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Non-LTE Revisited

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Abstract

The development of sophisticated techniques for quantum-mechanical computations has lead to the determination of large amounts of accurate atomic data by e.g. the Opacity and IRON Projects in recent years, stimulated by the demands of astrophysical and fusion research. Here, we report on the incorporation of such data in a new generation of non-LTE model atoms for a number of elements of astrophysical relevance. First applications are presented, indicating that significant improvement can be achieved in stellar parameter and elemental abundance studies when the ubiquitous non-LTE effects are addressed thoroughly with accurate atomic data. At best, stellar effective temperatures can be constrained to better than 1% and surface gravities to 0.05–0.10 dex. A high degree of redundancy is obtained by exploiting multiple independent indicators (ionization equilibria, Stark-broadened hydrogen lines). The uncertainties in abundance determinations can be reduced to typically 0.05–0.10 dex (random) and 0.07–0.12 dex (systematic 1σ-errors), even in supergiants. The new results demonstrate that even classical problems like the line formation for hydrogen still offer surprises, and they caution us not to trust apparently well-established assumptions.

1.1 Introduction

Virtually all our knowledge about stars and their evolution is derived by quantitative analyses of their spectra. These are based on model atmosphere techniques which have reached a high degree of sophistication in the recent years. The majority of the work has been performed under the assumption of local thermodynamic equilibrium (LTE), where the thermodynamic state of the atmospheric plasma is described via the Saha-Boltzmann equations as a function of the *local* temperature and electron density alone. However, this approximation strictly holds only in the limit that collisions, i.e. thermalizing processes, dominate, and that photon-mean-free-paths are small. For a more accurate physical description the *non-local* nature of the radiation field and its interaction with the stellar plasma has to be accounted for. This requires consideration of the detailed atomic processes for excitation and ionization, as expressed in the rate equations of statistical equilibrium (the non-LTE case).

While the efforts have concentrated on the development of efficient numerical algorithms for solving the non-LTE radiative transfer problem over many years, more recently the focus has shifted towards obtaining accurate atomic data. Vast amounts of radiative and collisional data from quantum-mechanical *ab-initio* calculations have been provided by the Opacity Project (Seaton et al. 1994) and the ongoing IRON Project (Hummer et al. 1993), supple-

Table 1.1. *Model atoms for non-LTE line-formation computations*

H I	Przybilla & Butler (in preparation)
He I/II	Husfeld et al. (1989)
C I/II	Przybilla, Butler & Kudritzki (2001)
N I/II	Przybilla & Butler (2001)
O I/II	Przybilla et al. (2000) + Becker & Butler (1988)
Mg I/II	Przybilla et al. (2001)
S II/III	Vrancken, Butler & Becker (1996)
Ti II	Becker (1998)
Fe II	Becker (1998)

mented by contributions from fusion research and state-of-the-art experiments. In particular, use of the *R*-matrix method in the close-coupling approximation allows for a reduction of the typical uncertainties in the data to $\sim$10% on the mean, in sharp contrast to the order-of-magnitude approximations widely used in astrophysics.

In the following we report on the impact that such accurate atomic data can have for stellar analyses. It has to be emphasized that a careful selection of the atomic data is essential for improving the standards: use of inaccurate or inappropriate atomic data in non-LTE studies will result in systematic errors that can go well beyond those introduced by assuming LTE.

1.2 Methods

The majority of the results presented here are obtained using the non-LTE line-formation package DETAIL/SURFACE (Giddings 1981; Butler & Giddings 1985, with significant modifications by one of us (K. B.), e.g. the inclusion of an ALI scheme) on the basis of prescribed classical model atmospheres. This hybrid approach allows us to perform detailed non-LTE line-formation calculations even for highly complex atoms/ions, like those of the Iron Group, with only moderate requirements on computing resources. Table 1.1 gives an overview of model atoms used in the present work. We rely on line-blanketed ATLAS9 model atmospheres (Kurucz 1993) for analyses of stars of spectral types late B to early A. These are a good choice for quantitative work in that temperature range, even for supergiants, as demonstrated by Przybilla (2002).

