.819 | 7.773 |
| Fe I | 5858.7778 | 24.800 | 0.49 | 23.045 | 24.335 | 7.848 | 7.812 | Fe II | 4893.8125 | 28.200 | 0.88 | 22.745 | 22.654 | 7.954 | 7.957 |
| Fe I | 5861.1084 | 16.000 | 0.46 | 16.344 | 17.314 | 7.788 | 7.755 | Fe II | 4993.3501 | 45.800 | 1.92 | 53.455 | 53.295 | 7.607 | 7.610 |
| Fe I | 5873.2124 | 30.600 | 0.31 | 27.167 | 28.567 | 7.883 | 7.848 | Fe II | 5000.7305 | 15.700 | 0.41 | 15.264 | 15.203 | 7.816 | 7.819 |
| Fe I | 5880.0273 | 19.800 | 0.42 | 23.519 | 24.809 | 7.694 | 7.662 | Fe II | 5100.6548 | 29.500 | 0.73 | 32.967 | 32.836 | 7.708 | 7.711 |
| Fe I | 5881.2798 | 25.400 | 0.31 | 25.657 | 27.036 | 7.793 | 7.758 | Fe II | 5132.6611 | 33.100 | 0.75 | 37.084 | 36.936 | 7.697 | 7.701 |
| Fe I | 5883.8164 | 83.700 | 1.29 | 81.140 | 83.050 | 7.847 | 7.812 | Fe II | 5256.9321 | 27.800 | 0.83 | 30.620 | 30.498 | 7.724 | 7.727 |
| Fe I | 5898.2153 | 23.100 | 0.34 | 21.574 | 22.878 | 7.843 | 7.806 | Fe II | 5264.8022 | 58.500 | 0.55 | 60.306 | 60.126 | 7.754 | 7.759 |
| Fe I | 5902.4731 | 21.700 | 0.75 | 26.920 | 28.457 | 7.659 | 7.624 | Fe II | 5284.1030 | 76.100 | 2.37 | 70.831 | 70.619 | 7.931 | 7.936 |
| Fe I | 5905.6714 | 73.200 | 1.25 | 76.534 | 79.310 | 7.740 | 7.689 | Fe II | 5325.5522 | 56.500 | 0.57 | 59.512 | 59.334 | 7.724 | 7.729 |
| Fe I | 5909.9722 | 51.800 | 0.51 | 46.706 | 48.805 | 7.913 | 7.865 | Fe II | 5414.0698 | 38.500 | 0.47 | 42.454 | 42.327 | 7.700 | 7.703 |
| Fe I | 5927.7886 | 58.400 | 1.08 | 59.874 | 62.434 | 7.771 | 7.721 | Fe II | 5425.2485 | 52.100 | 0.60 | 58.032 | 57.858 | 7.653 | 7.656 |
| Fe I | 5934.6543 | 92.800 | 1.26 | 95.428 | 97.078 | 7.757 | 7.729 | Fe II | 5534.8379 | 70.700 | 2.08 | 71.425 | 71.211 | 7.782 | 7.788 |
| Fe I | 5940.9912 | 32.900 | 0.74 | 28.988 | 30.514 | 7.896 | 7.857 | Fe II | 6084.1016 | 31.300 | 0.30 | 31.600 | 31.474 | 7.792 | 7.795 |
| Fe I | 5952.7178 | 81.300 | 2.45 | 75.320 | 77.251 | 7.913 | 7.877 | Fe II | 6149.2461 | 47.800 | 0.69 | 47.535 | 47.393 | 7.807 | 7.810 |
| Fe I | 5969.5620 | 7.200 | 0.29 | 6.331 | 6.749 | 7.862 | 7.831 | Fe II | 6238.3857 | 58.800 | 0.74 | 57.812 | 57.639 | 7.824 | 7.828 |
| Fe I | 5976.7769 | 85.800 | 1.14 | 83.332 | 85.033 | 7.844 | 7.814 | Fe II | 6247.5571 | 68.500 | 1.50 | 64.932 | 64.738 | 7.883 | 7.889 |
| Fe I | 5984.8149 | 100.400 | 1.54 | 108.225 | 112.034 | 7.693 | 7.643 | Fe II | 6369.4590 | 27.300 | 0.37 | 34.228 | 34.058 | 7.621 | 7.625 |
| Fe I | 5987.0649 | 85.900 | 0.81 | 86.722 | 90.713 | 7.787 | 7.724 | Fe II | 6456.3794 | 74.900 | 0.81 | 76.396 | 76.092 | 7.767 | 7.774 |
| Fe I | 6003.0112 | 99.900 | 1.49 | 96.344 | 97.911 | 7.857 | 7.832 | Fe II | 6516.0767 | 71.900 | 0.89 | 68.949 | 68.674 | 7.868 | 7.875 |


| $\beta \mathbf{H y i}$ |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m} \AA)$ |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m}$ ) |  | $\varepsilon_{\mathrm{Fe}}$ (dex) |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 4779.4390 | 41.600 | 1.10 | 41.387 | 44.550 | 7.415 | 7.342 |
| Fe I | 4787.8267 | 37.100 | 0.29 | 33.393 | 36.297 | 7.498 | 7.429 |
| Fe I | 4788.7568 | 66.600 | 0.95 | 59.486 | 62.683 | 7.588 | 7.507 |
| Fe I | 4789.6509 | 86.200 | 1.18 | 87.506 | 91.152 | 7.385 | 7.313 |
| Fe I | 4793.9614 | 6.700 | 0.25 | 7.178 | 8.120 | 7.376 | 7.316 |
| Fe I | 4794.3540 | 9.600 | 0.36 | 8.269 | 9.418 | 7.485 | 7.420 |
| Fe I | 4799.4058 | 29.000 | 0.64 | 27.852 | 30.506 | 7.439 | 7.373 |
| Fe I | 4802.8799 | 57.000 | 1.28 | 53.743 | 57.052 | 7.490 | 7.409 |
| Fe I | 4808.1479 | 21.200 | 0.59 | 20.436 | 22.631 | 7.433 | 7.369 |
| Fe I | 4809.9385 | 14.000 | 0.57 | 13.554 | 15.127 | 7.428 | 7.368 |
| Fe I | 4875.8770 | 50.400 | 1.54 | 51.757 | 54.944 | 7.379 | 7.309 |
| Fe I | 4882.1431 | 67.100 | 1.13 | 68.031 | 71.162 | 7.390 | 7.322 |
| Fe I | 4885.4302 | 68.000 | 1.06 | 68.580 | 71.887 | 7.397 | 7.321 |
| Fe I | 4892.8589 | 46.700 | 0.75 | 41.658 | 45.231 | 7.521 | 7.442 |
| Fe I | 4896.4385 | 31.600 | 0.64 | 28.320 | 30.951 | 7.493 | 7.426 |
| Fe I | 4907.7319 | 57.200 | 0.82 | 57.043 | 60.235 | 7.413 | 7.343 |
| Fe I | 4917.2300 | 60.600 | 0.74 | 52.429 | 56.315 | 7.590 | 7.503 |
| Fe I | 4918.0127 | 49.400 | 0.60 | 42.548 | 46.148 | 7.560 | 7.480 |
| Fe I | 4962.5718 | 48.900 | 0.51 | 48.491 | 52.141 | 7.419 | 7.340 |
| Fe I | 4966.0884 | 110.800 | 1.96 | 116.250 | 119.599 | 7.336 | 7.290 |
| Fe I | 4969.9175 | 72.600 | 1.39 | 69.513 | 73.950 | 7.472 | 7.383 |
| Fe I | 4985.2529 | 91.800 | 1.14 | 93.091 | 96.869 | 7.387 | 7.316 |
| Fe I | 4986.2227 | 41.300 | 0.42 | 41.779 | 45.264 | 7.399 | 7.325 |
| Fe I | 4993.6797 | 43.600 | 0.40 | 38.394 | 41.642 | 7.527 | 7.453 |
| Fe I | 4999.1123 | 25.500 | 0.48 | 27.180 | 29.901 | 7.365 | 7.299 |
| Fe I | 5002.7920 | 73.800 | 0.79 | 70.504 | 73.749 | 7.480 | 7.411 |
| Fe I | 5022.2354 | 92.400 | 0.43 | 95.142 | 99.106 | 7.362 | 7.289 |
| Fe I | 5023.4976 | 20.700 | 0.96 | 21.952 | 24.337 | 7.373 | 7.309 |
| Fe I | 5028.1260 | 79.900 | 1.15 | 80.418 | 83.944 | 7.399 | 7.325 |
| Fe I | 5029.6177 | 42.700 | 1.89 | 44.993 | 48.328 | 7.356 | 7.281 |
| Fe I | 5044.2109 | 66.800 | 0.19 | 65.400 | 68.770 | 7.443 | 7.364 |
| Fe I | 5048.4355 | 67.600 | 3.46 | 63.906 | 67.411 | 7.495 | 7.414 |
| Fe I | 5067.1494 | 64.100 | 0.26 | 56.620 | 60.427 | 7.572 | 7.489 |
| Fe I | 5074.7480 | 103.900 | 0.15 | 99.862 | 104.897 | 7.468 | 7.396 |
| Fe I | 5088.1533 | 29.600 | 0.94 | 27.237 | 29.898 | 7.470 | 7.403 |
| Fe I | 5090.7729 | 84.100 | 0.15 | 83.534 | 88.116 | 7.420 | 7.339 |
| Fe I | 5104.4375 | 27.600 | 0.79 | 26.041 | 28.743 | 7.450 | 7.382 |
| Fe I | 5129.6309 | 37.600 | 0.81 | 36.858 | 40.063 | 7.427 | 7.357 |
| Fe I | 5180.0557 | 40.000 | 0.25 | 37.030 | 40.827 | 7.477 | 7.392 |
| Fe I | 5198.7109 | 88.900 | 0.49 | 88.801 | 93.573 | 7.412 | 7.318 |
| Fe I | 5229.8447 | 106.100 | 0.31 | 104.765 | 108.565 | 7.431 | 7.372 |
| Fe I | 5242.4907 | 81.800 | 0.18 | 82.373 | 86.074 | 7.399 | 7.324 |
| Fe I | 5243.7764 | 54.800 | 1.09 | 51.419 | 55.230 | 7.484 | 7.401 |
| Fe I | 5253.4619 | 69.800 | 0.20 | 69.634 | 73.068 | 7.414 | 7.339 |
| Fe I | 5288.5249 | 51.200 | 0.42 | 54.422 | 58.019 | 7.336 | 7.257 |
| Fe I | 5293.9590 | 22.000 | 0.65 | 24.046 | 26.629 | 7.352 | 7.285 |
| Fe I | 5294.5474 | 8.400 | 0.43 | 9.478 | 10.710 | 7.350 | 7.288 |
| Fe I | 5295.3120 | 21.600 | 0.50 | 21.624 | 24.053 | 7.409 | 7.342 |
| Fe I | 5315.0698 | 26.600 | 0.29 | 24.521 | 27.125 | 7.465 | 7.397 |
| Fe I | 5320.0356 | 14.000 | 0.19 | 14.446 | 16.213 | 7.393 | 7.329 |
| Fe I | 5322.0405 | 56.300 | 0.21 | 55.215 | 58.927 | 7.437 | 7.346 |
| Fe I | 5326.1426 | 29.600 | 0.39 | 33.447 | 36.554 | 7.315 | 7.246 |
| Fe I | 5361.6250 | 37.900 | 0.21 | 31.960 | 35.237 | 7.548 | 7.469 |
| Fe I | 5379.5737 | 54.000 | 0.17 | 53.619 | 57.224 | 7.419 | 7.337 |
| Fe I | 5398.2793 | 64.400 | 0.44 | 64.193 | 68.951 | 7.414 | 7.320 |
| Fe I | 5400.5010 | 106.700 | 0.14 | 95.463 | 100.699 | 7.576 | 7.500 |
| Fe I | 5406.7749 | 28.600 | 0.71 | 22.145 | 24.578 | 7.579 | 7.511 |
| Fe I | 5436.2949 | 31.900 | 0.27 | 28.620 | 31.555 | 7.490 | 7.418 |
| Fe I | 5441.3389 | 24.000 | 0.25 | 23.809 | 26.367 | 7.415 | 7.348 |
| Fe I | 5452.0884 | 11.200 | 0.14 | 8.785 | 9.949 | 7.533 | 7.471 |
| Fe I | 5466.3960 | 70.500 | 0.15 | 67.958 | 72.296 | 7.460 | 7.375 |
| Fe I | 5466.9873 | 28.600 | 0.78 | 27.004 | 29.806 | 7.451 | 7.380 |
| Fe I | 5470.0928 | 18.300 | 0.25 | 16.880 | 18.924 | 7.457 | 7.390 |
| Fe I | 5472.7085 | 35.500 | 0.47 | 32.778 | 35.941 | 7.476 | 7.400 |
| Fe I | 5473.1626 | 13.000 | 0.49 | 14.239 | 15.963 | 7.361 | 7.298 |
| Fe I | 5473.9004 | 73.700 | 0.18 | 70.137 | 73.828 | 7.486 | 7.407 |
| Fe I | 5481.2432 | 54.000 | 0.89 | 48.986 | 52.844 | 7.522 | 7.435 |
| Fe I | 5483.0986 | 38.500 | 0.15 | 39.706 | 43.112 | 7.382 | 7.307 |
| Fe I | 5487.1450 | 29.200 | 0.44 | 27.952 | 30.886 | 7.441 | 7.370 |
| Fe I | 5494.4624 | 20.500 | 1.08 | 15.748 | 17.635 | 7.565 | 7.499 |
| Fe I | 5506.7788 | 113.600 | 0.19 | 107.149 | 112.551 | 7.551 | 7.432 |
| Fe I | 5522.4463 | 35.700 | 0.38 | 34.790 | 38.022 | 7.432 | 7.356 |
| Fe I | 5539.2798 | 12.600 | 0.19 | 14.114 | 15.876 | 7.349 | 7.285 |
| Fe I | 5543.9355 | 55.800 | 1.27 | 52.686 | 56.469 | 7.481 | 7.395 |
| Fe I | 5546.5059 | 44.400 | 0.24 | 39.290 | 42.846 | 7.525 | 7.444 |
| Fe I | 5546.9907 | 19.900 | 0.52 | 20.464 | 22.763 | 7.393 | 7.327 |


| $\beta \mathrm{Hyi}$ |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m}$ ) |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m}$ ) |  | $\varepsilon_{\mathrm{Fe}}$ (dex) |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 5554.8945 | 80.300 | 0.89 | 79.395 | 85.463 | 7.426 | 7.321 |
| Fe I | 5560.2114 | 43.800 | 0.37 | 42.325 | 46.106 | 7.443 | 7.361 |
| Fe I | 5567.3911 | 58.500 | 0.11 | 52.425 | 56.130 | 7.559 | 7.467 |
| Fe I | 5594.6553 | 59.700 | 3.98 | 58.481 | 63.360 | 7.435 | 7.338 |
| Fe I | 5618.6323 | 44.000 | 0.24 | 43.376 | 46.995 | 7.424 | 7.342 |
| Fe I | 5619.5952 | 27.400 | 0.15 | 22.510 | 25.039 | 7.540 | 7.470 |
| Fe I | 5636.6958 | 14.300 | 0.35 | 15.620 | 17.551 | 7.361 | 7.296 |
| Fe I | 5638.2622 | 69.600 | 0.22 | 67.624 | 71.409 | 7.452 | 7.370 |
| Fe I | 5641.4341 | 56.100 | 0.82 | 49.390 | 53.165 | 7.562 | 7.476 |
| Fe I | 5650.7056 | 28.300 | 0.18 | 25.207 | 29.209 | 7.492 | 7.388 |
| Fe I | 5651.4688 | 12.200 | 0.28 | 11.364 | 12.812 | 7.447 | 7.384 |
| Fe I | 5652.3174 | 18.400 | 0.45 | 17.907 | 19.985 | 7.426 | 7.361 |
| Fe I | 5655.1763 | 44.800 | 0.97 | 36.727 | 42.508 | 7.598 | 7.457 |
| Fe I | 5679.0229 | 50.500 | 0.20 | 45.672 | 50.300 | 7.514 | 7.414 |
| Fe I | 5680.2402 | 6.500 | 0.32 | 6.012 | 6.832 | 7.448 | 7.386 |
| Fe I | 5691.4971 | 32.400 | 0.32 | 31.155 | 34.387 | 7.441 | 7.363 |
| Fe I | 5701.5444 | 75.900 | 0.25 | 71.292 | 75.441 | 7.521 | 7.421 |
| Fe I | 5717.8325 | 54.000 | 0.19 | 52.315 | 56.253 | 7.448 | 7.360 |
| Fe I | 5731.7617 | 50.800 | 0.17 | 44.198 | 47.730 | 7.560 | 7.479 |
| Fe I | 5741.8477 | 25.100 | 0.19 | 24.217 | 26.848 | 7.434 | 7.364 |
| Fe I | 5742.9600 | 9.500 | 0.34 | 7.101 | 8.051 | 7.554 | 7.492 |
| Fe I | 5760.3438 | 16.900 | 0.32 | 19.365 | 21.685 | 7.330 | 7.263 |
| Fe I | 5838.3716 | 15.700 | 0.40 | 15.515 | 17.413 | 7.417 | 7.352 |
| Fe I | 5848.1265 | 33.700 | 0.39 | 35.924 | 39.739 | 7.357 | 7.274 |
| Fe I | 5849.6831 | 6.400 | 0.29 | 5.463 | 6.243 | 7.486 | 7.422 |
| Fe I | 5855.0757 | 20.100 | 0.27 | 19.729 | 22.143 | 7.421 | 7.351 |
| Fe I | 5858.7778 | 11.600 | 0.44 | 10.920 | 12.339 | 7.442 | 7.377 |
| Fe I | 5859.5864 | 69.800 | 0.83 | 70.917 | 76.010 | 7.389 | 7.292 |
| Fe I | 5873.2124 | 15.300 | 0.55 | 13.101 | 14.737 | 7.494 | 7.430 |
| Fe I | 5881.2798 | 15.700 | 0.35 | 12.289 | 13.886 | 7.543 | 7.477 |
| Fe I | 5883.8164 | 60.900 | 0.77 | 57.007 | 60.905 | 7.490 | 7.410 |
| Fe I | 5905.6714 | 52.400 | 0.82 | 51.870 | 56.937 | 7.421 | 7.318 |
| Fe I | 5909.9722 | 30.300 | 0.41 | 27.624 | 30.591 | 7.476 | 7.403 |
| Fe I | 5929.6763 | 36.100 | 0.40 | 28.161 | 31.255 | 7.597 | 7.520 |
| Fe I | 5930.1797 | 83.800 | 0.89 | 76.990 | 82.874 | 7.529 | 7.426 |
| Fe I | 5934.6543 | 71.100 | 0.84 | 68.573 | 72.411 | 7.459 | 7.384 |
| Fe I | 5952.7178 | 56.500 | 0.64 | 51.954 | 55.805 | 7.505 | 7.424 |
| Fe I | 5976.7769 | 62.500 | 0.79 | 58.849 | 62.605 | 7.485 | 7.408 |
| Fe I | 5984.8149 | 76.400 | 1.19 | 74.937 | 81.542 | 7.436 | 7.321 |
| Fe I | 5987.0649 | 63.000 | 0.58 | 58.749 | 65.132 | 7.495 | 7.370 |
| Fe I | 6003.0112 | 77.400 | 0.93 | 69.421 | 73.152 | 7.564 | 7.493 |
| Fe I | 6007.9595 | 56.300 | 0.68 | 55.422 | 60.176 | 7.429 | 7.329 |
| Fe I | 6008.5557 | 81.300 | 0.94 | 76.029 | 79.779 | 7.507 | 7.439 |
| Fe I | 6024.0576 | 98.300 | 1.21 | 90.092 | 95.639 | 7.536 | 7.451 |
| Fe I | 6027.0508 | 63.000 | 0.69 | 59.065 | 63.307 | 7.493 | 7.404 |
| Fe I | 6054.0732 | 7.200 | 0.30 | 5.820 | 6.614 | 7.513 | 7.451 |
| Fe I | 6056.0044 | 67.100 | 0.73 | 67.851 | 73.912 | 7.396 | 7.285 |
| Fe I | 6065.4819 | 110.900 | 1.57 | 102.632 | 107.468 | 7.561 | 7.471 |
| Fe I | 6078.4912 | 70.600 | 0.66 | 64.870 | 71.207 | 7.519 | 7.399 |
| Fe I | 6079.0078 | 40.500 | 0.33 | 36.758 | 40.572 | 7.493 | 7.408 |
| Fe I | 6082.7100 | 29.000 | 0.41 | 26.039 | 29.192 | 7.486 | 7.405 |
| Fe I | 6093.6431 | 27.100 | 0.34 | 22.602 | 25.339 | 7.530 | 7.455 |
| Fe I | 6096.6641 | 32.300 | 0.31 | 29.143 | 32.131 | 7.486 | 7.414 |
| Fe I | 6098.2441 | 13.700 | 0.28 | 10.747 | 12.185 | 7.538 | 7.472 |
| Fe I | 6127.9063 | 44.100 | 0.61 | 41.292 | 45.128 | 7.472 | 7.388 |
| Fe I | 6136.6147 | 123.100 | 1.47 | 118.443 | 124.024 | 7.484 | 7.396 |
| Fe I | 6137.6914 | 120.500 | 1.50 | 112.063 | 117.221 | 7.547 | 7.463 |
| Fe I | 6151.6172 | 44.200 | 0.72 | 40.266 | 44.200 | 7.501 | 7.410 |
| Fe I | 6157.7280 | 58.900 | 0.57 | 55.568 | 59.815 | 7.481 | 7.391 |
| Fe I | 6165.3599 | 40.900 | 0.36 | 37.903 | 41.606 | 7.478 | 7.395 |
| Fe I | 6180.2026 | 51.700 | 0.44 | 47.948 | 51.892 | 7.498 | 7.406 |
| Fe I | 6187.9893 | 43.400 | 0.42 | 40.501 | 44.023 | 7.473 | 7.397 |
| Fe I | 6213.4292 | 79.100 | 1.02 | 74.421 | 79.340 | 7.520 | 7.405 |
| Fe I | 6226.7344 | 23.800 | 0.19 | 21.568 | 24.071 | 7.472 | 7.403 |
| Fe I | 6229.2261 | 32.800 | 0.24 | 33.404 | 36.829 | 7.395 | 7.317 |
| Fe I | 6230.7222 | 130.100 | 1.47 | 123.490 | 129.174 | 7.504 | 7.423 |
| Fe I | 6232.6401 | 78.000 | 0.53 | 72.898 | 76.897 | 7.510 | 7.432 |
| Fe I | 6240.6460 | 43.100 | 0.40 | 41.162 | 45.084 | 7.455 | 7.365 |
| Fe I | 6252.5547 | 111.400 | 1.36 | 102.514 | 108.137 | 7.581 | 7.471 |
| Fe I | 6270.2236 | 46.600 | 0.36 | 47.795 | 51.726 | 7.382 | 7.295 |
| Fe I | 6271.2778 | 20.100 | 0.30 | 19.470 | 21.876 | 7.429 | 7.359 |
| Fe I | 6311.4995 | 23.100 | 0.25 | 20.798 | 23.395 | 7.476 | 7.402 |
| Fe I | 6315.8110 | 37.300 | 0.36 | 33.777 | 37.240 | 7.492 | 7.411 |
| Fe I | 6318.0181 | 103.600 | 2.01 | 96.339 | 101.838 | 7.553 | 7.444 |
| Fe I | 6338.8760 | 36.800 | 0.36 | 33.383 | 37.383 | 7.489 | 7.397 |
| Fe I | 6364.3638 | 23.000 | 0.23 | 19.109 | 21.690 | 7.524 | 7.446 |
| Fe I | 6380.7432 | 46.800 | 0.41 | 40.678 | 44.652 | 7.545 | 7.456 |


| $\beta \mathbf{H y i}$ |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m} \AA)$ |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m} \AA)$ |  | $\varepsilon_{\mathrm{Fe}}$ (dex) |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 6408.0176 | 86.700 | 0.74 | 84.847 | 88.938 | 7.443 | 7.370 |
| Fe I | 6430.8452 | 105.000 | 1.01 | 99.645 | 105.893 | 7.514 | 7.393 |
| Fe I | 6436.4058 | 6.700 | 0.27 | 5.064 | 5.821 | 7.543 | 7.477 |
| Fe I | 6469.1919 | 49.600 | 1.20 | 42.329 | 47.137 | 7.566 | 7.460 |
| Fe I | 6494.9805 | 143.900 | 4.37 | 136.945 | 144.153 | 7.496 | 7.407 |
| Fe I | 6495.7412 | 35.300 | 0.78 | 37.382 | 41.814 | 7.363 | 7.272 |
| Fe I | 6496.4658 | 58.100 | 0.70 | 54.005 | 59.346 | 7.494 | 7.385 |
| Fe I | 6518.3657 | 52.500 | 0.46 | 51.223 | 55.376 | 7.439 | 7.346 |
| Fe I | 6533.9282 | 29.800 | 0.47 | 26.149 | 29.282 | 7.503 | 7.423 |
| Fe I | 6569.2139 | 75.500 | 2.23 | 65.555 | 70.947 | 7.595 | 7.494 |
| Fe I | 6581.2090 | 13.600 | 0.44 | 13.926 | 16.231 | 7.397 | 7.314 |
| Fe I | 6597.5591 | 35.900 | 0.40 | 33.481 | 37.284 | 7.466 | 7.380 |
| Fe I | 6608.0249 | 12.400 | 0.29 | 13.452 | 15.462 | 7.366 | 7.292 |
| Fe I | 6627.5439 | 24.300 | 0.41 | 18.385 | 20.681 | 7.583 | 7.511 |
| Fe I | 6633.7485 | 60.000 | 0.54 | 51.575 | 56.182 | 7.586 | 7.488 |
| Fe I | 6667.7104 | 6.900 | 0.28 | 6.260 | 7.187 | 7.457 | 7.390 |
| Fe I | 6699.1411 | 6.400 | 0.37 | 6.304 | 7.246 | 7.417 | 7.350 |
| Fe I | 6703.5659 | 31.200 | 0.32 | 27.096 | 30.275 | 7.512 | 7.432 |
| Fe I | 6710.3179 | 11.700 | 0.36 | 11.964 | 14.009 | 7.398 | 7.315 |
| Fe I | 6713.0459 | 23.500 | 0.89 | 20.189 | 22.710 | 7.506 | 7.432 |
| Fe I | 6713.7427 | 15.900 | 0.30 | 11.851 | 13.513 | 7.569 | 7.499 |
| Fe I | 6716.2363 | 11.200 | 0.44 | 9.358 | 10.707 | 7.503 | 7.433 |
| Fe I | 6752.7065 | 28.800 | 0.29 | 29.387 | 32.725 | 7.395 | 7.315 |
| Fe I | 6786.8584 | 22.200 | 0.55 | 17.533 | 19.722 | 7.550 | 7.481 |
| Fe I | 6810.2622 | 42.100 | 0.41 | 40.729 | 44.905 | 7.440 | 7.350 |
| Fe II | 4893.8125 | 20.600 | 0.24 | 17.198 | 17.129 | 7.520 | 7.522 |
| Fe II | 4993.3501 | 43.900 | 0.74 | 47.487 | 47.345 | 7.321 | 7.324 |
| Fe II | 5000.7305 | 11.800 | 0.30 | 11.035 | 10.991 | 7.446 | 7.448 |
| Fe II | 5132.6611 | 27.200 | 0.41 | 30.774 | 30.651 | 7.316 | 7.320 |
| Fe II | 5234.6226 | 92.900 | 0.19 | 95.269 | 95.079 | 7.359 | 7.363 |
| Fe II | 5325.5522 | 50.800 | 0.20 | 53.415 | 53.255 | 7.345 | 7.349 |
| Fe II | 5414.0698 | 32.400 | 0.50 | 36.130 | 36.022 | 7.316 | 7.319 |
| Fe II | 5425.2485 | 47.600 | 1.25 | 51.952 | 51.797 | 7.303 | 7.307 |
| Fe II | 5534.8379 | 67.300 | 0.21 | 65.034 | 64.839 | 7.466 | 7.471 |
| Fe II | 6084.1016 | 27.000 | 0.22 | 25.600 | 25.498 | 7.448 | 7.451 |
| Fe II | 6113.3193 | 15.100 | 0.35 | 13.944 | 13.875 | 7.455 | 7.458 |
| Fe II | 6149.2461 | 44.400 | 0.41 | 41.190 | 41.067 | 7.489 | 7.492 |
| Fe II | 6238.3857 | 51.900 | 0.32 | 51.420 | 51.266 | 7.422 | 7.425 |
| Fe II | 6239.9429 | 15.800 | 0.27 | 14.989 | 14.929 | 7.441 | 7.443 |
| Fe II | 6247.5571 | 63.800 | 0.74 | 58.349 | 58.174 | 7.540 | 7.545 |
| Fe II | 6416.9189 | 45.200 | 0.35 | 26.897 | 30.221 | 7.541 | 7.544 |
| Fe II | 6416.9189 | 45.200 | 0.35 | 39.812 | 39.693 | 7.541 | 7.544 |
| Fe II | 6456.3794 | 73.200 | 0.53 | 69.131 | 68.924 | 7.504 | 7.509 |
| Fe II | 6516.0767 | 68.500 | 1.36 | 62.793 | 62.605 | 7.544 | 7.549 |


| $\beta$ Vir |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m}$ ) |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m} \AA)$ |  | $\varepsilon_{\mathrm{Fe}}$ (dex) |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 4787.8267 | 34.600 | 1.16 | 40.589 | 43.226 | 7.560 | 7.509 |
| Fe I | 4788.7568 | 69.100 | 1.31 | 68.735 | 71.524 | 7.699 | 7.634 |
| Fe I | 4793.9614 | 8.700 | 0.29 | 9.465 | 10.447 | 7.648 | 7.599 |
| Fe I | 4799.4058 | 33.100 | 0.73 | 35.348 | 37.846 | 7.639 | 7.586 |
| Fe I | 4808.1479 | 21.800 | 0.82 | 26.140 | 28.290 | 7.576 | 7.526 |
| Fe I | 4869.4634 | 18.700 | 0.57 | 22.216 | 24.095 | 7.586 | 7.538 |
| Fe I | 4892.8589 | 50.900 | 1.02 | 51.648 | 54.828 | 7.675 | 7.611 |
| Fe I | 4896.4385 | 35.000 | 0.75 | 36.291 | 38.772 | 7.661 | 7.607 |
| Fe I | 4907.7319 | 61.500 | 0.89 | 66.632 | 69.264 | 7.583 | 7.527 |
| Fe I | 4917.2300 | 67.900 | 0.78 | 63.006 | 66.392 | 7.791 | 7.721 |
| Fe I | 4918.0127 | 55.700 | 0.64 | 52.638 | 55.820 | 7.753 | 7.688 |
| Fe I | 4939.6865 | 99.400 | 1.80 | 92.630 | 96.995 | 7.873 | 7.753 |
| Fe I | 4962.5718 | 54.400 | 0.72 | 58.846 | 62.008 | 7.599 | 7.537 |
| Fe I | 4969.9175 | 79.200 | 1.51 | 81.318 | 85.061 | 7.650 | 7.579 |
| Fe I | 4986.2227 | 47.200 | 0.60 | 51.791 | 54.922 | 7.596 | 7.536 |
| Fe I | 4993.6797 | 50.700 | 0.67 | 48.086 | 50.993 | 7.745 | 7.684 |
| Fe I | 4994.1294 | 102.400 | 1.84 | 102.422 | 106.912 | 7.689 | 7.579 |
| Fe I | 4999.1123 | 30.000 | 0.55 | 35.437 | 38.023 | 7.565 | 7.513 |
| Fe I | 5002.7920 | 80.800 | 1.98 | 80.854 | 83.527 | 7.689 | 7.635 |
| Fe I | 5023.1860 | 33.800 | 0.96 | 38.456 | 41.218 | 7.589 | 7.534 |
| Fe I | 5023.4976 | 26.300 | 0.43 | 29.481 | 31.837 | 7.613 | 7.561 |
| Fe I | 5036.9214 | 22.900 | 0.59 | 22.393 | 24.447 | 7.704 | 7.649 |
| Fe I | 5048.4355 | 72.500 | 3.03 | 74.875 | 77.752 | 7.639 | 7.575 |
| Fe I | 5056.8413 | 25.600 | 0.32 | 23.596 | 25.592 | 7.742 | 7.690 |
| Fe I | 5067.1494 | 70.900 | 0.95 | 67.586 | 70.845 | 7.757 | 7.691 |
| Fe I | 5074.7480 | 113.800 | 1.77 | 114.582 | 118.492 | 7.680 | 7.626 |
| Fe I | 5079.2227 | 103.500 | 0.97 | 98.428 | 102.316 | 7.797 | 7.715 |
| Fe I | 5083.3384 | 108.600 | 1.32 | 106.939 | 111.395 | 7.730 | 7.624 |


| $\beta$ Vir |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m} \AA)$ |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m}$ ) |  | $\varepsilon_{\mathrm{Fe}}$ (dex) |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 5088.1533 | 34.800 | 0.27 | 35.508 | 38.017 | 7.674 | 7.621 |
| Fe I | 5090.7729 | 90.000 | 1.18 | 96.796 | 100.411 | 7.579 | 7.516 |
| Fe I | 5104.4375 | 33.100 | 0.43 | 34.331 | 36.915 | 7.662 | 7.607 |
| Fe I | 5107.6406 | 109.700 | 4.28 | 108.846 | 113.028 | 7.709 | 7.615 |
| Fe I | 5127.3594 | 93.100 | 1.75 | 93.342 | 97.843 | 7.684 | 7.569 |
| Fe I | 5129.6309 | 39.600 | 0.71 | 46.061 | 48.949 | 7.559 | 7.506 |
| Fe I | 5151.9106 | 93.100 | 1.53 | 89.739 | 94.165 | 7.777 | 7.663 |
| Fe I | 5159.0576 | 69.600 | 0.76 | 73.111 | 76.959 | 7.622 | 7.549 |
| Fe I | 5180.0557 | 45.000 | 0.45 | 47.077 | 50.620 | 7.647 | 7.579 |
| Fe I | 5197.9360 | 32.300 | 0.88 | 36.085 | 38.801 | 7.606 | 7.551 |
| Fe I | 5216.2739 | 121.200 | 3.81 | 122.077 | 126.505 | 7.673 | 7.586 |
| Fe I | 5225.5259 | 66.100 | 1.11 | 65.170 | 69.850 | 7.713 | 7.602 |
| Fe I | 5228.3760 | 62.000 | 0.65 | 51.945 | 55.026 | 7.897 | 7.832 |
| Fe I | 5229.8447 | 111.800 | 1.32 | 117.220 | 120.226 | 7.610 | 7.564 |
| Fe I | 5243.7764 | 60.300 | 0.91 | 62.223 | 65.429 | 7.651 | 7.586 |
| Fe I | 5247.0503 | 57.400 | 0.95 | 59.285 | 63.954 | 7.647 | 7.547 |
| Fe I | 5250.6455 | 99.700 | 1.66 | 96.429 | 100.657 | 7.756 | 7.671 |
| Fe I | 5267.2695 | 25.000 | 1.13 | 30.684 | 33.172 | 7.553 | 7.502 |
| Fe I | 5285.1274 | 29.600 | 0.65 | 25.593 | 27.818 | 7.788 | 7.732 |
| Fe I | 5293.9590 | 26.100 | 0.52 | 31.763 | 34.264 | 7.554 | 7.503 |
| Fe I | 5295.3120 | 26.100 | 0.64 | 29.258 | 31.699 | 7.613 | 7.559 |
| Fe I | 5307.3608 | 89.700 | 1.28 | 84.326 | 88.392 | 7.828 | 7.722 |
| Fe I | 5320.0356 | 16.200 | 0.18 | 19.343 | 21.140 | 7.590 | 7.539 |
| Fe I | 5361.6250 | 43.500 | 1.45 | 41.380 | 44.447 | 7.735 | 7.671 |
| Fe I | 5379.5737 | 59.600 | 0.69 | 63.610 | 66.747 | 7.604 | 7.538 |
| Fe I | 5397.6177 | 20.200 | 0.72 | 20.102 | 21.969 | 7.693 | 7.640 |
| Fe I | 5398.2793 | 71.500 | 0.50 | 76.426 | 80.364 | 7.598 | 7.524 |
| Fe I | 5401.2666 | 22.000 | 0.48 | 23.428 | 25.465 | 7.651 | 7.599 |
| Fe I | 5406.7749 | 32.900 | 0.47 | 29.861 | 32.247 | 7.760 | 7.705 |
| Fe I | 5409.1333 | 54.500 | 0.33 | 50.012 | 53.261 | 7.782 | 7.715 |
| Fe I | 5417.0332 | 31.100 | 0.45 | 29.868 | 32.325 | 7.719 | 7.662 |
| Fe I | 5436.2949 | 37.100 | 0.22 | 37.546 | 40.329 | 7.680 | 7.622 |
| Fe I | 5441.3389 | 27.300 | 0.31 | 31.770 | 34.272 | 7.585 | 7.533 |
| Fe I | 5452.0884 | 11.600 | 0.35 | 12.025 | 13.258 | 7.671 | 7.620 |
| Fe I | 5466.3960 | 77.800 | 0.58 | 80.513 | 84.043 | 7.641 | 7.575 |
| Fe I | 5466.9873 | 33.200 | 0.34 | 34.392 | 37.060 | 7.663 | 7.605 |
| Fe I | 5470.0928 | 23.600 | 0.19 | 23.434 | 25.527 | 7.694 | 7.641 |
| Fe I | 5472.7085 | 41.100 | 0.40 | 41.961 | 44.830 | 7.671 | 7.611 |
| Fe I | 5473.1626 | 16.500 | 0.44 | 19.718 | 21.503 | 7.589 | 7.539 |
| Fe I | 5473.9004 | 80.300 | 1.02 | 82.323 | 85.132 | 7.650 | 7.591 |
| Fe I | 5483.0986 | 44.300 | 0.40 | 49.587 | 52.584 | 7.579 | 7.520 |
| Fe I | 5487.1450 | 34.400 | 0.82 | 36.830 | 39.602 | 7.637 | 7.580 |
| Fe I | 5494.4624 | 24.500 | 0.74 | 21.493 | 23.438 | 7.772 | 7.718 |
| Fe I | 5501.4648 | 105.600 | 1.37 | 105.942 | 110.818 | 7.682 | 7.568 |
| Fe I | 5522.4463 | 41.300 | 0.17 | 44.214 | 47.136 | 7.627 | 7.567 |
| Fe I | 5543.1470 | 64.600 | 1.42 | 59.446 | 62.641 | 7.809 | 7.735 |
| Fe I | 5543.9355 | 61.800 | 0.37 | 63.662 | 66.872 | 7.651 | 7.584 |
| Fe I | 5546.5059 | 48.200 | 0.53 | 49.446 | 52.658 | 7.664 | 7.600 |
| Fe I | 5560.2114 | 48.300 | 0.62 | 52.954 | 56.274 | 7.596 | 7.533 |
| Fe I | 5567.3911 | 62.900 | 1.46 | 60.816 | 64.288 | 7.737 | 7.659 |
| Fe I | 5577.0249 | 12.200 | 0.27 | 12.067 | 13.620 | 7.696 | 7.632 |
| Fe I | 5587.5742 | 33.500 | 0.95 | 33.407 | 36.077 | 7.692 | 7.634 |
| Fe I | 5618.6323 | 51.200 | 0.51 | 53.618 | 56.739 | 7.639 | 7.574 |
| Fe I | 5619.5952 | 32.700 | 0.52 | 30.319 | 32.813 | 7.745 | 7.687 |
| Fe I | 5635.8223 | 28.100 | 1.05 | 23.178 | 25.221 | 7.815 | 7.761 |
| Fe I | 5641.4341 | 62.700 | 2.95 | 60.242 | 63.413 | 7.742 | 7.675 |
| Fe I | 5650.7056 | 32.700 | 0.48 | 34.668 | 38.909 | 7.645 | 7.561 |
| Fe I | 5653.8652 | 29.600 | 0.77 | 28.772 | 31.172 | 7.710 | 7.654 |
| Fe I | 5655.1763 | 47.500 | 0.51 | 47.886 | 53.744 | 7.682 | 7.572 |
| Fe I | 5701.5444 | 76.700 | 0.59 | 81.054 | 84.962 | 7.594 | 7.511 |
| Fe I | 5717.8325 | 62.500 | 1.14 | 63.439 | 66.778 | 7.670 | 7.601 |
| Fe I | 5838.3716 | 20.000 | 0.41 | 21.077 | 23.010 | 7.659 | 7.607 |
| Fe I | 5855.0757 | 23.700 | 0.30 | 27.242 | 29.708 | 7.600 | 7.545 |
| Fe I | 5858.7778 | 14.700 | 0.58 | 15.385 | 16.888 | 7.665 | 7.614 |
| Fe I | 5859.5864 | 78.300 | 0.92 | 84.264 | 88.420 | 7.586 | 7.510 |
| Fe I | 5861.1084 | 11.200 | 0.49 | 10.466 | 11.526 | 7.725 | 7.675 |
| Fe I | 5873.2124 | 17.600 | 0.40 | 18.334 | 20.037 | 7.667 | 7.616 |
| Fe I | 5879.4868 | 9.100 | 0.22 | 8.082 | 8.930 | 7.749 | 7.699 |
| Fe I | 5881.2798 | 17.300 | 0.28 | 17.634 | 19.336 | 7.679 | 7.627 |
| Fe I | 5883.8164 | 65.600 | 0.97 | 68.029 | 71.309 | 7.643 | 7.581 |
| Fe I | 5898.2153 | 13.000 | 0.18 | 14.528 | 16.071 | 7.631 | 7.577 |
| Fe I | 5905.6714 | 60.000 | 0.76 | 63.792 | 68.227 | 7.617 | 7.535 |
| Fe I | 5909.9722 | 32.700 | 0.27 | 34.614 | 37.461 | 7.647 | 7.588 |
| Fe I | 5916.2471 | 52.000 | 0.62 | 48.521 | 52.005 | 7.765 | 7.690 |
| Fe I | 5929.6763 | 40.300 | 0.65 | 37.333 | 40.273 | 7.753 | 7.691 |
| Fe I | 5930.1797 | 90.300 | 0.98 | 91.208 | 96.008 | 7.675 | 7.597 |
| Fe I | 5934.6543 | 75.700 | 0.85 | 80.465 | 83.470 | 7.604 | 7.547 |
| Fe I | 5940.9912 | 22.700 | 0.30 | 20.120 | 22.013 | 7.764 | 7.709 |


