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Jönsson, Henrik

2015

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Citation for published version (APA):

Jönsson, H. (2015). *The cosmic origin of fluorine and sulphur: Infrared spectroscopic studies of red giants*. Department of Astronomy and Theoretical Physics, Lund University.

Total number of authors:

1

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The cosmic origin of fluorine and sulphur: Infrared spectroscopic studies of red giants

Henrik Jönsson

Thesis for the degree of Doctor of Philosophy

Lund Observatory
Department of Astronomy and Theoretical Physics
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UNIVERSITY


To be presented, with the permission of the Faculty of Science of Lund University, for public criticism in the Lundmark lecture hall (Lundmarksalen) at the Department of Astronomy and Theoretical Physics on Friday, the 12th of June 2015 at 13:00. Faculty opponent: Prof. Livia Origlia

Organization LUND UNIVERSITY Department of Astronomy and Theoretical Physics Box 43 SE-221 00 LUND Sweden		Document name DOCTORAL DISSERTATION	
		Date of issue 2015-05-19	
		Sponsoring organization	
Author(s) Henrik Jönsson			
Title and subtitle The cosmic origin of fluorine and sulphur: Infrared spectroscopic studies of red giants			
Abstract Disregarding the small primordial traces of the lightest elements, all metals have been formed in stellar processes, which means that the relative amount of metals in the Universe increases for every stellar generation. This build-up of elements is called chemical evolution and might be used both to constrain stellar models as well as understanding the formation and evolution of stellar populations. In this thesis I determine abundances of two of the least studied elements, fluorine and sulphur, in three different stellar populations in the Milky Way using infrared spectroscopy of giants. Regarding fluorine the chemical evolution is very unclear because the number of previous observations are small. The cosmic origin of fluorine could still be one or more of three different sources: asymptotic giant branch stars, core-collapse supernovae, or the winds of Wolf-Rayet stars. If the latter is confirmed by observations, fluorine would make a great proxy for the determining whether the initial mass function in the Bulge is different from the solar neighborhood, which has been suggested in several other types of works, but not all. If confirmed, that would tell us that the central parts of our Galaxy have evolved differently than the local Disk. In the thesis I find that all the fluorine in the solar neighborhood most likely was produced by asymptotic giant branch stars, but at the same time find possible indications of fluorine production by Wolf-Rayet stars in the Bulge, indeed suggesting an initial mass function of the Bulge that is skewed towards more massive stars as compared to the solar neighborhood. When it comes to sulphur, there have been several proposed trends for metal-poor stars. Interestingly some of these observations cannot be explained with classic models of Galactic evolution, thereby questioning some of our understanding of the formation and evolution of the Milky Way. In this thesis I find a Galactic evolution-trend of sulphur following the expected trend from established models and cannot confirm any of the more exotic trends.			
Key words: Chemical evolution, near-infrared and mid-infrared spectroscopy, stellar abundances			
Classification system and/or index terms (if any):			
Supplementary bibliographical information:		Language English	
ISSN and key title:		ISBN 978-91-7623-373-3	
Recipient's notes		Number of pages 94	Price
		Security classification	

Distribution by

 Henrik Jönsson, Department of Astronomy and Theoretical Physics
 Box 43, SE-221 00 Lund, Sweden

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Date 2015-05-11

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Cover: IC 418 (the Spirograph nebula) is one of the planetary nebulae for which fluorine abundance has been determined (Zhang & Liu, 2005), thereby showing the creation of fluorine in asymptotic giant branch stars. The expelled outer layers of the previous giant star is clearly visible, as well as the remaining white dwarf star in the center.

Credits: NASA/ESA and The Hubble Heritage Team STScI/AURA

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Faculty of Science, Department of Astronomy and Theoretical Physics

ISBN 978-91-7623-373-3 (printed version)

ISBN 978-91-7623-374-0 (electronic version)

LUNFD6/(NFAS-1046)/1-94/(2015)

Printed in Sweden by E-husets Tryckeri, Lund University
Lund 2015

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List of publications

This thesis is based on the following publications:

- I **Sulphur abundances in halo giants from the [S I] line at 1082 nm and the S I triplet around 1045 nm**
H. Jönsson, N. Ryde, P. E. Nissen, R. Collet, K. Eriksson, M. Asplund, and B. Gustafsson
Astronomy & Astrophysics 530, A144 (2011)

- II **Chemical evolution of fluorine in the Bulge: High resolution K-band spectra of giants in three fields**
H. Jönsson, N. Ryde, G. M. Harper, K. Cunha, M. Schultheis, K. Eriksson, C. Kobayashi, V. V. Smith, and M. Zoccali
Astronomy & Astrophysics 564, A122 (2014)

- III **Fluorine in the solar neighborhood: Is it all produced in asymptotic giant branch stars?**
H. Jönsson, N. Ryde, G. M. Harper, M. J. Richter, K. H. Hinkle
The Astrophysical Journal Letters 789, L41 (2014)

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Popular summaries

Popular summary in English

Practically only the two lightest elements, hydrogen and helium, were formed during the Big Bang when our Universe was born. All other elements have been formed, and keep being formed, in different processes in different types of stars. This means that all atoms, except hydrogen and helium, that build up all things, plants, animals, and humans in our surroundings have been formed in stars.

When stars have formed new elements, these can either be locked up inside the star (or stellar remnant), or be expelled into space through different processes. These expelled left-overs are then used as starting material for the formation of new stars and celestial bodies in the eternal cosmic cycle. The continuous atom production in stars means two things on an astronomical scale: the amount of heavier elements is constantly increasing in the Universe, and the later an astronomical object, for example a star, is formed in the history of the Universe, the more heavy elements does it contain. The area of astronomical research tracing this build-up of different elements is called Galactic chemical evolution, and its results might be used in two different ways depending on if the stellar process (or processes) creating the studied element is known or not. For elements with unknown origin, determining the chemical evolution might tell us where and when the element was formed and in what kind of star (or stars), which might give us insight into the lives of stars and how they form and evolve. In case the formation process of the element already has been established, measuring the chemical evolution of the element in question in a stellar population with unknown history, might help to constrain the formation and evolution of that particular stellar population. In this thesis I make spectroscopic observations of stars to determine the uncertain chemical evolution of the elements fluorine and sulphur with the aim of understanding their cosmic origin.

Regarding fluorine, the chemical evolution is very unclear because the number of previous observations are small. The cosmic origin of fluorine could still be one or more of three different sources: asymptotic giant branch stars, which are solar-like stars in a later evo-

lutionary stage of their lives, core-collapse supernovae, which are the explosions ending massive stars' lives, or very massive stars called Wolf-Rayet stars. In the thesis I find that all the fluorine in the solar neighborhood most likely was produced by asymptotic giant branch stars. The picture on the cover of the thesis shows a planetary nebula, which is the end-result of the asymptotic giant branch phase: the former giant star has shrunk to the small white dwarf in the middle of the picture, and around it the elements the giant star has produced and expelled into its surroundings are clearly visible. In practice my result means that all the fluorine we come in contact with, including that in our toothpaste, likely has been formed like this in the sun's since long dead relatives, and that the other two possible production sites, Wolf-Rayet stars and core-collapse supernovae, do not seem to contribute much fluorine.

However, if the production of fluorine in the very massive Wolf-Rayet stars can be confirmed by further observations, the fluorine abundance would make a great proxy for determining the amount of massive stars that has existed and died in a particular stellar population with unknown history. In some, but not all, earlier studies of the central parts of our Galaxy - the Bulge - it has indeed been suggested that the relative amount of heavy stars has been larger in the Bulge than in the solar neighborhood. In the thesis I find possible indications of fluorine production by Wolf-Rayet stars in the Bulge, indicating that the central parts of our Galaxy possibly have evolved differently than the more outer part where we live.

When it comes to sulphur, its chemical evolution is expected to be similar to the rest of the alpha-elements¹ and mainly be formed in core-collapse supernovae, but observations have suggested several trends for the sulphur content in old Galactic stars, thereby questioning some of our understanding of the formation and evolution of our Galaxy. One of the trends might, for example, be explained if there were a large amount of really powerful supernovae - hypernovae - in the early history of our galaxy, but that is not confirmed in any other observations. In this thesis I find a Galactic evolution-trend of sulphur following the expected trend from established models and do not find any evidence for an amount of hypernovae contradicting other observations.

¹Alpha-elements are elements that would be possible to form by adding alpha-particles together, for example oxygen, magnesium, silicon, sulphur, calcium, and titanium.

Populärvetenskaplig sammanfattning på svenska

I Big Bang, då vårt Universum skapades, bildades i princip endast de två lättaste grundämnen, väte och helium. Alla andra grundämnen har skapats, och skapas fortfarande, i olika typer av stjärnor under olika utvecklingsfaser. Detta betyder att precis alla atomer, förutom väte och helium, som bygger upp alla saker, växter, djur och människor i vår omgivning, har bildats i stjärnor.

När stjärnor har bildat nya grundämnen kan dessa antingen bindas kvar i stjärnan (eller stjärnresten), eller genom olika processer kastas ut i rymden. Dessa utkastade rester används sedan till grund för bildandet av nya stjärnor och himlakroppar i det eviga kosmiska kretsloppet. Stjärnornas ständiga atomproduktion betyder därför, på en astronomisk skala, två saker: halten tyngre grundämnen ökar hela tiden i Universum, och ju senare ett astronomiskt objekt, till exempel en stjärna, bildats, desto större halt tunga grundämnen innehåller det. Den typ av astronomisk forskning som går ut på att mäta den ökande halten av tyngre grundämnen kallas galaktisk kemisk utveckling, och dess resultat kan användas på två olika sätt beroende på om den specifika stjärnprocess (eller processer) som bildar det studerade grundämnet är känd eller ej. För grundämnen med okänt ursprung kan bestämmandet av den galaktiska kemiska utvecklingen ge oss information om när och i vilken typ av stjärna (eller stjärnor) som grundämnet bildas, vilket i sin tur kan ge oss insikt i stjärnors liv och hur de bildas och utvecklas. Ifall ett grundämnes ursprung redan är fastställt, kan uppmätandet av den kemiska utvecklingen i en population stjärnor med hittills okänd historia hjälpa till att fastställa hur stjärnpopulationen i fråga har bildats och utvecklats. I den här avhandlingen bestämmer jag, genom spektroskopiska observationer av stjärnor, de tidigare okända galaktiska kemiska utvecklingstrenderna för grundämnena fluor och svavel med målet att förstå deras kosmiska ursprung.