For the modeling of early-type stars we use the non-LTE line-formation code FASTWIND (Santolaya-Rey, Puls & Herrero 1997, SPH97), which accounts for spherical extension and hydrodynamic mass-outflow. It has been updated for an approximate treatment of non-LTE line-blocking/blanketing recently (Puls et al. 2003). The line-formation computations with FASTWIND only comprise H+He features explicitly at present.

Testing of the models is performed on high-resolution and high-S/N Echelle data of several bright galactic main sequence stars and supergiants in the visual and near-IR spectral range. Complete wavelength coverage turns out to be essential in order to access all the strategic lines required for attaining the high degree of redundancy which allows us to put tight constraints on stellar parameters and chemical composition. In addition, medium-resolution K-band spectra have been adopted from the literature (Hanson, Conti & Rieke 1996; Wallace & Hinkle 1997).

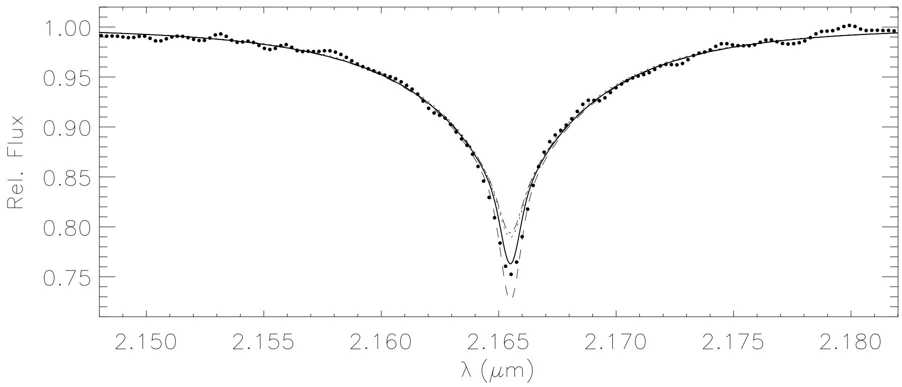

Fig. 1.1. Spectrum synthesis for Br_γ in Vega (A0 V, $T_{eff} = 9550$ K, $\log g = 3.95$, $\xi = 2$ km/s, $y = 0.09$) using different electron collision data for computation of non-LTE populations: ABBS00+PR78+PS69 (full line), J72 (dashed), PS69 (dotted) – see text for details. Further displayed are an LTE (dashed-dotted) and the observed profile (dots).

1.3 New Results on Hydrogen

Hydrogen attracted early interest for non-LTE studies, as it is the most abundant and therefore most important element in normal stars. Its simplicity allows for an almost complete analytical solution of the quantum-mechanical problem, and the atomic data are consequently of excellent quality. The only exception are particle collision data, which require the solution of a three-body problem, which has to be addressed numerically.

Several approaches to this problem have been published so far, they are mostly of an approximate or semi-empirical nature, as measurements for collisional cross-sections are available for only a few transitions involving the ground state. Recently, highly accurate results from *ab-initio* computations have also become available (Anderson et al. 2000, ABBS00), which motivated us to reconsider the non-LTE line-formation problem for hydrogen.

Three model atoms have been implemented, differing only in the electron collision data for excitation: two 'classical' models using data of Peterson & Strom (1969, PS69) and Johnson (1972, J72), and a new benchmark model comprising the data of ABBS00 for transitions between terms up to the $n = 5$ shell, of Percival & Richards (1978, PR78) for transitions between terms with $n > 5$, and PS69 data for the remainder. First tests on Vega show that all three model atoms give almost identical synthetic spectra for the lines of the Balmer series, which is not unexpected. However, examination of Br_γ reveals significant differences in the line core, see Fig. 1.1, and indeed the new model atom provides the best match between theory and observation. Apparently, the use of the PS69 data alone results in an overestimation of the collision rates, almost recovering detailed balance, whereas the J72 data underestimates the importance of the electron collisions, giving a too strong non-LTE effect. A similar scenario is suggested for other members of the Brackett series, and also for the Pfund series, where we do not have observations at our disposal.