| $\beta$ Vir |  |  |  |  |  |  |  | $\beta$ Vir |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m} \AA$ ) |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m} \AA)$ |  | $\varepsilon_{\mathrm{Fe}}$ (dex) |  |  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m} \AA)$ |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m} \AA)$ |  | $\varepsilon_{\mathrm{Fe}}$ (dex) |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE | el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 5952.7178 | 64.800 | 1.76 | 62.682 | 65.981 | 7.731 | 7.667 | Fe II | 4993.3501 | 54.300 | 1.12 | 59.041 | 58.923 | 7.579 | 7.582 |
| Fe I | 5956.6938 | 42.700 | 0.70 | 43.479 | 47.832 | 7.674 | 7.587 | Fe II | 5000.7305 | 18.000 | 0.32 | 16.503 | 16.454 | 7.740 | 7.742 |
| Fe I | 5976.7769 | 65.600 | 0.75 | 70.060 | 73.132 | 7.605 | 7.546 | Fe II | 5100.6548 | 35.800 | 0.75 | 36.411 | 36.338 | 7.676 | 7.677 |
| Fe I | 5987.0649 | 69.800 | 0.94 | 71.561 | 77.363 | 7.658 | 7.557 | Fe II | 5132.6611 | 34.900 | 0.43 | 41.064 | 40.982 | 7.550 | 7.551 |
| Fe I | 6003.0112 | 82.400 | 0.90 | 81.331 | 84.194 | 7.709 | 7.657 | Fe II | 5234.6226 | 107.100 | 1.27 | 111.295 | 111.184 | 7.609 | 7.611 |
| Fe I | 6005.5415 | 17.800 | 0.29 | 16.990 | 18.878 | 7.716 | 7.657 | Fe II | 5256.9321 | 29.900 | 0.58 | 33.917 | 33.849 | 7.594 | 7.595 |
| Fe I | 6007.9595 | 64.100 | 1.00 | 67.693 | 71.785 | 7.620 | 7.541 | Fe II | 5264.8022 | 65.700 | 0.77 | 66.827 | 66.694 | 7.663 | 7.666 |
| Fe I | 6008.5557 | 86.900 | 1.11 | 88.450 | 91.280 | 7.663 | 7.613 | Fe II | 5284.1030 | 82.400 | 2.56 | 77.581 | 77.426 | 7.805 | 7.809 |
| Fe I | 6024.0576 | 108.000 | 1.57 | 105.709 | 110.114 | 7.722 | 7.660 | Fe II | 5325.5522 | 63.600 | 0.58 | 66.025 | 65.893 | 7.633 | 7.636 |
| Fe I | 6027.0508 | 68.500 | 0.80 | 70.511 | 74.144 | 7.651 | 7.581 | Fe II | 5414.0698 | 42.900 | 0.29 | 47.586 | 47.491 | 7.584 | 7.586 |
| Fe I | 6056.0044 | 76.400 | 0.82 | 81.401 | 86.689 | 7.603 | 7.514 | Fe II | 5425.2485 | 60.000 | 0.34 | 64.509 | 64.380 | 7.586 | 7.589 |
| Fe I | 6065.4819 | 113.700 | 1.47 | 114.732 | 119.017 | 7.672 | 7.597 | Fe II | 5427.8159 | 8.500 | 0.32 | 11.065 | 11.054 | 7.546 | 7.546 |
| Fe I | 6078.4912 | 79.300 | 0.85 | 78.307 | 83.930 | 7.707 | 7.611 | Fe II | 5525.1172 | 22.200 | 0.47 | 28.800 | 28.714 | 7.517 | 7.519 |
| Fe I | 6079.0078 | 47.800 | 0.60 | 47.380 | 50.782 | 7.698 | 7.631 | Fe II | 5534.8379 | 80.900 | 1.39 | 78.569 | 78.412 | 7.744 | 7.748 |
| Fe I | 6082.7100 | 29.600 | 0.33 | 31.349 | 34.374 | 7.649 | 7.584 | Fe II | 5627.4888 | 19.700 | 0.81 | 20.029 | 19.969 | 7.680 | 7.682 |
| Fe I | 6093.6431 | 30.800 | 0.37 | 30.818 | 33.534 | 7.690 | 7.629 | Fe II | 6084.1016 | 37.200 | 0.39 | 35.691 | 35.584 | 7.725 | 7.727 |
| Fe I | 6096.6641 | 35.200 | 0.46 | 37.631 | 40.420 | 7.638 | 7.582 | Fe II | 6113.3193 | 22.500 | 0.49 | 20.952 | 20.889 | 7.735 | 7.737 |
| Fe I | 6098.2441 | 15.300 | 0.33 | 15.495 | 17.046 | 7.683 | 7.630 | Fe II | 6149.2461 | 56.800 | 0.55 | 54.132 | 54.024 | 7.750 | 7.753 |
| Fe I | 6127.9063 | 49.000 | 0.71 | 51.441 | 54.900 | 7.640 | 7.573 | Fe II | 6238.3857 | 65.000 | 0.51 | 65.246 | 65.116 | 7.685 | 7.687 |
| Fe I | 6136.6147 | 127.700 | 1.43 | 130.969 | 135.719 | 7.639 | 7.565 | Fe II | 6239.9429 | 23.700 | 0.25 | 23.044 | 22.975 | 7.709 | 7.711 |
| Fe I | 6136.9937 | 65.900 | 1.39 | 62.960 | 67.050 | 7.754 | 7.666 | Fe II | 6247.5571 | 79.200 | 1.08 | 72.728 | 72.583 | 7.833 | 7.837 |
| Fe I | 6137.6914 | 126.200 | 2.35 | 124.695 | 129.218 | 7.714 | 7.643 | Fe II | 6369.4590 | 31.700 | 0.28 | 38.484 | 38.369 | 7.536 | 7.538 |
| Fe I | 6151.6172 | 43.000 | 0.92 | 47.191 | 50.962 | 7.602 | 7.531 | Fe II | 6383.7222 | 15.900 | 0.19 | 13.983 | 13.955 | 7.766 | 7.767 |
| Fe I | 6157.7280 | 62.900 | 0.62 | 66.772 | 70.435 | 7.614 | 7.542 | Fe II | 6416.9189 | 56.900 | 0.36 | 36.237 | 39.474 | 7.783 | 7.786 |
| Fe I | 6165.3599 | 44.400 | 0.45 | 47.720 | 51.092 | 7.622 | 7.557 | Fe II | 6416.9189 | 56.900 | 0.36 | 52.707 | 52.602 | 7.783 | 7.786 |
| Fe I | 6173.3345 | 66.000 | 0.63 | 64.734 | 68.866 | 7.718 | 7.628 | Fe II | 6456.3794 | 87.700 | 0.99 | 84.591 | 84.422 | 7.756 | 7.760 |
| Fe I | 6180.2026 | 54.300 | 0.69 | 56.352 | 60.077 | 7.646 | 7.571 | Fe II | 6516.0767 | 78.100 | 1.37 | 76.303 | 76.151 | 7.729 | 7.733 |
| Fe I | 6187.9893 | 45.100 | 0.43 | 50.311 | 53.409 | 7.586 | 7.529 |  |  |  |  |  |  |  |  |
| Fe I | 6200.3125 | 72.400 | 0.72 | 68.972 | 72.909 | 7.767 | 7.679 |  |  |  |  |  |  |  |  |
| Fe I | 6213.4292 | 81.200 | 0.95 | 84.258 | 88.974 | 7.624 | 7.528 | $\eta$ Boo |  |  |  |  |  |  |  |
| Fe I | 6219.2803 | 88.100 | 1.04 | 87.320 | 92.110 | 7.707 | 7.606 |  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m}$ ) |  |  |  |  |  |
| Fe I | 6226.7344 | 25.700 | 0.30 | 28.526 | 30.973 | 7.621 | 7.566 |  |  |  |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m}$ ) |  | $\varepsilon_{\mathrm{Fe}}$ (dex) |  |
| Fe I | 6230.7222 | 133.000 | 1.48 | 136.803 | 141.618 | 7.637 | 7.570 | el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 6232.6401 | 80.500 | 0.83 | 84.783 | 87.949 | 7.611 | 7.551 | Fe I | 4787.8267 | 47.100 | 1.00 | 45.070 | 47.896 | 7.812 | 7.754 |
| Fe I | 6240.6460 | 42.500 | 0.52 | 48.246 | 51.989 | 7.569 | 7.500 | Fe I | 4788.7568 | 78.800 | 3.22 | 74.494 | 77.276 | 7.868 | 7.805 |
| Fe I | 6252.5547 | 114.300 | 1.33 | 114.282 | 119.542 | 7.690 | 7.594 | Fe I | 4799.4058 | 36.700 | 1.09 | 39.488 | 42.188 | 7.710 | 7.655 |
| Fe I | 6265.1323 | 84.800 | 0.98 | 82.799 | 87.525 | 7.734 | 7.632 | Fe I | 4869.4634 | 26.400 | 1.20 | 25.306 | 27.417 | 7.798 | 7.745 |
| Fe I | 6271.2778 | 20.900 | 0.43 | 25.209 | 27.611 | 7.575 | 7.520 | Fe I | 4872.9072 | 7.200 | 0.53 | 6.626 | 7.281 | 7.810 | 7.765 |
| Fe I | 6293.9243 | 13.500 | 0.27 | 12.745 | 14.130 | 7.721 | 7.666 | Fe I | 4875.8770 | 65.600 | 3.39 | 65.985 | 68.663 | 7.762 | 7.706 |
| Fe I | 6301.5000 | 115.000 | 3.35 | 120.189 | 123.144 | 7.619 | 7.577 | Fe I | 4892.8589 | 58.600 | 2.01 | 56.378 | 59.596 | 7.815 | 7.750 |
| Fe I | 6311.4995 | 24.600 | 0.44 | 26.121 | 28.704 | 7.651 | 7.590 | Fe I | 4896.4385 | 48.400 | 0.81 | 40.666 | 43.308 | 7.929 | 7.875 |
| Fe I | 6315.8110 | 40.800 | 0.56 | 43.033 | 46.272 | 7.643 | 7.579 | Fe I | 4903.3101 | 154.200 | 2.66 | 146.807 | 147.842 | 7.862 | 7.849 |
| Fe I | 6318.0181 | 106.900 | 1.36 | 108.064 | 113.156 | 7.668 | 7.575 | Fe I | 4938.8140 | 139.600 | 2.70 | 133.346 | 134.693 | 7.861 | 7.841 |
| Fe I | 6322.6851 | 73.200 | 0.58 | 70.492 | 74.516 | 7.750 | 7.662 | Fe I | 4962.5718 | 67.400 | 0.78 | 63.815 | 66.962 | 7.843 | 7.779 |
| Fe I | 6338.8760 | 43.200 | 0.48 | 43.801 | 47.558 | 7.678 | 7.603 | Fe I | 4969.9175 | 94.400 | 1.31 | 85.777 | 89.258 | 7.933 | 7.870 |
| Fe I | 6355.0283 | 68.800 | 0.69 | 63.512 | 67.351 | 7.806 | 7.721 | Fe I | 5014.9424 | 129.800 | 1.46 | 127.101 | 129.168 | 7.810 | 7.780 |
| Fe I | 6364.3638 | 28.600 | 0.23 | 26.789 | 29.438 | 7.734 | 7.670 | Fe I | 5022.2354 | 121.300 | 1.52 | 112.906 | 115.093 | 7.910 | 7.879 |
| Fe I | 6380.7432 | 51.900 | 0.32 | 50.898 | 54.495 | 7.710 | 7.639 | Fe I | 5029.6177 | 67.300 | 1.46 | 59.187 | 62.237 | 7.942 | 7.878 |
| Fe I | 6400.3169 | 58.900 | 0.82 | 56.140 | 61.022 | 7.750 | 7.647 | Fe I | 5036.9214 | 27.400 | 0.73 | 25.394 | 27.692 | 7.819 | 7.763 |
| Fe I | 6408.0176 | 91.500 | 0.68 | 97.849 | 100.979 | 7.584 | 7.529 | Fe I | 5049.8198 | 154.200 | 1.78 | 145.762 | 149.807 | 7.880 | 7.827 |
| Fe I | 6421.3501 | 111.100 | 1.59 | 104.220 | 109.131 | 7.829 | 7.729 | Fe I | 5056.8413 | 35.900 | 0.85 | 26.767 | 28.969 | 7.972 | 7.921 |
| Fe I | 6430.8452 | 107.500 | 1.17 | 111.293 | 117.151 | 7.619 | 7.514 | Fe I | 5068.7656 | 143.000 | 1.34 | 133.666 | 134.880 | 7.903 | 7.886 |
| Fe I | 6436.4058 | 8.100 | 0.21 | 7.338 | 8.181 | 7.738 | 7.685 | Fe I | 5072.6719 | 86.900 | 5.48 | 79.589 | 82.476 | 7.913 | 7.859 |
| Fe I | 6469.1919 | 55.300 | 0.41 | 53.864 | 58.231 | 7.718 | 7.634 | Fe I | 5090.7729 | 105.800 | 1.13 | 100.685 | 103.585 | 7.854 | 7.808 |
| Fe I | 6475.6240 | 48.000 | 0.66 | 47.530 | 51.218 | 7.700 | 7.624 | Fe I | 5127.3594 | 109.500 | 1.57 | 101.061 | 105.712 | 7.986 | 7.865 |
| Fe I | 6481.8696 | 59.100 | 0.52 | 58.688 | 62.835 | 7.699 | 7.613 | Fe I | 5133.6880 | 161.600 | 1.82 | 174.234 | 176.887 | 7.656 | 7.630 |
| Fe I | 6496.4658 | 65.700 | 0.82 | 66.624 | 71.256 | 7.673 | 7.588 | Fe I | 5159.0576 | 83.300 | 0.86 | 78.011 | 81.601 | 7.871 | 7.803 |
| Fe I | 6533.9282 | 34.900 | 0.35 | 35.049 | 38.055 | 7.687 | 7.623 | Fe I | 5180.0557 | 51.900 | 1.01 | 51.455 | 55.150 | 7.779 | 7.706 |
| Fe I | 6569.2139 | 83.200 | 2.37 | 79.436 | 83.882 | 7.754 | 7.678 | Fe I | 5187.9141 | 66.500 | 0.86 | 55.452 | 58.617 | 7.996 | 7.932 |
| Fe I | 6581.2090 | 14.000 | 0.28 | 16.456 | 18.700 | 7.603 | 7.534 | Fe I | 5198.7109 | 100.800 | 2.78 | 106.581 | 111.022 | 7.662 | 7.581 |
| Fe I | 6593.8696 | 79.200 | 0.64 | 78.598 | 83.261 | 7.703 | 7.604 | Fe I | 5217.3892 | 113.400 | 2.70 | 117.678 | 119.228 | 7.699 | 7.670 |
| Fe I | 6597.5591 | 42.300 | 0.33 | 44.009 | 47.577 | 7.655 | 7.586 | Fe I | 5229.8447 | 132.900 | 1.35 | 120.556 | 122.641 | 7.957 | 7.928 |
| Fe I | 6608.0249 | 13.200 | 0.19 | 16.682 | 18.702 | 7.565 | 7.504 | Fe I | 5236.2021 | 45.700 | 0.73 | 47.244 | 50.313 | 7.738 | 7.676 |
| Fe I | 6609.1099 | 62.300 | 0.47 | 60.027 | 64.063 | 7.740 | 7.653 | Fe I | 5242.4907 | 98.200 | 1.24 | 99.474 | 102.129 | 7.746 | 7.692 |
| Fe I | 6625.0215 | 9.700 | 0.27 | 10.995 | 12.726 | 7.627 | 7.554 | Fe I | 5243.7764 | 73.100 | 1.22 | 67.386 | 70.414 | 7.884 | 7.825 |
| Fe I | 6627.5439 | 27.100 | 0.20 | 25.544 | 27.856 | 7.729 | 7.672 | Fe I | 5253.4619 | 83.500 | 1.23 | 85.644 | 88.202 | 7.727 | 7.673 |
| Fe I | 6633.7485 | 66.900 | 0.60 | 63.710 | 67.633 | 7.751 | 7.676 | Fe I | 5263.3062 | 135.500 | 4.90 | 128.378 | 130.201 | 7.871 | 7.847 |
| Fe I | 6667.7104 | 8.500 | 0.16 | 9.277 | 10.319 | 7.647 | 7.593 | Fe I | 5267.2695 | 33.700 | 1.17 | 34.463 | 37.137 | 7.753 | 7.696 |
| Fe I | 6699.1411 | 8.500 | 0.19 | 9.345 | 10.406 | 7.643 | 7.589 | Fe I | 5281.7896 | 152.800 | 1.10 | 148.320 | 149.215 | 7.824 | 7.813 |
| Fe I | 6703.5659 | 30.900 | 0.25 | 33.387 | 36.528 | 7.634 | 7.568 | Fe I | 5285.1274 | 38.500 | 1.55 | 28.941 | 31.389 | 7.976 | 7.921 |
| Fe I | 6710.3179 | 12.000 | 0.27 | 14.172 | 16.178 | 7.603 | 7.535 | Fe I | 5288.5249 | 68.200 | 0.81 | 69.994 | 73.063 | 7.733 | 7.668 |
| Fe I | 6713.0459 | 28.100 | 0.90 | 27.878 | 30.368 | 7.695 | 7.636 | Fe I | 5293.9590 | 33.400 | 0.99 | 35.776 | 38.510 | 7.718 | 7.660 |
| Fe I | 6713.7427 | 20.400 | 0.17 | 17.262 | 19.074 | 7.787 | 7.729 | Fe I | 5295.3120 | 29.800 | 1.13 | 32.915 | 35.545 | 7.699 | 7.643 |
| Fe I | 6716.2363 | 14.700 | 0.23 | 13.625 | 15.105 | 7.731 | 7.675 | Fe I | 5315.0698 | 44.800 | 0.74 | 36.656 | 39.373 | 7.936 | 7.879 |
| Fe I | 6750.1514 | 71.300 | 0.37 | 69.883 | 74.265 | 7.721 | 7.627 | Fe I | 5322.0405 | 72.400 | 0.69 | 69.396 | 73.125 | 7.836 | 7.754 |
| Fe I | 6752.7065 | 34.600 | 0.42 | 38.983 | 42.098 | 7.594 | 7.532 | Fe I | 5326.1426 | 49.300 | 0.63 | 46.423 | 49.491 | 7.829 | 7.766 |
| Fe I | 6786.8584 | 23.300 | 0.43 | 24.024 | 26.227 | 7.671 | 7.616 | Fe I | 5339.9292 | 157.100 | 2.67 | 149.730 | 150.938 | 7.855 | 7.841 |
| Fe II | 4893.8125 | 27.400 | 0.39 | 24.794 | 24.720 | 7.758 | 7.760 | Fe I | 5373.7085 | 72.900 | 0.89 | 75.220 | 79.096 | 7.725 | 7.650 |


| $\eta \mathbf{B O O}$ |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m} \AA)$ |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m} \AA)$ |  | $\varepsilon_{\mathrm{Fe}}$ (dex) |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 5379.5737 | 69.600 | 1.09 | 69.198 | 72.307 | 7.778 | 7.713 |
| Fe I | 5389.4790 | 99.900 | 1.43 | 95.057 | 98.301 | 7.852 | 7.798 |
| Fe I | 5393.1670 | 141.800 | 0.97 | 143.490 | 144.939 | 7.748 | 7.729 |
| Fe I | 5397.6177 | 26.100 | 1.60 | 22.895 | 24.995 | 7.852 | 7.798 |
| Fe I | 5398.2793 | 82.000 | 0.85 | 81.166 | 84.724 | 7.786 | 7.718 |
| Fe I | 5401.2666 | 25.900 | 0.77 | 26.609 | 28.860 | 7.752 | 7.699 |
| Fe I | 5406.7749 | 36.600 | 1.23 | 33.635 | 36.206 | 7.834 | 7.778 |
| Fe I | 5409.1333 | 66.500 | 0.83 | 54.869 | 58.124 | 7.998 | 7.934 |
| Fe I | 5410.9097 | 158.100 | 3.92 | 157.467 | 162.505 | 7.776 | 7.727 |
| Fe I | 5417.0332 | 36.400 | 1.30 | 33.614 | 36.261 | 7.830 | 7.773 |
| Fe I | 5434.5234 | 167.200 | 1.11 | 162.444 | 166.098 | 7.842 | 7.787 |
| Fe I | 5441.3389 | 32.900 | 0.91 | 35.711 | 38.358 | 7.709 | 7.654 |
| Fe I | 5445.0420 | 127.000 | 0.87 | 122.883 | 125.905 | 7.825 | 7.785 |
| Fe I | 5452.0884 | 14.600 | 0.86 | 13.817 | 15.234 | 7.799 | 7.747 |
| Fe I | 5461.5493 | 25.100 | 0.86 | 22.991 | 24.990 | 7.825 | 7.773 |
| Fe I | 5466.3960 | 91.800 | 0.64 | 85.664 | 88.587 | 7.880 | 7.830 |
| Fe I | 5466.9873 | 44.100 | 0.50 | 38.630 | 41.538 | 7.883 | 7.822 |
| Fe I | 5470.0928 | 27.500 | 0.57 | 26.616 | 28.899 | 7.791 | 7.737 |
| Fe I | 5472.7085 | 53.400 | 0.62 | 46.758 | 49.743 | 7.904 | 7.844 |
| Fe I | 5473.1626 | 28.800 | 0.81 | 22.526 | 24.511 | 7.925 | 7.873 |
| Fe I | 5487.1450 | 50.900 | 1.04 | 41.087 | 43.990 | 7.963 | 7.906 |
| Fe I | 5494.4624 | 34.000 | 1.24 | 24.506 | 26.666 | 7.988 | 7.935 |
| Fe I | 5506.7788 | 132.900 | 0.82 | 124.388 | 129.167 | 7.957 | 7.852 |
| Fe I | 5522.4463 | 49.900 | 0.89 | 49.167 | 52.139 | 7.785 | 7.725 |
| Fe I | 5525.5435 | 67.500 | 0.56 | 66.554 | 69.617 | 7.789 | 7.726 |
| Fe I | 5536.5801 | 9.800 | 0.53 | 9.854 | 10.986 | 7.767 | 7.712 |
| Fe I | 5539.2798 | 23.500 | 0.39 | 21.600 | 23.632 | 7.821 | 7.767 |
| Fe I | 5543.9355 | 77.000 | 0.60 | 69.504 | 72.400 | 7.920 | 7.866 |
| Fe I | 5546.5059 | 60.400 | 0.60 | 54.336 | 57.498 | 7.891 | 7.828 |
| Fe I | 5546.9907 | 29.800 | 0.59 | 31.283 | 33.746 | 7.736 | 7.681 |
| Fe I | 5554.8945 | 99.800 | 1.64 | 96.822 | 101.384 | 7.819 | 7.743 |
| Fe I | 5569.6182 | 152.500 | 0.79 | 152.610 | 153.841 | 7.769 | 7.755 |
| Fe I | 5576.0889 | 128.700 | 0.78 | 119.544 | 121.488 | 7.908 | 7.882 |
| Fe I | 5577.0249 | 19.300 | 0.74 | 13.918 | 15.727 | 7.951 | 7.884 |
| Fe I | 5584.7646 | 51.500 | 1.27 | 48.281 | 51.472 | 7.835 | 7.771 |
| Fe I | 5618.6323 | 62.500 | 0.90 | 59.095 | 62.205 | 7.839 | 7.776 |
| Fe I | 5622.9453 | 11.900 | 0.51 | 7.711 | 8.568 | 7.983 | 7.933 |
| Fe I | 5638.2622 | 91.700 | 0.78 | 86.216 | 88.336 | 7.875 | 7.839 |
| Fe I | 5650.7056 | 37.900 | 1.79 | 38.443 | 43.146 | 7.758 | 7.665 |
| Fe I | 5653.8652 | 37.400 | 2.27 | 32.473 | 35.068 | 7.876 | 7.819 |
| Fe I | 5662.5161 | 108.300 | 6.16 | 112.599 | 114.663 | 7.708 | 7.674 |
| Fe I | 5679.0229 | 67.000 | 0.54 | 61.567 | 65.707 | 7.876 | 7.795 |
| Fe I | 5680.2402 | 10.800 | 0.54 | 10.016 | 11.055 | 7.808 | 7.758 |
| Fe I | 5691.4971 | 50.300 | 0.69 | 44.999 | 48.127 | 7.878 | 7.814 |
| Fe I | 5717.8325 | 75.900 | 0.94 | 69.271 | 72.383 | 7.902 | 7.843 |
| Fe I | 5720.8862 | 27.900 | 1.24 | 26.323 | 28.612 | 7.808 | 7.753 |
| Fe I | 5731.7617 | 70.200 | 0.82 | 60.307 | 63.083 | 7.966 | 7.915 |
| Fe I | 5741.8477 | 37.200 | 0.56 | 36.301 | 38.950 | 7.789 | 7.733 |
| Fe I | 5742.9600 | 17.500 | 0.60 | 11.749 | 12.939 | 7.980 | 7.932 |
| Fe I | 5760.3438 | 29.400 | 0.76 | 28.860 | 31.404 | 7.783 | 7.724 |
| Fe I | 5848.1265 | 47.800 | 1.15 | 51.116 | 54.728 | 7.704 | 7.633 |
| Fe I | 5853.1484 | 7.100 | 0.85 | 6.305 | 7.239 | 7.827 | 7.761 |
| Fe I | 5855.0757 | 31.700 | 0.67 | 30.761 | 33.436 | 7.791 | 7.732 |
| Fe I | 5858.7778 | 22.600 | 0.95 | 17.683 | 19.368 | 7.913 | 7.861 |
| Fe I | 5859.5864 | 98.700 | 0.78 | 89.112 | 92.536 | 7.934 | 7.881 |
| Fe I | 5861.1084 | 17.700 | 1.08 | 12.112 | 13.310 | 7.971 | 7.923 |
| Fe I | 5862.3564 | 118.100 | 1.60 | 107.127 | 110.554 | 7.934 | 7.888 |
| Fe I | 5873.2124 | 25.900 | 0.59 | 20.941 | 22.787 | 7.899 | 7.849 |
| Fe I | 5879.4868 | 9.900 | 0.97 | 9.399 | 10.363 | 7.796 | 7.747 |
| Fe I | 5905.6714 | 65.900 | 1.10 | 68.628 | 72.854 | 7.719 | 7.638 |
| Fe I | 5909.9722 | 43.500 | 0.84 | 38.732 | 41.827 | 7.866 | 7.803 |
| Fe I | 5927.7886 | 48.400 | 1.29 | 53.069 | 56.941 | 7.679 | 7.607 |
| Fe I | 5929.6763 | 44.100 | 1.10 | 41.662 | 44.654 | 7.819 | 7.759 |
| Fe I | 5930.1797 | 104.000 | 1.15 | 95.389 | 99.364 | 7.909 | 7.848 |
| Fe I | 5934.6543 | 85.400 | 1.25 | 85.832 | 88.123 | 7.762 | 7.719 |
| Fe I | 5956.6938 | 56.300 | 0.67 | 48.298 | 53.016 | 7.925 | 7.832 |
| Fe I | 5976.7769 | 86.400 | 0.96 | 75.505 | 78.082 | 7.971 | 7.930 |
| Fe I | 5984.8149 | 101.100 | 1.04 | 93.090 | 97.989 | 7.901 | 7.822 |
| Fe I | 5987.0649 | 85.800 | 0.82 | 75.758 | 81.285 | 7.953 | 7.851 |
| Fe I | 6007.9595 | 84.000 | 0.69 | 73.419 | 77.121 | 7.967 | 7.903 |
| Fe I | 6015.2437 | 8.700 | 0.96 | 7.466 | 8.465 | 7.845 | 7.783 |
| Fe I | 6027.0508 | 84.300 | 0.72 | 76.051 | 79.385 | 7.927 | 7.865 |
| Fe I | 6056.0044 | 89.600 | 0.66 | 85.765 | 90.469 | 7.836 | 7.755 |
| Fe I | 6079.0078 | 59.100 | 0.67 | 52.197 | 55.588 | 7.901 | 7.838 |
| Fe I | 6082.7100 | 46.600 | 0.95 | 35.212 | 38.567 | 7.994 | 7.925 |
| Fe I | 6093.6431 | 43.800 | 0.58 | 34.665 | 37.557 | 7.957 | 7.895 |
| Fe I | 6096.6641 | 47.000 | 0.48 | 41.962 | 44.783 | 7.869 | 7.813 |
| Fe I | 6098.2441 | 22.800 | 0.82 | 17.816 | 19.535 | 7.914 | 7.861 |


| $\eta$ Boo |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m}$ ) |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m}$ ( $)$ |  | $\varepsilon_{\mathrm{Fe}}(\mathrm{dex})$ |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 6127.9063 | 64.200 | 0.50 | 56.473 | 59.950 | 7.920 | 7.853 |
| Fe I | 6151.6172 | 55.800 | 1.26 | 52.384 | 56.448 | 7.837 | 7.758 |
| Fe I | 6157.7280 | 82.300 | 1.47 | 72.310 | 75.797 | 7.961 | 7.897 |
| Fe I | 6165.3599 | 52.200 | 0.80 | 52.603 | 56.080 | 7.762 | 7.695 |
| Fe I | 6173.3345 | 81.600 | 0.56 | 71.073 | 75.449 | 7.995 | 7.898 |
| Fe I | 6180.2026 | 70.700 | 0.68 | 62.138 | 66.104 | 7.944 | 7.862 |
| Fe I | 6187.9893 | 57.700 | 0.67 | 55.318 | 58.352 | 7.816 | 7.757 |
| Fe I | 6213.4292 | 95.100 | 0.93 | 91.601 | 96.422 | 7.842 | 7.744 |
| Fe I | 6219.2803 | 105.900 | 0.88 | 94.783 | 99.667 | 7.999 | 7.895 |
| Fe I | 6226.7344 | 35.400 | 0.60 | 32.152 | 34.797 | 7.840 | 7.783 |
| Fe I | 6229.2261 | 45.900 | 0.61 | 45.358 | 48.930 | 7.781 | 7.711 |
| Fe I | 6232.6401 | 94.000 | 0.74 | 90.673 | 93.285 | 7.830 | 7.783 |
| Fe I | 6240.6460 | 56.100 | 1.04 | 53.538 | 57.568 | 7.821 | 7.741 |
| Fe I | 6246.3179 | 121.900 | 1.10 | 123.827 | 124.826 | 7.742 | 7.725 |
| Fe I | 6270.2236 | 70.600 | 0.99 | 62.230 | 66.062 | 7.940 | 7.861 |
| Fe I | 6271.2778 | 33.800 | 1.20 | 28.493 | 31.174 | 7.888 | 7.827 |
| Fe I | 6301.5000 | 135.000 | 3.29 | 124.301 | 125.938 | 7.918 | 7.900 |
| Fe I | 6335.3301 | 110.300 | 1.00 | 108.425 | 113.772 | 7.806 | 7.704 |
| Fe I | 6336.8232 | 116.500 | 0.68 | 113.502 | 115.230 | 7.816 | 7.790 |
| Fe I | 6380.7432 | 64.900 | 0.65 | 55.907 | 59.602 | 7.943 | 7.872 |
| Fe I | 6393.6006 | 145.100 | 0.87 | 138.820 | 143.706 | 7.865 | 7.791 |
| Fe I | 6411.6479 | 134.800 | 0.57 | 135.470 | 136.151 | 7.761 | 7.752 |
| Fe I | 6430.8452 | 124.700 | 0.62 | 118.971 | 124.577 | 7.874 | 7.772 |
| Fe I | 6469.1919 | 70.100 | 0.96 | 58.572 | 62.913 | 7.984 | 7.905 |
| Fe I | 6494.9805 | 173.000 | 3.62 | 155.444 | 160.749 | 7.985 | 7.922 |
| Fe I | 6495.7412 | 64.700 | 1.07 | 53.013 | 57.311 | 7.988 | 7.908 |
| Fe I | 6496.4658 | 81.500 | 1.47 | 71.626 | 75.955 | 7.947 | 7.872 |
| Fe I | 6518.3657 | 72.100 | 1.21 | 66.182 | 70.332 | 7.888 | 7.805 |
| Fe I | 6533.9282 | 45.900 | 1.09 | 39.304 | 42.445 | 7.902 | 7.838 |
| Fe I | 6574.2266 | 30.500 | 0.82 | 23.914 | 27.237 | 7.922 | 7.842 |
| Fe I | 6581.2090 | 18.800 | 0.76 | 18.625 | 21.165 | 7.775 | 7.703 |
| Fe I | 6592.9126 | 133.000 | 2.61 | 122.629 | 126.683 | 7.944 | 7.877 |
| Fe I | 6593.8696 | 94.800 | 0.70 | 85.690 | 90.486 | 7.960 | 7.858 |
| Fe I | 6597.5591 | 47.900 | 0.84 | 48.668 | 52.219 | 7.755 | 7.687 |
| Fe I | 6608.0249 | 17.500 | 0.71 | 18.946 | 21.240 | 7.725 | 7.661 |
| Fe I | 6609.1099 | 76.700 | 0.74 | 66.074 | 70.441 | 7.988 | 7.895 |
| Fe I | 6625.0215 | 17.500 | 0.61 | 12.453 | 14.413 | 7.948 | 7.873 |
| Fe I | 6703.5659 | 41.400 | 0.66 | 37.463 | 40.943 | 7.850 | 7.779 |
| Fe I | 6710.3179 | 16.600 | 0.93 | 16.062 | 18.336 | 7.788 | 7.715 |
| Fe I | 6713.0459 | 42.500 | 0.96 | 31.650 | 34.253 | 7.994 | 7.939 |
| Fe I | 6713.7427 | 25.800 | 0.59 | 19.792 | 21.797 | 7.930 | 7.873 |
| Fe I | 6716.2363 | 23.200 | 0.66 | 15.712 | 17.400 | 7.991 | 7.936 |
| Fe I | 6739.5205 | 12.100 | 0.73 | 13.323 | 15.244 | 7.720 | 7.650 |
| Fe I | 6750.1514 | 83.600 | 0.66 | 76.611 | 81.156 | 7.916 | 7.820 |
| Fe I | 6752.7065 | 42.700 | 0.72 | 43.685 | 46.822 | 7.750 | 7.687 |
| Fe I | 6786.8584 | 30.900 | 0.82 | 27.266 | 29.605 | 7.853 | 7.799 |
| Fe I | 6810.2622 | 58.200 | 0.71 | 57.165 | 60.749 | 7.789 | 7.722 |
| Fe II | 4893.8125 | 38.200 | 1.40 | 33.333 | 33.266 | 7.878 | 7.880 |
| Fe II | 5197.5674 | 140.100 | 4.63 | 128.236 | 128.108 | 7.979 | 7.981 |
| Fe II | 5234.6226 | 130.600 | 1.58 | 123.247 | 123.124 | 7.908 | 7.911 |
| Fe II | 5264.8022 | 86.000 | 4.38 | 78.474 | 78.396 | 7.944 | 7.946 |
| Fe II | 5414.0698 | 60.200 | 2.74 | 58.589 | 58.472 | 7.805 | 7.807 |
| Fe II | 5425.2485 | 70.900 | 0.90 | 76.206 | 76.130 | 7.651 | 7.653 |
| Fe II | 5525.1172 | 36.300 | 0.55 | 38.040 | 37.964 | 7.731 | 7.733 |
| Fe II | 6084.1016 | 52.100 | 0.61 | 45.931 | 45.839 | 7.898 | 7.900 |
| Fe II | 6149.2461 | 71.000 | 0.66 | 65.602 | 65.536 | 7.886 | 7.887 |
| Fe II | 6238.3857 | 83.200 | 0.71 | 77.261 | 77.184 | 7.897 | 7.899 |
| Fe II | 6239.9429 | 40.600 | 0.90 | 31.185 | 31.123 | 7.980 | 7.981 |
| Fe II | 6369.4590 | 42.300 | 0.59 | 49.146 | 49.048 | 7.629 | 7.631 |
| Fe II | 6383.7222 | 27.400 | 0.60 | 19.641 | 19.621 | 7.994 | 7.994 |
| Fe II | 6416.9189 | 72.300 | 0.63 | 40.571 | 44.003 | 7.941 | 7.944 |
| Fe II | 6416.9189 | 72.300 | 0.63 | 64.188 | 64.060 | 7.941 | 7.944 |
| Fe II | 6456.3794 | 107.800 | 1.28 | 97.360 | 97.263 | 7.983 | 7.985 |
| Fe II | 6516.0767 | 99.300 | 2.31 | 89.161 | 88.983 | 7.982 | 7.986 |