När det gäller fluor är den galaktiska kemiska utvecklingstrenden väldigt osäker då det endast finns ett fåtal tidigare observationer. Fluors kosmiska ursprung kan fortfarande vara från en eller flera av tre olika källor: asymptotiska jättestjärnor, som är sollika stjärnor fast i ett senare utvecklingssteg, kärnkollapsande supernovor, som är de explosioner som innebär slutet för massiva stjärnors liv, eller så kallade Wolf-Rayet-stjärnor som är väldigt massiva stjärnor. I den här avhandlingen drar jag slutsatsen att allt fluor i solens astronomiska närhet sannolikt har bildats av asymptotiska jättestjärnor. Bilden på omslaget av avhandlingen visar en planetarisk nebulosa som är slutresultatet av den asymptotiska jättestjärnan; den tidigare jättestjärnan har krympt ihop till den lilla vita dvärg som syns mitt i bilden och runt omkring syns tydligt de ämnen stjärnan bildat och kastat ut i sin närhet. I praktiken innebär alltså mitt resultat att allt fluor vi stöter på, även det i vår tandkräm, sannolikt har bildats på detta vis av solens sedan länge döda släktingar, och att de andra två föreslagna produktionsställena - Wolf-Rayet stjärnor och kärnkollapsande supernovor - inte verkar bidra med särskilt mycket fluor.

Kan dock fluorproduktion i de väldigt massiva Wolf-Rayet-stjärnorna bekräftas genom vidare observationer, innebär detta att fluorhalten kan användas för att avgöra andelen massiva stjärnor som funnits och dött i en population stjärnor med okänd historia. I vissa tidigare arbeten, men inte alla, som undersökt de centrala delarna av vår galax - Bulben - har det precis föreslagits att andelen massiva stjärnor har varit större i Bulben än i solens astronomiska närhet. I den här avhandlingen hittar jag möjliga indikationer på flouerbildning i Wolf-Rayet-stjärnor i Bulben, vilket skulle innebära att de centrala delarna av vår Galax har utvecklats annorlunda än den mer yttre belägna delen där vi bor.

Gällande svavel förväntas dess galaktiska kemiska utveckling följa de andra alfaämnen², och främst bildas i kärnkollapsande supernovor, men tidigare utförda observationer har uppvisat flera olika svavelhaltstrender för gamla stjärnor, och ifrågasätter därmed en del av vår förståelse av bildandet och utvecklingen av vår galax. En av trenderna kan till exempel eventuellt förklaras om det skedde en stor mängd riktigt kraftiga supernovor - hypernovor - tidigt i vår galax historia. I den här avhandlingen bestämmer jag en svavelhaltstrend som följer vad man förväntar sig från etablerade modeller och hittar inga indikationer på att andelen hypernovor skulle vara så stor att den motsäger andra observationer.

²Alfaämnen är grundämnena som skulle vara möjliga att bilda genom att addera allt fler alfapartiklar, till exempel syre, magnesium, kisel, svavel, calcium och titan.

Preface and acknowledgements

This thesis consists of two parts. The first part consists of Chapters 1-3 and describes the concept of tracing the cosmic origin of fluorine and sulphur via stellar abundances, and gives a brief background to my research. The second part includes the three research papers, summaries of the same, and some of my thoughts about the future.

I would like to thank my supervisor, Nils Ryde, for never ending support and enthusiasm, and guiding me in the world of science. My assistant supervisor, Dainis Dravins, is thanked for helpful suggestions concerning both the thesis as well as the articles. Furthermore, I would like to thank the rest of the staff and students at Lund Observatory for brightening my days and helping with assorted problems and helpfully answering questions. Especially the SPOP-group has helped with suggestions on how to improve my work in several ways.

Bengt Edvardsson, Kjell Eriksson, Thomas Nordlander, and Bertil Pettersson at Uppsala Observatory are thanked for their swift and polite answers to my numerous e-mails concerning matters mostly related to computers and the MARCS/BSYN/EQWI/SME programs.

Carlos Abia, Karsten Brogaard, Hans Bruntt, Katia Cunha, and Rafael Fraga Guerço are thanked for fruitful and inspiring discussions comparing different types of stellar model atmospheres and different methodologies to determine stellar parameters.

Financially, this research has been supported by the Royal Physiographic Society in Lund, Stiftelsen Walter Gyllenbergs fond and Märta och Erik Holmbergs donation, but also by grants from the Swedish Research Council, Per Westlings minnesfond, and Jacob A. Letterstedts resestipendiefond.

Last, but certainly not least, I would like to acknowledge that the most important person for the existence of this thesis is Ulla, without whom I most likely not even would have started this line of work.

Chapter 1

Introduction

One of the large questions in astronomy today is how galaxies, and their different parts, form and evolve. To be able to get closer to the answer, advancements need to be made in several areas, both theoretical and observational as well as in the laboratory. In this thesis I present my first contributions to this area of research, by observationally tracing the evolution of the diagnostically interesting, but scarcely studied, elements fluorine and sulphur. As I will explain later in the thesis, determining the evolution of fluorine might help in understanding the evolution of the central parts - the Bulge - of our own Galaxy, the Milky Way, and the evolution of sulphur might help in understanding the formation of disc galaxies like our own. Both atomic and molecular spectral lines in the near- and mid-IR have been used, and further both LTE and non-LTE as well as 1D and 3D models are explored when determining abundances.

1.1 Chemical evolution

Almost all elements but hydrogen and helium are synthesized in different stars during different stages of their evolution. These elements are then either expelled into the interstellar medium (ISM) or confined in the endstage of the stars. New stars formed from this processed material contain an evolved set of elements, visible to us through spectral lines formed in their stellar atmospheres. Assuming that the stellar interiors do not pollute their own atmosphere during their life times, they will serve as markers of the elemental abundance in the ISM at the time when they were formed. This means two things: older stars have, on average, smaller metal content, and by observing stars formed at different times the build-up of elements in different stellar populations can be traced. This is called chemical evolution.

The most important objects/events expelling processed material into the ISM are the asymptotic giant branch stars (AGB-stars) and supernovae (SN), but within this thesis also the Wolf-Rayet stars (W-R stars) are discussed and might indeed play a role for the production of fluorine.

An AGB star is an evolved star with masses typically in the range of $1M_{\odot} \leq M_{\star} \leq 10M_{\odot}$, which means that our Sun will evolve into an AGB star late in its lifetime. During the AGB-phase, processed material from the inner layers of the star is dredged up into the atmosphere by thermal pulses, and at the end of the AGB-phase, the star sheds its outer envelopes through stellar winds, thereby enriching the ISM with the products of its nuclear reactions. The most important elements deposited into the cosmic cycle by this process are carbon, nitrogen, and the s-elements (Sr, Y, Zr, Nb, Ba, and La), but also fluorine. The cover of this thesis shows a planetary nebula, i.e. the end-product of this process. The expelled material is clearly visible as a sphere, and in the middle is the small, left-over star: a white dwarf.

SNe are explosive events with the stars showing an enormous increase in luminosity, in fact they might outshine an entire galaxy (Prialnik, 2000). Historically they have been sorted in different categories, and the types most important for this thesis and the chemical evolution of our Galaxy are the type Ia and type II.

SN type Ia are believed to occur due to mass transfer in a white-dwarf binary star system driving the receiving white dwarf to a thermonuclear explosion. The life time of such a system spans from 10^7 years to 10^{10} years and more (Matteucci, 2012). From a chemical evolution point of view these events are an unparalleled source of iron.

SN type II are associated with the end stages of massive ($\geq 10M_{\odot}$) stars' lives and are due to core collapse. These stars have relatively short life times of the order of 10^6 - 10^7 years (Prialnik, 2000), and are able to produce a plethora of elements. The most important elements created in these events are the alpha-elements (see Section 3.1), of which sulphur is one. However, fluorine is also proposed to be formed in SNe type II, via the exotic ν -process where the enormous neutrino flux during the core collapse might, even if the cross section of the reaction is very low, turn a significant part of the neon in the remaining stellar outer layers into fluorine (Woosley et al., 1990). Core collapse SNe with very large masses and high explosive energies have slightly different yields of elements and are sometimes referred to as hypernovae (Nakamura et al., 2001).

Very massive stars with initial masses over $30M_{\odot}$ are believed to show significant mass loss already during their main sequence phase (Prialnik, 2000). The mass loss is due to the gravitation not being able to stand against the enormous radiative pressure on the outer envelopes. The absorption lines we see in stellar spectra are due to absorption of light by atoms and molecules in the outer layers of the star. The more abundant the element in question is, the higher the absorption, and, consequently, the radiative pressure on the atoms/molecules would be higher. This means that a more metal-rich envelope would feel

an even greater radiation pressure and that this mass loss is metal-dependent, which means that a more metal-rich massive star would shed more outer layers as compared to a metal-poor star of similar starting-mass. The number of stars created with this high mass are low, but even so, there have been several indications for the W-R stars to have an impact on the chemical evolution of the Bulge (see Paper II). The most important elements believed to be expelled into the ISM by the W-R winds are carbon, nitrogen, and fluorine (see Paper II for further details). These stars end their lives in a core collapse SN explosion.

In general, more massive stars are more short-lived than less massive stars, meaning, for example, that the process of SN type II start to pollute the ISM in a particular stellar population after a relatively short time as compared to the AGB stars. Knowing the distribution of stars with different mass (the initial mass function, IMF), the rate at which stars form (the star formation rate, SFR), and the yields of the different stellar processes described above, means that the chemical evolution of a stellar population might be modeled. This field of research is called galactic chemical evolution modeling. As can be understood from the amount of information needed as input to these models, they have several degrees of freedom, but the observations of abundance trends in different stellar populations for different elements might constrain the models to be a very powerful tool in understanding the formation and evolution of galaxies. Observationally determining the uncertain abundance trends of the elements fluorine and sulphur is the subject of this thesis.

1.2 From spectra to abundances

The way the abundance of an element is determined on the basis of a stellar spectrum is by modeling or synthesizing the spectrum. This is done by calculating the radiative transfer through a model atmosphere of the star, which relies on that the *kind* of star is known, i.e. that there exists a reasonable estimate of the fundamental stellar atmospheric parameters: effective temperature (T_{eff}), surface gravity ($\log g$), iron abundance ($[\text{Fe}/\text{H}]^1$), and the microturbulence (v_{mic}). For weak lines the strength of the line, the equivalent width, is proportional to the abundance of the element in question and the atomic transition probability, the $\log gf$ -value, meaning the strength of the line can be used to determine the abundance of the element in question. If a line is stronger and closer to being saturated it starts to grow larger wings and its strength does not only depend on the abundance of the element, but on the often uncertain damping parameters of the line. Lines in-between weak and strong are affected by the microturbulence parameter. This parameter does not affect the stellar model as such, but affects the strength of spectral lines differently. Only strong lines are altered and weak lines are unaffected. As such, the microturbulence

¹The bracket notation is defined as: $[A/B] \equiv \log \left(\frac{N_A}{N_B} \right)_* - \log \left(\frac{N_A}{N_B} \right)_\odot$, where N is the number density. $[\text{Fe}/\text{H}]$ is the metallicity and, for example, $[\text{F}/\text{Fe}]$ is the fluorine abundance.

parameter can empirically be determined by forcing the weak and intermediately strong spectral lines of a particular species (often Fe I) to give the same abundance. Therefore it affects the calculated synthetic spectrum a lot, and specifically the lines on the verge to being categorized as strong. As an example, the 12.2 μm HF line used in Paper III is rather strong in some of the observed stars, and the uncertainty of the microturbulence is likely the reason why the star α Tau is showing discrepant fluorine abundances as derived from the weak 2.3 μm HF line and the stronger 12.2 μm HF line.