One has to ask, how the improved collision data affect the analysis in a true non-LTE situation. Corresponding results from our modeling of an early O-type main sequence star are

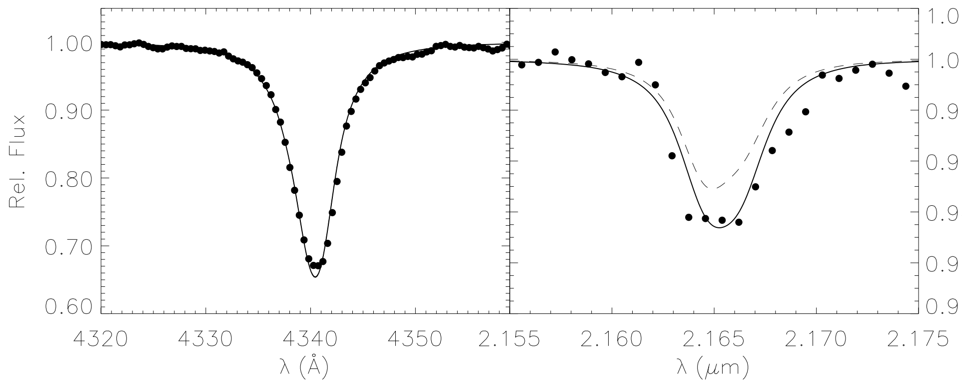

Fig. 1.2. Spectrum synthesis for H_γ (left) and Br_γ (right) in the O3.5 V((f+)) star HD 93250 ($T_{eff} = 46000$ K, $\log g = 3.96$, $y = 0.09$, $\dot{M} = 4 \times 10^{-6}\,M_\odot$, $v_\infty = 3250$ km/s, $\beta = 0.9$). Our new results (full line) are compared with those using the H model atom of SPH97 (dashed line) and observation (dots). The He II blends have been accounted for. Note that for H_γ both models predict virtually identical profiles.

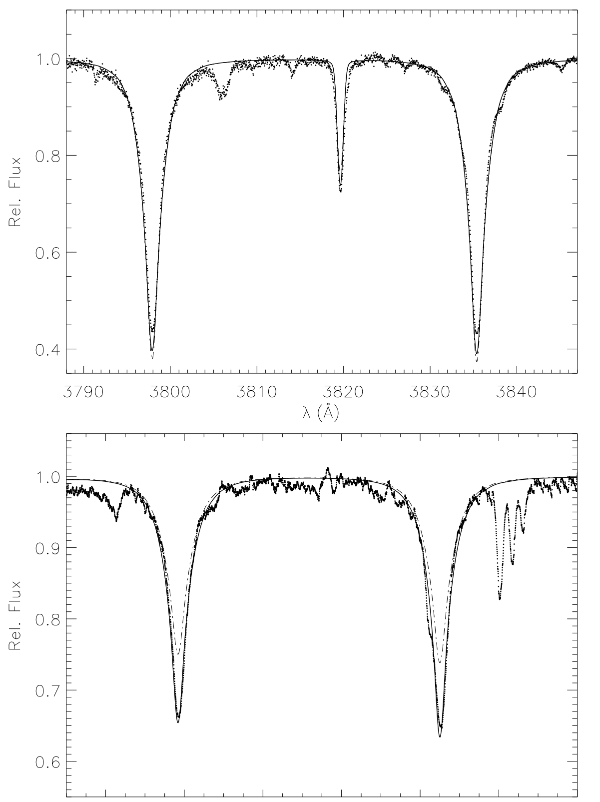

Fig. 1.3. Spectrum synthesis for H_9 and H_{10} (top) and Br_{13} and Br_{14} (bottom) in β Ori (B8 Ia, $T_{eff} = 12000$ K, $\log g = 1.75$, $\xi = 2$ km/s, $y = 0.135$). Non-LTE (solid line) and LTE (dashed-dotted line) computations are compared against observation (dots). Note that in the case of the Balmer lines both models are practically indistinguishable.

displayed in Fig. 1.2. While the Balmer lines are still insensitive to the different collisional data, a marked change in the equivalent width of Br_γ is obtained, by $\sim$30%. The new model atom hereby succeeds in reproducing the visual and IR lines at the same time (with stellar parameters determined from a standard analysis of the optical spectrum). For an even more pronounced non-LTE situation, such as an early O-type supergiant, changes by up to 60% in equivalent width are indicated for Br_γ.