| PrOCyOn |  |  |  |  |  |  |  |  |
| :--- | :--- | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | EW $_{\text {obs }}(\mathrm{m} \AA)$ |  | EW $_{\text {calc }}(\mathrm{mA})$ |  | $\varepsilon_{\mathrm{Fe}}(\mathrm{dex})$ |  |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |  |
| Fe I | 4799.4058 | 14.900 | 0.44 | 16.343 | 18.488 | 7.443 | 7.397 |  |
| Fe I | 4802.8799 | 44.700 | 0.41 | 42.303 | 46.283 | 7.475 | 7.445 |  |
| Fe I | 4882.1431 | 50.800 | 0.66 | 55.135 | 59.031 | 7.410 | 7.339 |  |
| Fe I | 4885.4302 | 57.800 | 0.70 | 59.828 | 63.987 | 7.436 | 7.366 |  |
| Fe I | 4892.8589 | 34.000 | 0.43 | 30.102 | 33.671 | 7.471 | 7.462 |  |
| Fe I | 4896.4385 | 17.700 | 0.52 | 17.568 | 19.806 | 7.461 | 7.435 |  |
| Fe I | 4905.1328 | 16.200 | 0.21 | 21.846 | 24.546 | 7.348 | 7.248 |  |
| Fe I | 4907.7319 | 39.200 | 0.36 | 43.013 | 46.804 | 7.422 | 7.358 |  |


| Procyon |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m} \AA)$ |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m}$ ) |  | $\varepsilon_{\mathrm{Fe}}(\mathrm{dex})$ |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 4917.2300 | 46.100 | 0.37 | 41.283 | 45.566 | 7.482 | 7.464 |
| Fe I | 4918.0127 | 34.700 | 0.33 | 31.004 | 34.641 | 7.471 | 7.460 |
| Fe I | 4938.8140 | 100.300 | 1.46 | 100.089 | 102.132 | 7.463 | 7.430 |
| Fe I | 4962.5718 | 35.900 | 0.33 | 36.973 | 40.899 | 7.451 | 7.404 |
| Fe I | 4969.9175 | 61.900 | 0.72 | 59.063 | 64.199 | 7.487 | 7.432 |
| Fe I | 4979.5859 | 5.600 | 0.2 | 5.419 | 6.236 | 7.46 | 7.438 |
| Fe I | 4985.2529 | 83.400 | 1.18 | 83.454 | 87.754 | 7.45 | 7.384 |
| Fe I | 4985.5469 | 86.300 | 1.32 | 86.853 | 89.910 | 7.452 | 7.399 |
| Fe I | 4986.2227 | 28.300 | 1.16 | 30.239 | 33.787 | 7.443 | 7.391 |
| Fe I | 4993.6797 | 27.200 | 0.45 | 27.046 | 30.253 | 7.461 | 7.429 |
| Fe I | 4994.1294 | 86.900 | 1.22 | 82.157 | 86.572 | 7.534 | 7.466 |
| Fe I | 5001.8633 | 112.500 | . 58 | 120.580 | 124.953 | 7.370 | 7.300 |
| Fe I | 5002.7920 | 55.000 | 0.45 | 57.455 | 61.449 | 7.433 | 7.370 |
| Fe I | 5014.9424 | 95.200 | 1.12 | 96.478 | 100.708 | 7.442 | 7.365 |
| Fe I | 5023.1860 | 17.600 | 0.31 | 19.517 | 22.103 | 7.438 | 7.385 |
| Fe I | 5028.1260 | 68.700 | 1.04 | 70.104 | 74.420 | 7.441 | 7.366 |
| Fe I | 5049.8198 | 111.600 | 1.34 | 108.907 | 112.857 | 7.501 | 7.439 |
| Fe I | 5056.8413 | 10.600 | 0.18 | 10.180 | 11.634 | 7.464 | 7.442 |
| Fe I | 5068.7656 | 100.000 | 1.05 | 99.974 | 102.014 | 7.460 | 7.428 |
| Fe I | 5088.1533 | 16.200 | 0.23 | 17.269 | 19.491 | 7.449 | 7.408 |
| Fe I | 5090.7729 | 72.500 | 0.68 | 71.977 | 77.146 | 7.466 | 7.392 |
| Fe I | 5127.3594 | 74.900 | 0.70 | 71.523 | 76.169 | 7.504 | 7.440 |
| Fe I | 5133.6880 | 120.200 | 1.96 | 124.939 | 129.470 | 7.409 | 7.345 |
| Fe I | 5151.9106 | 69.600 | 1.26 | 66.971 | 71.627 | 7.491 | 7.431 |
| Fe I | 5159.0576 | 52.300 | 0.46 | 50.853 | 55.882 | 7.472 | 7.419 |
| Fe I | 5180.0557 | 23.400 | 0.54 | 26.384 | 30.050 | 7.427 | 7.355 |
| Fe I | 5187.9141 | 32.700 | 0.29 | 29.397 | 32.883 | 7.472 | 7.459 |
| Fe I | 5194.9414 | 105.100 | 1.37 | 103.974 | 108.194 | 7.481 | 7.398 |
| Fe I | 5197.9360 | 19.500 | 0.75 | 17.806 | 20.234 | 7.466 | 7.454 |
| Fe I | 5198.7109 | 75.000 | 0.69 | 74.546 | 79.220 | 7.466 | 7.394 |
| Fe I | 5215.1802 | 95.000 | 1.29 | 95.372 | 98.627 | 7.455 | 7.402 |
| Fe I | 5216.2739 | 104.900 | 2.18 | 99.299 | 103.652 | 7.555 | 7.483 |
| Fe I | 5217.3892 | 83.900 | 0.75 | 86.289 | 89.511 | 7.426 | 7.365 |
| Fe I | 5225.5259 | 30.400 | 0.56 | 32.074 | 36.740 | 7.447 | 7.382 |
| Fe I | 5229.8447 | 94.900 | 0.92 | 88.294 | 92.165 | 7.537 | 7.499 |
| Fe I | 5235.3867 | 62.000 | 0.88 | 57.318 | 62.100 | 7.501 | 7.459 |
| Fe I | 5242.4907 | 71.200 | 0.67 | 71.575 | 76.063 | 7.455 | 7.383 |
| Fe I | 5243.7764 | 41.500 | 0.33 | 40.419 | 44.613 | 7.468 | 7.428 |
| Fel | 5247.0503 | 23.000 | 0.25 | 25.706 | 29.821 | 7.433 | 7.355 |
| Fe I | 5263.3062 | 90.400 | 0.94 | 94.358 | 97.679 | 7.402 | 7.335 |
| Fe I | 5273.1636 | 86.200 | 0.91 | 86.308 | 89.811 | 7.459 | 7.402 |
| Fe I | 5281.7896 | 107.800 | 1.44 | 109.340 | 110.780 | 7.439 | 7.415 |
| Fe I | 5293.9590 | 14.200 | 0.51 | 14.867 | 16.952 | 7.453 | 7.413 |
| Fe I | 5295.3120 | 14.300 | 0.24 | 13.573 | 15.530 | 7.465 | 7.444 |
| Fe I | 5307.3608 | 67.300 | 1.44 | 61.613 | 66.251 | 7.513 | 7.473 |
| Fe I | 5315.0698 | 15.400 | 0.31 | 15.648 | 17.802 | 7.458 | 7.424 |
| Fe I | 5339.9292 | 105.500 | 1.95 | 109.663 | 112.015 | 7.404 | 7.360 |
| FeI | 5373.7085 | 45.700 | 0.41 | 48.152 | 53.443 | 7.434 | 7.352 |
| Fe I | 5379.5737 | 39.200 | 0.31 | 41.038 | 45.246 | 7.443 | 7.384 |
| Fe I | 5389.4790 | 67.500 | 0.52 | 66.512 | 72.139 | 7.471 | 7.395 |
| Fe I | 5393.1670 | 100.600 | 1.39 | 105.530 | 108.125 | 7.390 | 7.338 |
| Fe I | 5398.2793 | 53.500 | 0.35 | 53.705 | 59.016 | 7.458 | 7.388 |
| Fe I | 5400.5010 | 90.200 | 1.19 | 81.749 | 87.526 | 7.544 | 7.494 |
| Fe I | 5406.7749 | 14.100 | 0.54 | 13.842 | 15.801 | 7.462 | 7.435 |
| Fe I | 5409.1333 | 33.000 | 0.36 | 28.799 | 32.358 | 7.472 | 7.464 |
| Fe I | 5417.0332 | 16.700 | 0.16 | 13.893 | 15.914 | 7.462 | 7.465 |
| Fe I | 5434.5234 | 127.100 | 1.58 | 124.681 | 128.009 | 7.502 | 7.443 |
| Fe I | 5436.2949 | 19.500 | 0.19 | 18.928 | 21.485 | 7.464 | 7.438 |
| Fe I | 5441.3389 | 13.000 | 0.22 | 14.974 | 17.035 | 7.428 | 7.370 |
| Fe I | 5445.0420 | 96.300 | 1.40 | 89.159 | 94.951 | 7.534 | 7.478 |
| Fe I | 5463.2754 | 92.900 | 1.32 | 92.448 | 98.349 | 7.465 | 7.380 |
| Fe I | 5466.3960 | 61.300 | 0.08 | 57.470 | 62.467 | 7.492 | 7.447 |
| Fe I | 5466.9873 | 17.800 | 0.77 | 15.486 | 17.678 | 7.466 | 7.461 |
| Fe I | 5470.0928 | 10.200 | 0.23 | 10.236 | 11.779 | 7.460 | 7.427 |
| Fe I | 5472.7085 | 22.800 | 0.15 | 22.193 | 25.134 | 7.464 | 7.435 |
| Fe I | 6003.0112 | 60.500 | 0.75 | 56.182 | 60.541 | 7.493 | 7.460 |
| Fe I | 6008.5557 | 62.100 | 0.95 | 62.625 | 66.979 | 7.454 | 7.394 |
| Fe I | 6027.0508 | 49.500 | 0.54 | 47.061 | 51.772 | 7.478 | 7.436 |
| Fe I | 6056.0044 | 57.300 | 0.54 | 57.008 | 63.696 | 7.463 | 7.372 |
| Fe I | 6079.0078 | 30.200 | 0.31 | 26.691 | 30.331 | 7.472 | 7.459 |
| Fe I | 6082.7100 | 10.800 | 0.32 | 11.179 | 12.984 | 7.454 | 7.412 |
| Fe I | 6093.6431 | 15.200 | 0.25 | 14.657 | 16.905 | 7.464 | 7.436 |
| Fe I | 6096.6641 | 16.600 | 0.37 | 17.826 | 20.234 | 7.446 | 7.400 |


| Procyon |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m} \AA)$ |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m}$ ) |  | $\varepsilon_{\mathrm{Fe}}$ (dex) |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 6098.2441 | 6.200 | 0.24 | 6.314 | 7.325 | 7.457 | 7.419 |
| Fe I | 6127.9063 | 30.400 | 0.45 | 29.057 | 32.796 | 7.468 | 7.436 |
| Fe I | 6136.9937 | 36.100 | 0.88 | 34.948 | 39.179 | 7.467 | 7.430 |
| Fe I | 6157.7280 | 42.200 | 0.53 | 43.331 | 48.039 | 7.450 | 7.386 |
| Fe I | 6165.3599 | 24.600 | 0.55 | 25.894 | 29.358 | 7.448 | 7.395 |
| Fe I | 6170.5059 | 56.500 | 0.33 | 48.102 | 54.291 | 7.508 | 7.479 |
| Fe I | 6173.3345 | 37.700 | 0.58 | 37.309 | 41.686 | 7.463 | 7.418 |
| Fe I | 6180.2026 | 26.100 | 0.30 | 30.158 | 33.962 | 7.412 | 7.333 |
| Fe I | 6187.9893 | 26.100 | 0.24 | 27.217 | 30.512 | 7.451 | 7.405 |
| Fe I | 6191.5576 | 108.600 | 1.18 | 102.390 | 107.103 | 7.550 | 7.484 |
| Fe I | 6200.3125 | 44.900 | 0.89 | 43.123 | 47.650 | 7.473 | 7.432 |
| Fe I | 6213.4292 | 56.000 | 0.76 | 58.508 | 63.596 | 7.430 | 7.349 |
| Fe I | 6219.2803 | 64.500 | 0.74 | 62.112 | 67.221 | 7.485 | 7.424 |
| Fe I | 6226.7344 | 10.400 | 0.38 | 12.080 | 13.869 | 7.426 | 7.364 |
| Fe I | 6232.6401 | 57.300 | 0.52 | 59.335 | 63.939 | 7.438 | 7.366 |
| Fe I | 6246.3179 | 87.000 | 0.86 | 88.230 | 91.525 | 7.445 | 7.392 |
| Fe I | 6253.8286 | 13.100 | 0.51 | 14.603 | 16.863 | 7.437 | 7.377 |
| Fe I | 6265.1323 | 62.700 | 0.73 | 57.023 | 62.117 | 7.506 | 7.466 |
| Fe I | 6270.2236 | 26.500 | 0.49 | 30.621 | 34.444 | 7.411 | 7.331 |
| Fe I | 6271.2778 | 9.800 | 0.30 | 9.626 | 11.128 | 7.462 | 7.432 |
| Fe I | 6290.9653 | 40.100 | 0.38 | 34.415 | 39.152 | 7.482 | 7.467 |
| Fe I | 6311.4995 | 9.200 | 0.34 | 9.445 | 10.983 | 7.456 | 7.415 |
| Fe I | 6315.8110 | 25.600 | 0.36 | 22.024 | 25.113 | 7.469 | 7.463 |
| Fe I | 6318.0181 | 87.400 | 1.68 | 82.725 | 87.818 | 7.522 | 7.454 |
| Fe I | 6322.6851 | 47.400 | 0.42 | 44.440 | 49.051 | 7.480 | 7.444 |
| Fe I | 6335.3301 | 78.100 | 1.08 | 75.307 | 80.628 | 7.496 | 7.422 |
| Fe I | 6336.8232 | 80.600 | 0.74 | 79.319 | 83.494 | 7.474 | 7.419 |
| Fe I | 6344.1479 | 31.200 | 0.83 | 27.097 | 30.757 | 7.473 | 7.463 |
| Fe I | 6355.0283 | 38.900 | 0.48 | 37.579 | 41.894 | 7.469 | 7.430 |
| Fe I | 6364.3638 | 11.800 | 0.39 | 12.363 | 14.460 | 7.452 | 7.402 |
| Fe I | 6380.7432 | 30.300 | 0.31 | 28.531 | 32.422 | 7.470 | 7.439 |
| Fe I | 6393.6006 | 104.200 | 1.01 | 101.942 | 106.857 | 7.494 | 7.416 |
| Fe I | 6400.0005 | 115.300 | 1.21 | 121.295 | 122.893 | 7.391 | 7.359 |
| Fe I | 6400.3169 | 25.500 | 1.08 | 24.074 | 27.863 | 7.468 | 7.437 |
| Fe I | 6408.0176 | 72.900 | 1.12 | 70.687 | 75.199 | 7.483 | 7.429 |
| Fe I | 6411.6479 | 94.700 | 0.79 | 96.792 | 99.683 | 7.434 | 7.386 |
| Fe I | 6430.8452 | 88.500 | 0.82 | 84.948 | 90.466 | 7.510 | 7.429 |
| Fe I | 6469.1919 | 40.700 | 0.80 | 32.351 | 37.185 | 7.477 | 7.480 |
| Fe I | 6475.6240 | 21.400 | 0.83 | 21.937 | 25.042 | 7.455 | 7.411 |
| Fe I | 6481.8696 | 29.900 | 0.24 | 30.580 | 34.593 | 7.455 | 7.404 |
| Fe I | 6494.9805 | 119.900 | 1.11 | 113.679 | 118.787 | 7.545 | 7.477 |
| Fe I | 6496.4658 | 47.200 | 0.79 | 43.742 | 49.482 | 7.484 | 7.436 |
| Fe I | 6518.3657 | 30.500 | 0.36 | 33.628 | 37.742 | 7.427 | 7.357 |
| Fe I | 6533.9282 | 18.500 | 0.27 | 17.244 | 19.912 | 7.468 | 7.443 |
| Fe I | 6592.9126 | 86.500 | 0.71 | 88.485 | 93.142 | 7.430 | 7.345 |
| Fe I | 6593.8696 | 54.700 | 0.43 | 52.537 | 57.606 | 7.479 | 7.426 |
| Fe I | 6597.5591 | 24.100 | 0.34 | 24.027 | 27.554 | 7.461 | 7.417 |
| Fe I | 6609.1099 | 36.200 | 0.43 | 32.936 | 37.048 | 7.476 | 7.453 |
| Fe I | 6633.7485 | 45.000 | 0.57 | 40.896 | 45.899 | 7.484 | 7.451 |
| Fe I | 6703.5659 | 12.600 | 0.23 | 12.935 | 14.988 | 7.456 | 7.414 |
| Fe I | 6713.0459 | 15.400 | 0.43 | 12.838 | 14.859 | 7.467 | 7.465 |
| Fe I | 6713.7427 | 11.200 | 0.32 | 7.255 | 8.495 | 7.435 | 7.465 |
| Fe I | 6716.2363 | 6.200 | 0.27 | 5.409 | 6.356 | 7.473 | 7.456 |
| Fe I | 6750.1514 | 44.400 | 0.34 | 42.743 | 47.440 | 7.472 | 7.428 |
| Fe I | 6804.2710 | 7.100 | 0.36 | 6.781 | 7.950 | 7.466 | 7.435 |
| Fe II | 4893.8125 | 26.200 | 0.25 | 20.073 | 20.053 | 7.446 | 7.446 |
| Fe II | 4993.3501 | 57.600 | 0.63 | 57.897 | 57.839 | 7.457 | 7.457 |
| Fe II | 5000.7305 | 15.000 | 0.35 | 12.665 | 12.640 | 7.464 | 7.464 |
| Fe II | 5132.6611 | 33.400 | 0.33 | 36.918 | 36.881 | 7.424 | 7.424 |
| Fe II | 5197.5674 | 117.300 | 1.31 | 117.181 | 117.181 | 7.462 | 7.462 |
| Fe II | 5256.9321 | 26.900 | 0.43 | 29.415 | 29.386 | 7.435 | 7.436 |
| Fe II | 5264.8022 | 71.100 | 0.64 | 67.882 | 67.814 | 7.498 | 7.499 |
| Fe II | 5284.1030 | 88.800 | 1.89 | 79.170 | 79.091 | 7.577 | 7.578 |
| Fe II | 5325.5522 | 67.700 | 0.79 | 66.943 | 66.876 | 7.470 | 7.470 |
| Fe II | 5414.0698 | 44.500 | 0.33 | 45.514 | 45.469 | 7.451 | 7.451 |
| Fe II | 5425.2485 | 63.000 | 0.54 | 65.150 | 65.085 | 7.431 | 7.432 |
| Fe II | 6084.1016 | 35.900 | 0.45 | 32.263 | 32.231 | 7.476 | 7.476 |
| Fe II | 6113.3193 | 21.700 | 0.23 | 17.457 | 17.422 | 7.463 | 7.463 |
| Fe II | 6129.6948 | 8.100 | 0.37 | 6.502 | 6.489 | 7.472 | 7.471 |
| Fe II | 6149.2461 | 63.600 | 0.62 | 54.924 | 54.869 | 7.522 | 7.522 |
| Fe II | 6238.3857 | 69.400 | 0.53 | 67.509 | 67.442 | 7.483 | 7.484 |
| Fe II | 6239.9429 | 23.700 | 0.54 | 20.506 | 20.486 | 7.471 | 7.471 |
| Fe II | 6383.7222 | 17.900 | 0.24 | 13.343 | 13.330 | 7.460 | 7.460 |
| Fe II | 6416.9189 | 61.300 | 0.48 | 53.302 | 53.249 | 7.516 | 7.517 |


| HD49933 |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m} \AA)$ |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m} \AA)$ |  | $\varepsilon_{\mathrm{Fe}}(\mathrm{dex})$ |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 4788.7568 | 26.200 | 0.82 | 24.949 | 28.096 | 7.072 | 992 |
| Fe I | 4789.6509 | 56.100 | 1.97 | 51.799 | 56.303 | 7.131 | 7.036 |
| Fe I | 4799.4058 | 6.000 | 0.31 | 6.568 | 7.628 | 6.997 | 6.924 |
| Fe I | 4872.1377 | 101.100 | 1.13 | 98.773 | 100.584 | 7.078 | 7.049 |
| Fe I | 4885.4302 | 32.400 | 0.33 | 35.739 | 39.754 | 6.964 | 6.877 |
| Fe I | 4892.8589 | 16.000 | 0.22 | 13.683 | 15.818 | 7.126 | 7.046 |
| Fe I | 4896.4385 | 7.300 | 0.29 | 7.154 | 8.299 | 7.050 | 6.976 |
| Fe I | 4903.3101 | 87.100 | 0.99 | 81.111 | 83.448 | 7.154 | 7.114 |
| Fe I | 4907.7319 | 20.100 | 0.83 | 21.578 | 24.410 | 6.998 | 6.921 |
| Fe I | 4917.2300 | 28.000 | 0.23 | 20.812 | 23.840 | 7.229 | 7.146 |
| Fe I | 4918.0127 | 20.300 | 0.74 | 14.210 | 16.409 | 7.240 | 7.163 |
| Fe I | 4938.8140 | 75.000 | 0.93 | 72.729 | 75.523 | 7.086 | 7.029 |
| Fe I | 4939.6865 | 50.100 | 0.84 | 45.822 | 49.969 | 7.136 | 7.043 |
| Fe I | 4950.1055 | 27.700 | 0.30 | 30.662 | 34.221 | 6.970 | 6.891 |
| Fe I | 4962.5718 | 18.200 | 0.30 | 17.886 | 20.465 | 7.050 | 6.971 |
| Fe I | 4967.8970 | 44.500 | 0.47 | 46.525 | 51.867 | 6.998 | 6.890 |
| Fe I | 4969.9175 | 39.800 | 0.32 | 35.104 | 39.621 | 7.143 | 7.044 |
| Fe I | 4985.2529 | 59.500 | 0.76 | 58.004 | 62.911 | 7.072 | 6.966 |
| Fe I | 4985.5469 | 59.600 | 0.76 | 60.738 | 64.137 | 7.016 | 6.942 |
| Fe I | 4986.2227 | 14.500 | 0.47 | 13.748 | 15.894 | 7.069 | 6.989 |
| Fe I | 4994.1294 | 60.200 | 1.22 | 56.726 | 60.670 | 7.121 | 7.029 |
| Fe I | 5001.8633 | 86.800 | 0.68 | 88.107 | 93.334 | 7.020 | 6.933 |
| Fe I | 5002.7920 | 33.000 | 0.29 | 32.893 | 36.548 | 7.042 | 6.961 |
| Fe I | 5014.9424 | 72.600 | 0.57 | 69.638 | 74.639 | 7.100 | 6.996 |
| Fe I | 5022.2354 | 59.900 | 0.62 | 59.482 | 64.444 | 7.049 | 6.942 |
| Fe I | 5028.1260 | 42.700 | 0.35 | 45.132 | 49.541 | 6.988 | 6.895 |
| Fe I | 5044.2109 | 25.500 | 0.39 | 27.657 | 30.902 | 6.986 | 6.909 |
| Fe I | 5048.4355 | 30.000 | 0.38 | 31.441 | 35.248 | 7.006 | 6.918 |
| Fe I | 5049.8198 | 87.200 | 0.80 | 81.128 | 84.596 | 7.171 | 7.098 |
| Fe I | 5067.1494 | 31.100 | 0.31 | 24.139 | 27.462 | 7.212 | 7.128 |
| Fe I | 5068.7656 | 75.200 | 0.49 | 72.289 | 75.066 | 7.098 | 7.043 |
| Fe I | 5072.6719 | 26.600 | 1.15 | 29.542 | 33.419 | 6.968 | 6.881 |
| Fe I | 5083.3384 | 65.900 | 0.64 | 60.753 | 64.425 | 7.162 | 7.075 |
| Fe I | 5088.1533 | 7.000 | 0.28 | 7.030 | 8.165 | 7.038 | 6.964 |
| Fe I | 5090.7729 | 50.900 | 0.30 | 46.552 | 51.782 | 7.129 | 7.022 |
| Fe I | 5104.4375 | 9.100 | 0.26 | 6.745 | 7.889 | 7.186 | 7.112 |
| Fe I | 5127.3594 | 48.300 | 0.55 | 45.523 | 49.643 | 7.102 | 7.010 |
| Fe I | 5133.6880 | 94.800 | 0.51 | 91.866 | 97.522 | 7.084 | 6.996 |
| Fe I | 5150.8394 | 57.800 | 0.45 | 56.506 | 60.434 | 7.070 | 6.979 |
| Fe I | 5151.9106 | 43.500 | 0.39 | 40.888 | 44.932 | 7.098 | 7.009 |
| Fe I | 5159.0576 | 30.800 | 0.40 | 28.009 | 31.974 | 7.107 | 7.013 |
| Fe I | 5162.2725 | 88.500 | 0.51 | 72.415 | 78.118 | 7.321 | 7.230 |
| Fe I | 5180.0557 | 12.700 | 0.21 | 11.673 | 13.733 | 7.084 | 6.998 |
| Fe I | 5187.9141 | 17.600 | 0.18 | 13.277 | 15.403 | 7.195 | 7.116 |
| Fe I | 5194.9414 | 79.700 | 1.02 | 77.538 | 81.192 | 7.092 | 7.003 |
| Fe I | 5195.4717 | 59.600 | 0.85 | 65.481 | 71.021 | 6.927 | 6.815 |
| Fe I | 5198.7109 | 48.400 | 0.71 | 48.276 | 52.531 | 7.043 | 6.953 |
| Fe I | 5215.1802 | 67.000 | 0.36 | 67.504 | 71.660 | 7.030 | 6.944 |
| Fe I | 5216.2739 | 76.600 | 0.53 | 73.215 | 76.987 | 7.122 | 7.031 |
| Fe I | 5217.3892 | 58.600 | 0.72 | 59.440 | 63.369 | 7.023 | 6.941 |
| Fe I | 5225.5259 | 15.900 | 0.51 | 13.683 | 16.155 | 7.122 | 7.031 |
| Fe I | 5228.3760 | 23.800 | 0.52 | 13.838 | 15.979 | 7.346 | 7.274 |
| Fe I | 5229.8447 | 69.700 | 0.42 | 61.265 | 65.735 | 7.207 | 7.122 |
| Fe I | 5232.9399 | 128.600 | 0.74 | 134.523 | 134.658 | 6.970 | 6.967 |
| Fe I | 5235.3867 | 37.400 | 0.32 | 33.576 | 37.811 | 7.127 | 7.031 |
| Fe I | 5242.4907 | 48.000 | 0.41 | 46.219 | 50.790 | 7.078 | 6.98 |
| Fe I | 5243.7764 | 21.900 | 0.28 | 20.177 | 23.165 | 7.090 | 7.005 |
| Fe I | 5250.6455 | 55.900 | 0.29 | 47.033 | 51.178 | 7.231 | 7.142 |
| Fe I | 5253.4619 | 29.000 | 0.23 | 31.933 | 35.679 | 6.972 | 6.889 |
| Fe I | 5263.3062 | 67.100 | 0.70 | 66.638 | 70.741 | 7.049 | 6.965 |
| Fe I | 5267.2695 | 5.400 | 0.35 | 5.747 | 6.737 | 7.011 | 6.934 |
| Fe I | 5281.7896 | 80.700 | 0.38 | 79.707 | 82.088 | 7.058 | 7.012 |
| Fe I | 5288.5249 | 16.800 | 0.34 | 21.093 | 24.134 | 6.909 | 6.829 |
| Fe I | 5307.3608 | 38.600 | 0.33 | 36.093 | 40.059 | 7.096 | 7.008 |
| Fe I | 5315.0698 | 8.000 | 0.26 | 6.299 | 7.376 | 7.156 | 7.080 |
| Fe I | 5322.0405 | 14.900 | 0.30 | 17.481 | 20.001 | 6.951 | 6.874 |
| Fe I | 5324.1787 | 113.900 | 0.37 | 114.694 | 116.915 | 7.030 | 6.998 |
| Fe I | 5326.1426 | 7.100 | 0.26 | 8.567 | 10.008 | 6.949 | 6.871 |
| Fe I | 5339.9292 | 79.600 | 0.43 | 79.687 | 83.007 | 7.038 | 6.973 |
| Fe I | 5364.8711 | 77.900 | 0.28 | 72.171 | 79.483 | 7.139 | 7.012 |
| Fe I | 5373.7085 | 25.400 | 0.24 | 26.026 | 30.018 | 7.024 | 6.927 |
| Fe I | 5379.5737 | 19.500 | 0.33 | 20.426 | 23.397 | 7.012 | 6.929 |
| FeI | 5389.4790 | 42.800 | 0.29 | 41.530 | 46.874 | 7.067 | 6.956 |
| Fe I | 5393.1670 | 76.100 | 0.25 | 76.292 | 79.720 | 7.036 | 6.967 |
| Fe I | 5398.2793 | 32.000 | 0.32 | 30.388 | 34.769 | 7.078 | 6.978 |
| Fe I | 5400.5010 | 61.800 | 0.34 | 55.273 | 61.346 | 7.167 | 7.049 |
| Fe I | 5405.7744 | 117.400 | 0.66 | 108.990 | 110.875 | 7.209 | 7.172 |


| HD49933 |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m} \AA)$ |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m}$ ) |  | $\varepsilon_{\mathrm{Fe}}$ (dex) |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 5409.1333 | 16.700 | 0.55 | 12.944 | 15.069 | 7.179 | 7.098 |
| Fe I | 5410.9097 | 79.200 | 1.06 | 80.402 | 88.451 | 7.020 | 6.883 |
| Fe I | 5417.0332 | 6.200 | 0.21 | 5.508 | 6.495 | 7.096 | 7.017 |
| Fe I | 5424.0679 | 105.300 | 0.74 | 95.011 | 101.943 | 7.182 | 7.089 |
| Fe I | 5434.5234 | 101.700 | 0.42 | 95.094 | 97.833 | 7.190 | 7.129 |
| Fe I | 5436.2949 | 11.000 | 0.69 | 7.814 | 9.161 | 7.210 | 7.134 |
| Fe I | 5445.0420 | 68.700 | 0.24 | 61.715 | 68.043 | 7.171 | 7.053 |
| Fe I | 5463.2754 | 64.100 | 0.54 | 64.442 | 70.971 | 7.034 | 6.909 |
| Fe I | 5466.3960 | 37.400 | 0.19 | 33.278 | 37.730 | 7.131 | 7.033 |
| Fe I | 5466.9873 | 7.700 | 0.24 | 6.152 | 7.221 | 7.148 | 7.072 |
| Fe I | 5472.7085 | 10.000 | 0.23 | 9.397 | 11.029 | 7.071 | 6.989 |
| Fe I | 5473.9004 | 37.900 | 0.21 | 37.017 | 41.499 | 7.060 | 6.961 |
| Fe I | 5483.0986 | 12.200 | 0.43 | 12.699 | 14.732 | 7.019 | 6.938 |
| Fe I | 5487.1450 | 6.700 | 0.36 | 7.595 | 8.914 | 6.980 | 6.900 |
| Fe I | 5501.4648 | 63.200 | 0.33 | 57.069 | 60.971 | 7.180 | 7.091 |
| Fe I | 5506.7788 | 74.000 | 0.48 | 66.981 | 70.730 | 7.207 | 7.119 |
| Fe I | 5522.4463 | 10.200 | 0.36 | 10.314 | 12.077 | 7.034 | 6.952 |
| Fe I | 5543.1470 | 23.900 | 0.31 | 18.440 | 21.293 | 7.199 | 7.114 |
| Fe I | 5543.9355 | 22.500 | 0.26 | 21.605 | 24.891 | 7.065 | 6.975 |
| Fe I | 5546.5059 | 15.700 | 0.31 | 12.758 | 14.835 | 7.153 | 7.072 |
| Fe I | 5553.5771 | 12.700 | 0.23 | 9.412 | 11.047 | 7.193 | 7.114 |
| Fe I | 5554.8945 | 42.500 | 0.39 | 42.672 | 48.712 | 7.036 | 6.915 |
| Fe I | 5560.2114 | 17.100 | 0.30 | 14.444 | 16.854 | 7.134 | 7.048 |
| Fe I | 5567.3911 | 14.000 | 0.25 | 16.271 | 18.724 | 6.958 | 6.879 |
| Fe I | 5569.6182 | 78.200 | 0.30 | 79.662 | 83.591 | 7.014 | 6.937 |
| Fe I | 5572.8423 | 98.000 | 1.54 | 93.725 | 97.225 | 7.105 | 7.053 |
| Fe I | 5576.0889 | 60.800 | 0.21 | 58.938 | 63.648 | 7.076 | 6.982 |
| Fe I | 5586.7554 | 103.100 | 0.63 | 107.512 | 109.930 | 6.979 | 6.936 |
| Fe I | 5600.2241 | 10.700 | 0.40 | 10.058 | 11.805 | 7.072 | 6.988 |
| Fe I | 5615.6440 | 118.600 | 3.19 | 121.160 | 123.005 | 7.009 | 6.983 |
| Fe I | 5618.6323 | 15.600 | 0.25 | 15.082 | 17.497 | 7.059 | 6.975 |
| Fe I | 5619.5952 | 7.700 | 0.25 | 5.628 | 6.613 | 7.190 | 7.115 |
| Fe I | 5638.2622 | 33.500 | 0.35 | 34.589 | 38.995 | 7.015 | 6.917 |
| Fe I | 5641.4341 | 20.600 | 0.22 | 19.166 | 22.183 | 7.083 | 6.994 |
| Fe I | 5650.7056 | 8.700 | 0.32 | 7.512 | 9.286 | 7.113 | 7.007 |
| Fe I | 5653.8652 | 8.300 | 0.26 | 5.202 | 6.127 | 7.262 | 7.189 |
| Fe I | 5662.5161 | 48.100 | 0.36 | 51.260 | 56.516 | 6.980 | 6.879 |
| Fe I | 5667.5181 | 13.200 | 0.38 | 8.517 | 9.996 | 7.262 | 7.186 |
| Fe I | 5679.0229 | 20.300 | 0.26 | 16.873 | 19.921 | 7.148 | 7.051 |
| Fe I | 5691.4971 | 8.600 | 0.29 | 8.858 | 10.446 | 7.025 | 6.941 |
| Fe I | 5701.5444 | 32.200 | 0.22 | 32.369 | 36.166 | 7.036 | 6.950 |
| Fe I | 5717.8325 | 22.600 | 0.28 | 21.540 | 24.787 | 7.070 | 6.980 |
| Fe I | 5731.7617 | 17.800 | 0.30 | 15.598 | 18.074 | 7.115 | 7.031 |
| Fe I | 5741.8477 | 6.400 | 0.26 | 6.097 | 7.165 | 7.063 | 6.985 |
| Fe II | 4893.8125 | 10.700 | 0.22 | 7.785 | 7.769 | 7.200 | 7.202 |
| Fe II | 4993.3501 | 31.200 | 1.18 | 32.266 | 32.234 | 7.015 | 7.016 |
| Fe II | 5100.6548 | 15.900 | 0.61 | 13.660 | 13.633 | 7.124 | 7.125 |
| Fe II | 5132.6611 | 16.000 | 0.35 | 16.626 | 16.593 | 7.018 | 7.019 |
| Fe II | 5197.5674 | 88.200 | 0.67 | 88.966 | 88.877 | 7.023 | 7.025 |
| Fe II | 5234.6226 | 93.500 | 0.75 | 85.000 | 84.915 | 7.234 | 7.235 |
| Fe II | 5256.9321 | 11.900 | 0.31 | 12.374 | 12.349 | 7.019 | 7.020 |
| Fe II | 5264.8022 | 45.100 | 0.75 | 41.750 | 41.708 | 7.114 | 7.115 |
| Fe II | 5284.1030 | 58.700 | 0.23 | 52.698 | 52.645 | 7.172 | 7.174 |
| Fe II | 5325.5522 | 39.700 | 0.27 | 40.778 | 40.737 | 7.016 | 7.017 |
| Fe II | 5414.0698 | 21.000 | 0.25 | 22.477 | 22.432 | 6.998 | 6.999 |
| Fe II | 5425.2485 | 35.900 | 0.22 | 38.965 | 38.926 | 6.971 | 6.972 |
| Fe II | 5534.8379 | 59.200 | 0.32 | 54.287 | 54.233 | 7.148 | 7.150 |
| Fe II | 5627.4888 | 6.700 | 0.29 | 6.347 | 6.334 | 7.066 | 7.067 |
|  |  |  |  |  |  |  |  |
| Arcturus |  |  |  |  |  |  |  |
|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m} \AA)$ |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m}$ ) |  | $\varepsilon_{\mathrm{Fe}}$ (dex) |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 4787.8267 | 86.000 | 3.18 | 79.676 | 82.395 | 7.081 | 7.020 |
| Fe I | 4793.9614 | 35.000 | 1.41 | 37.414 | 40.712 | 6.879 | 6.809 |
| Fe I | 4794.3540 | 52.500 | 2.00 | 53.288 | 57.115 | 6.914 | 6.837 |
| Fe I | 4802.8799 | 88.500 | 3.30 | 88.628 | 91.653 | 6.927 | 6.850 |
| Fe I | 4808.1479 | 63.100 | 2.39 | 60.846 | 64.251 | 6.978 | 6.905 |
| Fe I | 4809.9385 | 41.100 | 3.04 | 43.589 | 46.971 | 6.878 | 6.807 |
| Fe I | 4869.4634 | 55.900 | 2.85 | 50.149 | 53.578 | 7.049 | 6.979 |
| Fe I | 4873.7510 | 37.300 | 2.79 | 44.613 | 48.126 | 6.779 | 6.708 |
| Fe I | 4874.3530 | 57.500 | 3.17 | 53.237 | 56.756 | 7.018 | 6.946 |
| Fe I | 4885.4302 | 97.000 | 4.35 | 99.810 | 101.951 | 6.867 | 6.809 |
| Fe I | 4892.8589 | 74.700 | 7.62 | 66.937 | 71.210 | 7.093 | 7.009 |
| Fe I | 4896.4385 | 62.400 | 2.22 | 59.604 | 62.873 | 6.990 | 6.919 |
| Fe I | 4905.1328 | 63.200 | 1.18 | 64.198 | 67.719 | 6.908 | 6.828 |
| Fe I | 4918.0127 | 70.300 | 2.28 | 67.651 | 71.893 | 6.986 | 6.895 |