Furthermore, to account for the broadening of the spectral lines due to convective motions in the stellar atmosphere and rotation of the star, a macroturbulence (v_{mac}), needs to be assigned to the star when fitting a synthetic spectrum. However, just like the microturbulence it does not affect the stellar model, only the synthetic spectrum.

1.2.1 Stellar parameters

To achieve the goals presented in this thesis, spectroscopy of stars in the infrared (IR) wavelength region will be necessary. However, constraining the stellar parameters is a problem in IR spectroscopy since the most widely used methods of determining these parameters make use of spectral features in the visual wavelength region. The most often used method to determine the stellar parameters spectroscopically is based on Fe I and Fe II lines: forcing the abundance as derived from spectral lines from high excited states to agree with abundances derived from low excitation lines determines the temperature, forcing the abundances as derived from Fe I and Fe II lines to be the same determines the $\log g$, and, as mentioned earlier, forcing abundances as derived from the weak and strong lines to agree will determine the microturbulence.

There are also other spectral features that have been used to determine stellar parameters, for example the wings of the $\text{H}\alpha$ -line is temperature sensitive in dwarf stars (Barklem et al., 2002), and the 6162 \AA Ca I-line has been used to constrain the gravity in giants (Edvardsson, 1988). Non-spectroscopic methods are also used: for some of the very brightest and closest stars, the temperature might be determined by direct observations of the angular diameter of the star (see for example Mozurkewich et al., 2003), and for more distant stars the infrared flux method of combining photometric observations with a calibration to get temperatures is very common (see for example González Hernández & Bonifacio, 2009, for one such calibration). When it comes to determining gravities many nearby stars have parallaxes measured by the Hipparcos satellite, which gives a good estimate of the distance to the star in question, and together with its luminosity this can constrain the surface gravity of the star. Right now this method is only possible to use in the relatively nearby stellar sample of Hipparcos, but in the coming years this method would probably be one of the most widely used, since the satellite Gaia will measure parallaxes even more accurately for about one billion stars situated in all the main stellar components in our Galaxy.

The all-spectroscopic approaches have the advantage of being independent of photometry and estimations of the extinction, which may be uncertain at long distances and in obscured regions, like for example the Galactic Bulge studied in Paper II. Also an all-spectroscopic method means you can analyze nearby and distant stars in the same way and thereby get a homogeneously analyzed sample with smaller possible systematic uncertainties.

Different ways of determining the stellar parameters are used in this thesis: in Paper I we use stellar parameters taken from the literature, in Paper II we use parameters determined from optical spectra of the same stars, and in Paper III we use temperatures and gravities derived from angular diameter measurements (Mozurkewich et al., 2003) and parallaxes (van Leeuwen, 2007), and metallicities determined from archive optical spectra of our targets when such are available, and taken from the literature otherwise. The precision of the derived abundances depends on the stellar parameters, and having to take stellar parameters from different literature sources will certainly introduce systematic errors. For this reason it is obviously best if the stellar parameters could be reliably determined within the project or taken from the same source.

Neither of the methods used to determine the so important stellar parameters in Paper II or III are described in those papers, but instead we refer to other papers for a description: Jönsson et al. (in prep) and Ryde et al. (2015). Since it turns out that the first of those papers is still not published I, for completeness, describe the method below.

The method used in Paper II

I have chosen the spectroscopic method described above of using optical Fe I and Fe II lines and worked on finding the best suited lines for constraining the temperatures and gravities for red giant stars. This means that the lines should have accurate transition probabilities, as well as showing a range of lines strengths and excitation energies. I have used the program *Spectroscopy Made Easy* (SME) (Valenti & Piskunov, 1996) to simultaneously fit all selected lines with a synthetic spectrum while varying all the stellar parameters (T_{eff} , $\log g$, $[\text{Fe}/\text{H}]$, v_{mic} , and v_{mac}). To better constrain the gravity I have used gravity sensitive wings of three Ca I lines, but since the wings of these lines also depend on the abundance of calcium I have included four weaker Ca I-lines and also kept the $[\text{Ca}/\text{Fe}]$ as a free parameter. All line-data used in determining the stellar parameters in Paper II have been taken from the Gaia-ESO line list (Heiter et al. (in prep.)) with two exceptions: the Fe II-lines have been updated with astrophysical $\log gf$ -values from Meléndez & Barbuy (2009) and wavelength-data from Nave & Johansson (2013). I initially chose the Fe I and Ca I lines which, according to the Gaia-ESO line list group, have transition probabilities from laboratory measurements with excellent accuracy, but when it comes to Fe II I included all lines which are visible in my spectra.

To minimize the uncertainties in the derived stellar parameters, these initially selected lines have been carefully investigated for (known) blends in a grid of model atmospheres (using version 7.10 of the Uppsala EQWI code) and only the lines that could be considered unblended for K-giants are kept. However, all lines are typically blended with lines from the TiO-molecule for $T_{\text{eff}} \lesssim 3800$ K. At these low temperatures the TiO-molecule shows such a massive amount of lines that these lines define a pseudo-continuum. This means that even if the TiO line list can be fully trusted, there will be problems with the placement of the continuum, which makes a proper analysis of these stars very difficult. Therefore $T_{\text{eff}} \lesssim 3800$ is the present limit of my method of determining the stellar parameters, but this could possibly be lowered if another (perhaps iterative) method of placing the continuum is used, or if another spectral region not as affected by the TiO-molecule would be observed. One example of the blending from TiO of one of the chosen Fe I-lines can be seen in Figure 1.1.

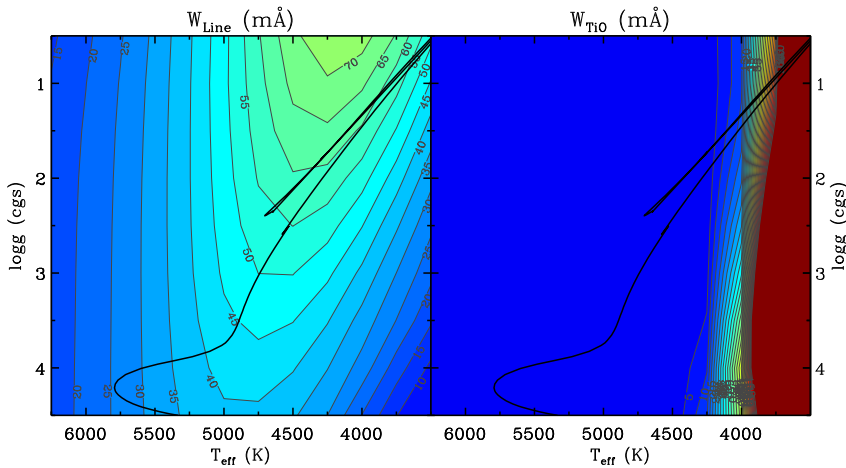


Figure 1.1: The left panel shows the equivalent width color coded and given in mÅ of the Fe I-line at 5855.0758 Å for different types of stars with solar metallicity. The right panel shows the total strength of TiO lines blending the Fe I-line, with the all-red region marking blending strengths more than 150 Å. All lines investigated show the same behavior: for $T_{\text{eff}} \lesssim 3800$ K the blending of TiO is so severe that the lines are impossible to use with the present method (see the text for details). Also shown, to guide the eye, are isochrones with $[\text{Fe}/\text{H}]=0.0$ and age 10 Gyr (Bressan et al., 2012).

The final line list consists of 39 lines in the wavelength range of the optical Bulge spectra, approximately 5800 Å to 6800 Å, and is presented together with the used data in Table 1.1. Regarding the broadening of spectral lines due to collisions with neutral hydrogen (van der Waals broadening) the data for all the listed lines are taken from Barklem & Asplund-Johansson (2005) and Barklem et al. (2000), with two exceptions: for the Fe I

line at 6793 Å values from Kurucz (2007) are used, and for the Ca I line at 5867 Å values from Smith (1988) are used.

Table 1.1: Atomic data for the spectral lines used in the determination of the stellar parameters (and calcium abundance). All atomic data are collected by the Gaia-ESO line list group and will be published in Heiter et al. (in prep.). For the three Ca I-lines marked with asterisks only the gravity-sensitive wings are used. The references are for wavelength, $\log gf$, and excitation energy respectively. In cases where several references are given for a quantity the value listed is a mean of the reference values.

Element	Wavelength (Å) (air)	$\log gf$	χ_{exc} (eV)	References
Fe I	5778.4533	-3.430	2.588	1, 2, 1
Fe I	5855.0758	-1.478	4.608	1, 2, 1
Fe I	6012.2098	-4.038	2.223	1, 3, 1
Fe I	6027.0508	-1.089	4.076	1, 4, 1
Fe I	6120.2464	-5.970	0.915	1, 5, 1
Fe I	6136.9938	-2.950	2.198	1, 4 & 6, 1
Fe I	6151.6173	-3.295	2.176	1, 3 & 4 & 6, 1
Fe I	6165.3598	-1.473	4.143	1, 4, 1
Fe I	6173.3343	-2.880	2.223	1, 6, 1
Fe I	6213.4294	-2.481	2.223	1, 4, 1
Fe I	6271.2779	-2.703	3.332	1, 2, 1
Fe I	6322.6850	-2.430	2.588	1, 4 & 7, 1
Fe I	6335.3299	-2.177	2.198	1, 4, 1
Fe I	6411.6480	-0.596	3.654	1, 3 & 4 & 8, 1
Fe I	6518.3657	-2.438	2.832	1, 2 & 4, 1
Fe I	6581.2092	-4.679	1.485	1, 3, 1
Fe I	6593.8695	-2.420	2.433	1, 4 & 6, 1
Fe I	6609.1097	-2.691	2.559	1, 4 & 7, 1
Fe I	6633.7487	-0.799	4.559	1, 4, 1
Fe I	6739.5204	-4.794	1.557	1, 3, 1
Fe I	6793.2582	-2.326	4.076	1, 2, 1
Fe I	6810.2622	-0.986	4.607	1, 4, 1
Fe I	6828.5912	-0.820	4.638	9, 10, 1
Fe I	6837.0056	-1.687	4.593	1, 2, 1
Fe I	6843.6554	-0.730	4.549	1, 11, 1
Fe II	5991.3721	-3.540	3.153	12, 13, 14
Fe II	6084.1030	-3.790	3.200	12, 13, 14
Fe II	6113.3192	-4.140	3.221	12, 13, 14
Fe II	6149.2459	-2.690	3.889	12, 13, 14
Fe II	6247.5590	-2.300	3.892	12, 13, 14