The current findings are encouraging, as they recover previous results in the optical, while they promise increased accuracy for analyses in the still developing field of IR spectroscopy. In particular, they will impact all stellar astrophysics where dust obscuration is of concern, e.g. studies of the early evolution stages of massive stars, or research on stars in the Galactic Center – and of course science with the NGST, which will operate in the IR.

A final example for non-LTE effects on hydrogen is given in Fig. 1.3. Our non-LTE computations succeed in simultaneously reproducing the pseudo-photospheric higher Balmer and Paschen lines in luminous supergiants, indicating a significant non-LTE strengthening of the Paschen lines. In BA-type supergiants the strength of the hydrogen lines tightly correlates with stellar luminosity, as the element becomes highly sensitive to ionization, allowing surface gravities to be determined to high precision, to $\sim$0.05 dex at best. Such an accuracy allows us to use BA-type supergiants as alternative distance indicators, via the flux-weighted gravity-luminosity relationship (Kudritzki, Bresolin & Przybilla 2003).

1.4 The Light Elements: CNO

Comprehensive model atoms for C I/II, N I/II and O I have been implemented recently (see Table 1.1). For the first time also detailed excitation cross-sections for electron collisions are accounted for in hundreds of transitions, as well as accurate radiative data, adopted from state-of-the-art quantum-mechanical *ab-initio* computations.

Similar non-LTE effects are at work in all three elements. Photoionizations depopulate the low-lying energy levels of the neutral species, while recombination cascades provide a significant overpopulation of the (quasi-)metastable states in the line-formation region. Moreover, photon losses – in particular in the tenuous atmospheres of the supergiants – lead to a drop of the line source function below the Planckian value. Both effects promote the non-LTE strengthening of the CNO lines of the neutral atoms at visual and near-IR wavelengths. Non-LTE abundances will therefore be systematically smaller than derived in LTE. Non-LTE strengthening is also found for the lines of the singly-ionized species.

The new results confirm these well-known facts from previous studies. However, for the first time practically *all* spectroscopic indicators are reproduced in a *quantitative* manner. Consistent results are obtained from lines of the different spin systems, simultaneously for the neutral *and* singly-ionized stages. A comparison of non-LTE and LTE abundances for individual lines in a few test objects is made in Fig. 1.4. In the main-sequence star Vega departures from LTE hardly affect the weaker C I and O I lines, whereas the strong lines of these species and the N I lines are subject to significant non-LTE effects. These strengthen in the supergiants, giving rise to non-LTE abundance corrections of typically $\sim$0.3 dex for the weak lines and of more than 1 dex for the strong lines. By accounting for non-LTE effects systematic trends of derived line abundance with equivalent width are removed and the statistical scatter from the weak lines is slightly reduced when compared to LTE analyses. Our results suggest that *absolute* abundances with 1σ-uncertainties of 0.05 to 0.10 dex (random) and 0.07 to 0.12 dex (systematic error) can be derived in main sequence to supergiant