Arcturus

|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m} \AA)$ |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m} \AA)$ |  | $\varepsilon_{\mathrm{Fe}}$ (dex) |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 4961.9136 | 62.700 | 1.73 | 61.240 | 64.667 | 6.961 | 6.887 |
| Fe I | 4962.5718 | 75.300 | 1.82 | 75.173 | 78.551 | 6.933 | 6.856 |
| Fe I | 4969.9175 | 98.900 | 3.01 | 91.839 | 96.368 | 7.084 | 6.990 |
| Fe I | 4979.5859 | 44.700 | 1.59 | 37.020 | 40.371 | 7.084 | 7.018 |
| Fe I | 4986.2227 | 67.500 | 1.47 | 67.592 | 71.602 | 6.928 | 6.839 |
| Fe I | 4999.1123 | 50.000 | 3.03 | 52.727 | 56.513 | 6.873 | 6.791 |
| Fe I | 5029.6177 | 89.400 | 3.92 | 84.737 | 87.901 | 7.040 | 6.967 |
| Fe I | 5031.9141 | 43.200 | 1.42 | 44.412 | 48.485 | 6.904 | 6.818 |
| Fe I | 5036.9214 | 64.800 | 2.47 | 61.378 | 64.950 | 7.002 | 6.927 |
| Fe I | 5048.4355 | 92.100 | 4.79 | 94.554 | 97.278 | 6.875 | 6.803 |
| Fe I | 5072.6719 | 90.500 | 3.44 | 87.788 | 90.972 | 6.989 | 6.919 |
| Fe I | 5088.1533 | 56.600 | 2.71 | 53.487 | 57.022 | 6.994 | 6.921 |
| Fe I | 5115.7769 | 37.800 | 3.50 | 43.473 | 46.998 | 6.813 | 6.740 |
| Fe I | 5143.7227 | 83.300 | 2.97 | 81.928 | 85.520 | 6.961 | 6.878 |
| Fe I | 5196.0591 | 98.300 | 2.36 | 102.314 | 106.800 | 6.851 | 6.750 |
| Fe I | 5243.7764 | 82.400 | 2.07 | 76.968 | 80.426 | 7.046 | 6.975 |
| Fe I | 5253.0210 | 70.100 | 2.14 | 66.049 | 69.967 | 7.013 | 6.933 |
| Fe I | 5267.2695 | 46.400 | 2.99 | 43.751 | 47.607 | 6.985 | 6.905 |
| Fe I | 5285.1274 | 38.200 | 2.15 | 36.711 | 40.431 | 6.962 | 6.882 |
| Fe I | 5288.5249 | 89.500 | 2.37 | 90.028 | 93.197 | 6.918 | 6.842 |
| Fe I | 5293.9590 | 49.000 | 1.51 | 49.887 | 53.816 | 6.912 | 6.830 |
| Fe I | 5294.5474 | 33.300 | 1.14 | 33.866 | 37.215 | 6.918 | 6.846 |
| Fe I | 5295.3120 | 40.500 | 2.06 | 41.231 | 45.160 | 6.915 | 6.831 |
| Fe I | 5315.0698 | 50.900 | 0.94 | 46.108 | 49.954 | 7.026 | 6.949 |
| Fe I | 5320.0356 | 48.000 | 0.80 | 44.618 | 48.340 | 6.997 | 6.923 |
| Fe I | 5326.1426 | 72.800 | 0.80 | 71.690 | 75.305 | 6.954 | 6.874 |
| Fe I | 5373.7085 | 79.200 | 1.54 | 79.264 | 83.789 | 6.929 | 6.827 |
| Fe I | 5379.5737 | 88.700 | 1.81 | 89.680 | 92.933 | 6.908 | 6.830 |
| Fe I | 5389.4790 | 99.500 | 1.73 | 96.893 | 100.930 | 6.983 | 6.898 |
| Fe I | 5398.2793 | 86.500 | 1.32 | 84.784 | 89.246 | 6.966 | 6.869 |
| Fe I | 5412.7837 | 34.700 | 1.32 | 34.399 | 37.968 | 6.937 | 6.859 |
| Fe I | 5417.0332 | 46.400 | 1.40 | 41.998 | 45.950 | 7.019 | 6.939 |
| Fe I | 5436.2949 | 56.600 | 2.06 | 51.032 | 54.932 | 7.040 | 6.964 |
| Fe I | 5441.3389 | 46.500 | 1.20 | 46.486 | 50.201 | 6.930 | 6.854 |
| Fe I | 5452.0884 | 31.300 | 1.92 | 32.049 | 35.296 | 6.914 | 6.843 |
| Fe I | 5460.8726 | 31.000 | 0.63 | 38.048 | 41.674 | 6.782 | 6.709 |
| Fe I | 5466.3960 | 97.200 | 1.38 | 91.552 | 94.971 | 7.041 | 6.978 |
| Fe I | 5466.9873 | 64.400 | 1.02 | 64.645 | 68.407 | 6.925 | 6.844 |
| Fe I | 5470.0928 | 38.700 | 1.32 | 33.901 | 37.668 | 7.031 | 6.952 |
| Fe I | 5473.1626 | 34.600 | 2.55 | 34.209 | 37.634 | 6.938 | 6.865 |
| Fe I | 5473.9004 | 98.600 | 2.69 | 99.502 | 101.636 | 6.911 | 6.860 |
| Fe I | 5483.0986 | 70.200 | 1.30 | 68.845 | 72.392 | 6.957 | 6.884 |
| Fe I | 5522.4463 | 61.000 | 0.71 | 62.071 | 65.684 | 6.909 | 6.831 |
| Fe I | 5524.2495 | 8.100 | 0.56 | 9.137 | 10.359 | 6.871 | 6.807 |
| Fe I | 5539.2798 | 41.200 | 0.48 | 43.964 | 47.683 | 6.874 | 6.799 |
| Fe I | 5543.9355 | 82.200 | 0.97 | 80.868 | 84.150 | 6.957 | 6.886 |
| Fe I | 5546.5059 | 71.400 | 1.69 | 63.325 | 67.082 | 7.093 | 7.022 |
| Fe I | 5549.9487 | 28.000 | 0.60 | 24.349 | 27.115 | 7.017 | 6.951 |
| Fe I | 5552.6919 | 8.700 | 0.65 | 7.299 | 9.147 | 7.016 | 6.905 |
| Fe I | 5560.2114 | 65.100 | 0.95 | 65.316 | 69.338 | 6.926 | 6.840 |
| Fe I | 5577.0249 | 12.200 | 0.66 | 11.944 | 14.986 | 6.941 | 6.819 |
| Fe I | 5584.7646 | 71.600 | 0.94 | 74.095 | 77.831 | 6.878 | 6.796 |
| Fe I | 5587.5742 | 59.600 | 0.91 | 51.586 | 55.529 | 7.087 | 7.013 |
| Fe I | 5600.2241 | 60.000 | 0.94 | 60.222 | 64.066 | 6.926 | 6.845 |
| Fe I | 5618.6323 | 68.800 | 0.70 | 71.580 | 75.110 | 6.874 | 6.793 |
| Fe I | 5622.9453 | 22.000 | 0.55 | 20.096 | 22.580 | 6.982 | 6.914 |
| Fe I | 5636.6958 | 44.300 | 0.41 | 46.867 | 50.667 | 6.879 | 6.802 |
| Fe I | 5638.2622 | 96.500 | 1.31 | 96.570 | 98.742 | 6.929 | 6.879 |
| Fe I | 5651.4688 | 28.900 | 0.43 | 24.556 | 27.406 | 7.035 | 6.966 |
| Fe I | 5652.3174 | 41.700 | 0.55 | 39.179 | 42.679 | 6.981 | 6.910 |
| Fe I | 5661.3447 | 39.700 | 0.86 | 42.166 | 45.833 | 6.879 | 6.802 |
| Fe I | 5662.5161 | 111.800 | 2.57 | 116.721 | 118.982 | 6.844 | 6.793 |
| Fe I | 5679.0229 | 68.000 | 0.64 | 63.313 | 68.669 | 7.024 | 6.916 |
| Fe I | 5691.4971 | 60.100 | 2.36 | 56.029 | 60.117 | 7.010 | 6.930 |
| Fe I | 5717.8325 | 78.900 | 1.76 | 79.564 | 83.139 | 6.917 | 6.836 |
| Fe I | 5731.7617 | 78.400 | 1.71 | 72.118 | 75.123 | 7.055 | 7.001 |
| Fe I | 5741.8477 | 47.900 | 0.44 | 48.363 | 52.059 | 6.921 | 6.845 |
| Fe I | 5742.9600 | 23.900 | 1.82 | 19.880 | 22.262 | 7.038 | 6.973 |
| Fe I | 5754.4023 | 41.600 | 3.26 | 42.432 | 46.172 | 6.913 | 6.838 |
| Fe I | 5759.2622 | 9.300 | 0.69 | 8.940 | 10.300 | 6.949 | 6.878 |
| Fe I | 5760.3438 | 47.200 | 1.57 | 53.152 | 57.091 | 6.813 | 6.734 |
| Fe I | 5838.3716 | 44.100 | 0.87 | 41.035 | 44.410 | 6.991 | 6.924 |
| Fe I | 5849.6831 | 24.500 | 0.62 | 21.628 | 24.247 | 7.004 | 6.936 |
| Fe I | 5853.1484 | 66.200 | 2.56 | 60.917 | 65.927 | 7.026 | 6.935 |
| Fe I | 5855.0757 | 36.300 | 0.92 | 35.331 | 39.213 | 6.951 | 6.867 |
| Fe I | 5858.7778 | 28.400 | 0.89 | 27.530 | 30.521 | 6.951 | 6.880 |
| Fe I | 5859.5864 | 93.200 | 1.90 | 90.694 | 94.670 | 6.978 | 6.899 |
| Fe I | 5861.1084 | 18.100 | 0.36 | 18.972 | 21.269 | 6.903 | 6.835 |
| Fe I | 5862.3564 | 103.900 | 2.73 | 105.286 | 108.879 | 6.904 | 6.827 |
| Fe I | 5883.8164 | 93.000 | 2.30 | 90.113 | 92.329 | 6.987 | 6.944 |

## Arcturus

|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m} \AA)$ |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m} \AA)$ |  | $\varepsilon_{\mathrm{Fe}}(\mathrm{dex})$ |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 5898.2153 | 20.100 | 0.63 | 18.502 | 21.218 | 6.978 | 6.897 |
| Fe I | 5905.6714 | 71.700 | 0.91 | 69.594 | 75.318 | 6.971 | 6.853 |
| Fe I | 5927.7886 | 57.200 | 0.90 | 55.605 | 61.037 | 6.961 | 6.852 |
| Fe I | 5934.6543 | 109.500 | 2.51 | 102.964 | 103.899 | 7.055 | 7.046 |
| Fe I | 5940.9912 | 41.000 | 1.29 | 35.150 | 38.499 | 7.049 | 6.982 |
| Fe I | 5952.7178 | 91.000 | 2.45 | 84.851 | 87.206 | 7.051 | 7.011 |
| Fe I | 5976.7769 | 97.400 | 2.19 | 93.392 | 94.718 | 7.007 | 6.987 |
| Fe I | 6007.9595 | 77.700 | 1.57 | 75.636 | 80.550 | 6.969 | 6.871 |
| Fe I | 6027.0508 | 95.700 | 2.27 | 89.910 | 93.852 | 7.044 | 6.969 |
| Fe I | 6034.0352 | 19.400 | 0.79 | 17.687 | 19.851 | 6.982 | 6.917 |
| Fe I | 6054.0732 | 19.500 | 0.41 | 14.769 | 16.632 | 7.080 | 7.019 |
| Fe I | 6056.0044 | 84.400 | 1.13 | 83.212 | 88.712 | 6.953 | 6.839 |
| Fe I | 6078.4912 | 86.200 | 1.22 | 78.556 | 84.834 | 7.076 | 6.958 |
| Fe I | 6079.0078 | 61.200 | 0.90 | 55.130 | 59.729 | 7.045 | 6.959 |
| Fe I | 6093.6431 | 44.800 | 0.57 | 39.065 | 43.357 | 7.046 | 6.960 |
| Fe I | 6096.6641 | 65.400 | 0.87 | 60.480 | 63.529 | 7.023 | 6.968 |
| Fe I | 6120.2466 | 68.800 | 1.84 | 62.532 | 68.416 | 7.039 | 6.937 |
| Fe I | 6127.9063 | 75.600 | 1.68 | 70.401 | 74.656 | 7.031 | 6.949 |
| Fe I | 6151.6172 | 118.400 | 2.88 | 110.305 | 115.261 | 7.088 | 6.993 |
| Fe I | 6165.3599 | 70.900 | 1.30 | 66.753 | 71.014 | 7.010 | 6.928 |
| Fe I | 6180.2026 | 114.600 | 2.26 | 107.529 | 111.660 | 7.069 | 6.989 |
| Fe I | 6187.3979 | 23.800 | 0.54 | 21.445 | 24.150 | 6.990 | 6.921 |
| Fe I | 6187.9893 | 77.200 | 1.17 | 74.601 | 77.227 | 6.979 | 6.929 |
| Fe I | 6199.5063 | 29.800 | 1.60 | 24.760 | 27.852 | 7.043 | 6.973 |
| Fe I | 6226.7344 | 52.800 | 0.46 | 52.172 | 55.680 | 6.942 | 6.874 |
| Fe I | 6229.2261 | 87.700 | 1.40 | 88.795 | 92.785 | 6.908 | 6.825 |
| Fe I | 6232.6401 | 117.500 | 2.24 | 113.899 | 116.342 | 6.996 | 6.953 |
| Fe I | 6240.6460 | 114.100 | 4.15 | 108.994 | 113.535 | 7.039 | 6.942 |
| Fe I | 6270.2236 | 103.900 | 2.57 | 104.528 | 108.432 | 6.917 | 6.836 |
| Fe I | 6271.2778 | 59.500 | 0.95 | 60.033 | 64.413 | 6.920 | 6.836 |
| Fe I | 5638.2622 | 96.500 | 1.31 | 96.570 | 98.742 | 6.929 | 6.879 |
| Fe I | 5651.4688 | 28.900 | 0.43 | 24.556 | 27.406 | 7.035 | 6.966 |
| Fe I | 5652.3174 | 41.700 | 0.55 | 39.179 | 42.679 | 6.981 | 6.910 |
| Fe I | 5661.3447 | 39.700 | 0.86 | 42.166 | 45.833 | 6.879 | 6.802 |
| Fe I | 5662.5161 | 111.800 | 2.57 | 116.721 | 118.982 | 6.844 | 6.793 |
| Fe I | 5679.0229 | 68.000 | 0.64 | 63.313 | 68.669 | 7.024 | 6.916 |
| Fe I | 5691.4971 | 60.100 | 2.36 | 56.029 | 60.117 | 7.010 | 6.930 |
| Fe I | 5717.8325 | 78.900 | 1.76 | 79.564 | 83.139 | 6.917 | 6.836 |
| Fe I | 5731.7617 | 78.400 | 1.71 | 72.118 | 75.123 | 7.055 | 7.001 |
| Fe I | 5741.8477 | 47.900 | 0.44 | 48.363 | 52.059 | 6.921 | 6.845 |
| Fe I | 5742.9600 | 23.900 | 1.82 | 19.880 | 22.262 | 7.038 | 6.973 |
| Fe I | 5754.4023 | 41.600 | 3.26 | 42.432 | 46.172 | 6.913 | 6.838 |
| Fe I | 5759.2622 | 9.300 | 0.69 | 8.940 | 10.300 | 6.949 | 6.878 |
| Fe I | 5760.3438 | 47.200 | 1.57 | 53.152 | 57.091 | 6.813 | 6.734 |
| Fe I | 5838.3716 | 44.100 | 0.87 | 41.035 | 44.410 | 6.991 | 6.924 |
| Fe I | 5849.6831 | 24.500 | 0.62 | 21.628 | 24.247 | 7.004 | 6.936 |
| Fe I | 5853.1484 | 66.200 | 2.56 | 60.917 | 65.927 | 7.026 | 6.935 |
| Fe I | 5855.0757 | 36.300 | 0.92 | 35.331 | 39.213 | 6.951 | 6.867 |
| Fe I | 5858.7778 | 28.400 | 0.89 | 27.530 | 30.521 | 6.951 | 6.880 |
| Fe I | 5859.5864 | 93.200 | 1.90 | 90.694 | 94.670 | 6.978 | 6.899 |
| Fe I | 5861.1084 | 18.100 | 0.36 | 18.972 | 21.269 | 6.903 | 6.835 |
| Fe I | 5862.3564 | 103.900 | 2.73 | 105.286 | 108.879 | 6.904 | 6.827 |
| Fe I | 5883.8164 | 93.000 | 2.30 | 90.113 | 92.329 | 6.987 | 6.944 |
| Fe I | 5898.2153 | 20.100 | 0.63 | 18.502 | 21.218 | 6.978 | 6.897 |
| Fe I | 5905.6714 | 71.700 | 0.91 | 69.594 | 75.318 | 6.971 | 6.853 |
| Fe I | 5927.7886 | 57.200 | 0.90 | 55.605 | 61.037 | 6.961 | 6.852 |
| Fe I | 5934.6543 | 109.500 | 2.51 | 102.964 | 103.899 | 7.055 | 7.046 |
| Fe I | 5940.9912 | 41.000 | 1.29 | 35.150 | 38.499 | 7.049 | 6.982 |
| Fe I | 5952.7178 | 91.000 | 2.45 | 84.851 | 87.206 | 7.051 | 7.011 |
| Fe I | 5976.7769 | 97.400 | 2.19 | 93.392 | 94.718 | 7.007 | 6.987 |
| Fe I | 6007.9595 | 77.700 | 1.57 | 75.636 | 80.550 | 6.969 | 6.871 |
| Fe I | 6027.0508 | 95.700 | 2.27 | 89.910 | 93.852 | 7.044 | 6.969 |
| Fe I | 6034.0352 | 19.400 | 0.79 | 17.687 | 19.851 | 6.982 | 6.917 |
| Fe I | 6054.0732 | 19.500 | 0.41 | 14.769 | 16.632 | 7.080 | 7.019 |
| Fe I | 6056.0044 | 84.400 | 1.13 | 83.212 | 88.712 | 6.953 | 6.839 |
| Fe I | 6078.4912 | 86.200 | 1.22 | 78.556 | 84.834 | 7.076 | 6.958 |
| Fe I | 6079.0078 | 61.200 | 0.90 | 55.130 | 59.729 | 7.045 | 6.959 |
| Fe I | 6093.6431 | 44.800 | 0.57 | 39.065 | 43.357 | 7.046 | 6.960 |
| Fe I | 6096.6641 | 65.400 | 0.87 | 60.480 | 63.529 | 7.023 | 6.968 |
| Fe I | 6120.2466 | 68.800 | 1.84 | 62.532 | 68.416 | 7.039 | 6.937 |
| Fe I | 6127.9063 | 75.600 | 1.68 | 70.401 | 74.656 | 7.031 | 6.949 |
| Fe I | 6151.6172 | 118.400 | 2.88 | 110.305 | 115.261 | 7.088 | 6.993 |
| Fe I | 6165.3599 | 70.900 | 1.30 | 66.753 | 71.014 | 7.010 | 6.928 |
| Fe I | 6180.2026 | 114.600 | 2.26 | 107.529 | 111.660 | 7.069 | 6.989 |
| Fe I | 6187.3979 | 23.800 | 0.54 | 21.445 | 24.150 | 6.990 | 6.921 |
| Fe I | 6187.9893 | 77.200 | 1.17 | 74.601 | 77.227 | 6.979 | 6.929 |
| Fe I | 6199.5063 | 29.800 | 1.60 | 24.760 | 27.852 | 7.043 | 6.973 |
| Fe I | 6226.7344 | 52.800 | 0.46 | 52.172 | 55.680 | 6.942 | 6.874 |
| Fe I | 6229.2261 | 87.700 | 1.40 | 88.795 | 92.785 | 6.908 | 6.825 |


| Arcturus |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m}$ ) |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m}$ ) |  | $\varepsilon_{\mathrm{Fe}}$ (dex) |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 6232.6401 | 117.500 | 2.24 | 113.899 | 116.342 | 6.996 | 6.953 |
| Fe I | 6240.6460 | 114.100 | 4.15 | 108.994 | 113.535 | 7.039 | 6.942 |
| Fe I | 6270.2236 | 103.900 | 2.57 | 104.528 | 108.432 | 6.917 | 6.836 |
| Fe I | 6271.2778 | 59.500 | 0.95 | 60.033 | 64.413 | 6.920 | 6.836 |
| Fe I | 6311.4995 | 80.000 | 0.94 | 73.235 | 77.415 | 7.060 | 6.981 |
| Fe I | 6315.8110 | 68.700 | 2.72 | 63.703 | 67.841 | 7.026 | 6.947 |
| Fe I | 6338.8760 | 53.700 | 1.68 | 47.931 | 53.257 | 7.042 | 6.939 |
| Fe I | 6380.7432 | 77.600 | 1.50 | 69.042 | 73.527 | 7.092 | 7.012 |
| Fe I | 6408.0176 | 124.100 | 3.11 | 125.523 | 128.085 | 6.906 | 6.857 |
| Fe I | 6495.7412 | 53.300 | 2.00 | 51.564 | 57.357 | 6.963 | 6.849 |
| Fe I | 6518.3657 | 111.400 | 2.45 | 111.741 | 116.155 | 6.924 | 6.842 |
| Fe I | 6533.9282 | 51.800 | 0.82 | 44.975 | 49.261 | 7.059 | 6.980 |
| Fe I | 6581.2090 | 97.000 | 1.10 | 91.500 | 97.444 | 7.036 | 6.921 |
| Fe I | 6591.3130 | 17.200 | 0.39 | 14.410 | 16.525 | 7.025 | 6.952 |
| Fe I | 6597.5591 | 52.300 | 0.50 | 48.694 | 53.451 | 6.999 | 6.907 |
| Fe I | 6608.0249 | 75.700 | 1.99 | 73.155 | 78.157 | 6.977 | 6.885 |
| Fe I | 6627.5439 | 41.800 | 0.31 | 34.885 | 38.293 | 7.069 | 7.002 |
| Fe I | 6633.7485 | 81.100 | 1.17 | 74.731 | 78.830 | 7.043 | 6.974 |
| Fe I | 6699.1411 | 15.000 | 0.21 | 13.503 | 15.503 | 6.985 | 6.912 |
| Fe I | 6703.5659 | 90.300 | 1.50 | 84.348 | 88.787 | 7.044 | 6.960 |
| Fe I | 6710.3179 | 92.400 | 1.75 | 87.900 | 93.910 | 7.015 | 6.901 |
| Fe I | 6732.0649 | 14.200 | 0.39 | 16.048 | 18.341 | 6.864 | 6.787 |
| Fe I | 6733.1504 | 38.200 | 0.35 | 50.127 | 54.605 | 6.697 | 6.604 |
| Fe I | 6739.5205 | 75.900 | 1.16 | 81.016 | 86.834 | 6.837 | 6.731 |
| Fe I | 6746.9536 | 26.900 | 0.12 | 28.562 | 32.056 | 6.893 | 6.817 |
| Fe I | 6786.8584 | 43.800 | 0.74 | 40.084 | 43.381 | 7.002 | 6.938 |
| Fe I | 6804.2710 | 25.000 | 0.69 | 23.096 | 26.097 | 6.979 | 6.902 |
| Fe II | 4993.3501 | 46.700 | 2.21 | 46.386 | 44.135 | 6.938 | 6.997 |
| Fe II | 5234.6226 | 78.200 | 1.06 | 87.000 | 82.700 | 6.714 | 6.816 |
| Fe II | 5256.9321 | 22.500 | 0.91 | 23.455 | 22.359 | 6.899 | 6.935 |
| Fe II | 5264.8022 | 42.100 | 0.88 | 46.712 | 44.488 | 6.810 | 6.865 |
| Fe II | 5284.1030 | 61.900 | 2.53 | 61.942 | 58.546 | 6.929 | 7.014 |
| Fe II | 5325.5522 | 40.900 | 0.64 | 45.798 | 43.576 | 6.802 | 6.857 |
| Fe II | 5414.0698 | 21.600 | 0.87 | 29.769 | 28.433 | 6.670 | 6.704 |
| Fe II | 5425.2485 | 36.100 | 1.19 | 44.231 | 42.005 | 6.715 | 6.766 |
| Fe II | 6084.1016 | 22.900 | 0.60 | 19.637 | 18.596 | 7.043 | 7.084 |
| Fe II | 6238.3857 | 33.700 | 0.98 | 33.112 | 31.505 | 6.947 | 6.997 |
| Fe II | 6247.5571 | 38.200 | 0.45 | 38.918 | 36.924 | 6.910 | 6.967 |
| Fe II | 6369.4590 | 19.200 | 0.39 | 23.721 | 22.148 | 6.777 | 6.825 |
| Fe II | 6456.3794 | 48.100 | 0.75 | 47.714 | 44.971 | 6.940 | 7.012 |
| Fe II | 6516.0767 | 52.900 | 0.61 | 55.906 | 51.574 | 6.862 | 6.962 |


| $\mu$ Leo |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m} \AA)$ |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m} \AA)$ |  | $\varepsilon_{\mathrm{Fe}}$ (dex) |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 4793.9614 | 57.100 | 1.44 | 57.476 | 58.470 | 7.692 | 7.669 |
| Fe I | 4794.3540 | 76.200 | 1.99 | 70.507 | 71.726 | 7.828 | 7.802 |
| Fe I | 4802.5234 | 45.600 | 2.63 | 38.213 | 40.014 | 7.864 | 7.821 |
| Fe I | 4802.8799 | 101.700 | 3.18 | 108.419 | 109.073 | 7.546 | 7.526 |
| Fe I | 4808.1479 | 77.900 | 2.73 | 79.418 | 80.301 | 7.664 | 7.641 |
| Fe I | 4809.9385 | 61.000 | 3.65 | 65.081 | 66.005 | 7.607 | 7.584 |
| Fe I | 4874.3530 | 69.000 | 4.58 | 71.826 | 72.772 | 7.633 | 7.609 |
| Fe I | 4875.8770 | 109.200 | 2.46 | 112.334 | 112.446 | 7.633 | 7.628 |
| Fe I | 4892.8589 | 92.700 | 3.56 | 91.748 | 92.675 | 7.720 | 7.701 |
| Fe I | 4907.7319 | 115.100 | 2.19 | 117.355 | 117.121 | 7.654 | 7.658 |
| Fe I | 4917.2300 | 108.800 | 2.11 | 101.932 | 102.962 | 7.845 | 7.828 |
| Fe I | 4918.0127 | 89.200 | 2.99 | 92.680 | 93.616 | 7.627 | 7.604 |
| Fe I | 4935.4141 | 17.700 | 1.68 | 23.947 | 24.637 | 7.517 | 7.498 |
| Fe I | 4961.9136 | 81.000 | 2.50 | 81.642 | 82.467 | 7.685 | 7.665 |
| Fe I | 4962.5718 | 92.900 | 2.00 | 99.646 | 100.348 | 7.560 | 7.541 |
| Fe I | 4969.9175 | 119.800 | 4.98 | 121.350 | 122.576 | 7.673 | 7.649 |
| Fe I | 4992.7852 | 31.500 | 2.72 | 38.823 | 39.778 | 7.532 | 7.510 |
| Fe I | 4999.1123 | 83.000 | 3.66 | 75.880 | 76.802 | 7.865 | 7.847 |
| Fe I | 5025.3027 | 45.200 | 3.95 | 54.200 | 55.250 | 7.504 | 7.480 |
| Fe I | 5029.6177 | 107.100 | 3.91 | 103.218 | 103.946 | 7.793 | 7.777 |
| Fe I | 5031.9141 | 68.100 | 1.28 | 69.527 | 70.729 | 7.668 | 7.640 |
| Fe I | 5036.9214 | 76.300 | 2.64 | 79.294 | 80.338 | 7.629 | 7.602 |
| Fe I | 5048.4355 | 115.400 | 4.29 | 117.719 | 117.837 | 7.652 | 7.648 |
| Fe I | 5067.1494 | 114.900 | 1.61 | 106.577 | 107.005 | 7.873 | 7.872 |
| Fe I | 5072.6719 | 112.800 | 3.89 | 114.319 | 114.663 | 7.671 | 7.662 |
| Fe I | 5088.1533 | 75.600 | 2.81 | 77.041 | 77.819 | 7.668 | 7.649 |
| Fe I | 5109.6519 | 104.200 | 4.57 | 101.728 | 102.652 | 7.751 | 7.733 |
| Fe I | 5115.7769 | 64.000 | 2.01 | 65.271 | 66.265 | 7.672 | 7.649 |
| Fe I | 5143.7227 | 91.800 | 3.25 | 95.449 | 96.608 | 7.611 | 7.581 |


| $\mu$ Leo |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m} \AA)$ |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m} \AA)$ |  | $\varepsilon_{\mathrm{Fe}}(\mathrm{dex})$ |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 5213.8062 | 34.000 | 2.79 | 37.918 | 38.771 | 7.612 | 7.593 |
| Fe I | 5243.7764 | 102.500 | 3.12 | 101.668 | 102.076 | 7.717 | 7.709 |
| Fe I | 5253.0210 | 81.600 | 3.78 | 81.814 | 83.144 | 7.695 | 7.665 |
| Fe I | 5279.6499 | 33.600 | 2.83 | 48.324 | 49.361 | 7.391 | 7.370 |
| Fe I | 5285.1274 | 60.500 | 2.03 | 62.276 | 63.418 | 7.662 | 7.636 |
| Fe I | 5288.5249 | 111.600 | 3.47 | 111.310 | 111.869 | 7.706 | 7.694 |
| Fe I | 5293.9590 | 75.500 | 1.99 | 73.681 | 74.727 | 7.740 | 7.718 |
| Fe I | 5294.5474 | 55.400 | 0.88 | 56.868 | 57.910 | 7.670 | 7.648 |
| Fe I | 5295.3120 | 59.800 | 2.59 | 66.728 | 67.951 | 7.550 | 7.521 |
| Fe I | 5320.0356 | 69.900 | 1.74 | 67.222 | 68.246 | 7.757 | 7.736 |
| Fe I | 5321.1079 | 82.000 | 1.07 | 89.930 | 90.930 | 7.533 | 7.505 |
| Fe I | 5373.7085 | 100.000 | 2.10 | 107.495 | 108.471 | 7.555 | 7.529 |
| Fe I | 5379.5737 | 110.800 | 1.77 | 110.923 | 111.480 | 7.697 | 7.685 |
| Fe I | 5386.3330 | 71.300 | 3.51 | 79.011 | 79.809 | 7.538 | 7.516 |
| Fe I | 5398.2793 | 106.900 | 1.94 | 114.087 | 115.123 | 7.568 | 7.543 |
| Fe I | 5406.7749 | 77.500 | 1.77 | 68.659 | 69.634 | 7.885 | 7.871 |
| Fe I | 5412.7837 | 59.900 | 0.83 | 60.058 | 61.221 | 7.697 | 7.672 |
| Fe I | 5417.0332 | 69.500 | 2.06 | 67.962 | 68.997 | 7.732 | 7.711 |
| Fe I | 5432.9478 | 105.100 | 3.18 | 96.909 | 97.987 | 7.866 | 7.852 |
| Fe I | 5436.2949 | 78.800 | 1.69 | 76.660 | 77.513 | 7.745 | 7.728 |
| Fe I | 5441.3389 | 68.100 | 2.11 | 71.723 | 72.594 | 7.624 | 7.603 |
| Fe I | 5452.0884 | 58.000 | 4.84 | 54.665 | 55.724 | 7.769 | 7.748 |
| Fe I | 5460.8726 | 52.200 | 1.10 | 58.969 | 60.172 | 7.559 | 7.533 |
| Fe I | 5466.3960 | 122.500 | 1.32 | 122.262 | 122.384 | 7.704 | 7.702 |
| Fe I | 5466.9873 | 91.700 | 1.27 | 84.981 | 85.926 | 7.855 | 7.838 |
| Fe I | 5470.0928 | 67.600 | 1.50 | 59.764 | 60.984 | 7.862 | 7.840 |
| Fe I | 5473.1626 | 58.700 | 2.96 | 59.033 | 59.993 | 7.693 | 7.673 |
| Fe I | 5473.9004 | 126.800 | 3.54 | 125.618 | 124.993 | 7.722 | 7.735 |
| Fe I | 5483.0986 | 88.600 | 1.93 | 93.014 | 93.388 | 7.610 | 7.598 |
| Fe I | 5522.4463 | 81.300 | 1.73 | 85.822 | 86.167 | 7.603 | 7.590 |
| Fe I | 5524.2495 | 23.400 | 0.65 | 23.459 | 24.110 | 7.698 | 7.681 |
| Fe I | 5525.5435 | 99.800 | 1.29 | 101.728 | 101.830 | 7.660 | 7.655 |
| Fe I | 5536.5801 | 54.600 | 1.16 | 60.250 | 61.480 | 7.583 | 7.557 |
| Fe I | 5539.2798 | 69.500 | 0.81 | 66.561 | 67.643 | 7.763 | 7.741 |
| Fe I | 5543.9355 | 104.200 | 1.27 | 105.046 | 105.046 | 7.683 | 7.682 |
| Fe I | 5554.8945 | 131.500 | 2.14 | 131.312 | 132.505 | 7.703 | 7.684 |
| Fe I | 5577.0249 | 40.900 | 0.55 | 32.816 | 34.985 | 7.882 | 7.829 |
| Fe I | 5600.2241 | 76.000 | 6.40 | 84.592 | 85.103 | 7.519 | 7.499 |
| Fe I | 5618.6323 | 93.200 | 0.90 | 95.132 | 95.418 | 7.659 | 7.650 |
| Fe I | 5619.2246 | 50.100 | 2.35 | 59.600 | 60.692 | 7.502 | 7.478 |
| Fe I | 5636.6958 | 75.600 | 2.55 | 69.384 | 70.441 | 7.833 | 7.813 |
| Fe I | 5638.2622 | 130.800 | 1.90 | 122.634 | 121.903 | 7.850 | 7.872 |
| Fe I | 5650.7056 | 64.500 | 2.29 | 61.565 | 66.199 | 7.761 | 7.666 |
| Fe I | 5651.4688 | 40.300 | 3.88 | 48.785 | 49.781 | 7.517 | 7.495 |
| Fe I | 5652.3174 | 52.600 | 3.64 | 64.088 | 64.866 | 7.461 | 7.439 |
| Fe I | 5653.8652 | 63.200 | 2.71 | 67.469 | 68.427 | 7.612 | 7.589 |
| Fe I | 5655.1763 | 72.400 | 1.36 | 75.461 | 81.668 | 7.639 | 7.524 |
| Fe I | 5661.3447 | 57.800 | 2.65 | 67.197 | 67.944 | 7.504 | 7.482 |
| Fe I | 5677.6846 | 40.800 | 0.41 | 49.876 | 50.842 | 7.510 | 7.488 |
| Fe I | 5679.0229 | 93.700 | 0.94 | 91.565 | 93.054 | 7.743 | 7.713 |
| Fe I | 5696.0894 | 53.100 | 0.48 | 53.334 | 54.534 | 7.695 | 7.670 |
| Fe I | 5698.0200 | 75.800 | 6.13 | 66.379 | 67.458 | 7.896 | 7.877 |
| Fe I | 5717.8325 | 107.000 | 2.46 | 104.402 | 104.507 | 7.752 | 7.753 |
| Fe I | 5741.8477 | 69.500 | 1.87 | 73.056 | 73.719 | 7.625 | 7.607 |
| Fe I | 5742.9600 | 51.100 | 3.18 | 41.541 | 42.475 | 7.894 | 7.877 |
| Fe I | 5754.4023 | 74.000 | 3.69 | 65.422 | 66.553 | 7.878 | 7.858 |
| Fe I | 5759.2622 | 26.100 | 1.33 | 24.552 | 25.364 | 7.741 | 7.719 |
| Fe I | 5760.3438 | 69.700 | 3.38 | 75.440 | 76.511 | 7.578 | 7.552 |
| Fe I | 5849.6831 | 46.100 | 1.58 | 42.417 | 43.460 | 7.775 | 7.754 |
| Fe I | 5853.1484 | 81.600 | 3.26 | 75.723 | 77.506 | 7.822 | 7.786 |
| Fe I | 5855.0757 | 62.900 | 1.37 | 61.995 | 63.260 | 7.718 | 7.693 |
| Fe I | 5859.5864 | 129.400 | 3.03 | 122.514 | 122.760 | 7.814 | 7.816 |
| Fe I | 5862.3564 | 136.000 | 3.39 | 143.528 | 143.672 | 7.593 | 7.586 |
| Fe I | 5880.0273 | 36.700 | 2.36 | 47.139 | 48.150 | 7.477 | 7.455 |
| Fe I | 5902.4731 | 39.300 | 2.90 | 50.796 | 52.098 | 7.454 | 7.427 |
| Fe I | 5905.6714 | 92.300 | 2.66 | 98.995 | 100.197 | 7.573 | 7.540 |
| Fe I | 5929.6763 | 76.000 | 2.24 | 74.551 | 75.456 | 7.729 | 7.711 |
| Fe I | 5930.1797 | 127.600 | 2.37 | 127.998 | 128.641 | 7.694 | 7.683 |
| Fe I | 5934.6543 | 124.600 | 2.87 | 131.814 | 130.380 | 7.582 | 7.601 |
| Fe I | 5952.7178 | 119.300 | 4.22 | 110.282 | 109.733 | 7.869 | 7.887 |
| Fe I | 5961.9180 | 10.800 | 0.94 | 13.227 | 13.693 | 7.593 | 7.574 |
| Fe I | 5969.5620 | 27.100 | 1.54 | 20.000 | 20.619 | 7.885 | 7.869 |
| Fe I | 5976.7769 | 122.300 | 3.42 | 119.778 | 118.475 | 7.745 | 7.771 |
| Fe I | 5984.8149 | 128.800 | 3.45 | 124.377 | 125.760 | 7.769 | 7.750 |
| Fe I | 6003.0112 | 134.600 | 2.68 | 134.098 | 132.639 | 7.708 | 7.732 |