Continued on next page

Table 1.1 – continued from previous page

Element	Wavelength (Å) (air)	$\log gf$	χ_{exc} (eV)	References
Fe II	6432.6772	-3.570	2.891	12, 13, 14
Fe II	6456.3805	-2.050	3.903	12, 13, 14
Ca I	5867.5620	-1.570	2.933	15, 15, 15
Ca I*	6122.2170	-0.380	1.886	16, 17, 16
Ca I*	6162.1730	-0.170	1.899	16, 17, 16
Ca I	6166.4390	-1.142	2.521	18 & 19, 18, 18 & 19
Ca I	6169.0420	-0.797	2.523	18 & 19, 18, 18 & 19
Ca I*	6439.0750	0.390	2.526	18 & 19, 18, 18 & 19
Ca I	6499.6500	-0.818	2.523	18 & 19, 18, 18 & 19

References. (1) Kurucz (2007); (2) Bard & Kock (1994); (3) Bard et al. (1991) (4) O’Brian et al. (1991); (5) Blackwell et al. (1986); (6) Blackwell et al. (1982a) (7) Blackwell et al. (1982b); (8) Den Hartog et al. (2014); (9) Fuhr et al. (1988) (10) May et al. (1974); (11) Ruffoni et al. (2014); (12) Nave & Johansson (2013) (13) Meléndez & Barbuy (2009); (14) Kurucz (2013); (15) Smith (1988) (16) Smith & O’Neill (1975); (17) Aldenius et al. (2009) (18) Smith & Raggett (1981); (19) Smith (1981)

To test the accuracy of the method of determining the stellar parameters I have tested it against two stellar samples of red giant stars with independently determined stellar parameters with high accuracy, thus comprising a good set of bench-mark stars to test against. I have used 29 nearby giants with temperatures determined from angular diameter measurements (Mozurkewich et al., 2003), which is one of the most accurate methods, independent of the surface gravity, and 79 giants from the Kepler field with unprecedentedly well-determined surface gravities, determined from asteroseismology (Thygesen et al., 2012; Huber et al., 2014). I find that I am able to retrieve the temperatures of the Mozurkewich-stars with a standard deviation of the same order of magnitude as the uncertainties of those measurements, 67 K, and the gravities of the Kepler-stars with a standard deviation of 0.13 dex compared to the seismic value.

To get an idea of the impact that the signal-to-noise ratio (S/N) might have on the determination of the stellar parameters, I simulated a range of red giant spectra of different S/N . As a typical red giant spectrum, I chose to degrade the Arcturus spectrum of Hinkle et al. (2000) using the IDL-routine `x_addnoise`² to 100 realizations each of S/N 10, 15, 20, 25, 30, 35, 40, 45, 50, 55, 60, 65, 70, and 75 respectively (i.e. 1400 individual spectra) and analyzed them using the same method. The routine injects random noise drawn from a gaussian distribution corresponding to the demanded S/N into every datapoint

²<http://www.ucolick.org/~xavier/IDL/>

of the reduced spectrum. Depending on the detector used and the reduction process of the spectrum this might or might not represent realistic noise. However, this method can still be used to give a hint of some properties of the determined stellar parameters as a function of S/N. The results from the analysis can be seen in Figure 1.2. The horizontal line in each panel represents the value as determined from the original, high-S/N, atlas spectrum. Three conclusions can be directly drawn from this investigation:

- The spread in the results for $S/N \gtrsim 45$ are of the same order, for example giving uncertainties in temperatures below 50 K. This means that, as for determining stellar parameters for Arcturus-like stars, the observation time might be limited to a value reaching about this S/N. However, a higher S/N might be needed for cooler, more metal-rich stars where the line-blending is more serious. Furthermore a higher value might be needed to determine the abundance(s) of interest in the particular program: possibly one is forced to use very weak lines or just one line, making the abundance very sensitive to the noise.
- The spread in results seems to “explode” for $S/N \lesssim 20$, meaning that one should preferably, if possible, stay above this value.
- At the same time, for all S/N bins the “original” high-S/N parameters are, in the mean, derived, except for v_{mic} starting to show systematically higher values for $S/N \lesssim 15$. Also it is mainly the “whiskers” of the box-plots that grow for lower S/N - the box-sizes are of more similar sizes - meaning that the analysis of the majority of the spectra with even the lowest S/N results in reasonable values for the stellar parameters (the box marks the interquartile range, holding 50% of the data, while the whiskers extend out to the minimum/maximum values).

1.2.2 Modeling spectra

As always in computer models, simplifying assumptions are made in the modeling of the stellar atmosphere and the synthetic spectrum. The most severe assumption often made when modeling stellar atmospheres is the assumption of hydrostatic equilibrium where convection is treated in the mixing-length formulation. These models are usually referred to as 1D models as opposed to 3D hydrodynamical models where convective inhomogeneities are treated more physically. When it comes to calculating a synthetic spectrum, an often used simplification is the assumption of local thermodynamic equilibrium (LTE). In LTE the level population of the atoms is distributed due to the Boltzmann distribution and the ionization of elements is determined by the Saha equation. This means that in LTE, the energy distribution of matter and radiation is locally determined, and maintained by collisions. In synthesis referred to as “non-LTE” one or both of these assumptions are relaxed.

Obviously, non-LTE 3D analyses are more physical and describe a stellar atmosphere in a better way than LTE 1D models. However, the simplifying assumptions might in some kinds of stars, and for some spectral lines, describe the situation just as well as the more advanced models. Often LTE 1D models are used even when it is not known whether these assumptions are valid due to lack of better models; 3D models are emerging, but they are still not available for all kinds of stars and not widely spread, mostly since they are much more computationally demanding. Non-LTE modeling is made for some lines for one atomic species at a time and demands a lot more in terms of atomic data, like collisional cross sections, which often are lacking and are difficult to measure and/or calculate. Once a non-LTE model atom has been set up, non-LTE corrections are usually tabulated by specifying the abundance correction needed for the element in question when using a specific line in a star with specific stellar parameters. It should be noted that during recent years it has been realized that in some cases LTE 3D modeling show results less accurate than non-LTE 1D modeling: what seems to be needed to improve abundance determinations is the full non-LTE 3D treatment (Bergemann et al., 2012), which is very computationally challenging.

1.3 The evolution of infrared spectroscopy

The field of observational astrophysics has always benefitted from new technological advancements. For example new materials for mirrors in combination with fast computers have resulted in telescopes with adaptive optics compensating in real-time for fluctuations in the earth's atmosphere and the possibilities to build larger telescopes, the arrival of the CCD as light detector was of course a revolution for optical astronomy, the space based observatories have been able to detect objects never seen before, just to mention a few. Another recent advancement in observational astrophysics is the arrival of better detectors for IR light opening up a new wavelength range for spectroscopic stellar abundance analysis. There is a lot to win to explore the IR wavelengths, for example there are in general fewer spectral lines in the IR than in the visual region which means that fewer lines are blended, and some elements only reveal themselves through spectral lines in the IR. One such element is fluorine studied in this thesis. Furthermore the extinction of light due to dust does not affect the IR light as much as visual, meaning that IR observations are more time-efficient than visual when observing dust-obscured stellar populations like the Bulge (see Paper II). However, since the IR region has been less extensively used than the visual, the performance of IR diagnostics are less well tested. Doubtless, now is the optimal time to explore spectral lines and their usefulness of these less-explored spectral windows to space, since many of the observatories around the world are currently building high-resolution IR spectrometers, see Table 1.2. These next-generation IR spectrometers build upon the experiences from the present generation, being both technologically better with, for example, more efficient detectors, but more importantly they are cross-dispersed, offer-

ing a much wider wavelength-coverage, multiplying the usefulness of the instrument. For example the upgraded CRIRES+ spectrometer planned for 2017 will be able to record a stellar spectrum of the entire K-band in one observation, as opposed to the current, non-upgraded, CRIRES where it would take ten observations in ten different settings to record the entire K-band. With E-ELT not built yet, CRIRES+ is the instrument in the list planned for the largest presently available telescope, but since the IR spectral region, as described, has a lot to offer, there can be much interesting science made using the instruments already available at smaller telescopes: IGRINS and GIANO.

Table 1.2: Some new/planned IR spectrometers at large observatories.

Instrument	R	Telescope	Diam. (m)	Observatory	Coverage (μm)	Available
IGRINS	40000	H. Smith	2.7	McDonald	1.45-2.45	now
GIANO	50000	TNG	3.6	La Palma	0.95-2.45	now
ISHELL	80000	IRTF	3.0	Mauna Kea	1.20-5.00	2015
SPIRou	73500	CFHT	3.6	Mauna Kea	0.95-2.45	2017
CRIRES+	100000	VLT	8.2	Paranal	0.95-5.30	2017
HIRES	100000	E-ELT	39.3	Armazones	0.35-2.45	2024