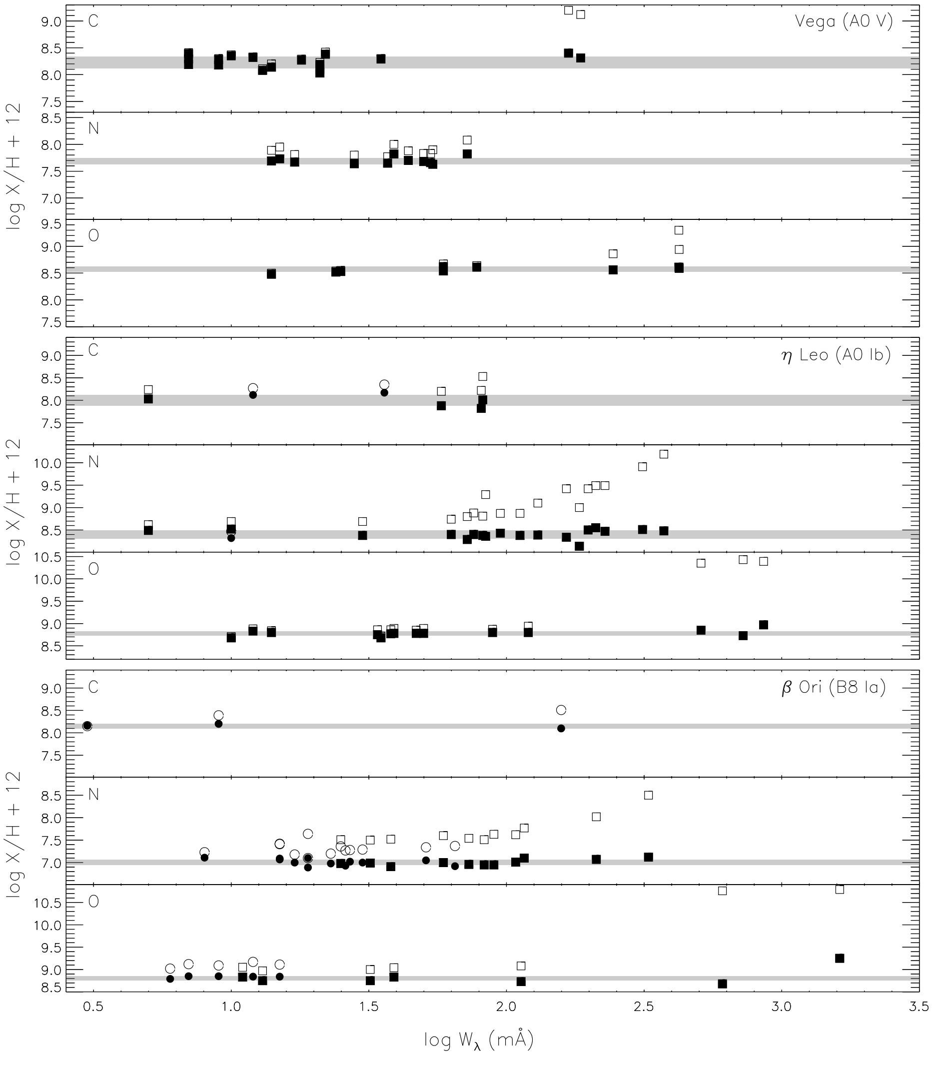

Fig. 1.4. Comparison of LTE and non-LTE abundances (open/filled symbols) for CNO from our best fits of unblended spectral lines in three bright galactic objects on the usual logarithmic scale. Abundances for the neutral (boxes) and singly-ionized species (circles) are displayed as a function of equivalent width. The gray band spans the uncertainty range associated with the mean abundances ($\pm 1\sigma$ random errors).

stars alike. In particular, the new models indicate much higher nitrogen abundances from the analysis of N I lines in BA-type supergiants than derived previously, by a factor of $\sim$2. The refined collisional excitation data (Frost et al. 1998) allow for a realistic treatment of the processes trying to restore detailed balance. It turns out that the non-LTE departures are drastically dampened in comparison to the case with less elaborate data. These findings have significant consequences for the interpretation of the deduced abundance ratios in

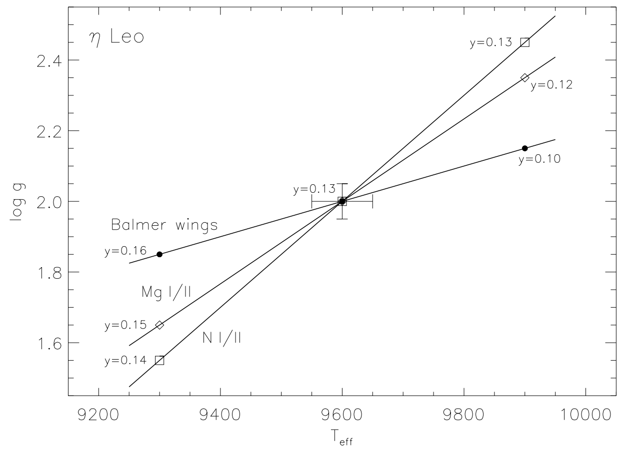

Fig. 1.5. Fit diagram of temperature- and gravity-sensitive spectral lines in the (T_{eff}, $\log g$)-plane for η Leo. Along the curves either the computed spectral lines of two different ionization stages of the elements indicated or the synthetic profiles of the higher Balmer lines agree with the observations. The curves are parameterized by surface helium abundance y (by number); a $\xi = 4$ km/s is adopted.

terms of chemical mixing in the course of massive star evolution (Przybilla et al. 2003). In particular, high accuracy in the abundance determination allows one to distinguish objects evolving from the main sequence to the red supergiant stage from stars on a blue-loop with high confidence, based on the observed abundance patterns.