| $\mu$ Leo |  |  |  |  |  |  |  | HD107328 |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m}$ ) |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m} \AA)$ |  | $\varepsilon_{\mathrm{Fe}}$ (dex) |  |  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m} \AA)$ |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m}$ A $)$ |  | $\varepsilon_{\mathrm{Fe}}$ (dex) |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE | el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 6007.9595 | 107.700 | 3.34 | 105.004 | 105.744 | 7.748 | 7.737 | Fe I | 4873.7510 | 40.300 | 1.38 | 39.586 | 44.933 | 7.134 | 7.031 |
| Fe I | 6008.5557 | 147.900 | 4.42 | 142.824 | 141.270 | 7.775 | 7.800 | Fe I | 4896.4385 | 67.400 | 1.41 | 58.513 | 63.879 | 7.299 | 7.193 |
| Fe I | 6015.2437 | 62.900 | 1.23 | 66.114 | 67.670 | 7.637 | 7.606 | Fe I | 4918.0127 | 75.100 | 1.37 | 68.962 | 75.286 | 7.243 | 7.116 |
| Fe I | 6024.0576 | 149.800 | 3.41 | 151.168 | 151.168 | 7.684 | 7.683 | Fe I | 4961.9136 | 63.100 | 1.11 | 58.994 | 64.686 | 7.202 | 7.088 |
| Fe I | 6027.0508 | 113.600 | 1.93 | 117.074 | 117.662 | 7.638 | 7.624 | Fe I | 4962.5718 | 77.600 | 1.04 | 76.473 | 82.229 | 7.143 | 7.023 |
| Fe I | 6034.0352 | 40.200 | 0.61 | 39.121 | 40.001 | 7.723 | 7.704 | Fe I | 4986.2227 | 70.600 | 1.28 | 68.745 | 74.886 | 7.157 | 7.032 |
| Fe I | 6056.0044 | 110.900 | 1.68 | 116.428 | 117.485 | 7.607 | 7.583 | Fe I | 4999.1123 | 54.300 | 1.70 | 52.643 | 58.427 | 7.153 | 7.039 |
| Fe I | 6078.4912 | 120.600 | 2.25 | 111.902 | 113.606 | 7.846 | 7.823 | Fe I | 5031.9141 | 44.400 | 0.86 | 44.873 | 50.761 | 7.111 | 6.997 |
| Fe I | 6079.0078 | 90.100 | 2.47 | 83.551 | 84.395 | 7.824 | 7.814 | Fe I | 5036.9214 | 64.600 | 1.28 | 55.797 | 61.859 | 7.290 | 7.174 |
| Fe I | 6093.6431 | 72.700 | 1.50 | 66.255 | 67.538 | 7.828 | 7.805 | Fe I | 5088.1533 | 56.900 | 1.60 | 53.300 | 58.895 | 7.190 | 7.081 |
| Fe I | 6096.6641 | 89.200 | 1.80 | 84.976 | 84.976 | 7.784 | 7.788 | Fe I | 5115.7769 | 42.400 | 1.28 | 39.800 | 45.176 | 7.171 | 7.067 |
| Fe I | 6120.2466 | 83.600 | 2.00 | 75.941 | 78.129 | 7.850 | 7.808 | Fe I | 5143.7227 | 81.000 | 1.75 | 73.715 | 80.387 | 7.273 | 7.133 |
| Fe I | 6127.9063 | 102.200 | 2.75 | 95.950 | 96.821 | 7.822 | 7.810 | Fe I | 5267.2695 | 47.600 | 1.80 | 44.142 | 49.878 | 7.188 | 7.076 |
| Fe I | 6151.6172 | 125.800 | 3.40 | 126.910 | 128.843 | 7.679 | 7.642 | Fe I | 5285.1274 | 42.800 | 1.08 | 37.071 | 42.464 | 7.235 | 7.127 |
| Fe I | 6165.3599 | 95.000 | 1.71 | 92.174 | 93.105 | 7.756 | 7.739 | Fe I | 5293.9590 | 51.900 | 0.94 | 49.396 | 55.377 | 7.168 | 7.054 |
| Fe I | 6187.9893 | 103.600 | 2.17 | 99.150 | 98.853 | 7.786 | 7.797 | Fe I | 5294.5474 | 35.900 | 0.64 | 30.416 | 35.244 | 7.233 | 7.133 |
| Fe I | 6200.3125 | 151.400 | 2.68 | 142.565 | 143.860 | 7.850 | 7.830 | Fe I | 5295.3120 | 43.700 | 1.24 | 41.719 | 47.462 | 7.160 | 7.047 |
| Fe I | 6220.7798 | 75.000 | 2.57 | 79.862 | 80.344 | 7.603 | 7.590 | Fe I | 5320.0356 | 50.200 | 0.55 | 41.245 | 46.923 | 7.287 | 7.181 |
| Fe I | 6221.6719 | 51.700 | 1.37 | 44.309 | 46.252 | 7.828 | 7.795 | Fe I | 5326.1426 | 75.900 | 0.51 | 69.670 | 75.811 | 7.248 | 7.122 |
| Fe I | 6226.7344 | 73.500 | 2.54 | 76.549 | 77.166 | 7.639 | 7.624 | Fe I | 5373.7085 | 82.800 | 0.93 | 82.386 | 89.550 | 7.128 | 6.980 |
| Fe I | 6229.2261 | 110.100 | 2.00 | 106.897 | 108.086 | 7.766 | 7.743 | Fe I | 5412.7837 | 35.200 | 0.67 | 34.646 | 39.869 | 7.132 | 7.026 |
| Fe I | 6232.6401 | 148.800 | 3.09 | 144.027 | 143.883 | 7.770 | 7.774 | Fe I | 5417.0332 | 50.000 | 0.80 | 42.558 | 48.361 | 7.262 | 7.151 |
| Fe I | 6240.6460 | 126.800 | 4.34 | 123.802 | 125.433 | 7.766 | 7.731 | Fe I | 5436.2949 | 59.400 | 1.18 | 51.873 | 57.894 | 7.263 | 7.149 |
| Fe I | 6253.8286 | 62.400 | 1.30 | 64.049 | 65.290 | 7.667 | 7.641 | Fe I | 5441.3389 | 50.100 | 0.64 | 46.675 | 52.444 | 7.186 | 7.076 |
| Fe I | 6270.2236 | 123.600 | 2.72 | 123.324 | 124.444 | 7.705 | 7.683 | Fe I | 5466.9873 | 67.700 | 0.84 | 62.039 | 68.325 | 7.231 | 7.108 |
| Fe I | 6271.2778 | 84.700 | 3.04 | 82.076 | 83.495 | 7.753 | 7.725 | Fe I | 5470.0928 | 41.400 | 0.77 | 34.251 | 39.597 | 7.264 | 7.155 |
| Fe I | 6290.5430 | 53.900 | 1.23 | 46.677 | 48.022 | 7.833 | 7.809 | Fe I | 5473.1626 | 35.600 | 1.42 | 33.329 | 38.353 | 7.167 | 7.065 |
| Fe I | 6311.4995 | 96.700 | 1.20 | 92.124 | 93.432 | 7.794 | 7.769 | Fe I | 5483.0986 | 74.800 | 0.88 | 69.349 | 75.379 | 7.224 | 7.108 |
| Fe I | 6315.8110 | 93.500 | 1.50 | 88.636 | 89.441 | 7.797 | 7.784 | Fe I | 5522.4463 | 64.700 | 0.67 | 62.567 | 68.604 | 7.161 | 7.043 |
| Fe I | 6322.6851 | 153.800 | 2.41 | 146.690 | 148.022 | 7.815 | 7.795 | Fe I | 5525.5435 | 79.100 | 0.56 | 79.302 | 85.363 | 7.116 | 6.990 |
| Fe I | 6338.8760 | 76.700 | 1.65 | 76.926 | 78.256 | 7.696 | 7.668 | Fe I | 5539.2798 | 42.900 | 0.28 | 40.606 | 46.354 | 7.164 | 7.055 |
| Fe I | 6408.0176 | 160.800 | 3.04 | 161.813 | 161.651 | 7.687 | 7.689 | Fe I | 5543.9355 | 85.200 | 0.65 | 82.542 | 88.469 | 7.172 | 7.051 |
| Fe I | 6496.4658 | 106.200 | 1.54 | 100.939 | 101.856 | 7.793 | 7.782 | Fe I | 5549.9487 | 25.600 | 0.58 | 21.543 | 25.434 | 7.222 | 7.124 |
| Fe I | 6509.6157 | 34.500 | 3.33 | 45.102 | 46.211 | 7.475 | 7.451 | Fe I | 5552.6919 | 9.000 | 0.54 | 7.939 | 10.284 | 7.182 | 7.054 |
| Fe I | 6569.2139 | 124.100 | 1.74 | 118.441 | 118.678 | 7.784 | 7.785 | Fe I | 5560.2114 | 69.200 | 0.86 | 67.226 | 73.713 | 7.158 | 7.032 |
| Fe I | 6591.3130 | 40.500 | 0.48 | 34.623 | 35.694 | 7.826 | 7.804 | Fe I | 5577.0249 | 14.900 | 0.28 | 13.122 | 17.019 | 7.189 | 7.048 |
| Fe I | 6597.5591 | 80.200 | 1.62 | 78.357 | 79.389 | 7.734 | 7.716 | Fe I | 5584.7646 | 74.800 | 0.96 | 72.030 | 78.550 | 7.175 | 7.045 |
| Fe I | 6608.0249 | 96.900 | 3.00 | 91.138 | 92.998 | 7.812 | 7.777 | Fe I | 5600.2241 | 61.500 | 0.87 | 60.900 | 67.144 | 7.131 | 7.011 |
| Fe I | 6633.7485 | 106.600 | 1.70 | 104.863 | 104.968 | 7.729 | 7.729 | Fe I | 5618.6323 | 73.800 | 0.52 | 72.583 | 78.723 | 7.144 | 7.020 |
| Fe I | 6653.8511 | 43.900 | 0.52 | 55.459 | 56.189 | 7.474 | 7.456 | Fe I | 5622.9453 | 23.300 | 0.41 | 17.421 | 20.789 | 7.281 | 7.185 |
| Fe I | 6667.4180 | 62.200 | 0.99 | 62.054 | 63.645 | 7.703 | 7.673 | Fe I | 5636.6958 | 47.400 | 0.44 | 43.574 | 49.516 | 7.192 | 7.081 |
| Fe I | 6699.1411 | 39.000 | 0.81 | 33.103 | 34.127 | 7.828 | 7.806 | Fe I | 5651.4688 | 29.600 | 0.38 | 24.671 | 28.821 | 7.235 | 7.138 |
| Fe I | 6703.5659 | 110.900 | 2.79 | 103.238 | 104.810 | 7.852 | 7.824 | Fe I | 5652.3174 | 43.800 | 0.61 | 38.801 | 44.142 | 7.217 | 7.113 |
| Fe I | 6704.4795 | 29.700 | 1.15 | 42.541 | 43.498 | 7.424 | 7.403 | Fe I | 5661.3447 | 41.700 | 0.35 | 42.051 | 47.677 | 7.113 | 7.006 |
| Fe I | 6725.3560 | 57.800 | 1.48 | 65.229 | 65.954 | 7.559 | 7.541 | Fe I | 5679.0229 | 73.700 | 0.51 | 66.310 | 74.255 | 7.264 | 7.109 |
| Fe I | 6732.0649 | 34.200 | 0.85 | 37.241 | 38.314 | 7.632 | 7.607 | Fe I | 5691.4971 | 65.900 | 1.81 | 56.650 | 63.085 | 7.295 | 7.174 |
| Fe I | 6733.1504 | 66.600 | 1.22 | 77.994 | 78.702 | 7.480 | 7.453 | Fe I | 5717.8325 | 85.600 | 1.27 | 81.406 | 87.722 | 7.201 | 7.076 |
| Fe I | 6739.5205 | 89.700 | 1.73 | 95.866 | 98.123 | 7.578 | 7.532 | Fe I | 5720.8862 | 31.000 | 0.76 | 32.530 | 37.738 | 7.087 | 6.981 |
| Fe I | 6745.9556 | 36.500 | 0.29 | 44.908 | 46.059 | 7.524 | 7.499 | Fe I | 5731.7617 | 82.400 | 0.81 | 73.301 | 78.988 | 7.294 | 7.189 |
| Fe I | 6746.9536 | 48.700 | 0.37 | 48.140 | 49.578 | 7.710 | 7.684 | Fe I | 5741.8477 | 54.000 | 0.72 | 48.381 | 54.300 | 7.226 | 7.114 |
| Fe I | 6750.1514 | 155.900 | 2.30 | 147.586 | 149.077 | 7.856 | 7.833 | Fe I | 5754.4023 | 42.700 | 1.94 | 39.016 | 44.794 | 7.191 | 7.081 |
| Fe I | 6786.8584 | 67.400 | 1.25 | 66.641 | 67.178 | 7.714 | 7.704 | Fe I | 5759.2622 | 11.900 | 0.43 | 9.146 | 11.059 | 7.250 | 7.157 |
| Fe I | 6796.1235 | 70.400 | 1.72 | 65.148 | 66.342 | 7.801 | 7.780 | Fe I | 5760.3438 | 51.400 | 1.23 | 50.133 | 56.520 | 7.144 | 7.026 |
| Fe I | 6804.2710 | 51.700 | 0.53 | 47.430 | 48.596 | 7.786 | 7.764 | Fe I | 5838.3716 | 46.700 | 0.59 | 39.109 | 44.543 | 7.263 | 7.160 |
| Fe I | 6810.2622 | 89.000 | 1.09 | 91.050 | 91.416 | 7.664 | 7.654 | Fe I | 5849.6831 | 24.900 | 0.49 | 19.025 | 22.676 | 7.273 | 7.175 |
| Fe II | 4993.3501 | 47.000 | 4.03 | 53.401 | 52.099 | 7.531 | 7.562 | Fe I | 5855.0757 | 38.300 | 0.43 | 36.500 | 42.245 | 7.157 | 7.043 |
| Fe II | 5000.7305 | 20.800 | 1.33 | 17.982 | 17.647 | 7.805 | 7.819 | Fe I | 5858.7778 | 31.000 | 0.52 | 26.706 | 31.162 | 7.217 | 7.116 |
| Fe II | 5100.6548 | 39.400 | 3.67 | 33.564 | 32.809 | 7.864 | 7.888 | Fe I | 5861.1084 | 19.800 | 0.40 | 18.368 | 21.712 | 7.162 | 7.067 |
| Fe II | 5234.6226 | 88.500 | 1.01 | 95.802 | 93.012 | 7.527 | 7.592 | Fe I | 5898.2153 | 21.500 | 0.54 | 19.332 | 23.180 | 7.182 | 7.075 |
| Fe II | 5264.8022 | 51.600 | 1.19 | 54.799 | 53.462 | 7.616 | 7.650 | Fe I | 5902.4731 | 25.900 | 0.79 | 26.542 | 31.300 | 7.104 | 6.997 |
| Fe II | 5325.5522 | 54.400 | 0.79 | 53.829 | 52.465 | 7.715 | 7.751 | Fe I | 5905.6714 | 75.300 | 1.01 | 73.136 | 81.534 | 7.160 | 6.998 |
| Fe II | 5414.0698 | 30.000 | 1.01 | 37.507 | 36.664 | 7.475 | 7.496 | Fe I | 5927.7886 | 60.400 | 0.83 | 58.255 | 66.124 | 7.160 | 7.013 |
| Fe II | 5425.2485 | 43.400 | 2.10 | 52.149 | 50.778 | 7.467 | 7.500 | Fe I | 5940.9912 | 40.000 | 0.77 | 34.242 | 39.404 | 7.235 | 7.132 |
| Fe II | 6247.5571 | 46.100 | 1.31 | 48.289 | 46.974 | 7.641 | 7.676 | Fe I | 5952.7178 | 93.000 | 1.62 | 35.305 | 90.943 | 7.265 | 7.161 |
| Fe II | 6369.4590 | 21.500 | 1.33 | 29.932 | 28.920 | 7.427 | 7.452 | Fe I | 5969.5620 | 9.800 | 0.62 | 7.039 | 8.501 | 7.277 | 7.189 |
| Fe II | 6416.9189 | 55.800 | 0.87 | 69.523 | 70.942 | 7.432 | 7.396 | Fe I | 6007.9595 | 80.600 | 1.02 | 79.217 | 86.861 | 7.146 | 6.999 |
| Fe II | 6416.9189 | 55.800 | 0.87 | 31.981 | 31.231 | 7.432 | 7.396 | Fe I | 6034.0352 | 19.400 | 0.38 | 17.208 | 20.389 | 7.186 | 7.092 |
| Fe II | 6456.3794 | 58.400 | 2.00 | 57.483 | 55.701 | 7.723 | 7.769 | Fe I | 6056.0044 | 89.700 | 1.10 | 87.926 | 96.728 | 7.152 | 6.985 |
|  |  |  |  |  |  |  |  | Fe I | 6078.4912 | 90.400 | 1.01 | 83.320 | 92.887 | 7.251 | 7.072 |
| HD107328 |  |  |  |  |  |  |  | Fe I | 6079.0078 | 65.200 | 0.65 | 57.763 | 64.829 | 7.256 | 7.127 |
|  |  |  |  |  |  |  |  | Fe I | 6093.6431 | 47.600 | 0.55 | 40.541 | 46.814 | 7.256 | 7.135 |
|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m} \AA)$ |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m} \AA)$ |  | $\varepsilon_{\mathrm{Fe}}$ (dex) |  | Fe I | 6096.6641 | 67.200 | 0.71 | 59.499 | 65.384 | 7.259 | 7.154 |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE | Fe I | 6127.9063 | 77.900 | 1.15 | 71.012 | 78.207 | 7.249 | 7.114 |
| Fe I | 4793.9614 | 37.500 | 0.57 | 31.188 | 36.014 | 7.248 | 7.150 | Fe I | 6165.3599 | 72.100 | 0.71 | 67.168 | 74.301 | 7.212 | 7.079 |
| Fe I | 4808.1479 | 63.400 | 1.54 | 56.638 | 62.308 | 7.254 | 7.142 | Fe I | 6187.9893 | 79.000 | 0.95 | 74.078 | 79.912 | 7.210 | 7.103 |
| Fe I | 4809.9385 | 42.500 | 2.30 | 39.978 | 45.122 | 7.170 | 7.069 | Fe I | 6226.7344 | 55.800 | 0.75 | 50.304 | 56.458 | 7.220 | 7.108 |


| HD107328 |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m}$ ) |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m} \AA)$ |  | $\varepsilon_{\mathrm{Fe}}$ (dex) |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 6229.2261 | 90.900 | 1.00 | 82.898 | 90.500 | 7.274 | 7.128 |
| Fe I | 6271.2778 | 61.600 | 0.64 | 55.516 | 62.659 | 7.230 | 7.101 |
| Fe I | 6290.5430 | 27.400 | 0.49 | 20.243 | 24.687 | 7.292 | 7.182 |
| Fe I | 6315.8110 | 70.400 | 0.87 | 63.574 | 70.559 | 7.246 | 7.117 |
| Fe I | 6338.8760 | 56.800 | 0.46 | 51.006 | 58.695 | 7.228 | 7.084 |
| Fe I | 6495.7412 | 55.300 | 1.47 | 55.086 | 63.463 | 7.124 | 6.972 |
| Fe I | 6496.4658 | 82.300 | 1.09 | 74.066 | 82.663 | 7.267 | 7.113 |
| Fe I | 6533.9282 | 54.600 | 0.44 | 46.520 | 53.227 | 7.268 | 7.145 |
| Fe I | 6569.2139 | 94.700 | 1.36 | 88.570 | 96.481 | 7.223 | 7.088 |
| Fe I | 6591.3130 | 17.500 | 0.28 | 14.750 | 17.836 | 7.212 | 7.110 |
| Fe I | 6597.5591 | 57.500 | 0.46 | 51.834 | 59.104 | 7.223 | 7.091 |
| Fe I | 6633.7485 | 84.600 | 0.99 | 77.610 | 85.005 | 7.241 | 7.113 |
| Fe I | 6699.1411 | 15.900 | 0.28 | 13.821 | 16.753 | 7.194 | 7.092 |
| Fe I | 6746.9536 | 27.100 | 0.36 | 21.088 | 25.780 | 7.263 | 7.150 |
| Fe I | 6786.8584 | 47.000 | 0.66 | 39.451 | 45.087 | 7.259 | 7.155 |
| Fe I | 6804.2710 | 25.800 | 0.38 | 23.761 | 28.287 | 7.171 | 7.062 |
| Fe I | 6810.2622 | 68.800 | 0.92 | 64.371 | 71.683 | 7.198 | 7.068 |
| Fe II | 4993.3501 | 49.300 | 1.57 | 55.600 | 53.616 | 6.979 | 7.020 |
| Fe II | 5000.7305 | 15.000 | 1.05 | 15.370 | 14.822 | 7.106 | 7.127 |
| Fe II | 5100.6548 | 36.700 | 1.73 | 32.912 | 31.677 | 7.212 | 7.245 |
| Fe II | 5256.9321 | 25.500 | 0.61 | 29.432 | 28.327 | 7.014 | 7.041 |
| Fe II | 5284.1030 | 69.300 | 1.98 | 73.492 | 70.597 | 7.028 | 7.090 |
| Fe II | 5534.8379 | 69.000 | 4.23 | 69.136 | 66.413 | 7.117 | 7.178 |
| Fe II | 6084.1016 | 27.300 | 0.36 | 26.380 | 25.268 | 7.146 | 7.178 |
| Fe II | 6113.3193 | 16.800 | 0.81 | 14.752 | 14.144 | 7.198 | 7.224 |
| Fe II | 6149.2461 | 34.000 | 0.42 | 35.591 | 34.321 | 7.079 | 7.111 |
| Fe II | 6238.3857 | 40.800 | 0.70 | 45.468 | 43.719 | 7.009 | 7.048 |
| Fe II | 6247.5571 | 45.500 | 0.68 | 52.621 | 50.549 | 6.958 | 7.000 |
| Fe II | 6456.3794 | 55.200 | 0.75 | 63.470 | 60.737 | 6.942 | 6.995 |
| Fe II | 6516.0767 | 63.600 | 2.32 | 69.014 | 65.231 | 7.012 | 7.086 |

## $\beta$ Gem

|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m} \AA)$ |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m} \AA)$ |  | $\varepsilon_{\mathrm{Fe}}$ (dex) |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 4779.4390 | 78.900 | 7.98 | 87.227 | 90.111 | 7.389 | 7.319 |
| Fe I | 4793.9614 | 30.800 | 1.74 | 39.900 | 42.857 | 7.391 | 7.337 |
| Fe I | 4794.3540 | 53.500 | 4.05 | 50.459 | 54.141 | 7.638 | 7.568 |
| Fe I | 4799.4058 | 72.000 | 4.50 | 71.120 | 74.161 | 7.599 | 7.532 |
| Fe I | 4808.1479 | 67.300 | 2.44 | 65.691 | 68.858 | 7.614 | 7.547 |
| Fe I | 4809.9385 | 50.600 | 4.09 | 50.968 | 53.934 | 7.573 | 7.514 |
| Fe I | 4869.4634 | 61.000 | 4.65 | 57.023 | 60.024 | 7.664 | 7.600 |
| Fe I | 4874.3530 | 54.600 | 6.03 | 56.367 | 59.648 | 7.544 | 7.478 |
| Fe I | 4917.2300 | 96.700 | 2.90 | 92.561 | 96.018 | 7.667 | 7.595 |
| Fe I | 4918.0127 | 79.700 | 3.12 | 82.672 | 86.027 | 7.519 | 7.448 |
| Fe I | 4935.4141 | 13.200 | 1.48 | 13.355 | 14.644 | 7.574 | 7.526 |
| Fe I | 4961.9136 | 70.500 | 1.85 | 69.559 | 72.684 | 7.600 | 7.533 |
| Fe I | 4962.5718 | 79.900 | 1.79 | 89.585 | 92.738 | 7.381 | 7.313 |
| Fe I | 4979.5859 | 46.200 | 2.74 | 44.794 | 47.755 | 7.608 | 7.550 |
| Fe I | 4992.7852 | 20.100 | 1.64 | 26.972 | 29.127 | 7.402 | 7.355 |
| Fe I | 4999.1123 | 62.800 | 4.95 | 65.615 | 68.779 | 7.521 | 7.455 |
| Fe I | 5023.1860 | 68.300 | 2.86 | 67.696 | 70.960 | 7.593 | 7.524 |
| Fe I | 5031.9141 | 53.700 | 2.22 | 59.320 | 62.706 | 7.466 | 7.401 |
| Fe I | 5036.9214 | 55.100 | 3.45 | 64.247 | 67.700 | 7.395 | 7.329 |
| Fe I | 5058.4966 | 26.300 | 3.08 | 36.889 | 39.623 | 7.349 | 7.300 |
| Fe I | 5109.6519 | 95.300 | 3.54 | 92.663 | 96.223 | 7.634 | 7.561 |
| Fe I | 5115.7769 | 42.700 | 1.67 | 50.972 | 54.110 | 7.416 | 7.359 |
| Fe I | 5159.0576 | 95.500 | 4.26 | 103.568 | 107.547 | 7.430 | 7.349 |
| Fe I | 5228.3760 | 86.100 | 4.00 | 83.108 | 86.301 | 7.641 | 7.576 |
| Fe I | 5243.7764 | 82.500 | 3.43 | 92.497 | 95.555 | 7.377 | 7.309 |
| Fe I | 5253.0210 | 61.000 | 2.66 | 62.139 | 66.317 | 7.558 | 7.477 |
| Fe I | 5267.2695 | 56.600 | 3.79 | 58.614 | 61.960 | 7.540 | 7.473 |
| Fe I | 5285.1274 | 51.000 | 2.73 | 51.707 | 54.949 | 7.566 | 7.502 |
| Fe I | 5293.9590 | 54.600 | 2.16 | 62.686 | 66.055 | 7.418 | 7.354 |
| Fe I | 5294.5474 | 47.100 | 2.15 | 41.564 | 44.644 | 7.686 | 7.626 |
| Fe I | 5295.3120 | 48.800 | 2.95 | 56.420 | 59.830 | 7.428 | 7.366 |
| Fe I | 5315.0698 | 65.600 | 1.36 | 61.229 | 64.519 | 7.667 | 7.602 |
| Fe I | 5320.0356 | 50.400 | 3.78 | 52.911 | 56.288 | 7.531 | 7.467 |
| Fe I | 5326.1426 | 78.200 | 3.78 | 79.501 | 82.986 | 7.552 | 7.476 |
| Fe I | 5373.7085 | 92.600 | 2.44 | 98.587 | 102.481 | 7.465 | 7.385 |
| Fe I | 5379.5737 | 98.500 | 1.72 | 100.102 | 103.518 | 7.545 | 7.471 |
| Fe I | 5386.3330 | 59.600 | 2.26 | 68.036 | 71.391 | 7.414 | 7.349 |
| Fe I | 5398.2793 | 94.500 | 1.84 | 104.992 | 108.800 | 7.385 | 7.304 |
| Fe I | 5406.7749 | 63.300 | 2.78 | 58.078 | 61.264 | 7.682 | 7.620 |
| Fe I | 5409.1333 | 82.800 | 3.33 | 79.777 | 83.101 | 7.640 | 7.574 |
| Fe I | 5412.7837 | 42.800 | 1.07 | 49.199 | 52.395 | 7.453 | 7.395 |
| Fe I | 5417.0332 | 54.900 | 2.57 | 57.509 | 60.856 | 7.529 | 7.465 |


| $\beta$ Gem |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m}$ ) |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m} \AA)$ |  | $\varepsilon_{\mathrm{Fe}}(\mathrm{dex})$ |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 5436.2949 | 68.100 | 2.25 | 66.629 | 69.915 | 7.609 | 7.544 |
| Fe I | 5436.5879 | 106.200 | 3.09 | 109.957 | 115.259 | 7.500 | 7.389 |
| Fe I | 5460.8726 | 35.700 | 1.28 | 40.948 | 44.316 | 7.475 | 7.413 |
| Fe I | 5466.9873 | 74.000 | 5.41 | 72.485 | 76.060 | 7.612 | 7.537 |
| Fe I | 5470.0928 | 46.200 | 2.00 | 48.933 | 52.223 | 7.526 | 7.464 |
| Fe I | 5473.1626 | 49.100 | 3.22 | 46.837 | 49.933 | 7.624 | 7.564 |
| Fe I | 5483.0986 | 80.600 | 2.81 | 82.485 | 85.565 | 7.543 | 7.479 |
| Fe I | 5487.1450 | 63.900 | 3.29 | 65.523 | 68.899 | 7.548 | 7.482 |
| Fe I | 5491.8315 | 30.500 | 2.21 | 29.715 | 32.159 | 7.598 | 7.544 |
| Fe I | 5536.5801 | 30.900 | 0.74 | 40.842 | 44.345 | 7.380 | 7.320 |
| Fe I | 5539.2798 | 47.700 | 1.32 | 52.338 | 55.738 | 7.490 | 7.427 |
| Fe I | 5543.1470 | 93.800 | 2.46 | 96.241 | 99.835 | 7.525 | 7.442 |
| Fe I | 5543.9355 | 87.500 | 2.07 | 95.763 | 98.623 | 7.415 | 7.346 |
| Fe I | 5546.5059 | 83.400 | 3.66 | 79.088 | 82.469 | 7.668 | 7.599 |
| Fe I | 5549.9487 | 36.700 | 1.28 | 31.246 | 33.926 | 7.693 | 7.637 |
| Fe I | 5560.2114 | 80.700 | 2.11 | 82.360 | 85.702 | 7.548 | 7.481 |
| Fe I | 5584.7646 | 82.100 | 2.08 | 82.386 | 86.178 | 7.574 | 7.494 |
| Fe I | 5622.9453 | 30.600 | 1.23 | 25.910 | 28.317 | 7.685 | 7.630 |
| Fe I | 5636.6958 | 49.500 | 1.75 | 55.353 | 58.886 | 7.467 | 7.402 |
| Fe I | 5638.2622 | 102.700 | 1.55 | 113.213 | 115.406 | 7.381 | 7.325 |
| Fe I | 5650.7056 | 52.800 | 1.03 | 53.568 | 60.460 | 7.564 | 7.438 |
| Fe I | 5651.4688 | 37.500 | 1.34 | 37.867 | 40.630 | 7.572 | 7.517 |
| Fe I | 5652.3174 | 52.400 | 1.28 | 52.821 | 55.895 | 7.572 | 7.512 |
| Fe I | 5655.1763 | 72.800 | 1.97 | 67.314 | 76.493 | 7.695 | 7.512 |
| Fe I | 5661.3447 | 54.900 | 0.69 | 56.281 | 59.431 | 7.553 | 7.491 |
| Fe I | 5679.0229 | 83.800 | 1.50 | 83.172 | 87.642 | 7.592 | 7.504 |
| Fe I | 5680.2402 | 30.200 | 0.95 | 25.969 | 28.227 | 7.677 | 7.624 |
| Fe I | 5691.4971 | 72.500 | 2.43 | 70.758 | 74.170 | 7.615 | 7.546 |
| Fe I | 5696.0894 | 37.800 | 1.49 | 42.747 | 45.915 | 7.480 | 7.420 |
| Fe I | 5698.0200 | 51.900 | 9.06 | 51.896 | 55.444 | 7.580 | 7.513 |
| Fe I | 5705.4644 | 67.500 | 1.58 | 75.843 | 79.003 | 7.415 | 7.348 |
| Fe I | 5717.8325 | 86.500 | 1.02 | 95.210 | 98.357 | 7.408 | 7.336 |
| Fe I | 5720.8862 | 38.800 | 1.82 | 47.501 | 50.749 | 7.408 | 7.350 |
| Fe I | 5754.4023 | 48.100 | 3.09 | 50.856 | 54.391 | 7.527 | 7.461 |
| Fe I | 5760.3438 | 54.600 | 2.96 | 61.886 | 65.627 | 7.439 | 7.370 |
| Fe I | 5849.6831 | 31.100 | 2.06 | 28.150 | 30.731 | 7.645 | 7.588 |
| Fe I | 5855.0757 | 49.200 | 1.77 | 52.136 | 55.701 | 7.523 | 7.456 |
| Fe I | 5858.7778 | 36.200 | 2.25 | 39.380 | 42.299 | 7.515 | 7.458 |
| Fe I | 5859.5864 | 104.700 | 3.05 | 113.539 | 117.051 | 7.429 | 7.358 |
| Fe I | 5861.1084 | 28.400 | 2.25 | 29.145 | 31.542 | 7.563 | 7.510 |
| Fe I | 5881.2798 | 32.000 | 2.54 | 38.692 | 41.649 | 7.439 | 7.383 |
| Fe I | 5883.8164 | 106.400 | 3.39 | 104.640 | 107.433 | 7.613 | 7.560 |
| Fe I | 5902.4731 | 31.000 | 1.27 | 40.587 | 43.830 | 7.378 | 7.321 |
| Fe I | 5905.6714 | 83.900 | 2.40 | 90.742 | 95.217 | 7.453 | 7.362 |
| Fe I | 5929.6763 | 67.600 | 1.83 | 65.014 | 68.508 | 7.629 | 7.563 |
| Fe I | 5930.1797 | 115.200 | 3.31 | 119.023 | 123.340 | 7.518 | 7.443 |
| Fe I | 5934.6543 | 111.700 | 4.32 | 119.231 | 121.293 | 7.451 | 7.408 |
| Fe I | 5952.7178 | 103.800 | 4.82 | 98.955 | 101.806 | 7.671 | 7.619 |
| Fe I | 5976.7769 | 106.000 | 2.59 | 107.919 | 110.121 | 7.545 | 7.502 |
| Fe I | 5984.8149 | 112.500 | 6.45 | 115.630 | 120.952 | 7.529 | 7.439 |
| Fe I | 6003.0112 | 118.600 | 2.82 | 121.088 | 123.182 | 7.538 | 7.499 |
| Fe I | 6007.9595 | 87.700 | 4.08 | 96.356 | 100.371 | 7.423 | 7.340 |
| Fe I | 6015.2437 | 31.800 | 1.95 | 42.351 | 46.642 | 7.376 | 7.307 |
| Fe I | 6027.0508 | 102.000 | 3.05 | 105.889 | 109.843 | 7.508 | 7.432 |
| Fe I | 6093.6431 | 62.000 | 1.31 | 56.634 | 60.442 | 7.682 | 7.609 |
| Fe I | 6096.6641 | 77.000 | 2.40 | 73.045 | 76.168 | 7.655 | 7.596 |
| Fe I | 6120.2466 | 42.600 | 2.93 | 43.112 | 49.047 | 7.571 | 7.469 |
| Fe I | 6127.9063 | 78.500 | 2.82 | 85.206 | 89.221 | 7.452 | 7.373 |
| Fe I | 6139.6440 | 16.100 | 1.26 | 19.225 | 21.601 | 7.484 | 7.420 |
| Fe I | 6151.6172 | 111.300 | 4.45 | 105.749 | 112.022 | 7.691 | 7.566 |
| Fe I | 6157.7280 | 106.600 | 2.28 | 102.179 | 106.215 | 7.662 | 7.587 |
| Fe I | 6165.3599 | 80.200 | 2.62 | 81.362 | 85.375 | 7.558 | 7.480 |
| Fe I | 6180.2026 | 110.900 | 4.42 | 108.347 | 113.930 | 7.630 | 7.520 |
| Fe I | 6187.3979 | 22.400 | 1.61 | 21.882 | 24.395 | 7.593 | 7.530 |
| Fe I | 6187.9893 | 91.200 | 1.54 | 87.366 | 90.347 | 7.652 | 7.597 |
| Fe I | 6220.7798 | 58.900 | 1.18 | 67.157 | 70.617 | 7.426 | 7.363 |
| Fe I | 6226.7344 | 67.000 | 1.00 | 63.640 | 67.202 | 7.643 | 7.576 |
| Fe I | 6229.2261 | 87.900 | 2.44 | 90.346 | 95.302 | 7.531 | 7.433 |
| Fe I | 6232.6401 | 118.600 | 2.38 | 128.719 | 132.291 | 7.413 | 7.348 |
| Fe I | 6240.6460 | 99.400 | 4.68 | 105.188 | 111.192 | 7.458 | 7.336 |
| Fe I | 6253.8286 | 48.000 | 1.39 | 54.943 | 58.637 | 7.448 | 7.381 |
| Fe I | 6270.2236 | 102.600 | 2.86 | 106.659 | 111.919 | 7.499 | 7.394 |
| Fe I | 6271.2778 | 59.200 | 1.68 | 66.507 | 70.903 | 7.444 | 7.368 |
| Fe I | 6290.5430 | 28.500 | 2.17 | 26.298 | 29.383 | 7.629 | 7.561 |
| Fe I | 6293.9243 | 28.000 | 0.90 | 28.007 | 30.575 | 7.580 | 7.522 |
| Fe I | 6311.4995 | 72.100 | 1.63 | 74.489 | 79.244 | 7.534 | 7.445 |
| Fe I | 6315.8110 | 76.600 | 2.65 | 77.472 | 81.464 | 7.563 | 7.485 |