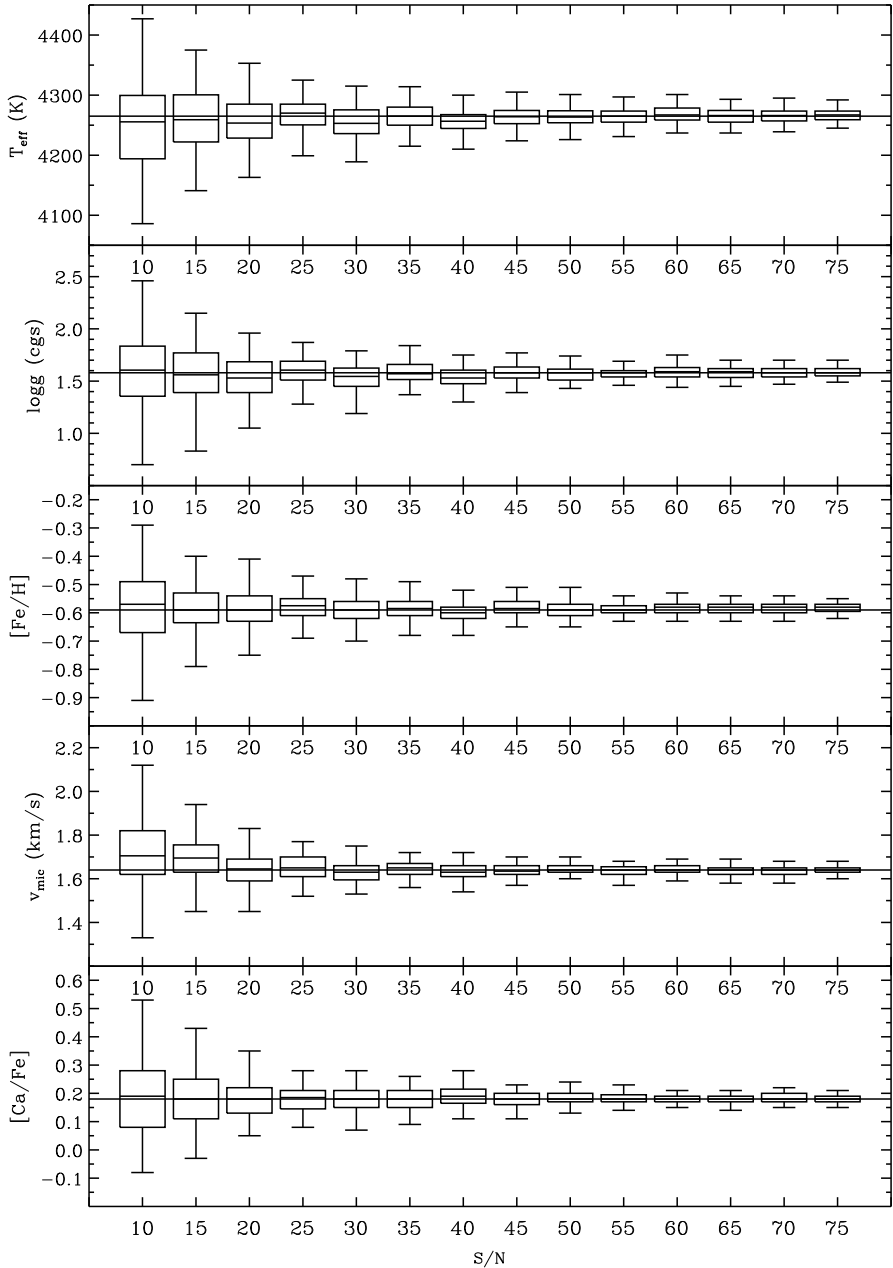


Figure 1.2: Results from determining the stellar parameters for Arcturus spectra with different injected S/N. The horizontal line crossing each panel represents the value as determined from the original, high-S/N, atlas spectrum. The horizontal line in the boxes shows the median of the data, the lower and upper boundaries of the boxes show the lower and upper quartiles of the data, and the whiskers extend to the lowest and highest value of the data.

Chapter 2

Fluorine

The cosmic origin of fluorine is unknown, not because it is astrophysically un-interesting, but simply because it is hard to determine. On the contrary fluorine is a very interesting element, perhaps surprisingly because it is so fragile and therefore hard to make. Fluorine is easily destroyed in stellar interiors, which means that in order to make cosmic fluorine the fluorine that is produced in a stellar process has to be saved from destruction quickly after its production. This sensitivity and need for fine-tuning makes fluorine a great probe for the physical conditions during different stages of stellar evolution. Furthermore, as I will describe in Section 2.4 the fluorine abundance trend might help constrain the relative amount of massive stars that have been responsible for the chemical evolution of a particular stellar population. In Paper II we determine the chemical evolution of fluorine in the Bulge, and in Paper III we determine the chemical evolution of fluorine in the solar neighborhood.

2.1 Chemical evolution of fluorine

Even if the observational data for fluorine is scarce, there are several theoretically proposed sites for fluorine production: AGB stars, SNe type II, and/or W-R stars (see Paper II for a more thorough description of the processes involved). The production of fluorine in AGB stars has been observationally proven by direct measurements in AGB stars, by measurements in post AGB stars, planetary nebulae, carbon enhanced metal-poor stars, and Ba stars (Jorissen et al., 1992; Abia et al., 2009, 2010; Werner et al., 2005; Zhang & Liu, 2005; Otsuka et al., 2008; Schuler et al., 2007; Lucatello et al., 2011; Alves-Brito et al., 2011), while the other two processes are more uncertain. This means that fluorine *is* produced in AGB stars, but it is uncertain whether they are the dominant producers of

cosmic fluorine or if one of the other two processes is more significant. The uncertainties of the amount of fluorine produced in SNe type II and W-R stars are mainly due to lack of observational data. More observations of fluorine abundances in “known” stellar populations might, together with chemical evolution models, constrain the yields of these processes. As described in Section 2.3, the previous confusion on the data for the spectral lines used in fluorine abundance determination means that possibly even the observational trend of fluorine in the solar neighborhood is unknown. Paper III is our first publication in a project trying to determine exactly this.

2.2 Previous works on fluorine

Following the pioneering work of Jorissen et al. (1992) where fluorine was for the first time detected in a star, there have been claims for either of the above possible production sites of fluorine to be important in the solar neighborhood. To mention two recent works Recio-Blanco et al. (2012) find evidence for AGB stars being the most important producer of fluorine in the solar neighborhood, while Nault & Pilachowski (2013) argue they are not, instead favoring the ν -process in SNe type II. As we will see, our work on determining the chemical evolution of fluorine in the solar neighborhood (see Paper III and Chapter 4), corroborates Recio-Blanco et al. (2012) and we find that the production of fluorine by AGB stars most likely is enough to explain the fluorine abundance in the solar neighborhood.

When it comes to fluorine in the Bulge, as is determined in Paper II, there has been only one such study before: Cunha et al. (2008). From their fluorine abundances they find indications of W-R stars being relatively more important in the chemical evolution of the Bulge than in the local disk, and as described in Paper III and Chapter 4, we possibly find the same.

2.3 Fluorine diagnostics

There are several spectral lines of fluorine arising from atomic transitions in the optical wavelength region, however they have only been detected in extreme helium stars and R Coronae Borealis stars (Pandey, 2006; Pandey et al., 2008). Some UV-lines arising from highly ionized fluorine have been used in extremely hot post-AGB stars (Werner et al., 2005; Zhang & Liu, 2005; Otsuka et al., 2008), but for more “normal” stars suitable for determining the galactic chemical evolution of fluorine only IR molecular lines from the HF molecule can be used. The line list for the HF molecule have never been properly published, but only shared via private communication. Furthermore there have been two line lists used in the literature, one by Tipping (for example used in Jorissen et al. (1992),

Cunha et al. (2008), etc.) and one by Sauval (used in Lucatello et al. (2011), D’Orazi et al. (2013), and Nault & Pilachowski (2013)). They differ by 0.25 eV in excitation energy, owing to two different definitions of dissociation energies. The Tipping list uses the energy of the energy potential, D_e , and the list by Sauval uses the true energy required for dissociation, D_0 , see Figure 2.1.

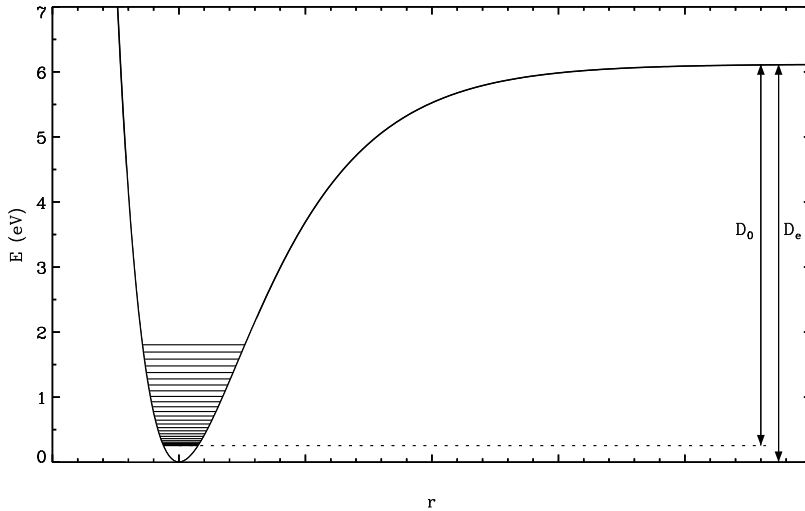


Figure 2.1: A general Morse potential showing the potential energy of a diatomic molecule versus the distance between the two atoms. Some energy states as well as the difference between the two dissociation energies discussed in the text are marked. For HF $D_e = 6.12$ eV is the energy of the energy potential and $D_0 = 5.87$ is the energy needed for dissociation from the lowest energy state.

It does not matter which list is used in the analysis as long as the corresponding partition function is used, which I show below. Assuming LTE the number density of a lower level of a certain transition can be calculated with

$$\frac{n_{\text{lower}}}{n_{\text{total}}} = \frac{g_{\text{lower}}}{Q(T)} \cdot e^{-\frac{\chi_{\text{lower}}}{kT}}, \quad (2.1)$$

where g is the statistical weight, χ is the excitation energy, k is Boltzmann’s constant, T is the temperature, and Q is the partition function:

$$Q(T) = \sum_i g_i \cdot e^{-\frac{\chi_i}{kT}}. \quad (2.2)$$

If the dissociation energy is defined like in the list of Sauval the lowest energy state would have energy 0 eV, while it would have $\chi_0 = D_e - D_0$ in the Tipping list, and all the other energy states would have $\chi_{i,Tipping} = \chi_{i,Sauval} + \chi_0$. Using this in Equation 2.1 gives

$$\frac{n_{\text{lower},Tipping}}{n_{\text{total},Tipping}} = \frac{g_{\text{lower}}}{Q(T)_{Tipping}} \cdot e^{-\frac{\chi_{\text{lower},Tipping}}{kT}} = \frac{g_{\text{lower}}}{Q(T)_{Tipping}} \cdot e^{-\frac{\chi_0}{kT}} \cdot e^{-\frac{\chi_{\text{lower},Sauval}}{kT}}. \quad (2.3)$$

As for the partition function, Equation 2.2, would become

$$Q(T)_{Tipping} = \sum_i g_i \cdot e^{-\frac{\chi_{i,Tipping}}{kT}} = e^{-\frac{\chi_0}{kT}} \cdot \sum_i g_i \cdot e^{-\frac{\chi_{i,Sauval}}{kT}} = e^{-\frac{\chi_0}{kT}} \cdot Q(T)_{Sauval}. \quad (2.4)$$

Inserting Equation 2.4 into 2.3 gives

$$\frac{n_{\text{lower},Tipping}}{n_{\text{total},Tipping}} = \frac{g_{\text{lower}}}{Q(T)_{Sauval}} \cdot e^{-\frac{\chi_{\text{lower},Sauval}}{kT}} = \frac{n_{\text{lower},Sauval}}{n_{\text{total},Sauval}}, \quad (2.5)$$

meaning that the difference in dissociation energy cancels out as long as matching excitation energies and partition functions are used. Consequently, both the Tipping and Sauval line lists are possible to use for determining fluorine abundance *as long as the corresponding partition function is used*. None of the previous works on fluorine have specified which partition function they use, but the most commonly used computer programs for deriving a stellar abundance from a spectrum (MOOG, BSYN, and SME) comes with the partition function of the Sauval list pre-installed. The partition functions are often buried rather deep in the program code and one would therefore guess that most previous works on fluorine using the Tipping list have been using a mis-matching partition function, deriving abundances almost 0.3 dex too high!

To clarify this situation we derived a new line list for the HF-molecule compatible with the partition function already built into MOOG, BSYN, and SME. In Paper II we present the part of the list for the often used vibrational-rotational K-band lines around 2 μm , while we in Paper III present data for previously never used pure rotational lines around 12 μm and use one of them for abundance analysis. We find that the abundances as derived from the two lines agree well, giving credibility to our derived line list.

In parallel with our project there have been other calculations of HF transition probabilities, including more lines, and they are available for download from the **High-resolution TRANsmission molecular absorption database (HITRAN)**¹. They were used

¹<https://www.cfa.harvard.edu/hitran/>

in Maiorca et al. (2014) that came out during the review-process of our Paper III, where we present our second part of the HF line list. However, HITRAN defines the statistical weight in a way not compatible with the partition function built into most spectral synthesis programs used to determine stellar abundances (MOOG, BSYN, and SME): instead of using only the “standard” $g = 2J + 1$, they recommend an extra nuclear factor of 4, $g = 4 \cdot (2J + 1)$ (Šimečková et al., 2006). To avoid to, once again, run into problems with the partition function, Maiorca et al. (2014), slightly inconsistently, use the A-values from HITRAN but ignore the recommended nuclear factor of 4 in the statistical weight when they derive their $\log gf$ -values. In the end they arrive at a line list very similar to ours, meaning that the derived stellar abundances will be the same using either of the line lists.

2.4 Fluorine in the Bulge

Classically the Galactic Bulge was thought to be formed by mergers of smaller dwarf galaxies, which is what one would expect from cosmological models. However, during the last years it has been shown that the Bulge is a complex environment with a dynamically formed bar and possibly several different stellar populations. The existence of a bar has been shown by the general morphology (Weiland et al., 1994), the kinematics of the stars (Howard et al., 2008; Kunder et al., 2012), and the recent discovery of two red clump populations towards the Bulge (McWilliam & Zoccali, 2010). At the same time it has been repeatedly shown that the metal-poor stars in the Bulge might be behaving kinematically differently (Ness et al., 2013; Dékány et al., 2013), possibly indicating an old merger-formed component. Which stellar populations really are present in the Bulge, and what it would mean for the formation of it, have been addressed in a multitude of papers, but our picture and understanding of the Bulge is still sketchy.

For example the trends of alpha-elements have been used to, via chemical evolution models, estimate the star formation history of the Bulge (see Section 3.1 for a description of the concept). Some works doing this have found surprisingly different oxygen and magnesium trends that possibly can be explained if W-R stars played an important role in the chemical enrichment of the Bulge (for example Lecureur et al., 2007). There have also been other more recent studies finding other indications for the need for relatively more massive stars to explain the chemical evolution of the Bulge (Johnson et al., 2014; Grieco et al., 2015, for example). Given that the yield of fluorine from W-R winds is high enough, the fluorine trend in the Bulge might be used as a proxy of the importance of W-R stars in the chemical evolution of the Bulge. This is exactly the question we address in Paper II. However, our results are inconclusive mainly due to the uncertainty of the yields of fluorine production by W-R winds and the ν -process (see Paper II and Chapter 4). Measuring the fluorine abundance of more Bulge stars might settle this issue, but to find the possible uniqueness of the chemical evolution of the Bulge it has to be compared

to fluorine trends of the solar neighborhood, which is what we determine in Paper III. As can be seen in Figure 2.2, our fluorine abundances from the solar neighborhood in Paper III unfortunately are few and in a narrow metallicity-range, making it hard to see a possible difference to the Bulge trend. The uncertainties in the abundances as derived from the Bulge stars are of course larger due to lower S/N in those spectra, but disregarding all upper limits (downward-pointing triangles) and the possibly systematically different re-analyzed stars of Cunha et al. (2008) (blue squares), the Bulge abundances might follow the possible thick-disk trend in the solar neighborhood (so far only sampled by one single star, Arcturus!). Obviously, also the trend in the solar neighborhood needs to be traced better to draw conclusions from this kind of comparison, which we are doing in an ongoing project (see Chapter 5).

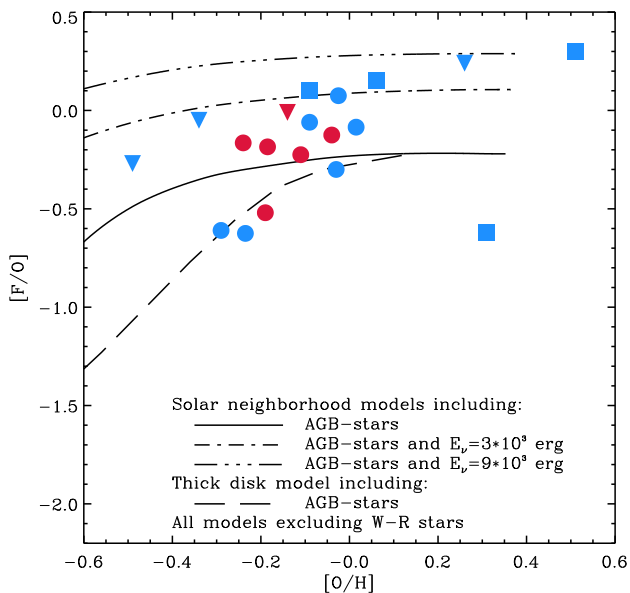


Figure 2.2: The abundances from the Bulge in blue (Paper II) overplotted on the abundances from the solar neighborhood in red (Paper III). The blue squares mark the results from the re-analyzed stars from Cunha et al. (2008), which due to different stellar parameters, might show systematic differences with respect to the other results. As for the results from the solar neighborhood, I have plotted the mean fluorine abundance as derived from the $2.3 \mu\text{m}$ and $12.2 \mu\text{m}$ lines. Furthermore, the value for α Tau is shown as an upper limit, because in this case the lower value as derived from the weak $2.3 \mu\text{m}$ line is more reliable than the higher value derived from the stronger $12.2 \mu\text{m}$ line, being sensitive to the adopted microturbulence. Also shown are the solar neighborhood chemical evolution models of Kobayashi et al. (2011).

Chapter 3

Sulphur

The element sulphur is, just like fluorine, not much studied before, and, just like for fluorine, its cosmic origin has been investigated and debated in the current literature. Sulphur is one of the diagnostically important alpha-elements, like for example oxygen and magnesium, that has been used to constrain the chemical evolution of our Galaxy. When investigating other galaxies one interesting type of object is the so called damped Lyman α -systems believed to be spiral galaxies, just like our own, in the making. It turns out sulphur possibly would be the a suitable alpha-element to measure in these systems because it is volatile, meaning that it is not depleted on dust (Wolfe et al., 2005; Nissen et al., 2007). When determining abundances of these distant systems one uses spectroscopy of the integrated light from the entire (proto-) galaxy, and only the abundance of the element in gas-phase can be inferred. In case of the other, more well-studied, alpha-elements one would then have to estimate the amount of the element locked up in dust to get the total alpha-elemental abundance of the system. This would not be necessary for sulphur because of its volatile properties, thereby giving lower uncertainty to the alpha-determination. However, to be able to use sulphur to determine the chemical evolution of other galaxies, the chemical evolution of sulphur in our own Galaxy needs to be understood. This is the subject of Paper I.

3.1 Chemical evolution of alpha-elements

Alpha-elements are elements like for example oxygen, magnesium, silicon, and sulphur that would be possible to produce by adding α -particles together. Models show that SNe type II produce higher or equal amounts of the alpha-elements as compared to iron (higher amount in the case of oxygen and roughly the same amount in the case of magnesium,

silicon, and sulphur).

In SN type Ia, on the other hand, significantly more iron is produced as compared to the alpha-elements. Due to the different life times of the stars leading to the two types of SNe - all SN type II go off “shortly” after star formation whereas it takes considerably longer time for a SN type Ia to occur - it is expected that old stars that formed out of ISM mainly polluted by SNe type II have a larger $[\alpha/\text{Fe}]$ than younger stars also polluted by gas processed in SNe type Ia. Since older stars, on average, have a lower metal content, and therefore lower $[\text{Fe}/\text{H}]$, an $[\alpha/\text{Fe}]$ vs. $[\text{Fe}/\text{H}]$ plot for a particular stellar population is expected to show the “knee-like” behavior, schematically shown overplotted onto the data of Fig. 3.1. A slow star-formation history, like in dwarf galaxies, would result in a short plateau whereas a faster star-formation history, like suggested for the Galactic Bulge, would lead to a longer plateau. The height of the plateau would depend on the yield from, and amount of, SNe type II, meaning that a successful chemical evolution model of abundance data like this would depend on and constrain parameters such as SNe yields, nucleosynthesis, the star-formation rate, and the initial mass-function of the stellar population at the same time. Obviously models depending on such a number of variables might have problem with the uniqueness of the successful parameters but it might also be a very powerful tool for testing our understanding of the formation of stellar systems like our Galaxy, subcomponents of the Galaxy, or other galaxies.

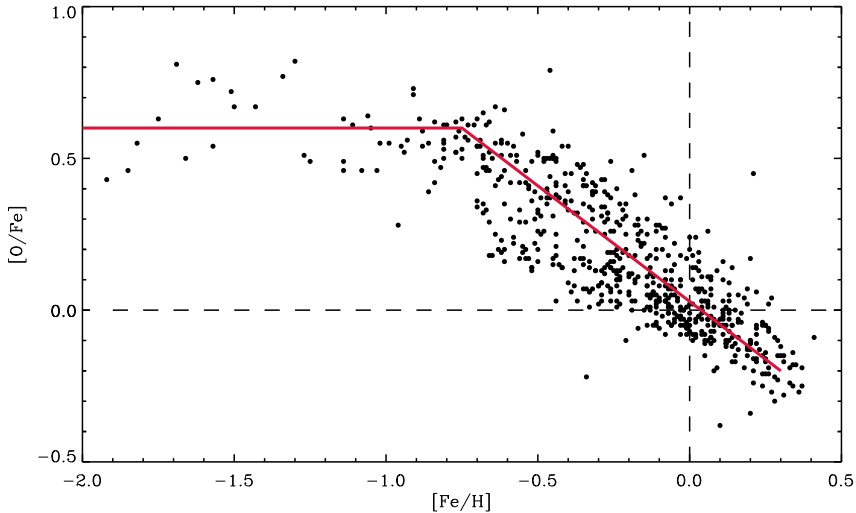


Figure 3.1: $[\text{O}/\text{Fe}]$ vs. $[\text{Fe}/\text{H}]$ with data from Bensby et al. (2014). The red line was added to make the knee-form more obvious and does not represent any real chemical evolution model.