| $\beta$ Gem |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m}$ ) |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m} \AA)$ |  | $\varepsilon_{\mathrm{Fe}}$ (dex) |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 6338.8760 | 63.000 | 4.61 | 68.803 | 73.117 | 7.471 | 7.389 |
| Fe I | 6380.7432 | 79.600 | 5.01 | 84.540 | 88.803 | 7.487 | 7.404 |
| Fe I | 6475.6240 | 105.700 | 2.03 | 101.342 | 107.354 | 7.669 | 7.547 |
| Fe I | 6481.8696 | 117.300 | 1.86 | 118.459 | 125.486 | 7.558 | 7.430 |
| Fe I | 6495.7412 | 67.300 | 3.75 | 73.663 | 78.532 | 7.464 | 7.375 |
| Fe I | 6496.4658 | 91.300 | 2.52 | 93.157 | 97.751 | 7.547 | 7.462 |
| Fe I | 6518.3657 | 107.300 | 4.28 | 113.624 | 119.604 | 7.464 | 7.356 |
| Fe I | 6569.2139 | 109.800 | 2.91 | 109.120 | 113.195 | 7.591 | 7.524 |
| Fe I | 6574.2266 | 89.400 | 3.18 | 94.145 | 102.332 | 7.487 | 7.338 |
| Fe I | 6581.2090 | 73.500 | 5.35 | 79.649 | 86.575 | 7.465 | 7.347 |
| Fe I | 6591.3130 | 29.300 | 2.22 | 25.242 | 27.647 | 7.675 | 7.618 |
| Fe I | 6597.5591 | 67.800 | 1.61 | 69.915 | 73.984 | 7.542 | 7.466 |
| Fe I | 6608.0249 | 68.300 | 2.12 | 68.928 | 74.517 | 7.569 | 7.470 |
| Fe I | 6633.7485 | 88.600 | 1.33 | 95.168 | 98.927 | 7.467 | 7.395 |
| Fe I | 6667.4180 | 33.400 | 1.65 | 39.118 | 43.320 | 7.469 | 7.395 |
| Fe I | 6667.7104 | 27.300 | 1.26 | 23.830 | 26.129 | 7.664 | 7.608 |
| Fe I | 6699.1411 | 21.300 | 1.53 | 23.900 | 26.206 | 7.511 | 7.455 |
| Fe I | 6703.5659 | 90.500 | 1.51 | 85.042 | 90.470 | 7.686 | 7.581 |
| Fe I | 6710.3179 | 77.500 | 3.15 | 75.721 | 82.665 | 7.613 | 7.488 |
| Fe I | 6725.3560 | 45.800 | 3.24 | 52.450 | 55.857 | 7.458 | 7.398 |
| Fe I | 6739.5205 | 62.000 | 1.92 | 69.303 | 75.907 | 7.451 | 7.346 |
| Fe I | 6745.9556 | 27.200 | 2.34 | 32.357 | 35.324 | 7.465 | 7.405 |
| Fe I | 6746.9536 | 28.200 | 1.26 | 27.470 | 30.761 | 7.596 | 7.526 |
| Fe I | 6750.1514 | 131.900 | 3.75 | 128.010 | 134.747 | 7.656 | 7.524 |
| Fe I | 6752.7065 | 69.600 | 13.08 | 66.635 | 70.142 | 7.635 | 7.570 |
| Fe I | 6786.8584 | 53.100 | 2.96 | 54.352 | 57.699 | 7.557 | 7.497 |
| Fe I | 6796.1235 | 50.000 | 0.76 | 52.877 | 56.735 | 7.526 | 7.457 |
| Fe II | 4993.3501 | 57.700 | 3.53 | 62.180 | 60.901 | 7.477 | 7.505 |
| Fe II | 5100.6548 | 34.800 | 3.63 | 39.531 | 38.718 | 7.464 | 7.483 |
| Fe II | 5256.9321 | 28.200 | 1.81 | 36.137 | 35.394 | 7.377 | 7.392 |
| Fe II | 5264.8022 | 55.400 | 3.07 | 65.875 | 64.520 | 7.342 | 7.367 |
| Fe II | 5284.1030 | 78.200 | 7.02 | 80.116 | 78.238 | 7.536 | 7.579 |
| Fe II | 5534.8379 | 67.600 | 1.52 | 77.248 | 75.438 | 7.366 | 7.401 |
| Fe II | 6149.2461 | 47.700 | 1.93 | 45.433 | 44.499 | 7.634 | 7.658 |
| Fe II | 6247.5571 | 61.700 | 0.52 | 63.354 | 61.869 | 7.543 | 7.576 |
| Fe II | 6369.4590 | 34.000 | 2.28 | 38.273 | 37.158 | 7.478 | 7.503 |
| Fe II | 6416.9189 | 56.700 | 1.26 | 60.976 | 65.145 | 7.499 | 7.422 |
| Fe II | 6416.9189 | 56.700 | 1.26 | 43.516 | 42.579 | 7.499 | 7.422 |
| Fe II | 6456.3794 | 69.200 | 1.61 | 74.652 | 72.760 | 7.464 | 7.502 |
| Fe II | 6516.0767 | 79.800 | 5.35 | 76.680 | 74.159 | 7.644 | 7.699 |


| $\epsilon$ Vir |  |  |  |  |  |  |  |  |
| :--- | :--- | :--- | :--- | :---: | :---: | :---: | :---: | :---: |
|  |  | EW $_{\text {obs }}$ | $(\mathrm{mA})$ | EW $_{\text {calc }}$ |  | $(\mathrm{mA})$ | $\varepsilon_{\text {Fe }}($ dex $)$ |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |  |
| Fe I | 4793.9614 | 29.300 | 0.83 | 35.075 | 39.103 | 7.469 | 7.388 |  |
| Fe I | 4794.3540 | 43.800 | 1.14 | 44.072 | 49.078 | 7.594 | 7.494 |  |
| Fe I | 4799.4058 | 70.800 | 1.17 | 65.594 | 69.855 | 7.721 | 7.622 |  |
| Fe I | 4802.5234 | 30.300 | 1.81 | 25.372 | 29.163 | 7.723 | 7.627 |  |
| Fe I | 4808.1479 | 60.900 | 1.62 | 59.984 | 64.430 | 7.620 | 7.522 |  |
| Fe I | 4809.9385 | 45.400 | 1.89 | 46.221 | 50.405 | 7.582 | 7.495 |  |
| Fe I | 4869.4634 | 56.300 | 1.78 | 52.136 | 56.363 | 7.692 | 7.599 |  |
| Fe I | 4874.3530 | 50.400 | 2.46 | 50.754 | 55.288 | 7.592 | 7.497 |  |
| Fe I | 4877.6045 | 59.000 | 4.75 | 51.748 | 56.370 | 7.753 | 7.656 |  |
| Fe I | 4961.9136 | 63.600 | 1.01 | 64.070 | 68.524 | 7.589 | 7.490 |  |
| Fe I | 4986.2227 | 77.500 | 1.56 | 76.565 | 81.021 | 7.620 | 7.522 |  |
| Fe I | 4992.7852 | 20.800 | 1.08 | 24.504 | 27.471 | 7.499 | 7.426 |  |
| Fe I | 4999.1123 | 62.500 | 2.03 | 60.959 | 65.407 | 7.634 | 7.535 |  |
| Fe I | 5023.1860 | 64.100 | 1.42 | 62.929 | 67.376 | 7.626 | 7.528 |  |
| Fe I | 5023.4976 | 61.300 | 0.97 | 53.377 | 57.767 | 7.770 | 7.676 |  |
| Fe I | 5025.3027 | 37.100 | 2.30 | 38.930 | 42.827 | 7.560 | 7.478 |  |
| Fe I | 5031.9141 | 51.000 | 1.24 | 54.992 | 59.580 | 7.514 | 7.419 |  |
| Fe I | 5036.9214 | 57.500 | 1.26 | 58.242 | 63.101 | 7.584 | 7.480 |  |
| Fe I | 5058.4966 | 30.200 | 1.31 | 33.062 | 36.817 | 7.534 | 7.454 |  |
| Fe I | 5088.1533 | 63.900 | 1.05 | 61.686 | 65.974 | 7.648 | 7.555 |  |
| Fe I | 5104.4375 | 63.300 | 0.79 | 58.934 | 63.506 | 7.694 | 7.596 |  |
| Fe I | 5115.7769 | 50.100 | 0.73 | 46.207 | 50.610 | 7.681 | 7.589 |  |
| Fe I | 5180.0557 | 75.200 | 0.76 | 68.935 | 74.605 | 7.740 | 7.613 |  |
| Fe I | 5197.9360 | 57.800 | 1.90 | 60.925 | 65.652 | 7.534 | 7.436 |  |
| Fe I | 5236.2021 | 66.400 | 3.91 | 68.518 | 73.203 | 7.554 | 7.451 |  |
| Fe I | 5253.0210 | 55.300 | 1.22 | 55.003 | 60.777 | 7.606 | 7.490 |  |
| Fe I | 5267.2695 | 56.500 | 2.62 | 54.380 | 58.980 | 7.645 | 7.548 |  |
| Fe I | 5285.1274 | 53.900 | 0.73 | 47.900 | 52.407 | 7.726 | 7.631 |  |
| Fe I | 5293.9590 | 58.900 | 1.33 | 58.100 | 62.811 | 7.617 | 7.517 |  |
| Fe I | 5294.5474 | 35.600 | 1.02 | 37.360 | 41.557 | 7.562 | 7.477 |  |
| Fe I | 5295.3120 | 52.400 | 1.24 | 52.331 | 57.005 | 7.601 | 7.504 |  |
|  |  |  |  |  |  |  |  |  |


| $\epsilon$ Vir |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m} \AA$ ) |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m} \AA)$ |  | $\varepsilon_{\mathrm{Fe}}$ (dex) |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 5320.0356 | 50.600 | 0.60 | 48.123 | 52.766 | 7.651 | 7.556 |
| Fe I | 5326.1426 | 77.200 | 1.71 | 73.488 | 78.429 | 7.685 | 7.572 |
| Fe I | 5401.2666 | 51.600 | 0.70 | 46.545 | 50.925 | 7.706 | 7.614 |
| Fe I | 5406.7749 | 61.700 | 0.85 | 53.939 | 58.439 | 7.760 | 7.668 |
| Fe I | 5412.7837 | 40.800 | 0.34 | 45.548 | 49.998 | 7.499 | 7.412 |
| Fe I | 5417.0332 | 57.800 | 1.36 | 53.426 | 58.009 | 7.690 | 7.596 |
| Fe I | 5436.2949 | 68.000 | 0.54 | 62.047 | 66.646 | 7.724 | 7.629 |
| Fe I | 5441.3389 | 56.700 | 0.47 | 56.714 | 61.246 | 7.600 | 7.506 |
| Fe I | 5452.0884 | 36.600 | 0.81 | 35.490 | 39.654 | 7.624 | 7.536 |
| Fe I | 5466.9873 | 72.700 | 0.45 | 66.752 | 71.776 | 7.732 | 7.621 |
| Fe I | 5470.0928 | 50.800 | 0.71 | 45.334 | 49.818 | 7.712 | 7.620 |
| Fe I | 5472.7085 | 76.300 | 0.58 | 68.410 | 72.854 | 7.768 | 7.677 |
| Fe I | 5473.1626 | 45.100 | 0.83 | 43.085 | 47.346 | 7.642 | 7.554 |
| Fe I | 5483.0986 | 78.100 | 0.83 | 76.994 | 81.475 | 7.623 | 7.527 |
| Fe I | 5487.1450 | 67.300 | 1.62 | 61.042 | 65.707 | 7.729 | 7.633 |
| Fe I | 5494.4624 | 55.100 | 1.46 | 46.552 | 51.044 | 7.776 | 7.684 |
| Fe I | 5522.4463 | 69.600 | 0.76 | 70.781 | 75.139 | 7.575 | 7.479 |
| Fe I | 5528.8979 | 40.700 | 2.02 | 33.932 | 37.702 | 7.744 | 7.662 |
| Fe I | 5539.2798 | 44.600 | 0.32 | 47.549 | 52.309 | 7.539 | 7.445 |
| Fe I | 5549.9487 | 32.500 | 0.34 | 27.869 | 31.526 | 7.706 | 7.622 |
| Fe I | 5552.6919 | 19.200 | 0.30 | 14.473 | 17.209 | 7.759 | 7.662 |
| Fe I | 5560.2114 | 76.900 | 0.71 | 76.912 | 81.648 | 7.600 | 7.500 |
| Fe I | 5577.0249 | 22.700 | 0.53 | 22.840 | 27.094 | 7.596 | 7.487 |
| Fe I | 5584.7646 | 73.200 | 0.56 | 76.090 | 81.380 | 7.537 | 7.422 |
| Fe I | 5587.5742 | 67.400 | 0.89 | 60.124 | 64.999 | 7.753 | 7.651 |
| Fe I | 5600.2241 | 71.500 | 0.87 | 69.684 | 74.211 | 7.638 | 7.541 |
| Fe I | 5618.6323 | 79.100 | 1.09 | 80.020 | 84.498 | 7.580 | 7.480 |
| Fe I | 5619.5952 | 62.900 | 0.53 | 54.445 | 59.179 | 7.773 | 7.676 |
| Fe I | 5622.9453 | 25.900 | 0.39 | 22.905 | 26.177 | 7.676 | 7.593 |
| Fe I | 5636.6958 | 48.500 | 0.41 | 50.404 | 55.328 | 7.561 | 7.462 |
| Fe I | 5651.4688 | 37.200 | 0.68 | 34.960 | 38.801 | 7.649 | 7.566 |
| Fe I | 5652.3174 | 50.500 | 0.56 | 48.915 | 53.226 | 7.633 | 7.544 |
| Fe I | 5661.3447 | 48.500 | 0.37 | 52.237 | 56.656 | 7.523 | 7.434 |
| Fe I | 5679.0229 | 83.000 | 0.60 | 77.525 | 83.540 | 7.713 | 7.589 |
| Fe I | 5691.4971 | 72.900 | 1.84 | 65.971 | 70.784 | 7.746 | 7.646 |
| Fe I | 5698.0200 | 41.800 | 3.90 | 47.103 | 51.990 | 7.491 | 7.398 |
| Fe I | 5741.8477 | 60.900 | 0.81 | 58.089 | 62.663 | 7.658 | 7.563 |
| Fe I | 5742.9600 | 33.200 | 1.91 | 26.814 | 30.196 | 7.746 | 7.667 |
| Fe I | 5754.4023 | 45.100 | 1.75 | 46.121 | 51.019 | 7.579 | 7.482 |
| Fe I | 5760.3438 | 60.500 | 2.35 | 56.618 | 61.810 | 7.680 | 7.573 |
| Fe I | 5838.3716 | 53.200 | 0.73 | 47.832 | 52.447 | 7.707 | 7.615 |
| Fe I | 5849.6831 | 26.500 | 0.56 | 25.020 | 28.529 | 7.637 | 7.552 |
| Fe I | 5853.1484 | 42.200 | 1.27 | 40.054 | 46.847 | 7.642 | 7.513 |
| Fe I | 5855.0757 | 47.900 | 0.79 | 48.527 | 53.444 | 7.587 | 7.488 |
| Fe I | 5858.7778 | 37.300 | 0.64 | 36.101 | 40.157 | 7.626 | 7.540 |
| Fe I | 5861.1084 | 24.800 | 0.33 | 26.609 | 29.931 | 7.554 | 7.476 |
| Fe I | 5880.0273 | 29.100 | 1.00 | 33.836 | 37.721 | 7.491 | 7.411 |
| Fe I | 5881.2798 | 36.500 | 0.50 | 35.900 | 39.978 | 7.613 | 7.527 |
| Fe I | 5898.2153 | 32.400 | 0.70 | 29.753 | 33.619 | 7.662 | 7.573 |
| Fe I | 5905.6714 | 85.800 | 1.50 | 84.749 | 90.641 | 7.621 | 7.500 |
| Fe I | 5927.7886 | 72.500 | 0.96 | 70.348 | 76.299 | 7.643 | 7.523 |
| Fe I | 5940.9912 | 52.700 | 0.61 | 43.913 | 48.416 | 7.777 | 7.686 |
| Fe I | 5969.5620 | 13.600 | 0.36 | 11.177 | 12.862 | 7.701 | 7.629 |
| Fe I | 6007.9595 | 93.300 | 2.79 | 90.380 | 95.945 | 7.655 | 7.547 |
| Fe I | 6034.0352 | 25.300 | 0.55 | 25.383 | 28.617 | 7.598 | 7.520 |
| Fe I | 6054.0732 | 27.800 | 0.36 | 21.957 | 24.810 | 7.747 | 7.673 |
| Fe I | 6079.0078 | 76.500 | 1.13 | 70.026 | 75.216 | 7.726 | 7.626 |
| Fe I | 6082.7100 | 87.100 | 1.33 | 79.266 | 86.441 | 7.771 | 7.614 |
| Fe I | 6093.6431 | 58.800 | 0.84 | 52.814 | 58.037 | 7.720 | 7.615 |
| Fe I | 6096.6641 | 71.900 | 0.88 | 67.587 | 72.208 | 7.686 | 7.594 |
| Fe I | 6098.2441 | 41.600 | 0.72 | 33.092 | 37.016 | 7.779 | 7.695 |
| Fe I | 6120.2466 | 35.400 | 0.67 | 34.347 | 41.785 | 7.621 | 7.479 |
| Fe I | 6127.9063 | 85.400 | 1.23 | 79.136 | 84.819 | 7.728 | 7.612 |
| Fe I | 6165.3599 | 78.900 | 0.93 | 75.532 | 81.217 | 7.669 | 7.552 |
| Fe I | 6187.3979 | 20.300 | 0.81 | 18.490 | 21.753 | 7.653 | 7.560 |
| Fe I | 6187.9893 | 83.300 | 1.21 | 80.989 | 85.612 | 7.646 | 7.553 |
| Fe I | 6199.5063 | 22.600 | 0.36 | 19.432 | 23.024 | 7.687 | 7.589 |
| Fe I | 6226.7344 | 60.700 | 0.93 | 58.512 | 63.531 | 7.643 | 7.544 |
| Fe I | 6229.2261 | 87.200 | 0.77 | 82.673 | 89.376 | 7.696 | 7.554 |
| Fe I | 6240.6460 | 98.200 | 1.87 | 95.986 | 103.881 | 7.649 | 7.476 |
| Fe I | 6270.2236 | 98.900 | 1.24 | 98.103 | 105.148 | 7.617 | 7.469 |
| Fe I | 6271.2778 | 61.100 | 1.13 | 60.446 | 66.497 | 7.613 | 7.496 |
| Fe I | 6290.5430 | 23.500 | 0.32 | 22.083 | 26.041 | 7.637 | 7.538 |
| Fe I | 6293.9243 | 33.900 | 0.87 | 26.075 | 29.631 | 7.782 | 7.695 |
| Fe I | 6311.4995 | 70.700 | 0.57 | 67.455 | 73.964 | 7.666 | 7.536 |
| Fe I | 6315.8110 | 76.100 | 1.13 | 71.844 | 77.502 | 7.687 | 7.571 |
| Fe I | 6338.8760 | 70.000 | 0.76 | 64.471 | 70.306 | 7.709 | 7.594 |


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|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m} \AA)$ |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m}$ A $)$ |  | $\varepsilon_{\mathrm{Fe}}$ (dex) |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 6495.7412 | 79.200 | 2.50 | 69.036 | 75.614 | 7.793 | 7.670 |
| Fe I | 6496.4658 | 94.400 | 1.50 | 87.236 | 93.400 | 7.733 | 7.620 |
| Fe I | 6533.9282 | 67.300 | 0.40 | 58.832 | 64.227 | 7.763 | 7.660 |
| Fe I | 6574.2266 | 87.600 | 1.05 | 83.190 | 93.682 | 7.691 | 7.480 |
| Fe I | 6581.2090 | 74.300 | 0.78 | 70.044 | 79.056 | 7.684 | 7.510 |
| Fe I | 6591.3130 | 24.700 | 0.36 | 23.278 | 26.634 | 7.637 | 7.552 |
| Fe I | 6597.5591 | 68.900 | 0.71 | 65.655 | 71.287 | 7.662 | 7.554 |
| Fe I | 6608.0249 | 59.300 | 0.46 | 61.062 | 68.532 | 7.566 | 7.432 |
| Fe I | 6627.5439 | 56.800 | 0.31 | 47.998 | 52.629 | 7.770 | 7.681 |
| Fe I | 6633.7485 | 96.400 | 1.32 | 89.221 | 94.714 | 7.728 | 7.632 |
| Fe I | 6667.4180 | 29.300 | 0.15 | 33.313 | 38.826 | 7.513 | 7.407 |
| Fe I | 6667.7104 | 25.800 | 0.20 | 21.965 | 25.160 | 7.700 | 7.616 |
| Fe I | 6699.1411 | 21.400 | 0.41 | 22.034 | 25.268 | 7.582 | 7.498 |
| Fe I | 6703.5659 | 82.200 | 1.10 | 77.317 | 84.685 | 7.699 | 7.551 |
| Fe I | 6710.3179 | 68.100 | 1.53 | 66.152 | 75.173 | 7.637 | 7.471 |
| Fe I | 6713.7427 | 42.400 | 0.19 | 33.657 | 38.031 | 7.782 | 7.689 |
| Fe I | 6746.9536 | 20.300 | 0.19 | 23.123 | 27.364 | 7.524 | 7.423 |
| Fe I | 6752.7065 | 66.200 | 1.18 | 62.572 | 67.499 | 7.670 | 7.574 |
| Fe I | 6786.8584 | 53.500 | 0.75 | 50.145 | 54.984 | 7.664 | 7.572 |
| Fe I | 6804.2710 | 34.600 | 0.77 | 34.729 | 39.153 | 7.597 | 7.504 |
| Fe II | 4993.3501 | 61.000 | 1.86 | 67.052 | 65.931 | 7.453 | 7.478 |
| Fe II | 5000.7305 | 30.100 | 1.31 | 24.536 | 24.102 | 7.750 | 7.763 |
| Fe II | 5100.6548 | 43.000 | 0.36 | 45.144 | 44.346 | 7.548 | 7.567 |
| Fe II | 5132.6611 | 43.700 | 0.65 | 49.575 | 48.698 | 7.460 | 7.479 |
| Fe II | 5136.7949 | 31.600 | 0.72 | 36.711 | 36.062 | 7.470 | 7.485 |
| Fe II | 5256.9321 | 42.300 | 0.72 | 41.856 | 41.116 | 7.611 | 7.629 |
| Fe II | 5264.8022 | 69.800 | 1.08 | 71.181 | 69.991 | 7.567 | 7.595 |
| Fe II | 5325.5522 | 70.700 | 0.78 | 70.386 | 69.209 | 7.608 | 7.636 |
| Fe II | 5414.0698 | 46.800 | 0.74 | 52.312 | 51.387 | 7.468 | 7.488 |
| Fe II | 5425.2485 | 62.500 | 0.77 | 68.937 | 67.718 | 7.448 | 7.474 |
| Fe II | 5427.8159 | 6.300 | 0.63 | 7.451 | 7.429 | 7.504 | 7.506 |
| Fe II | 5525.1172 | 33.700 | 1.09 | 33.841 | 33.275 | 7.596 | 7.611 |
| Fe II | 6084.1016 | 46.900 | 0.37 | 40.092 | 39.267 | 7.759 | 7.781 |
| Fe II | 6113.3193 | 31.100 | 0.76 | 25.402 | 24.904 | 7.754 | 7.771 |
| Fe II | 6149.2461 | 58.900 | 0.62 | 52.447 | 51.520 | 7.750 | 7.775 |
| Fe II | 6238.3857 | 69.400 | 0.69 | 63.038 | 61.863 | 7.745 | 7.775 |
| Fe II | 6247.5571 | 75.900 | 1.26 | 70.302 | 68.924 | 7.727 | 7.761 |
| Fe II | 6369.4590 | 40.600 | 0.52 | 44.849 | 43.755 | 7.502 | 7.525 |
| Fe II | 6416.9189 | 61.400 | 0.38 | 57.238 | 62.899 | 7.682 | 7.570 |
| Fe II | 6416.9189 | 61.400 | 0.38 | 50.693 | 49.748 | 7.682 | 7.570 |
| Fe II | 6456.3794 | 86.800 | 1.08 | 81.426 | 79.751 | 7.719 | 7.759 |
| Fe II | 6516.0767 | 85.900 | 1.00 | 82.555 | 80.463 | 7.672 | 7.721 |


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|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m} \AA)$ |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m}$ ) |  | $\varepsilon_{\mathrm{Fe}}$ (dex) |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 4793.9614 | 28.700 | 0.92 | 34.434 | 38.218 | 7.485 | 7.363 |
| Fe I | 4794.3540 | 41.800 | 1.31 | 43.459 | 48.234 | 7.578 | 7.429 |
| Fe I | 4799.4058 | 67.900 | 1.21 | 68.135 | 72.330 | 7.605 | 7.466 |
| Fe I | 4802.5234 | 29.600 | 1.87 | 25.403 | 28.867 | 7.710 | 7.638 |
| Fe I | 4808.1479 | 57.500 | 1.80 | 61.647 | 66.003 | 7.527 | 7.372 |
| Fe I | 4809.9385 | 42.600 | 2.00 | 46.724 | 50.732 | 7.528 | 7.399 |
| Fe I | 4869.4634 | 53.000 | 2.15 | 53.272 | 57.405 | 7.605 | 7.479 |
| Fe I | 4874.3530 | 47.100 | 2.46 | 51.336 | 55.739 | 7.527 | 7.380 |
| Fe I | 4961.9136 | 60.000 | 0.95 | 66.394 | 70.707 | 7.482 | 7.333 |
| Fe I | 4962.5718 | 78.400 | 1.41 | 87.605 | 91.829 | 7.424 | 7.311 |
| Fe I | 4986.2227 | 73.000 | 1.34 | 80.208 | 84.608 | 7.467 | 7.329 |
| Fe I | 4992.7852 | 17.700 | 1.33 | 24.195 | 26.913 | 7.429 | 7.339 |
| Fe I | 4999.1123 | 59.300 | 1.69 | 63.326 | 67.656 | 7.529 | 7.377 |
| Fe I | 5023.1860 | 60.900 | 1.52 | 65.496 | 69.825 | 7.519 | 7.371 |
| Fe I | 5023.4976 | 58.100 | 0.87 | 55.057 | 59.329 | 7.670 | 7.571 |
| Fe I | 5031.9141 | 49.100 | 1.17 | 56.884 | 61.364 | 7.457 | 7.317 |
| Fe I | 5036.9214 | 54.700 | 1.31 | 59.524 | 64.281 | 7.516 | 7.347 |
| Fe I | 5058.4966 | 29.300 | 1.04 | 32.716 | 36.230 | 7.535 | 7.419 |
| Fe I | 5088.1533 | 59.900 | 1.21 | 64.012 | 68.170 | 7.529 | 7.390 |
| Fe I | 5104.4375 | 60.300 | 0.89 | 61.109 | 65.568 | 7.594 | 7.453 |
| Fe I | 5115.7769 | 48.500 | 0.55 | 46.682 | 50.907 | 7.645 | 7.540 |
| Fe I | 5180.0557 | 70.200 | 0.90 | 72.276 | 77.716 | 7.568 | 7.351 |
| Fe I | 5197.9360 | 53.800 | 2.04 | 63.213 | 67.825 | 7.430 | 7.305 |
| Fe I | 5236.2021 | 63.700 | 3.39 | 71.531 | 76.097 | 7.455 | 7.314 |
| Fe I | 5253.0210 | 52.300 | 1.27 | 55.212 | 60.806 | 7.556 | 7.357 |
| Fe I | 5267.2695 | 55.600 | 2.65 | 56.177 | 60.601 | 7.599 | 7.463 |
| Fe I | 5285.1274 | 49.400 | 0.83 | 49.141 | 53.414 | 7.615 | 7.494 |


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| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m} \AA)$ |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m} \AA)$ |  | $\varepsilon_{\mathrm{Fe}}$ (dex) |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 5293.9590 | 54.800 | 1.08 | 60.080 | 64.672 | 7.507 | 7.351 |
| Fe I | 5294.5474 | 34.200 | 0.81 | 37.163 | 41.110 | 7.550 | 7.426 |
| Fe I | 5295.3120 | 47.900 | 0.96 | 53.970 | 58.472 | 7.492 | 7.343 |
| Fe I | 5320.0356 | 48.300 | 0.71 | 48.745 | 53.215 | 7.602 | 7.472 |
| Fe I | 5326.1426 | 74.000 | 1.49 | 76.709 | 81.519 | 7.554 | 7.369 |
| Fe I | 5401.2666 | 48.800 | 0.78 | 47.575 | 51.768 | 7.634 | 7.524 |
| Fe I | 5406.7749 | 58.300 | 1.07 | 55.598 | 59.912 | 7.661 | 7.563 |
| Fe I | 5412.7837 | 39.100 | 0.31 | 46.551 | 50.820 | 7.463 | 7.334 |
| Fe I | 5417.0332 | 53.400 | 1.64 | 55.070 | 59.535 | 7.578 | 7.441 |
| Fe I | 5432.9478 | 80.100 | 1.22 | 86.459 | 91.491 | 7.487 | 7.326 |
| Fe I | 5436.2949 | 60.400 | 3.62 | 64.464 | 68.945 | 7.533 | 7.387 |
| Fe I | 5441.3389 | 51.500 | 0.62 | 58.594 | 63.004 | 7.475 | 7.338 |
| Fe I | 5452.0884 | 36.800 | 1.09 | 35.229 | 39.143 | 7.642 | 7.541 |
| Fe I | 5460.8726 | 25.400 | 0.56 | 35.378 | 39.661 | 7.393 | 7.302 |
| Fe I | 5461.5493 | 47.500 | 0.65 | 41.580 | 45.492 | 7.724 | 7.670 |
| Fe I | 5466.9873 | 66.100 | 0.42 | 69.265 | 74.160 | 7.547 | 7.367 |
| Fe I | 5470.0928 | 43.200 | 1.26 | 46.316 | 50.619 | 7.549 | 7.413 |
| Fe I | 5487.1450 | 60.900 | 1.10 | 63.375 | 67.926 | 7.563 | 7.419 |
| Fe I | 5491.8315 | 27.600 | 1.09 | 26.733 | 29.803 | 7.630 | 7.541 |
| Fe I | 5494.4624 | 51.800 | 1.03 | 47.421 | 51.713 | 7.694 | 7.613 |
| Fe I | 5528.8979 | 29.900 | 2.29 | 34.135 | 37.677 | 7.518 | 7.402 |
| Fe I | 5539.2798 | 39.700 | 0.30 | 48.147 | 52.735 | 7.447 | 7.316 |
| Fe I | 5543.9355 | 85.300 | 0.72 | 94.372 | 98.407 | 7.434 | 7.322 |
| Fe I | 5546.5059 | 79.700 | 1.28 | 77.335 | 81.836 | 7.656 | 7.542 |
| Fe I | 5549.9487 | 28.900 | 0.40 | 27.349 | 30.695 | 7.645 | 7.553 |
| Fe I | 5552.6919 | 15.800 | 0.42 | 14.400 | 16.842 | 7.660 | 7.555 |
| Fe I | 5560.2114 | 71.300 | 0.62 | 80.651 | 85.255 | 7.434 | 7.312 |
| Fe I | 5573.1021 | 71.400 | 2.91 | 83.091 | 87.556 | 7.392 | 7.301 |
| Fe I | 5636.6958 | 40.300 | 0.17 | 51.248 | 56.009 | 7.402 | 7.298 |
| Fe I | 5651.4688 | 33.700 | 1.15 | 35.241 | 38.854 | 7.578 | 7.466 |
| Fe I | 5652.3174 | 46.400 | 0.91 | 50.057 | 54.233 | 7.540 | 7.411 |
| Fe I | 5653.8652 | 59.700 | 0.98 | 54.317 | 58.785 | 7.710 | 7.638 |
| Fe I | 5655.1763 | 71.600 | 0.92 | 65.841 | 76.559 | 7.728 | 8.158 |
| Fe I | 5661.3447 | 44.500 | 0.73 | 53.694 | 57.985 | 7.436 | 7.319 |
| Fe I | 5680.2402 | 19.900 | 0.43 | 23.162 | 25.996 | 7.521 | 7.413 |
| Fe I | 5691.4971 | 65.800 | 1.81 | 68.780 | 73.483 | 7.553 | 7.396 |
| Fe I | 5741.8477 | 50.600 | 1.61 | 60.081 | 64.465 | 7.432 | 7.314 |
| Fe I | 5742.9600 | 27.700 | 2.10 | 26.541 | 29.622 | 7.637 | 7.549 |
| Fe I | 5754.4023 | 50.100 | 1.78 | 46.566 | 51.228 | 7.676 | 7.576 |
| Fe I | 5838.3716 | 50.500 | 0.54 | 48.613 | 53.013 | 7.645 | 7.539 |
| Fe I | 5848.1265 | 76.300 | 1.08 | 72.167 | 77.516 | 7.687 | 7.568 |
| Fe I | 5849.6831 | 26.200 | 0.46 | 24.433 | 27.608 | 7.653 | 7.563 |
| Fe I | 5853.1484 | 41.900 | 1.26 | 38.339 | 44.632 | 7.675 | 7.510 |
| Fe I | 5855.0757 | 46.500 | 0.66 | 49.901 | 54.596 | 7.545 | 7.392 |
| Fe I | 5858.7778 | 36.400 | 0.49 | 36.289 | 40.098 | 7.612 | 7.505 |
| Fe I | 5861.1084 | 24.300 | 0.35 | 26.382 | 29.411 | 7.559 | 7.454 |
| Fe I | 5873.2124 | 46.800 | 0.69 | 40.976 | 44.930 | 7.719 | 7.663 |
| Fe I | 5879.4868 | 24.800 | 1.30 | 19.114 | 21.476 | 7.760 | 7.735 |
| Fe I | 5881.2798 | 39.700 | 0.66 | 36.314 | 40.126 | 7.678 | 7.597 |
| Fe I | 5898.2153 | 37.800 | 1.59 | 29.967 | 33.558 | 7.773 | 7.752 |
| Fe I | 5902.4731 | 30.300 | 0.65 | 38.199 | 42.396 | 7.442 | 7.319 |
| Fe I | 5905.6714 | 81.600 | 1.25 | 89.293 | 95.094 | 7.471 | 7.305 |
| Fe I | 5909.9722 | 74.100 | 0.81 | 74.450 | 80.313 | 7.603 | 7.389 |
| Fe I | 5927.7886 | 64.400 | 1.35 | 73.639 | 79.352 | 7.441 | 7.294 |
| Fe I | 5929.6763 | 68.600 | 0.83 | 63.073 | 67.820 | 7.712 | 7.634 |
| Fe I | 5940.9912 | 49.300 | 0.77 | 44.615 | 48.920 | 7.699 | 7.621 |
| Fe I | 6007.9595 | 88.600 | 2.50 | 95.245 | 100.469 | 7.491 | 7.341 |
| Fe I | 6015.2437 | 25.300 | 0.30 | 34.623 | 39.842 | 7.410 | 7.295 |
| Fe I | 6034.0352 | 24.700 | 0.37 | 25.117 | 28.064 | 7.600 | 7.504 |
| Fe I | 6054.0732 | 26.600 | 0.33 | 21.657 | 24.252 | 7.732 | 7.692 |
| Fe I | 6079.0078 | 72.000 | 1.01 | 73.220 | 78.227 | 7.588 | 7.441 |
| Fe I | 6082.7100 | 82.800 | 1.17 | 81.921 | 88.948 | 7.627 | 7.283 |
| Fe I | 6093.6431 | 55.700 | 0.70 | 54.546 | 59.548 | 7.631 | 7.494 |
| Fe I | 6096.6641 | 68.700 | 0.82 | 70.128 | 74.525 | 7.584 | 7.458 |
| Fe I | 6098.2441 | 39.700 | 0.70 | 33.346 | 37.010 | 7.738 | 7.693 |
| Fe I | 6120.2466 | 35.100 | 0.60 | 32.012 | 38.662 | 7.670 | 7.457 |
| Fe I | 6127.9063 | 79.700 | 1.07 | 82.925 | 88.406 | 7.550 | 7.361 |
| Fe I | 6151.6172 | 93.200 | 1.66 | 100.239 | 108.249 | 7.472 | 7.191 |
| Fe I | 6165.3599 | 74.400 | 0.78 | 79.010 | 84.503 | 7.524 | 7.335 |
| Fe I | 6187.3979 | 20.500 | 0.90 | 17.474 | 20.319 | 7.697 | 7.618 |
| Fe I | 6187.9893 | 79.400 | 1.04 | 84.706 | 89.070 | 7.513 | 7.382 |
| Fe I | 6226.7344 | 57.200 | 0.81 | 60.156 | 65.034 | 7.556 | 7.405 |
| Fe I | 6229.2261 | 82.100 | 0.69 | 85.948 | 92.417 | 7.536 | 7.264 |