Once we have a galactic chemical evolution model of the Milky Way that is able to reproduce observations, one can use the model tuned for other galaxies and other evolutionary stages, and thus infer the star-forming history of other stages of galaxy evolution. As described above, sulphur would be a good choice for representing the alpha-elements in the case of damped Lyman α -systems, because there are suitable spectral lines available, and sulphur is not believed to be depleted on dust, removing the extra uncertainty of estimating the ratio of alpha-elements in gas and in dust, which is needed to determine the entire alpha abundance in the system. For the same reason zinc could possibly be used as a proxy of the iron abundance, the two elements evolving in lock-step with each other. An $[\alpha/\text{Fe}]$ vs. $[\text{Fe}/\text{H}]$ plot of systems like these might tell us the average star-forming history and discriminate whether they truly are the progenitors of galaxies like ours.

3.2 Works on sulphur previous to Paper I

Sulphur is the least studied alpha-element, but during recent years there has been a number of sulphur studies, and at the time of Paper I, there were several suggestions for the trends in the Galactic $[\text{S}/\text{Fe}]$ vs. $[\text{Fe}/\text{H}]$ plot. Three studies conducted at that time are shown in Figure 3.2. The works all agree on the trend for disk stars (by which we mean stars with $[\text{Fe}/\text{H}] \geq -1$) but differ for halo stars (i.e. stars with $[\text{Fe}/\text{H}] \leq -1$).

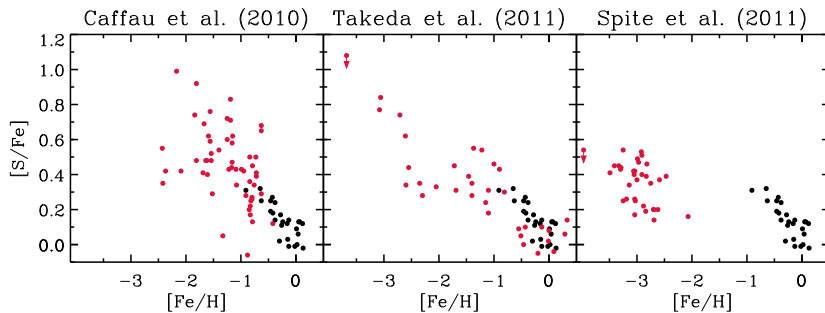


Figure 3.2: $[\text{S}/\text{Fe}]$ vs. $[\text{Fe}/\text{H}]$ from Caffau et al. (2005, 2010), Takeda & Takada-Hidai (2011), and Spite et al. (2011), respective. Black symbols in all panels from Chen et al. (2002).

The panels show in turn the scattered trend of Caffau et al. (2005, 2010), the zig-zag trend of Takeda & Takada-Hidai (2011), and the flat trend of Spite et al. (2011). Interestingly enough the three works show different trends for halo stars. Moreover, Caffau et al. (2005, 2010) and Takeda & Takada-Hidai (2011) show sulphur-trends that differ from those of other alpha-elements. These are not expected from models of chemical evolution. It

has been suggested that the trend of Caffau et al. (2005, 2010) might be modeled by a scenario involving really massive SNe type II (hypernovae) in the early history of the Galaxy (Nakamura et al., 2001) or with a model where the iron deposition into the ISM from SNe is time-delayed as compared to sulphur (Ramaty et al., 2000). However, there is no suggestion on how to interpret the trend found by Takeda & Takada-Hidai (2011). As it will turn out, and as is described in Chapter 4 and Paper I, we find a trend corroborating the alpha-typical trend of Spite et al. (2011).

3.3 Sulphur diagnostics

The different results on the Galactic chemical evolution of sulphur described in Sect. 3.2 might be caused by the fact that different studies use different lines as sulphur diagnostics: Caffau et al. (2005) used as many diagnostics as possible of a multiplet around 675 nm, a doublet around 869 nm, and a triplet around 923 nm, Caffau et al. (2010) and Takeda & Takada-Hidai (2011) used a triplet around 1045 nm, while Spite et al. (2011) used the triplet around 923 nm. A list of sulphur lines including the ones used in these works and this thesis can be seen in Table 3.1. Since sulphur is placed just below oxygen in the periodic table they have electron structure and energy levels resembling each other. Since oxygen is a more commonly known and used alpha-element I have listed the analogous oxygen lines next to the sulphur lines in the table.

Ideally, abundances determined from different spectral lines should of course agree, but the disagreement on the trend in the $[S/Fe]$ vs $[Fe/H]$ plot might have its cause in the diagnostic used through possible blends for some of the sulphur lines in certain stars, the non-LTE corrections of Takeda et al. (2005), or due to the fact that some of the lines used become very weak in halo stars making them hard to distinguish from the noise in the spectra. The latter is certainly the case for the 675 nm and 869 nm lines, adding great uncertainty to the sulphur abundance determinations from these lines in metal-poor stars. The 923 nm lines are the strongest in Table 3.1, making them suitable for usage in halo stars, but they show large non-LTE effects making the modeling and abundance determination hard and possibly imprecise. For these reasons I have chosen to observe the slightly weaker, but likely less non-LTE sensitive, 1045 nm triplet lines, and also the $[S\ I]$ -line that is formed under LTE conditions.

To rule out possible blends in the diagnostics used in this thesis, I have calculated synthetic equivalent widths for all relevant lines in the vicinity of the sulphur lines in an extensive grid of model atmospheres spanning from hot to warm stars and from dwarfs to giants (see Paper I for details). The results are shown in contour plots in Figures 1-3 in Paper I. They show that neither of the two diagnostics used in the article are blended for our metal-poor giants, but caution should be shown for certain other stellar parameters. E.g., for solar-metallicity dwarfs with temperatures of 4500 K the strength of the blending

Table 3.1: Atomic data for some visual and near-IR sulphur transitions. The first four lines in the table have been collected by the Gaia-ESO line-list group and will be published in Heiter et al. (in prep.), and the rest are taken from the VALD database (Valenti & Piskunov, 1996; Ryabchikova et al., 1997; Kupka et al., 1999, 2000). The references are for wavelength, $\log gf$, and excitation energy respectively. In cases where several references are given for a quantity the value listed is a mean of the reference values.

Element	Wavelength (nm) (air)	$\log gf$	χ_{exc} (eV)	References	O analogue (nm) (air)
S I	674.3600	-0.700	7.870	1, 1, 2	615.60
S I	675.7171	-0.310	7.870	1, 1, 2	615.67
S I	869.3980	-0.850	7.870	2, 2, 2	926.08
S I	869.4710	0.101	7.870	2, 3 & 4, 2	926.09
S I	921.2863	0.470	6.525	2, 2, 2	777.19
S I	922.8093	0.320	6.525	2, 2, 2	777.41
S I	923.7538	0.010	6.525	2, 2, 2	777.54
S I	1045.5449	0.250	6.860	5, 5, 5	844.62
S I	1045.6757	-0.447	6.860	5, 5, 5	844.64
S I	1045.9406	0.030	6.860	5, 5, 5	844.67
[S I]	1082.1176	-8.704	0.000	1, 6, 1	630.03

References. (1) Kurucz (2004); (2) Biemont et al. (1993)

(3) Zatsarinny & Bartschat (2006); (4) Froese Fischer & Tachiev (2012)

(5) Zerne et al. (1997); (6) Froese Fischer & Tachiev (2012)

Fe I line would be roughly equal to that of the 1045.5 nm S I triplet line. Also, the neighboring Cr I and [S I] lines might become unresolvable and therefore blend when observing at lower spectral resolution. This type of investigation should also be made for the other diagnostics that have been used in the literature making it possible to check whether blends have influenced the results in some of the previous, disagreeing, studies.

In Paper I we conclude that the 1082 nm [S I] line can be regarded as a preferred sulphur diagnostic when observable, since it is situated in a wavelength region with almost no telluric lines, it is almost always blend-free (see Figure 1 in Paper I), it shows small differences when modeled using 1D and 3D models, at least for our giants, and it is formed under LTE conditions. The 1082 nm [S I] line also has the advantage of not being as sensitive to temperature, and hence to the adopted T_{eff} , as the other used diagnostics, stemming from more highly excited transitions. The 1045 nm triplet is also situated in a wavelength region with few telluric lines, but it is not as blend-free (see Figures 2-3 in Paper I) and have larger 3D and non-LTE corrections. However, it has the advantage of being much stronger than the [S I] line and therefore visible in more types of stars.

3.4 Works on sulphur after Paper I

After the publication of Paper I, the authors of Takeda & Takada-Hidai (2011) have re-analyzed their data (Takeda & Takada-Hidai, 2012) and found that the “high” [S/Fe]-values determined for the most metal-poor stars was because of the lines used were too weak thereby giving the noise in the spectra large influence on the abundance. In the second article they also expand their metal-poor stellar sample and conclude that the trend they are determining is very close to that of Spite et al. (2011).

Matroziis et al. (2013) have used the 1082 nm [S I] line in more giants and furthermore re-analyzed our sample of stars from Paper I using, when possible, new, homogeneously determined, stellar parameters. They were able to derive homogeneous parameters for six of the ten stars in Paper I, and use interquartile mean values from the literature for the remaining four stars. In the end the [S/Fe] they derive are close to those determined in Paper I (see their Table 4), meaning that their conclusion is the same as ours: the chemical evolution of sulphur is alpha-like. However, their total sample is larger and the homogeneously determined parameters gives slightly less scatter. Furthermore they find that their trend is systematically higher than the corresponding trend as derived by Spite et al. (2011) and Nissen et al. (2007) from the 923 nm S I triplet. Since the 1082 nm [S I] line, as described in Paper I, is not believed to be affected by non-LTE nor 3D-effects Matroziis et al. (2013) conclude that their result probably is the most trustworthy, but that this needs to be investigated further.

Furthermore there have been several studies of sulphur abundances of stars in star clusters (see Kacharov et al., 2015, and references therein). The conclusion from these studies is also that sulphur most likely is behaving as a typical alpha-element.

It seems a consensus has been reached that the evolution of sulphur is alpha-typical and most earlier claims of high [S/Fe]-values for halo stars can be explained by problems with the used spectral lines. However, there still are some unexplained rather high values of Caffau et al. (2010), Takeda & Takada-Hidai (2012), and Kacharov et al. (2015) that might point towards a more complicated origin of sulphur.

Chapter 4

Main results and author contributions

Paper I:

Sulphur abundances in halo giants from the [S I] line at 1082 nm and the S I triplet around 1045 nm

H. Jönsson, N. Ryde, P. E. Nissen, R. Collet, K. Eriksson, M. Asplund, and B. Gustafsson

Astronomy & Astrophysics 530, A144 (2011)

In this paper we determine the sulphur abundance in ten halo giants using two sets of observed lines: the [S I] line at 1082 nm and the S I triplet around 1045 nm analyzing them with the Uppsala 1D LTE programs MARCS, BSYN and EQWI. The 1082 nm [S I] line is formed under conditions close to LTE. The 1045 nm triplet is, however, likely not, but there are non-LTE corrections available in the literature. We have also tried to estimate the 3D effects for both diagnostics by inter- and extrapolating in the very coarse grid of 3D models calculated for our kind of stars. Due to the small wavelength coverage of the IR spectrometer used (CRIRES at VLT) we have not been able to determine the stellar parameters of the stars in a consistent way, but are forced to take the parameters from three literature sources, which could introduce systematic errors.

The paper makes three main points:

- The 1082 nm [S I] line is usable as a sulphur diagnostic in giants down to $[\text{Fe}/\text{H}] =$

–2.3 and an extensive search for blending lines shows no blends. The line also shows small non-LTE and 3D effects. This result adds important information on what lines are useful for abundance determination in different kinds of stars.

- In comparing the abundance results from the 1082 nm [S I] line and the non-LTE corrected values deduced from the 1045 nm triplet, we are able to conclude that the non-LTE corrections for the 1045 nm triplet from Takeda et al. (2005) perform well in our 1D model. It *might*, however, be argued that they perform worse when 3D models are used. It should, however, be noted that the very coarse grid of available 3D models for our kind of metal-poor giants only makes it possible to give qualitative ballpark-estimations of the 3D effects.
- Some previous works have found an alpha-like trend for sulphur, while others have found peculiarly high sulphur abundances for low-metallicity stars, that possibly could imply that very massive supernovae, hypernovae, played an important role in the halo-phase of chemical evolution of the Milky Way. We find a flat trend in the [S/Fe] vs. [Fe/H] plot for halo stars, implying “standard” explosive nucleosynthesis in type II supernovae and that no exotic hypernovae are needed.

My contribution:

The observations were all made before I took over the lead of the project, so I had no part in preparing or executing them. The CRIRES pipeline is deemed stable enough to produce science data and therefore the pipeline was used to reduce the data when possible. As described in the paper, unfortunately half the data needed to be manually re-reduced, which was done by me. The specifically tailored 1D model atmospheres and synthetic spectra were computed by me using MARCS/BSYN, as well as the measurements of equivalent widths. The 3D models and the 3D-1D corrections were calculated by Remo Collet. As the first author of the paper, I did in principle all of the writing and analysis/discussion, with appreciated help and suggestions from the other authors and the anonymous referee.

Paper II: Chemical evolution of fluorine in the Bulge: High resolution K-band spectra of giants in three fields

H. Jönsson, N. Ryde, G. M. Harper, K. Cunha, M. Schultheis, K. Eriksson, C. Kobayashi, V. V. Smith, and M. Zoccali
Astronomy & Astrophysics 564, A122 (2014)

In this paper we determine the fluorine abundance in 13 Bulge giants using the $2.3\ \mu\text{m}$ HF molecular line. Eight of the spectra were observed for this project with CRIRES at VLT, and five were previously published, but re-analyzed here. The K -band is smitten by telluric lines, which can be removed by dividing the spectrum with that of a fast rotating O-star showing, in principle, only telluric absorption lines. The stellar parameters cannot be determined by the narrow wavelength range of CRIRES, but was instead derived from optical spectra of the very same stars recorded using UVES at VLT.

The paper makes three main points:

- We present a new line list for the HF molecule, the only proxy for fluorine abundance in stellar atmospheres. Prior to our paper there have been two sets of data used in the literature. Neither has been properly published, but only shared via private communication. It turns out a majority of the previous works most likely have used an incorrect partition function in their analysis leading to fluorine abundances about 0.3 dex too high.
- Some previous works determining trends of alpha-elements in the Bulge have proposed that W-R stars might have been important in the chemical evolution of the Bulge, thereby indicating that the amount of massive stars have been relatively larger in the Bulge than in the solar neighborhood. This can potentially be tested by tracing the fluorine abundance in the Bulge, and was the motivation behind the project. However, the existing chemical evolution models were not able to reproduce our results, making our conclusion on this matter ambiguous.
- The new line list implying lower abundances revealed the need for improving chemical evolution models. However, to do so, more observations of “known” stellar populations are needed.

My contribution

The observations were all made before I took over the lead of the project, so I had no

part in preparing or executing them. The CRIRES pipeline produced spectra with poor wavelength-calibration in the K -band, so I re-reduced them manually using the ESO tools Gasgano and ESOREX. Furthermore I did the removal of telluric lines. I analyzed all spectra using the software SME and MARCS-models, but Katia Cunha also analyzed the five previously published spectra using MOOG and the new line list. As described in the paper our derived abundances agree very well.

The HF line list was calculated by Graham Harper and the chemical evolution models were made by Chiaki Kobayashi.

I devised a method based on a line list of Fe I, Fe II, and Ca I lines to determine the stellar parameters from the optical spectra using SME. As described in Section 1.2.1 of this thesis, I did a lot of testing of this method against benchmark stars, both against stars with temperatures determined from angular diameter measurements, but also against Kepler stars with well determined $\log g$ (this will be further described in a forthcoming paper where I explore the optical spectra from the Bulge stars further). The method of determining the stellar parameters for giants was incorporated in the Gaia-ESO UVES-pipeline of the LUMBA node. As the first author of the paper, I did in principle all of the writing and analysis/discussion, with appreciated help and suggestions from the other authors and the anonymous referee.

Paper III:

Fluorine in the solar neighborhood: Is it all produced in asymptotic giant branch stars?

H. Jönsson, N. Ryde, G. M. Harper, M. J. Richter, K. H. Hinkle
The Astrophysical Journal Letters 789, L41 (2014)

In this paper we determine the fluorine abundance in seven solar neighborhood giants using the often used vibrational-rotational $2.3 \mu\text{m}$ HF molecular line and a never before used purely rotational HF line at $12.2 \mu\text{m}$. The paper was published in rapid communication succeeding the previous paper and is a follow-up on the first and last main points made in that paper: since we have found it likely that most previous works have determined fluorine abundances about 0.3 dex too high, even the evolution of fluorine in the most known stellar populations of the thin and thick disks is uncertain and needs to be determined.

The paper makes two main points:

- By comparing our determined fluorine abundances to existing chemical evolution models of the solar neighborhood we draw the conclusion that all the fluorine likely has been produced by asymptotic giant branch stars, and that the exotic ν -process in type II supernovae is probably not needed.
- The never before used $12.2 \mu\text{m}$ HF line is stronger and possible to use to trace the evolution of fluorine in more metal-poor stars than the often used $2.3 \mu\text{m}$ line, which is weaker and becomes impossible to use for lower metallicities.

My contribution

This project was initiated and led by me from beginning to end. As the first author of the paper, I did in principle all of the writing and analysis/discussion, with appreciated help and suggestions from the other authors and the anonymous referee. The HF line list was calculated by Graham Harper. The spectra were taken from archives (the $2.3 \mu\text{m}$ spectra from the FTS-archive of Ken Hinkle and the $12.2 \mu\text{m}$ spectra from the TEXES-archive of Matt Richter), and therefore we could not choose the metallicities of the stars, but ended up with a narrow metallicity range, weakening the conclusion. As described in Chapter 5 in this thesis, I am leading a follow-up on this study where I, as PI, have applied for and been awarded telescope time on the Mayall telescope at Kitt Peak Observatory and on the NOT at Roque de los Muchachos Observatory.

Chapter 5

Personal reflections and future prospects

As has been shown in this thesis, the present development in IR spectrometers opens up new possibilities for stellar abundance analysis. The new high resolution cross-dispersed spectrometers will make it possible to determine abundances in stars that are inaccessible using optical spectroscopy. The wider wavelength-coverage will make the problems with determining the stellar parameters, as I have faced in my work, less severe. As has been shown by, for example, the ongoing APOGEE-survey, the same spectroscopic approaches used in the optical region to determine stellar parameters might be used in the IR, given that the observed spectra contain enough parameter-sensitive lines (Shetrone et al., 2015). This of course relies on that the line data we have can be trusted, which is often not the case. I would say that this is the largest challenge for IR spectroscopy right now: when doing spectroscopy in the optical region there is a collected experience of which lines are good to use for abundance determination, while that is not the case in the less explored IR region. During my work I have run into problems with known and unknown blending lines, of known and unknown strengths, arising from known and unknown transitions, and the only way forward is to keep testing the untested lines with the goal of finding out which might be useful. This exploration has, together with the above described immediate science goals, been part of my thesis work.

Regarding the direct questions addressed in the three papers: the chemical evolution of fluorine in the Bulge and in the solar neighborhood, and the chemical evolution of sulphur in metal-poor stars, there are several future prospects I have chosen to pursue.

Due to the problems with the HF line list described in Section 2.3 and the limited spread in metallicity of our stellar sample in Paper III, the fluorine trend is still not well determined even in the solar neighborhood, leading to uncertainties in the fluorine yields of the processes producing cosmic fluorine. While this thesis was being printed I was ob-

serving new local disk giants¹ using the Phoenix spectrometer at the 4m Mayall telescope at Kitt Peak National Observatory in Tucson and also using the FIES spectrometer at the Nordic Optical Telescope at Observatorio del Roque de los Muchachos on La Palma. The Phoenix spectra cover the 2.3 μm HF line and the FIES spectra are optical (3700-7300 Å) and will be used to determine the stellar parameters. In this project we have concentrated on the more metal-rich end of the fluorine trend ($[\text{Fe}/\text{H}] > -0.5$), with the plans of applying for more observational time for tracing the more metal-poor part of the trend using the more suitable mid-IR lines used in Paper III. A suitable instrument for this would be the spectrometer TEXES that from time to time is offered as a visiting instrument on the Gemini observatory on Hawaii.

When it comes to the fluorine trend in the Bulge, as traced in Paper II, we already have more data taken in the same manner as is done in Paper II (the spectrometer CRIRES at VLT on Paranal) in another Bulge field closer to the Galactic center: the Sagittarius field. The stellar parameters have already been determined from optical UVES/VLT spectra, so if nothing unexpected happens that paper will be out during the autumn.

Regarding sulphur, the discussion is less diversified than at the time of Paper I (see Section 3.4), meaning that this issue is most likely solved, and the Galactic evolution of sulphur is likely understood well enough to not pose any hinder to using sulphur as a tracer for alpha-elements in damped Lyman α -systems.

¹Given that the weather was good enough...

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