| $\xi$ Hya |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m} \AA)$ |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m} \AA$ ) |  | $\varepsilon_{\mathrm{Fe}}(\mathrm{dex})$ |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 6240.6460 | 92.800 | 1.85 | 100.22 | 107.996 | 7.46 | 7.225 |
| FeI | 6271.2778 | 57.200 | 0.96 | 61.872 | 67.694 | 7.525 | 7.321 |
| Fel | 6293.9243 | 30.900 | 0.39 | 26.197 | 29.468 | 7.718 | 7.659 |
| Fe I | 6311.4995 | 66.600 | 0.62 | 69.174 | 75.435 | 7.563 | 7.324 |
| Fe I | 6315.8110 | 72.200 | 1.13 | 74.955 | 80.338 | 7.559 | 7.376 |
| Fe I | 6338.8760 | 65.700 | 0.61 | 67.389 | 73.090 | 7.579 | 7.391 |
| Fe I | 6380.7432 | 84.600 | 0.93 | 82.269 | 87.988 | 7.653 | 7.494 |
| Fe I | 6495.7412 | 65.800 | 1.73 | 72.279 | 78.564 | 7.495 | 7.29 |
| Fel | 6496.4658 | 99.500 | 1.29 | 91.982 | 97.957 | 7.739 | 7.66 |
| Fe I | 6533.9282 | 60.600 | 0.73 | 60.972 | 66.130 | 7.603 | 7.456 |
| Fe I | 6591.3130 | 22.700 | 0.46 | 23.158 | 26.227 | 7.598 | 7.487 |
| Fe I | 6597.5591 | 64.300 | 0.68 | 68.525 | 73.921 | 7.535 | 7.368 |
| Fel | 6608.0249 | 55.800 | 0.39 | 61.522 | 68.663 | 7.510 | 7.244 |
| Fe I | 6627.5439 | 54.700 | 0.29 | 49.219 | 53.615 | 7.709 | 7.641 |
| Fe I | 6633.7485 | 91.200 | 0.83 | 93.773 | 98.917 | 7.567 | 7.427 |
| Fe I | 6667.4180 | 30.400 | 1.42 | 32.053 | 37.055 | 7.576 | 7.406 |
| Fe I | 6667.7104 | 24.100 | 0.34 | 21.796 | 24.712 | 7.670 | 7.588 |
| Fel | 6699.1411 | 21.200 | 0.35 | 21.874 | 24.800 | 7.59 | 7.482 |
| Fe I | 6703.5659 | 77.600 | 0.89 | 79.876 | 87.011 | 7.568 | 7.247 |
| Fel | 6713.7427 | 41.800 | 0.28 | 34.099 | 38.185 | 7.761 | 7.728 |
| Fe I | 6746.9536 | 19.800 | 0.17 | 21.906 | 25.621 | 7.553 | 7.401 |
| Fe I | 6752.7065 | 62.500 | 1.28 | 65.145 | 69.898 | 7.563 | 7.424 |
| Fel | 6786.8584 | 51.200 | 0.37 | 51.179 | 55.751 | 7.610 | 7.492 |
| Fe II | 5000.7305 | 25.300 | 1.43 | 24.716 | 24.351 | 7.626 | 7.635 |
| Fe II | 5100.6548 | 38.900 | 0.94 | 46.757 | 46.066 | 7.434 | 7.452 |
| Fe II | 5256.9321 | 38.200 | 0.79 | 43.259 | 42.620 | 7.495 | 7.512 |
| Fe II | 5264.8022 | 63.900 | 1.19 | 75.271 | 74.232 | 7.361 | 7.386 |
| Fe II | 5325.5522 | 64.300 | 0.68 | 74.399 | 73.372 | 7.389 | 7.416 |
| Fe II | 5534.8379 | 78.200 | 3.00 | 87.297 | 85.922 | 7.413 | 7.448 |
| Fe II | 6084.1016 | 41.300 | 0.31 | 41.591 | 40.856 | 7.603 | 7.620 |
| Fe II | 6113.3193 | 27.300 | 0.74 | 25.931 | 25.498 | 7.647 | 7.657 |
| Fe II | 6149.2461 | 52.200 | 0.63 | 55.354 | 54.536 | 7.541 | 7.561 |
| Fe II | 6238.3857 | 62.500 | 0.51 | 66.821 | 65.769 | 7.518 | 7.544 |
| Fe II | 6247.5571 | 68.900 | 1.00 | 74.682 | 73.506 | 7.488 | 7.518 |
| Fe II | 6369.4590 | 34.000 | 0.51 | 46.511 | 45.554 | 7.337 | 7.357 |
| Fe II | 6416.9189 | 56.000 | 0.26 | 59.474 | 64.928 | 7.546 | 7.365 |
| Fe II | 6416.9189 | 56.000 | 0.26 | 53.471 | 52.629 | 7.546 | 7.365 |
| Fe II | 6416.9189 | 56.000 | 0.26 | 59.474 | 64.928 | 7.546 | 7.678 |
| Fe II | 6416.9189 | 56.000 | 0.26 | 53.471 | 52.629 | 7.546 | 7.678 |
| Fe II | 6416.9189 | 56.000 | 0.26 | 59.474 | 64.928 | 7.665 | 7.365 |
| Fe II | 6416.9189 | 56.000 | 0.26 | 53.471 | 52.629 | 7.665 | 7.365 |
| Fe II | 6416.9189 | 56.000 | 0.26 | 59.474 | 64.928 | 7.665 | 7.678 |
| Fe II | 6416.9189 | 56.000 | 0.26 | 53.471 | 52.629 | 7.665 | 7.678 |
| Fe II | 6456.3794 | 79.800 | 0.91 | 86.701 | 85.252 | 7.469 | 7.504 |
| Fe II | 6516.0767 | 85.400 | 1.94 | 87.282 | 85.403 | 7.572 | 7.610 |

## 61 Cyg B

|  |  | EW $_{\text {obs }}(\mathrm{m} \AA)$ |  | EW $_{\text {calc }}(\mathrm{mA})$ |  | $\varepsilon_{\mathrm{Fe}}(\mathrm{dex})$ |  |
| :--- | :--- | :---: | :---: | :---: | :---: | :---: | :---: |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 4787.8267 | 59.100 | 3.94 | 51.399 | 51.399 | 7.189 | 7.189 |
| Fe I | 4802.8745 | 37.500 | 5.25 | 33.817 | 33.851 | 7.141 | 7.140 |
| Fe I | 4875.8770 | 69.500 | 3.87 | 77.490 | 77.490 | 6.973 | 6.973 |
| Fe I | 4905.1328 | 36.900 | 2.19 | 33.694 | 33.728 | 7.133 | 7.132 |
| Fe I | 4917.2300 | 57.600 | 2.70 | 57.852 | 57.968 | 7.067 | 7.065 |
| Fe I | 4918.0127 | 35.500 | 3.32 | 41.730 | 41.814 | 6.962 | 6.961 |
| Fe I | 5002.7920 | 101.800 | 6.30 | 116.493 | 116.493 | 6.935 | 6.934 |
| Fe I | 5159.0576 | 54.200 | 10.08 | 69.183 | 69.322 | 6.879 | 6.877 |
| Fe I | 5196.0591 | 102.800 | 11.34 | 96.200 | 96.393 | 7.137 | 7.135 |
| Fe I | 5223.1826 | 37.400 | 3.57 | 51.101 | 51.152 | 6.836 | 6.835 |
| Fe I | 5235.3867 | 57.900 | 5.46 | 77.682 | 77.838 | 6.805 | 6.803 |
| Fe I | 5243.7764 | 46.600 | 1.78 | 51.724 | 51.776 | 6.992 | 6.992 |
| Fe I | 5253.4619 | 87.900 | 6.11 | 112.808 | 112.808 | 6.822 | 6.822 |
| Fe I | 5288.5249 | 53.700 | 4.07 | 67.150 | 67.217 | 6.879 | 6.878 |
| Fe I | 5295.3120 | 16.900 | 2.25 | 14.922 | 14.937 | 7.136 | 7.136 |
| Fe I | 5398.2793 | 58.900 | 4.89 | 68.540 | 68.677 | 6.951 | 6.949 |
| Fe I | 5400.5010 | 100.500 | 2.00 | 131.611 | 131.875 | 6.815 | 6.811 |
| Fe I | 5436.2949 | 21.100 | 2.86 | 20.860 | 20.881 | 7.077 | 7.076 |
| Fe I | 5436.5879 | 88.100 | 4.01 | 81.849 | 81.849 | 7.160 | 7.160 |
| Fe I | 5466.3960 | 85.200 | 5.46 | 74.958 | 75.108 | 7.183 | 7.182 |
| Fe I | 5473.9004 | 70.100 | 3.12 | 80.633 | 80.795 | 6.936 | 6.933 |
| Fe I | 5483.0986 | 27.000 | 4.32 | 34.447 | 34.481 | 6.907 | 6.906 |
| Fe I | 5543.1470 | 54.700 | 3.16 | 51.421 | 51.472 | 7.130 | 7.129 |
| Fe I | 5560.2114 | 23.800 | 3.67 | 34.387 | 34.456 | 6.848 | 6.846 |
| Fe I | 5584.7646 | 25.900 | 3.81 | 38.063 | 38.101 | 6.813 | 6.812 |
| Fe I | 5618.6323 | 38.700 | 1.84 | 37.504 | 37.542 | 7.093 | 7.092 |
| Fe I | 5636.6958 | 17.000 | 1.30 | 15.380 | 15.395 | 7.126 | 7.125 |
| Fe I | 5638.2622 | 64.100 | 1.07 | 73.305 | 73.452 | 6.946 | 6.944 |

61 Cyg B

|  |  | $\mathrm{EW}_{\text {obs }}\left(\mathrm{m}\right.$ A ${ }^{\text {a }}$ |  | $\mathrm{EW}_{\text {calc }}(\mathrm{mA}$ ) |  | $\varepsilon_{\text {Fe }}$ (dex) |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| el | (air) | EW | ${ }_{\text {EWW }}$ | nLTE | LTE |  |  |
| Fe | 5641.4341 | 48.900 | 3.34 | 44.763 | 44.853 | 7.14 | 7.1 |
| Fe I | . 0229 | 9.500 | 11 | 35.314 | 35.420 |  |  |


| Fe I | 5679.0229 | 39.500 | 1.11 | 35.314 | 35.420 | 7.142 | 7.14 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| Fe I | 5691.4971 | 27.200 | 2.45 | 23.123 | 23.169 | 7.172 | 7.171 |


| Fe I | 5701.5444 | 107.500 | 5.08 | 120.396 | 120.396 | 6.931 | 6.931 |
| :--- | :--- | :---: | :---: | :---: | :---: | :---: | :---: |


| Fe I | 5705.4644 | 20.900 | 1.33 | 27.089 | 27.143 | 6.910 | 6.909 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |


| Fe I | 5717.8325 | 48.900 | 2.45 | 48.137 | 48.233 | 7.083 | 7.081 |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Fe I | 5720.8862 | 9.300 | 0.56 | 9.443 | 9.462 | 7.062 | 7.061 |


| Fe I | 5754.4023 | 15.000 | 1.66 | 12.836 | 12.849 | 7.154 | 7.154 |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: | :---: |


| Fe I | 5760.3438 | 16.400 | 1.63 | 19.019 | 19.038 | 6.985 | 6.985 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |


| Fe I | 5848.1265 | 27.500 | 0.96 | 23.800 | 23.872 | 7.159 | 7.158 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| Fe I | 5853.1484 | 24.400 | 2.60 | 19.934 | 19.954 | 7.195 | 7.194 |


| Fe I | 5855.0757 | 12.400 | 1.17 | 11.031 | 11.042 | 7.129 | 7.129 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |


| Fe I | 5905.6714 | 30.900 | 0.88 | 42.315 | 42.442 | 6.870 | 6.868 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| Fe I | 5909.9722 | 40.900 | 1.94 | 35.351 | 35.351 | 7.173 | 7.173 |


| Fe I | 5916.2471 | 66.800 | 1.83 | 65.258 | 65.258 | 7.095 | 7.095 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |


| Fe I | 5927.7886 | 31.000 | 0.95 | 25.441 | 25.518 | 7.188 | 7.187 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |


| Fe I | 5934.6543 | 70.700 | 3.60 | 86.684 | 86.684 | 6.897 | 6.896 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| Fe | 5940.9912 | 9.500 | 1.39 | 9.903 | 9.913 | 7.049 | 7.048 |


| Fe I | 5940.9912 | 9.500 | 1.39 | 9.903 | 9.913 | 7.049 | 7.048 |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Fe I | 5952.7178 | 46.600 | 1.42 | 56.030 | 56.030 | 6.937 | 6.937 |


| Fe I | 5956.6938 | 95.700 | 3.58 | 94.140 | 94.140 | 7.094 | 7.094 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |


| Fe I | 5976.7769 | 61.000 | 2.05 | 67.966 | 67.966 | 6.984 | 6.983 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| Fe I | 5984.8149 | 57.500 | 2.36 | 76.110 | 76.339 | 6.858 | 6.855 |


| Fe I | 5987.0649 | 44.600 | 0.90 | 49.544 | 49.743 | 6.999 | 6.996 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| Fe I | 6003.0112 | 83.100 | 1.93 | 89.141 | 89.141 | 7.007 | 7.007 |


| Fe I | 6005.5415 | 27.500 | 1.66 | 23.981 | 23.981 | 7.160 | 7.160 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |


| Fe I | 6007.9595 | 40.800 | 2.05 | 44.872 | 45.007 | 7.001 | 6.998 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |


| Fe I | 6008.5557 | 86.300 | 2.69 | 102.443 | 102.443 | 6.914 | 6.913 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| Fe I | 6012.2100 | 24.600 | 1.90 | 25.926 | 25.952 | 7.035 | 7.035 |


| Fe I | 6020.1685 | 78.600 | 5.66 | 80.997 | 81.241 | 7.044 | 7.042 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |


| Fe I | 6024.0576 | 89.200 | 2.52 | 104.496 | 104.705 | 6.926 | 6.924 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Fe I | 6027.0508 | 49.700 | 0.91 | 63.701 | 63.765 | 6.877 | 6.876 |


| Fe I | 6056.0044 | 49.500 | 2.33 | 63.502 | 63.693 | 6.890 | 6.887 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |


| Fe I | 6079.0078 | 22.400 | 0.47 | 23.729 | 23.777 | 7.037 | 7.036 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |


| Fe I | 6082.7100 | 53.200 | 0.97 | 48.458 | 48.507 | 7.159 | 7.158 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |


| Fe I | 6093.6431 | 12.000 | 0.58 | 12.662 | 12.687 | 7.042 | 7.041 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| Fe I | 6096.6641 | 27.100 | 0.73 | 25.159 | 25.159 | 7.114 | 7.114 |


| Fe I | 6127.9063 | 34.000 | 1.72 | 36.191 | 36.227 | 7.029 | 7.028 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| Fe I | 6136.9937 | 102.600 | 4.84 | 92.938 | 92.938 | 7.195 | 7.195 |


| Fe I | 6136.9937 | 102.600 | 4.84 | 92.938 | 92.938 | 7.195 | 7.195 |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Fe I | 6151.6172 | 59.900 | 3.67 | 69.647 | 69.647 | 6.909 | 6.908 |


| Fe I | 6157.7280 | 52.700 | 1.46 | 57.410 | 57.467 | 7.003 | 7.002 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| Fe I | 6165.3599 | 36.800 | 1.65 | 32.033 | 32.065 | 7.161 | 7.160 |


| Fe I | 6165.3599 | 36.800 | 1.65 | 32.033 | 32.065 | 7.161 | 7.160 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| Fe I | 6173.3345 | 82.500 | 2.22 | 95.448 | 95.448 | 6.893 | 6.892 |


| Fe I | 6180.2026 | 55.400 | 3.83 | 69.810 | 69.810 | 6.841 | 6.841 |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Fe I | 6187.9893 | 38.200 | 1.69 | 39.031 | 39.031 | 7.056 | 7.056 |
| Fe I | 6200.3125 | 91.400 | 2.57 | 93.198 | 93.198 | 7.047 | 7.047 |
| Fe I | 6220.7798 | 18.800 | 2.09 | 20.852 | 20.852 | 7.012 | 7.012 |
| Fe I | 6229.2261 | 45.000 | 5.05 | 46.651 | 46.651 | 7.039 | 7.039 |
| Fe I | 6232.6401 | 80.500 | 3.27 | 100.902 | 100.902 | 6.860 | 6.860 |
| Fe I | 6240.6460 | 75.500 | 3.98 | 69.813 | 69.813 | 7.161 | 7.161 |
| Fe I | 6254.2578 | 120.000 | 5.93 | 131.369 | 131.369 | 6.955 | 6.955 |
| Fe I | 6265.1323 | 113.500 | 3.27 | 134.454 | 134.454 | 6.858 | 6.858 |
| Fe I | 6270.2236 | 57.500 | 2.58 | 66.851 | 66.851 | 6.921 | 6.921 |
| Fe I | 6297.7925 | 98.400 | 2.04 | 109.330 | 109.330 | 6.939 | 6.938 |
| Fe I | 6315.8110 | 31.300 | 1.91 | 27.959 | 27.987 | 7.142 | 7.141 |
| Fe I | 6322.6851 | 84.500 | 3.17 | 96.147 | 96.147 | 6.919 | 6.919 |
| Fe I | 6355.0283 | 77.700 | 1.63 | 77.785 | 77.785 | 7.069 | 7.069 |
| Fe I | 6358.6968 | 111.600 | 2.31 | 109.001 | 109.001 | 7.104 | 7.104 |
| Fe I | 6364.3638 | 9.600 | 1.08 | 8.969 | 8.996 | 7.103 | 7.102 |
| Fe I | 6380.7432 | 32.100 | 2.00 | 34.163 | 34.197 | 7.029 | 7.029 |
| Fe I | 6400.3169 | 123.800 | 4.96 | 116.224 | 116.224 | 7.159 | 7.159 |
| Fe I | 6408.0176 | 102.400 | 3.45 | 124.217 | 124.217 | 6.879 | 6.878 |
| Fe I | 6475.6240 | 61.300 | 2.85 | 61.185 | 61.185 | 7.072 | 7.072 |
| Fe I | 6481.8696 | 82.300 | 4.24 | 83.879 | 83.879 | 7.047 | 7.047 |
| Fe I | 6496.4658 | 40.400 | 1.66 | 39.830 | 39.950 | 7.080 | 7.077 |
| Fe I | 6518.3657 | 71.200 | 4.11 | 72.513 | 72.513 | 7.051 | 7.051 |
| Fe I | 6569.2139 | 61.600 | 2.09 | 55.331 | 55.497 | 7.152 | 7.151 |
| Fe I | 6574.2266 | 67.200 | 2.41 | 62.702 | 62.765 | 7.153 | 7.152 |
| Fe I | 6581.2090 | 43.400 | 0.94 | 43.521 | 43.565 | 7.068 | 7.067 |
| Fe I | 6593.8696 | 107.500 | 3.95 | 116.300 | 116.300 | 6.973 | 6.973 |
| Fe I | 6608.0249 | 29.300 | 2.81 | 28.184 | 28.212 | 7.097 | 7.096 |
| Fe I | 6609.1099 | 79.900 | 1.93 | 78.973 | 78.973 | 7.083 | 7.083 |
| Fe I | 6627.5439 | 10.200 | 0.47 | 9.574 | 9.584 | 7.102 | 7.102 |
| Fe I | 6633.7485 | 40.500 | 0.57 | 39.392 | 39.471 | 7.089 | 7.088 |
| Fe I | 6710.3179 | 37.000 | 2.87 | 39.508 | 39.548 | 7.017 | 7.017 |
| Fe I | 6733.1504 | 21.500 | 1.16 | 17.976 | 18.012 | 7.174 | 7.173 |
| Fe I | 6739.5205 | 29.400 | 1.10 | 33.278 | 33.311 | 6.981 | 6.981 |
| Fe I | 6750.1514 | 84.100 | 2.17 | 99.061 | 99.061 | 6.876 | 6.876 |
|  |  |  |  |  |  |  |  |


| $\epsilon$ Eri |  |  |  |  |  |  |  | $\epsilon$ Eri |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m} \AA)$ |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m}$ ¢ $)$ |  | $\varepsilon_{\mathrm{Fe}}$ (dex) |  |  |  | $\mathrm{EW}_{\text {obs }}(\mathrm{m}$ ) |  | $\mathrm{EW}_{\text {calc }}(\mathrm{m} \AA)$ |  | $\varepsilon_{\mathrm{Fe}}$ (dex) |  |
| el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE | el | $\lambda$ (air) | EW | $\sigma$ EW | nLTE | LTE | nLTE | LTE |
| Fe I | 4787.8267 | 62.100 | 1.16 | 60.670 | 61.594 | 7.388 | 7.387 | Fe I | 5861.1084 | 13.200 | 0.29 | 13.412 | 13.784 | 7.352 | 7.352 |
| Fe I | 4793.9614 | 17.100 | 0.83 | 17.945 | 18.405 | 7.333 | 7.332 | Fe I | 5873.2124 | 13.200 25.700 | 0.45 | 24.076 | 24.693 | 7.398 | 7.397 |
| Fe I | 4799.4058 | 48.400 | 1.01 | 49.217 | 50.068 | 7.344 | 7.344 | Fe I | 5881.2798 | 17.000 | 0.65 | 20.700 | 21.274 | 7.252 | 7.245 |
| Fe I | 4808.1479 | 40.200 | 1.52 | 40.079 | 40.855 | 7.363 | 7.363 | Fe I | 5909.9722 | 46.200 | 0.48 | 52.049 | 53.111 | 7.249 | 7.240 |
| Fe I | 4875.8770 4892.8589 | 81.900 67.300 | 1.29 1.47 | 88.390 68.316 | 89.464 | 7.261 | 7.255 | Fe I | 5927.7886 | 52.300 | 0.65 | 59.863 | 61.398 | 7.241 | 7.227 |
| Fe I | 4896.4385 | 46.900 | 1.53 | 46.904 | 47.715 | 7.360 | 7.360 | Fe I | 5940.9912 | 26.400 | 0.31 | 25.763 | 26.397 | 7.376 | 7.376 |
| Fe I | 4917.2300 | 76.900 | 1.42 | 85.709 | 87.103 | 7.234 | 7.219 | Fe I | 5952.7178 | 78.900 | 1.81 | 87.072 | 88.398 | 7.247 | 7.237 |
| Fe I | 4918.0127 | 69.500 | 2.49 | 69.638 | 70.914 | 7.358 | 7.358 | Fe I | 6003.0112 | 107.700 | 2.06 | 119.237 | 120.685 | 7.231 | 7.218 |
| Fe I | 4979.5859 | 26.400 | 1.12 | 22.747 | 23.282 | 7.453 | 7.447 | Fe I | 6012.2100 | 37.600 | 0.81 | 31.660 | 32.639 | 7.495 | 7.478 |
| Fe I | 5023.1860 | 48.000 | 1.92 | 49.568 | 50.580 | 7.333 | 7.333 |  | 6034.0352 | 9.900 | 0.26 | 12.836 | 13.192 | 7.232 | 7.223 |
| Fe I | 5023.4976 | 41.600 | 1.26 | 37.873 | 38.685 | 7.430 | 7.426 | Fe I | 6079.0078 | 56.500 | 0.86 | 57.526 | 58.880 | 7.343 | 7.343 |
| Fe I | 5031.9141 | 36.400 | 0.50 | 40.438 | 41.348 | 7.285 | 7.282 | Fe I | 6082.7100 | 57.000 | 0.81 | 53.693 | 55.013 | 7.434 | 7.427 |
| Fe I | 5054.6426 | 50.100 | 1.63 | 54.637 | 55.525 | 7.256 | 7.247 | I | 6093.6431 | 36.700 | 0.48 | 36.471 | 37.406 | 7.365 | 7.364 |
| Fe I | 5067.1494 | 85.100 | 1.44 | 92.260 | 93.665 | 7.261 | 7.254 | Fe I | 6096.6641 | 51.500 | 0.36 | 50.781 | 51.765 | 7.372 | 7.372 |
| Fe I | 5088.1533 | 47.300 | 1.75 | 45.902 | 46.791 | 7.386 | 7.385 | Fe I | 6098.2441 | 21.800 | 0.28 | 18.299 | 18.807 | 7.460 | 7.453 |
| Fe I | 5109.6519 | 87.900 | 1.09 | 85.879 | 87.364 | 7.388 | 7.387 |  | 6120.2466 | 17.500 | 0.35 | 14.934 | 15.753 | 7.448 | 7.440 |
| Fe I | 5129.6309 | 59.000 | 2.22 | 64.240 | 65.285 | 7.279 | 7.276 | Fe I | 6127.9063 | 58.200 | 0.92 | 66.746 | 68.039 | 7.222 | 7.204 |
| Fe I | 5228.3760 | 72.100 | 0.98 | 67.018 | 68.177 | 7.443 | 7.437 |  | 6151.6172 | 69.900 | 1.51 | 70.949 | 72.694 | 7.338 | 7.336 |
| Fe I | 5247.0503 | 97.900 | 2.42 | 93.933 | 96.838 | 7.452 | 7.453 | Fe I | 6165.3599 | 54.300 | 0.74 | 61.638 | 62.896 | 7.238 | 7.225 |
| Fe I | 5253.0210 | 34.400 | 1.26 | 31.542 | 32.417 | 7.427 | 7.422 |  | 10.5059 | 93.000 | 1.97 | 95.332 | 97.676 | 7.331 | 7.330 |
| Fe I | 5285.1274 | 33.100 | 1.04 | 31.930 | 32.682 | 7.384 | 7.383 |  | 6173.3345 | 93.000 | 26 | 91.127 | 93.272 | 7.395 | 7.395 |
| Fe I | 5293.9590 | 34.200 | 1.29 | 39.915 | 40.771 | 7.241 | 7.231 |  | 6180.2026 | 76.000 | 1.28 | 77.749 | 79.336 | 7.326 | 7.324 |
| Fe I | 5315.0698 | 40.600 | 1.32 | 41.068 | 41.949 | 7.351 | 7.351 | Fe I | 6187.3979 | 8.800 | 0.13 | 7.883 | 8.160 | 7.414 | 7.412 |
| Fe I | 5320.0356 | 31.300 | 0.55 | 28.359 | 29.027 | 7.429 | 7.425 | Fe I | 6187.9893 | 63.900 | 0.80 | 68.032 | 69.209 | 7.295 | 7.293 |
| Fe I | 5322.0405 | 81.700 | 1.51 | 87.262 | 88.862 | 7.250 | 7.229 |  | 6199.506 | 8.400 | 0.17 | 8.221 | 8.528 | 7.371 | 7.370 |
| Fe I | 5326.1426 | 54.400 | 1.07 | 54.847 | 55.796 | 7.351 | 7.351 |  | 6200.3125 | 96.200 | 1.32 | 95.065 | 97.005 | 7.380 | 7.380 |
| Fe I | 5361.6250 | 56.200 | 2.29 | 52.155 | 53.274 | 7.429 | 7.424 |  | 6226.734 | 39.400 | 0.26 | 39.677 | 40.570 | 7.355 | 7.355 |
| Fe I | 5401.2666 | 31.700 | 0.54 | 29.618 | 30.315 | 7.406 | 7.403 | Fe | 6229.2261 | 55.500 | 0.77 | 59.213 | 60.483 | 7.283 | 7.277 |
| Fe I | 5409.1333 | 66.200 | 1.13 | 63.695 | 64.863 | 7.400 | 7.398 |  | 6240.646 | 71.400 | 1.13 | 71.395 | 73.076 | 7.360 | 7.360 |
| Fe I | 5412.7837 | 23.300 | 0.62 | 29.159 | 29.876 | 7.225 | 7.213 | Fe | 6265.132 | 114.200 | 1.62 | 121.176 | 124.283 | 7.264 | 7.238 |
| Fe I | 5417.0332 | 37.300 | 1.66 | 37.142 | 38.016 | 7.363 | 7.363 | Fe I | 6271.2778 | 36.600 | 0.71 | 39.277 | 40.202 | 7.306 | 7.304 |
| Fe I | 5432.9478 | 80.500 | 1.33 | 78.216 | 79.812 | 7.393 | 7.392 | Fe I | 6293 | 15.200 | 0.24 | 13.927 | 14.358 | 7.406 | 7.404 |
| Fe I | 5436.2949 | 47.100 | 0.71 | 46.926 | 47.933 | 7.363 | 7.363 | Fe I | 6297.7925 | 101.200 | 1.15 | 102.549 | 105.071 | 7.338 | 7.336 |
| Fe I | 5441.3389 | 35.300 | 0.98 | 39.922 | 40.778 | 7.270 | 7.265 | Fe I | 6311.4995 | 45.300 | 0.46 | 43.097 | 44.157 | 7.407 | 7.404 |
| Fe I | 5452.0884 | 20.300 | 0.31 | 18.724 | 19.224 | 7.407 | 7.405 | Fe I | 6315.8110 | 52.300 | 0.64 | 55.433 | 56.564 | 7.305 | 7.303 |
| Fe I | 5460.8726 | 14.300 | 0.20 | 18.229 | 18.754 | 7.227 | 7.214 | Fe I | 6322.6851 | 98.200 | 1.13 | 97.518 | 99.610 | 7.372 | 7.372 |
| Fe I | 5466.9873 | 44.200 | 1.01 | 46.632 | 47.535 | 7.309 | 7.308 | Fe I | 6338.8760 | 49.600 | 0.26 | 52.195 | 53.643 | 7.317 | 7.316 |
| Fe I | 5470.0928 | 33.600 | 0.52 | 28.896 | 29.637 | 7.460 | 7.452 | Fe I | 6355.0283 | 90.200 | 1.63 | 86.302 | 88.063 | 7.431 | 7.425 |
| Fe I | 5472.7085 | 55.100 | 0.82 | 51.497 | 52.494 | 7.429 | 7.424 | Fe I | 6364.3638 | 35.300 | 0.56 | 30.436 | 31.345 | 7.459 | 7.450 |
| Fe I | 5473.1626 | 25.000 | 0.92 | 25.579 | 26.208 | 7.346 | 7.346 | I | 6380.7432 | 60.200 | 0.62 | 65.528 | 66.865 | 7.273 | 7.267 |
| Fe I | 5483.0986 | 55.500 | 1.15 | 61.068 | 62.124 | 7.258 | 7.250 | Fe I | 6469.1919 | 67.700 | 0.84 | 66.058 | 67.891 | 7.384 | 7.384 |
| Fe I | 5487.1450 | 45.200 | 0.62 | 45.801 | 46.783 | 7.349 | 7.349 | Fe I | 6481.8696 | 85.800 | 0.83 | 83.845 | 85.907 | 7.398 | 7.397 |
| Fe I | 5522.4463 | 53.000 | 0.63 | 54.136 | 55.185 | 7.338 | 7.338 | Fe I | 6495.7412 | 51.100 | 2.55 | 58.102 | 59.714 | 7.251 | 7.238 |
| Fe I | 5524.2495 | 6.000 | 0.24 | 5.783 | 5.950 | 7.377 | 7.377 | Fe I | 6496.4658 | 77.000 | 2.18 | 85.143 | 87.237 | 7.252 | 7.235 |
| Fe I | 5539.2798 | 23.600 | 0.41 | 28.103 | 28.794 | 7.249 | 7.241 | Fe I | 6518.3657 | 76.800 | 0.96 | 82.389 | 84.156 | 7.258 | 7.240 |
| Fe I | 5543.9355 | 74.800 | 0.86 | 79.838 | 81.136 | 7.278 | 7.271 | Fe I | 6533.9282 | 45.500 | 0.41 | 41.286 | 42.345 | 7.440 | 7.433 |
| Fe I | 5546.5059 | 62.200 | 0.90 | 62.448 | 63.657 | 7.356 | 7.356 | Fe I | 6574.2266 | 58.200 | 0.73 | 53.009 | 55.046 | 7.478 | 7.458 |
| Fe I | 5549.9487 | 13.700 | 0.68 | 13.528 | 13.903 | 7.367 | 7.367 | Fe I | 6581.2090 | 39.300 | 0.32 | 41.726 | 43.284 | 7.307 | 7.303 |
| Fe I | 5560.2114 | 59.000 | 0.94 | 67.221 | 68.523 | 7.232 | 7.217 | Fe I | 6591.3130 | 13.500 | 0.15 | 11.562 | 11.920 | 7.441 | 7.436 |
| Fe I | 5567.3911 | 87.700 | 1.65 | 83.118 | 84.555 | 7.450 | 7.441 | I | 6593.8696 | 110.100 | 2.08 | 111.865 | 114.616 | 7.334 | 7.331 |
| Fe I | 5600.2241 | 47.600 | 0.40 | 52.941 | 54.021 | 7.259 | 7.251 | Fe I | 6597.5591 | 51.100 | 0.51 | 51.551 | 52.873 | 7.352 | 7.353 |
| Fe I | 5618.6323 | 61.700 | 0.44 | 65.544 | 66.678 | 7.290 | 7.286 | Fe I | 6608.0249 | 33.900 | 0.21 | 35.258 | 36.386 | 7.330 | 7.329 |
| Fe I | 5619.5952 | 44.600 | 0.36 | 37.551 | 38.396 | 7.494 | 7.481 | Fe I | 6609.1099 | 87.000 | 1.45 | 83.457 | 85.422 | 7.428 | 7.423 |
| Fe I | 5622.9453 | 11.300 | 0.30 | 10.714 | 11.023 | 7.387 | 7.387 | Fe I | 6625.0215 | 41.000 | 1.78 | 36.261 | 37.890 | 7.464 | 7.450 |
| Fe I | 5636.6958 | 28.100 | 0.74 | 30.553 | 31.272 | 7.303 | 7.301 | Fe I | 6627.5439 | 34.500 | 0.27 | 29.424 | 30.178 | 7.473 | 7.463 |
| Fe I | 5641.4341 | 78.100 | 0.88 | 74.557 | 75.846 | 7.420 | 7.416 | Fe I | 6633.7485 | 76.600 | 1.31 | 78.703 | 80.391 | 7.329 | 7.328 |
| Fe I | 5650.7056 | 41.600 | 0.25 | 39.069 | 40.655 | 7.406 | 7.402 | Fe I | 6667.4180 | 12.900 | 0.11 | 15.406 | 15.981 | 7.265 | 7.257 |
| Fe I | 5651.4688 | 22.900 | 0.42 | 19.775 | 20.282 | 7.445 | 7.440 | Fe I | 6667.7104 | 14.000 | 0.15 | 10.735 | 11.067 | 7.497 | 7.485 |
| Fe I | 5652.3174 | 33.600 | 0.51 | 30.411 | 31.127 | 7.432 | 7.427 | Fe I | 6699.1411 | 10.300 | 0.22 | 10.786 | 11.120 | 7.337 | 7.336 |
| Fe I | 5655.1763 | 60.300 | 1.08 | 57.515 | 59.849 | 7.403 | 7.400 | Fe I | 6703.5659 | 54.300 | 0.51 | 52.242 | 53.527 | 7.403 | 7.400 |
| Fe I | 5661.3447 | 30.200 | 0.30 | 33.681 | 34.474 | 7.283 | 7.279 | Fe I | 6710.3179 | 35.100 | 0.18 | 38.042 | 39.545 | 7.295 | 7.289 |
| Fe I | 5679.0229 | 71.200 | 0.86 | 73.763 | 75.499 | 7.324 | 7.323 | Fe | 6732.0649 | 9.700 | 0.24 | 12.902 | 13.301 | 7.216 | 7.201 |
| Fe I | 5680.2402 | 14.000 | 0.35 | 11.608 | 11.930 | 7.456 | 7.450 | Fe | 6746.9536 | 8.700 | 0.22 | 9.979 | 10.362 | 7.292 | 7.288 |
| Fe I | 5691.4971 | 49.400 | 0.53 | 48.868 | 49.916 | 7.370 | 7.370 | Fe I | 6750.1514 | 94.000 | 1.05 | 97.706 | 100.109 | 7.296 | 7.285 |
| Fe I | 5698.0200 | 22.100 | 0.38 | 27.532 | 28.209 | 7.223 | 7.210 | Fe I | 6752.7065 | 42.300 | 0.72 | 44.394 | 45.532 | 7.319 | 7.318 |
| Fe I | 5701.5444 | 108.900 | 1.89 | 115.451 | 117.567 | 7.267 | 7.253 | Fe I | 6786.8584 | 32.800 | 0.46 | 31.453 | 32.226 | 7.388 | 7.387 |
| Fe I | 5705.4644 | 49.600 | 0.44 | 54.390 | 55.500 | 7.270 | 7.264 | Fe I | 6804.2710 | 18.400 | 0.23 | 19.084 | 19.654 | 7.339 | 7.339 |
| Fe I | 5717.8325 | 73.200 | 1.40 | 79.041 | 80.408 | 7.265 | 7.255 | Fe I | 6810.2622 | 57.200 | 1.07 | 61.805 | 63.195 | 7.284 | 7.279 |
| Fe I | 5731.7617 | 71.200 | 0.97 | 66.680 | 67.833 | 7.440 | 7.434 | Fe II | 5325.5522 | 29.200 | 1.12 | 25.064 | 24.742 | 7.483 | 7.494 |
| Fe I | 5741.8477 | 43.000 | 0.44 | 39.403 | 40.248 | 7.434 | 7.429 | Fe II | 5425.2485 | 20.900 | 0.74 | 23.659 | 23.355 | 7.270 | 7.271 |
| Fe I | 5754.4023 | 22.300 | 0.94 | 26.654 | 27.337 | 7.249 | 7.241 | Fe II | 5534.8379 | 34.100 | 0.60 | 34.660 | 34.181 | 7.345 | 7.344 |
| Fe I | 5759.2622 | 9.000 | 0.38 | 7.248 | 7.464 | 7.464 | 7.457 | Fe II | 6084.1016 | 8.600 | 0.20 | 7.516 | 7.405 | 7.431 | 7.434 |
| Fe I | 5760.3438 | 30.900 | 0.71 | 36.347 | 37.165 | 7.242 | 7.232 | Fe II | 6149.2461 | 14.300 | 0.54 | 14.102 | 13.949 | 7.369 | 7.369 |
| Fe I | 5838.3716 | 29.700 | 0.34 | 29.669 | 30.367 | 7.361 | 7.361 | Fe II | 6238.3857 | 20.800 | 0.32 | 20.268 | 20.028 | 7.379 | 7.380 |
| Fe I | 5849.6831 | 11.200 | 0.48 | 11.828 | 12.169 | 7.332 | 7.331 | Fe II | 6247.5571 | 27.400 | 0.18 | 25.281 | 24.957 | 7.425 | 7.430 |
| Fe I | 5853.1484 | 20.100 | 0.29 | 18.880 | 19.687 | 7.397 | 7.396 | Fe II | 6369.4590 | 6.400 | 0.15 | 8.691 | 8.529 | 7.203 | 7.211 |
| Fe I | 5855.0757 | 28.400 | 0.53 | 32.408 | 33.239 | 7.275 | 7.271 | Fe II | 6456.3794 | 35.000 | 0.19 | 33.637 | 33.173 | 7.397 | 7.399 |
| Fe I | 5858.7778 | 19.700 | 0.43 | 19.812 | 20.341 | 7.357 | 7.357 | Fe II | 6516.0767 | 30.400 | 0.32 | 30.798 | 30.135 | 7.349 | 7.348 |

## E | List of publications

## Refereed

1- Non-LTE iron abundances in cool stars: The role of hydrogen collisions (submitted to Astronomische Nachrichten)

2- The role of Hydrogen collisions in non-LTE iron abundances: Introducing the quantum fitting method (in prep.)

## Non-refereed conference proceedings

1- Non-LTE iron abundance determination of a sample of Kepler red giants (EAS Publications Series, Vol. 63, 2013, pp.407-409).

2- NLTE iron abundance determination in red giants (SF2A-2013: Proceedings of the Annual meeting of the French Society of Astronomy and Astrophysics. Eds.: L. Cambresy, F. Martins, E. Nuss, A. Palacios, pp.119-121)

# Non-LTE iron abundances in cool stars: The role of hydrogen collisions 

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In the aim of determining accurate iron abundances in stars, this work is meant to empirically calibrate H-collisions crosssections with iron, where no quantum mechanical calculations have been published yet. Thus, a new iron model atom has been developed, which includes hydrogen collisions for excitation, ionization and charge transfer processes. We show that collisions with hydrogen leading to charge transfer are important for an accurate non-LTE modeling. We apply our calculations on several benchmark stars including the Sun, the metal-rich star $\alpha$ Cen A and the metal-poor star HD140283.

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## 1 Introduction

Iron plays an important role in studying the atmospheres of cool stars. It is often used as a proxy to the total metal content and metallicities in stars.

Neutral iron lines, Fe I, have been shown to be subject to non-LTE effects (Lind et al. 2012; Mashonkina et al. 2011; Thévenin \& Idiart 1999). This deviation from LTE grows towards lower metallicities, due to a decreasing number of electrons donated by metals which decreases the collisional rates. Thus, a non-LTE modeling of the spectra of these stars becomes important, which in turn requires a good knowledge of a bulk of atomic data for each atom under consideration. A common problem in non-LTE calculations comes from uncertainties in the underlying atomic data, of which, in cool stars, the inelastic neutral hydrogen collisional rates are the most significant source.

Quantum calculations for hydrogen collisional rates have recently been calculated for a small number of elements including Li (Belyaev \& Barklem 2003), Na (Barklem et al. 2010), Mg (Belyaev et al. 2012), Al (Belyaev 2013) and Si (Belyaev et al. 2014). For iron, however, no quantum calculations have been published yet.
In the lack of quantum data, a common practice is to estimate the hydrogen collisional rates using the classical Drawin approximation (Drawin 1968, 1969) which is a modified version of Thomson (1912) classical $\mathrm{e}^{-}+$atom ionization rate equation, extended by Drawin to that of same atoms $(A+A)$ excitation and ionization collisions, where $A$ corresponds to an element species.
Drawin's approximation was then rewritten by Steenbock

[^34]\& Holweger (1984) for inelastic H + atom collisions, which was then reviewed and re-derived by Lambert (1993). Both their approaches apply only to allowed excitation collisional transitions due to the dependence of the collisional rates on the transition's oscillator strength $f$-value in Drawin's equation.

Upon comparison with quantum calculations, the Drawin approximation has been shown to overestimate the collisional rates by several orders of magnitude (Barklem et al. 2011), which is commonly treated by applying a multiplicative scaling fudge factor $S_{H}$ to the Drawin rate equation by using different calibration methods on reference stars.

Recent non-LTE abundance studies using quantum calculations revealed that charge transfer (CT) process, i.e. $A+\mathrm{H} \rightleftharpoons A^{+}+\mathrm{H}^{-}$, can play a more important role than excitation (Lind et al. 2011; Osorio et al. 2015). To our knowledge, no study has yet tested the inclusion of $\mathrm{H}+\mathrm{Fe}$ charge transfer collision in their non-LTE calculations, which was an important reason that motivated this work.

In this article, we aim at testing the role of the different $\mathrm{H}+\mathrm{Fe}$ collisional processes including excitation, ionization and charge transfer in non-LTE calculations, using a newly developed iron model atom, and starting from well defined non-spectroscopic atmospheric parameters for a set of benchmark stars.

## 2 Method

We performed non-LTE, 1D modeling of Fe I and Fe II spectral lines using the radiative transfer code MULTI2. 3 (Carlsson 1986, 1992), which solves the statistical equilibrium and radiative transfer equations simultaneously for the
element in question, through the Accelerated Lambda Iteration (ALI) approximation (Scharmer 1981). In the sections below, we present the observational data including the spectra and measured equivalent widths in Sect. 2.1, the model atmospheres and atmospheric parameters adopted for the stars under study in Sect. 2.2, and the newly developed Fe I/Fe II model atom used in the non-LTE calculations in Sect. 2.3.

### 2.1 Observational data

The spectra of the stars in this work were obtained from the Gaia-ESO survey collaboration. They were observed by the UVES spectrograph of the VLT, and reduced by the standard UVES pipeline version 3.2 (Ballester et al. 2000). All the spectra have high signal to noise ratios ( $\mathrm{S} / \mathrm{N}>110$ ), and a high resolution of $R=70000$.

The equivalent widths (EW) for each star were measure automatically using a Gaussian fitting method with the Automated Equivalent Width Measurement code Robospect (Waters \& Hollek 2013). The Fe I and Fe II linelist chosen in the analysis is a subset of the Gaia-ESO survey "golden" linelist (v4 Heiter et al. (2015)), which was tested on the Sun. All lines that are blended and whose relative errors $\left(\frac{\sigma E W}{E W}\right)>0.3$, were removed from the linelist. In addition, only lines with EW between $10 \AA$ and $100 \AA$ in the Solar spectrum were included. The final number of lines used for each star is $\sim 100 \mathrm{Fe}$ I lines and 10 Fe II lines.

### 2.2 Model atmospheres

Three benchmark stars of different metallicities and stellar parameters were considered in this study, namely the Sun, the metal-rich dwarf $\alpha$ Centauri A and the metal-poor halo subgiant HD140283. Their atmospheric parameters were adopted from the study of the Gaia benchmark stars by Jofré et al. (2014), where the effective temperatures $T_{\text {eff }}$ and surface gravities $\log g$ were determined homogeneously and independently from spectroscopic models, while the stellar metallicities were determined spectroscopically from Fe I lines by fixing $T_{\text {eff }}$ and $\log g$ to the previous values and applying a line-by-line non-LTE correction to each line. The parameters are listed in Table 1.

1D MARCS (Gustafsson et al. 2008) atmospheric models were interpolated to the atmospheric parameters of each star using the code interpol_marcs. $f$ written by Thomas Masseron ${ }^{1}$, except for the Solar case where the reference Solar MARCS model was used. Background line opacities except iron, calculated for each star as a function of its atmospheric parameters and sampled to ~ 153000 wavelength points using the MARCS opacity package, were also employed in the MULTI2 . 3 calculations.

[^35]Table 1 Atmospheric parameters of the stars used in this study, adopted from Jofré et al. (2014).

| Star | $T_{\text {eff }}$ | $\log g$ | $[\mathrm{Fe} / \mathrm{H}]$ |
| :---: | :---: | :---: | :---: |
| Sun | 5777 | 4.43 | +0.00 |
| $\alpha$ Cen A | 5840 | 4.31 | +0.26 |
| HD140283 | 5720 | 3.67 | -2.36 |

### 2.3 Model atom

A new iron model atom including Fe I and Fe II energy levels, as well as the Fe III ground level has been developed with the most up-to-date atomic data available, including radiative and collisional transitions for all the levels.

### 2.3.1 Energy levels

The Fe I and Fe II energy levels were adopted from the NIST database ${ }^{2}$ from the calculations of Nave et al. (1994) and Nave \& Johansson (2013) respectively and supplemented by the predicted high-lying Fe I levels from Peterson \& Kurucz (2015) up to an excitation energy of 8.392 eV . The model was completed with the ground Fe III energy level. In order to reduce the large number of energy levels (initially 1939 fine structure levels), all the levels in our iron model atom, except the ground and first ionized states of Fe I and Fe II, were grouped into mean term levels from their respective fine structure levels using the code FORMATO (Merle et al., in prep.). In addition, all mean levels above 5 eV and lying within an energy interval of $0.0124 \mathrm{eV}\left(100 \mathrm{~cm}^{-1}\right)$ were combined into superlevels. The excitation potential of each superlevel is a weighted mean by the statistical weights of the excitation potentials of its corresponding mean levels.

The final number of levels in the model atom is 135 Fe I levels (belonging to 911 fine structure levels and 203 spectroscopic terms) and 127 Fe II levels (belonging to 1027 fine structure levels and 189 terms).

### 2.3.2 Radiative transitions

For our Fe I/Fe II model, we used the VALD3 (Ryabchikova et al. 2011) interface database ${ }^{3}$ to extract all the Fe I and Fe II radiative bound-bound transitions. In addition, the UV and IR lines corresponding to transitions from and to the predicted high lying levels have also been included in the model (Peterson \& Kurucz 2015). Individual transitions belonging to levels that have been combined to superlevels have also been combined into superlines using FORMATO. The superline total transition probability is a weighted average of $g f$-values of individual transitions, combined via the relation of Martin et al. (1988). Our final FeI/FeII model includes 9816 FeI (belonging to 81162 lines) and 16745

[^36]FeII (belonging to 113964 transitions) super transitions combined from the individual lines.

In addition to the b-b transitions, Fe I and Fe II energy levels were coupled via photoionization to the Fe II and Fe III ground levels respectively. For Fe I levels, the corresponding photoionization cross-section tables were calculated by Bautista (1997) for 52 LS terms and those for Fe II by Nahar \& Pradhan (1994) for 86 LS terms, and were extracted from the NORAD ${ }^{4}$ database (Nahar \& Collaboration). For the rest of the levels, the hydrogenic approximation was used to calculate threshold cross-sections via Kramer's semi-classical relation (Travis \& Matsushima 1968). All the photoionization energies extracted from NORAD were shifted to match the threshold ionization energies in NIST due to existing energy differences between their theoretical values (Verner et al. 1994). Sharp crosssection resonance peaks in the tables were smoothed as a function of photon frequencies and then using an opacity sampling method they were resampled to a maximum of 200 frequency points per transition.

### 2.3.3 Collisional transitions

All levels in our iron model were coupled via electron and neutral hydrogen atom collisional transitions. $\mathrm{e}^{-}$ b-b effective collisional strengths were included from the calculations of Pelan \& Berrington (1997) for the ground and first excited states of Fe I, and from Zhang \& Pradhan (1995) and Bautista \& Pradhan (1996) for 142 Fe II fine structure levels. For the rest of the levels, the Seaton (1962a) and Seaton (1962b) impact approximations were used to calculate the cross-sections for the allowed and forbidden transitions respectively. In addition, $\mathrm{e}^{-}$ ionization collisional transitions were included using the semi-classical approximation of Bely \& van Regemorter (1970).

For the H collisions, Lambert (1993) derivation of the Drawin approximation was used to calculate the rate coefficients $\langle\sigma v\rangle$, with the oscillator strength $f$ set to 1 for all transitions. This was motivated by the approach adopted by Steenbock (1985) who set the $Q$-factor ${ }^{5}$ in their $\mathrm{Mg}+\mathrm{H}$ rate equations equal to 1 for forbidden transitions. Another attempt to remove the oscillator strength dependence from the rate equations was by Collet et al. (2005), who set a constant $f=10^{-3}$ in the van Regemorter (1962) equation for the $\mathrm{e}^{-}$collisions for all transitions. In addition, recent quantum calculations for Mg and other elements found large H-collisional rates for forbidden transitions, which were comparable to the allowed ones (Feautrier et al.

[^37]2014).

We also adopt the Drawin approximation for charge transfer H collisions in the absence of any other suitable approximation.

All the levels in the model were coupled with b-b, b-f and charge transfer $\left(\mathrm{Fe}+\mathrm{H} \rightleftharpoons \mathrm{Fe}^{+}+\mathrm{H}^{-}\right) \mathrm{H}$ collisions. The rates were scaled with a different global multiplicative scaling factor, as follows:

- $\mathrm{S}_{\mathrm{H}}$ : multiplicative factor for b-b and b-f H collision rates.
- $\mathrm{S}_{\mathrm{H}}(\mathrm{CT})$ : multiplicative factor for charge transfer H collision rates.
Several modified model atoms were created using different scaling factors for each H collisional process. $\mathrm{S}_{\mathrm{H}}$ was varied between 0.0001 and 10 , in multiplication steps of 10 , while $\mathrm{S}_{\mathrm{H}}(\mathrm{CT})$ was varied between 0.1 and 10 in multiplication steps of 10 , in addition to the $S_{H}(C T)=0$ models.


## 3 non-LTE calculations and results

Non-LTE calculations were performed for each atomic model with a given $\mathrm{S}_{\mathrm{H}}$ and $\mathrm{S}_{\mathrm{H}}(\mathrm{CT})$. Thus, a total of 24 models were computed for each star. The calculated EW(calc) for each model were compared to the measured EW(obs) using the $\chi^{2}$ test:
$\chi^{2}=\frac{1}{\mathrm{~N}_{\text {lines }}} \sum_{\text {lines }}\left(\frac{\mathrm{EW}(\mathrm{calc})-\mathrm{EW}(\mathrm{obs})}{\sigma \mathrm{EW}(\mathrm{obs})}\right)^{2}$
where $\mathrm{N}_{\text {lines }}$ is the total number of lines used in the $\chi^{2}$ test. The variation of $\chi^{2}$ as a function of $S_{H}$ and $S_{H}(C T)$ for each star is shown in Fig. 1. The LTE $\chi^{2}$ are also shown for comparison.

For the Sun, it can be seen that when charge transfer rates are neglected, the best fit is obtained at $S_{H}=0.01$. Upon including charge transfer rates, smaller $\mathrm{S}_{\mathrm{H}}$ values are needed. For the metal-rich star $\alpha$ Cen A, larger values of $\mathrm{S}_{\mathrm{H}}$ and $\mathrm{S}_{\mathrm{H}}(\mathrm{CT})$ are favored. For the metal-poor star HD140283, large variations in $\chi^{2}$ are obtained with $S_{H}$ and $\mathrm{S}_{\mathrm{H}}(\mathrm{CT})$ showing that charge transfer process plays an important role in producing the best-fit. Similar to the Sun, the best fit is also obtained at $\mathrm{S}_{\mathrm{H}}=0.01$ upon neglecting the charge transfer rates, while smaller values of $\mathrm{S}_{\mathrm{H}}$ are needed when including them.

Comparing to recent studies, Mashonkina et al. (2011) and Bergemann et al. (2012) used Fe I/Fe II model atoms in their non-LTE abundance determinations, which are comparable to our model. Their calculations were also tested on benchmark stars including the Sun and HD140283, where they used the Drawin approximation scaled with an $\mathrm{S}_{\mathrm{H}}$-factor for the excitation and ionization H collisional rates. Charge transfer rates were not included in their calculations. They could not find a single $\mathrm{S}_{\mathrm{H}}$-factor that


Fig. $1 \quad \chi^{2}$ as a function of scaling factors $\mathrm{S}_{\mathrm{H}}$ and $\mathrm{S}_{\mathrm{H}}(\mathrm{CT})$ for the Sun, HD140283 and $\alpha$ Cen A. The dotted lines represent the $\chi^{2}$ values obtained in LTE.
would fit all stars. For metal-poor stars, Mashonkina et al. (2011) determined a value of $\mathrm{S}_{\mathrm{H}}=0.1$ while Bergemann et al. (2012) determined an optimum value of $S_{H}=1$. For solar-metallicity stars, both studies found that different $\mathrm{S}_{\mathrm{H}}$ values had no significant effect on the calculated abundances.

Similarly, we could not find a single set of $\mathrm{S}_{\mathrm{H}}$ values that would ensure a best fit for all stars. We could, however, note that including charge transfer H collisional rates is important in iron non-LTE calculations. When neglecting charge transfer rates, however, a large value of $S_{H}$ is needed for $\alpha$ Cen A ( $\mathrm{S}_{\mathrm{H}}>1$ ), while a smaller value is needed for the Sun and HD140283 ( $\mathrm{S}_{\mathrm{H}} \leq 0.01$ ), which is not in accordance with previous studies.

## 4 Conclusions

We performed iron non-LTE spectral line calculations for three benchmark stars with well determined atmospheric parameters, using hydrogen collisions for excitation and ionization processes, and including charge transfer rates for the first time. We show that the charge transfer rates are important to include in the non-LTE calculations, especially for the metal-poor star. They were found, however, to play a less important role with increasing metallicity for the Sun and the metal-rich star $\alpha$ Cen A, where non-LTE effects are of smaller magnitude. No single set of values for the scaling factors $\mathrm{S}_{\mathrm{H}}$ and $\mathrm{S}_{\mathrm{H}}(\mathrm{CT})$ was obtained for the different types of stars. This demonstrates the inability of the Drawin approximation to reproduce the correct behavior and magnitudes of hydrogen collision rates (see Barklem et al. (2011)). In the lack of quantum calculations for the hy-
drogen collision rates, more efficient models than the classical Drawin approximation are required. We are working on such a method based on semi-empirical fitting of the available quantum data for other chemical species.

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# NON-LTE IRON ABUNDANCE DETERMINATION OF A SAMPLE OF KEPLER RED GIANTS 

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#### Abstract

In the aim of calibrating non-LTE effects in atoms, particularly iron, for which quantum mechanical calculations for collisions with neutral hydrogen do not exist, we re-analyzed a sample of Kepler K red giant stars and determined both LTE and non-LTE FeI and FeII abundances, using asteroseismic fundamental atmospheric parameters. 1D, spherical MARCS model atmospheres were used for the abundance determinations. FeI and FeII lines with reliable oscillator strength values were selected. Results show better mutual agreement in abundances between neutral and singly ionized Fe lines as a function of equivalent width and excitation potential in NLTE as compared to that in LTE.


Keywords: Iron abundances, NLTE, Red Giants

## 1 Introduction

The study of iron abundances in cool stars plays an important role in understanding the Galactic chemical evolution, since there exists a wealth of Fe spectral lines even in metal-poor stars, which makes it a proxy for the total metal content in the star. Iron is also an important opacity contributor in the stellar atmosphere of late-type stars. Moreover, iron lines are used to derive fundamental atmospheric parameters (Effective temperature $T_{\text {eff }}$, surface gravity $\log g$ and microturbulent velocity $\xi$ ) of the star.

In stellar atmospheres, the statistical equilibrium of neutral iron can deviate from thermodynamic equilibrium due to the deviation of the mean intensity of ionizing radiation $J_{\nu}$ from the Planck function $B_{\nu}$ (Mashonkina et al. 2011), and thus it is important to perform non-local thermodynamic equilibrium (NLTE) line formation calculations in order to accurately determine abundances.

In his review, Asplund (2005) described NLTE as the case where "Everything depends on everything, everywhere". And thus in order to correctly synthesize and model stellar spectra to determine NLTE abundances, one has to take into account accurate atomic data including all possible radiative and collisional transitions between the corresponding levels of a model atom of the element under study, especially the collisions with neutral hydrogen which become important in metal poor stars where $\mathrm{n}_{H} / \mathrm{n}_{e} \sim 10^{5}$. However, collisional rates with hydrogen are usually treated using the semi-classical Drawin approximation (Drawin 1969) which is based on classical rather than quantum mechanics, and has been shown to overestimate the collisional rates up to 5 orders of magnitude (Belyaev \& Barklem 2003). And since quantum mechanical data are not yet available for iron, we attempt to calibrate these collisional rates by accurately modelling and determining NLTE FeI/FeII abundances.

## 2 Method

For this study, we selected a sample of bright Kepler red giants which have reliable asteroseismic fundamental atmospheric parameters, $T_{\text {eff }}$ and $\log g$. We used high resolution ( $\mathrm{R}=67000$ ) spectra (Thygesen et al. 2012) from the FIES (FIber-fed Echelle Spectrograph) spectrograph of the NOT (Nordic Optical Telescope) at La Palma,

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Fig. 1. Diagnostic plots of the results for FeI and FeII in LTE (left column) and NLTE (right column): abundances versus excitation potential and equivalent width for one of the sample stars of KIC ID 1726211.
to measure equivalent widths of a well selected list of non-blended lines from the inspect database* (Bergemann et al. 2012). The chosen lines have up-to-date averaged experimental oscillator strengths values from Gehren et al. (2001). Spherical 1D model atmospheres were interpolated ${ }^{\dagger}$ from the MARCS database (Gustafsson et al. 2008) and used with an FeI/FeII model atom (Thévenin \& Idiart 1999) to determine NLTE abundances using the spectral synthesis code MULTI2.2 (Carlsson 1986) and a curve-of-growth technique, while LTE abundances were calculated using the TURBOSPECTRUM code (Alvarez \& Plez 1998), (Plez 2012).

## 3 Results and Conclusions

Our LTE results show less deviations with respect to the mean in FeI abundances as a function of excitation potential and equivalent width ( $\sim 0.25$ dex) as compared to that of previous work on these stars. Bruntt et al. (2011) calculated LTE abundances and imposed ionization equilibrium between FeI and FeII lines to derive atmospheric parameters $\left(T_{\text {eff }}, \log g\right.$ and $\left.\xi\right)$. The deviations from the mean in their plots are up to 0.5 dex. It is important to note that there is also a difference of up to 400 K in $T_{\text {eff }}, 0.23$ dex in $\log g$ and 0.2 dex in metallicity, between our asteroseismic and their spectroscopic values of atmospheric parameters. This can have serious consequences on the further abundance determination using these parameters, and thus they have to be carefully chosen.

Our results also show better mutual agreement between FeI and FeII lines in NLTE as compared to LTE (see Fig.1) as a function of equivalent width and excitation potential, without imposing ionization equilibrium between the singly and ionized iron lines.

Future work aims at improving our results by calculating more accurate NLTE abundances, using a better and more complete iron model atom with up-to-date atomic data, and using the updated version of MULTI

[^39](MULTI2.3). This will allow us to quantify the effects of collision with neutral hydrogen and electrons, leading to more accurate iron abundance determinations in giant stars.

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# NLTE IRON ABUNDANCE DETERMINATION IN RED GIANTS 

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#### Abstract

Our aim is to perform Non-LTE iron abundance calculations on a sample of Kepler red giants with reliable fundamental atmospheric parameters from asteroseismology, specifically $\log g$, in order to calibrate for unknown atomic collisional effects with neutral hydrogen for which quantum mechanical data does not yet exist. Preliminary results show better mutual agreement between FeI and FeII lines as compared to LTE, as well as less FeI abundance dispersion than that of previous work.


## 1 Introduction

Iron is often considered as a proxy for the total metal content in a star, due to the wealth of lines in the optical spectrum. Its contribution to the opacity in the atmospheres of cool stars is large. Iron is also of prime interest for the understanding of the Galactic chemical evolution. Neutral iron line formation is known to deviate from local thermodynamic equilibrium (LTE) (See Asplund 2005) and thus it is vital to perform non-LTE calculations to accurately determine abundances

In order to correctly synthesize and model stellar spectra, one has to take into account accurate atomic data including all possible radiative and collisional transitions between the corresponding levels of a model atom of the element under study. This data is not always available, or of high enough quality. Specifically, the inelastic collisions with neutral hydrogen have been considered as the main source of uncertainty in atomic modelling (Barklem et al. 2011). It is usually treated using the semi-classical Drawin approximation (Drawin 1969), which is based on classical rather than quantum mechanics, and has been shown to overestimate the collisional rates up to 5 orders of magnitudes (Belyaev \& Barklem 2003). And since

[^40]quantum mechanical collisional data are not yet available for iron, we attempt at calibrating these collisional rates by accurately modelling and determining NLTE FeI/FeII abundances.

## 2 Method

For this study, we selected a sample of bright Kepler red giants which have reliable asteroseismic fundamental atmospheric parameters, $T_{\text {eff }}$ and $\log g$. We used high resolution ( $\mathrm{R}=67000$ ) spectra (Thygesen et al. 2012) from the FIES (FIber-fed Echelle Spectrograph) spectrograph of the NOT (Nordic Optical Telescope) at La Palma. We measured equivalent widths of a well selected non-blended lines from the INSPECT database ${ }^{3}$ (Bergemann et al. 2012). We have chosen the most accurate $\log g f$ values based on the experimental averaged values of Gehren et al. (2001). Spherical 1D model atmospheres were interpolated ${ }^{4}$ from the MARCS database (Gustafsson et al. 2008) and used with an FeI/FeII model atom (Thévenin \& Idiart 1999) to determine NLTE abundances using the spectral synthesis code MULTI2.2 (Carlsson 1986) and a curve-of-growth technique, while LTE abundances were calculated using the TURBOSPECTRUM code (Alvarez \& Plez 1998; Plez 2012). The inelastic collisions with neutral hydrogen have been treated using the semi-classical Drawin approximation (Drawin 1969) with a scaling fudge factor of $\mathrm{S}_{H}=1$.

## 3 Results and conclusions

Bruntt et al. (2011) used the same spectra to derive LTE abundances imposing ionization equilibrium between FeI and FeII lines to derive atmospheric parameters ( $T_{\text {eff }}, \log g$ and the microturbulent velocity $\xi$ ). Their method leads to a deviations in FeI abundance as a function of excitation potential and equivalent width of up to 0.5 dex with respect to the mean. It is important to note that there is a difference of up to 400 K in $T_{\text {eff }}, 0.23$ dex in $\log g$ and 0.2 dex in metallicity, between the asteroseismic and their spectroscopic values of atmospheric parameters. These differences have serious consequences on the abundance determination and thus have to be carefully chosen.

Our results show a better mutual agreement between FeI and FeII lines in NLTE as compared to LTE as a function of equivalent width and excitation potential. They also show less deviations with respect to the mean in LTE as compared to Bruntt et al. (2011) and even less deviations in NLTE (of up to $\sim 0.25$ dex). This shows that a more careful selection of lines with good $\log \mathrm{g} f$ values, and starting with asteroseismic parameters leads to different less dispersed abundances.

Future work, aims at improving the obtained results (less dispersion, better ionization equilibrium) by using a more complete iron model atom with up-todate atomic data and an updated version of the NLTE spectral synthesis code

[^41]MULTI2.3 in order to be able to calibrate the uncertain collisional effects of iron with neutral hydrogen and electrons. This should result in more accurate iron abundance determinations in red giants.

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[^1]:    ${ }^{1}$ See however the very recent, unpublished, results of Paul Barklem (private communication, 2015) presented in Chapter 7

[^2]:    ${ }^{1}$ Turbulent velocities include macro- and micro- turbulent velocities which correspond to both non-thermal components of the gas velocity which can cause broadening of the stellar spectral lines (explained in Sec. 2.3)

[^3]:    $\overline{{ }^{3} \text { expressed in units of erg } \cdot \mathrm{s}^{-1} \cdot \mathrm{~cm}^{-2} \cdot \mathrm{~Hz}^{-1}}$
    ${ }^{4}$ expressed in units of erg $\cdot \mathrm{s}^{-1} \cdot \mathrm{~cm}^{-2} \cdot \mathrm{~Hz}^{-1}$

[^4]:    ${ }^{5}$ expressed in units of dyne $\cdot \mathrm{cm}^{2} \cdot \mathrm{~Hz}^{-1}$
    ${ }^{6}$ expressed in $\mathrm{cm}^{2} \cdot \mathrm{~g}^{-1}$
    ${ }^{7}$ expressed in erg $\cdot \mathrm{s}^{-1} \cdot \mathrm{rad}^{2} \cdot \mathrm{~Hz}^{-1} \cdot \mathrm{~g}^{-1}$
    ${ }^{8}$ expressed in same units as $I_{\nu}$, and is proportional to the number of photons emitted per unit optical depth interval.

[^5]:    ${ }^{9}$ i.e. the physical variables such as temperature, density, etc., depend on the vertical geometric or optical depth only. A good approximation for stars with photospheres relatively thin with respect to the stellar diameter. For giant stars, however, the assumption of spherical atmospheres is more appropriate, due to their extended atmospheres.

[^6]:    ${ }^{10}$ Also denoted excitation potential (measured in eV).

[^7]:    ${ }^{11}$ Also denoted as Bremsstrahlung, important at high temperatures where the plasma is highly ionized.

[^8]:    $12 \int_{0}^{\infty} \phi(\nu) \mathrm{d} \nu=1$

[^9]:    ${ }^{13}$ Each transition from level $i$ to level $j$ is balanced by its opposite from $j$ to $i$.
    ${ }^{14}$ Inelastic collisions are those with transfer of energy to the target atom/ion and are more important to spectral line formation than elastic collisions (Pradhan and Nahar, 2011).
    ${ }^{15}$ Given its name by M.J. Seaton (1953)

[^10]:    ${ }^{16}$ Resonances result from incident electrons with insufficient energy to re-escape the atom's potential well, that become 'bound' in a doubly excited resonant state.

[^11]:    ${ }^{17}$ http://www.usm.uni-muenchen.de/people/ip/iron-project.html

[^12]:    ${ }^{18}$ transitions which are observed in the laboratory and which obey the quantum selection rules, unlike the forbidden transitions which violate it and whose probabilities of occurance are much smaller than allowed ones (Garstang, 1961)

[^13]:    ${ }^{19}$ http://vald.astro.uu.se/

[^14]:    ${ }^{20}$ http://marcs.astro.uu.se/
    ${ }^{21}$ http://www.oact.inaf.it/castelli/

[^15]:    ${ }^{1}$ Starting from the assumption that all particles (electrons and hydrogen atoms included) can be described by a single local kinetic energy $T$, i.e. $\frac{1}{2} m_{e} v_{e}^{2}=\frac{1}{2} m_{\mathrm{H}} v_{\mathrm{H}}^{2}=k_{\mathrm{B}} T$

[^16]:    ${ }^{2}$ Electrons in an atom which have the same principal and orbital quantum numbers, but not necessarily the same magnetic orbital and magnetic spin quantum numbers (see Chapter 4).

[^17]:    ${ }^{1}$ http://kurucz.harvard.edu/atoms.html

[^18]:    ²http://www.nist.gov/pml/data/asd.cfm

[^19]:    ${ }^{3}$ http://cdsweb.u-strasbrg.fr/OP.htx
    ${ }^{4}$ http://www.astronomy.ohio-state.edu/~csur/NORAD/norad.html
    ${ }^{5}$ The threshold energy of an atomic level is the minimum energy required for ionization.

[^20]:    ${ }^{6}$ http://kurucz.harvard.edu/atoms/2600/

[^21]:    ${ }^{1} \nu \sin i$ is referred to as the line of sight rotational velocity of the star, where $\nu$ is the rotational velocity at the equator of the star and $i$ is the angle of inclination between its axis of inclination and the line of sight toward the Earth.

[^22]:    ${ }^{2}$ The term $f_{\text {bol }}$ refers to the bolometric flux which is the total radiative flux from the star received at the Earth.
    ${ }^{3}$ Center for High Angular Resolution Astronomy: http://www.chara.gsu.edu/
    ${ }^{4}$ The Very Large Telescope Interferometer: https://www.eso.org/sci/facilities/paranal/telescopes/vlti.html
    ${ }^{5}$ The Two Micron All Sky Survey at IPAC: http://www.ipac.caltech.edu/2mass/

[^23]:    ${ }^{6}$ Excitation potential (EP) of an absorption line is the energy of its lower level.

[^24]:    ${ }^{7}$ The large frequency spacing for the Sun varies with both $n$ and $l$, but is in general around $135.229 \mu \mathrm{~Hz}$ (Bazot et al., 2011).

[^25]:    ${ }^{8}$ http://kepler.nasa.gov/Mission
    ${ }^{9}$ http://sci.esa.int/corot/
    ${ }^{10}$ https://cnes.fr/fr

[^26]:    ${ }^{11}$ In this dissertation, MULTI2.3 (Carlsson, 1986) was used for spectral synthesis and equivalent width calculations. See appendix B for details on the code and chapter 2 for details on the theory of stellar atmospheres employed by the code.

[^27]:    ${ }^{12}$ http://sci.esa.int/gaia/

[^28]:    ${ }^{13}$ http://www.eso.org/sci/facilities/paranal/instruments/uves.html
    ${ }^{14}$ http://www.eso.org/public/teles-instr/vlt/
    ${ }^{15} \mathrm{http}: / /$ simbad.u-strasbg.fr/simbad/
    ${ }^{16}$ http://obswww.unige.ch/gcpd/gcpd.html (Mermilliod et al., 1997)

[^29]:    ${ }^{17}$ http://sci.esa.int/hipparcos/

[^30]:    ${ }^{1}$ http://marcs.astro.uu.se/software.php

[^31]:    ${ }^{2}$ http://www.ifa.hawaii.edu/users/watersc1/robospect/

[^32]:    ${ }^{1}$ https://staggergrid.wordpress.com/

[^33]:    ${ }^{1}$ http://physics.nist.gov/cuu/Constants/index.html
    ${ }^{2}$ http://nssdc.gsfc.nasa.gov/planetary/factsheet/sunfact.html

[^34]:    $\star$ Corresponding author: rana.ezzeddine@umontpellier.fr

[^35]:    ${ }^{1} \mathrm{http}: / /$ marcs.astro.uu.se/software.php

[^36]:    ${ }^{2}$ http://www.nist.gov/pml/data/asd.cfm
    ${ }^{3}$ http://vald.inasan.ru/~vald3/php/vald.php

[^37]:    ${ }^{4}$ http://www.astronomy.ohio-state.edu/~csur/NORAD/norad.html
    ${ }^{5} Q=\left(\frac{\chi_{\mathrm{H}}^{\infty}}{\Delta E^{\mathrm{A}}}\right)^{2} f$, where $\chi_{\mathrm{H}}^{\infty}=13.6 \mathrm{eV}$ is the ionization potential of hydrogen, $\Delta E^{\mathrm{A}}$ is the transition energy of atom $A$ and $f$ is the oscillator strength of the transition.

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[^39]:    *www.inspect-stars.net
    $\dagger$ Masseron code: http://marcs.astro.uu.se/software.php

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[^41]:    ${ }^{3}$ WWW. inspect-stars.net
    ${ }^{4}$ Masseron code: http://marcs.astro.uu.se/software.php