1.5 Stellar Parameters

The progress in non-LTE line-formation computations described so far both *relies on* and *allows for* the determination of precise stellar parameters. Our approach is purely spectroscopic and requires access to a number of strategic lines spread over the entire visual and near-IR spectral range. The Stark-broadened (higher) Balmer series members act as surface gravity indicators. These may be complemented by the Paschen lines. Multiple non-LTE ionization equilibria (e.g. N I/II, O I/II, and also several of the heavier metals) help us to constrain the stellar effective temperature. Here spectral lines of two (or more) ionization stages of an element have to be brought into simultaneous agreement with observation. The general procedure is schematically illustrated in Fig. 1.5: the intersection of the different loci in the (T_{eff}, $\log g$)-plane determines the values of these fundamental parameters. Note that secondary parameters such as the helium abundance and metallicity have to be explicitly accounted for at the same time, if high accuracy is desired. This applies in particular to analyses of objects close to the Eddington limit, see Przybilla (2002) for details.

The impact of improved atomic data for the stellar parameter determination is enormous. Applications of the new non-LTE model atoms result in simultaneous agreement of all independent stellar parameter indicators under consideration, which we interpret as the absence of systematic errors to a large extent. An optimistic evaluation of the uncertainties involved in the parameter determination suggests that effective temperatures can be constrained to better than 1% and surface gravities to $\sim$0.05–0.10 dex for objects of spectral types late B to early A, even in the supergiant regime. This is a significant improvement with regard to the current standard. The redundancy inherent in our approach turns out to be highly advantageous, and the gain in accuracy in this crucial step of stellar analyses justifies the additional effort. More work is clearly needed in order to improve the standards for analyses of objects of other spectral types.

1.6 Stellar Abundances: The Whole Picture

With accurate stellar parameters at our disposal we can extend the discussion of non-LTE abundance analyses to a much broader scope. Model atoms based on accurate atomic data are available for a number of α-process and Iron Group elements (see Table 1.1), with additional work on s-process elements currently being undertaken. Results from the non-LTE analysis of two bright BA-type supergiants are displayed in Fig. 1.6, and they are compared with findings obtained under the assumption of LTE. Non-LTE line-formation computations recover an abundance distribution of the heavier elements close to the solar standard, only the light elements depart from this as a result of mixing processes occurring in the course of stellar evolution. Accounting for non-LTE reduces the random errors and removes systematic trends, such as misleading 'abundance patterns' introduced by the assumption of LTE. In particular, LTE analyses tend to overestimate the abundances of the light and α–process elements in most cases, and to underestimate the Iron Group abundances; this systematic effect strengthens with increasing luminosity. This behavior is a consequence of the atomic structure of the ions under consideration. The Iron Group elements are characterized by a partially filled 3d electron shell which gives rise to a highly complex term structure with many low-lying and closely spaced (metastable) energy levels. Typically, these are the lower states of the observed transitions, and overionization may lead to non-LTE weakening of the lines. The few outer electrons of the lighter chemical species on the other hand couple to only a small number of terms in the ground state configuration, which are usually separated by an energy gap of several eV from the next excited terms (the lower levels of the observed features in this case). Recombination cascades lead to an overpopulation of these (quasi-)metastable states in the line-formation region, as collisional processes become ineffective in depopulating these due to the large energy gap, resulting in a non-LTE strengthening of the lines in the visual and near-IR.

Pronounced non-LTE abundance corrections are found for the strong lines, amounting up to $\sim$2 dex in extreme cases. On the mean, however, these are smaller, of the order of typically 0.1 dex on the main sequence and 0.3 dex in supergiants. Contrary to well-established assumptions, marked (by a factor of $\sim$2) non-LTE corrections are also found for weak lines ($W_\lambda \simeq 10$ mÅ) in several cases (O II, S II/III, Ti II). The statistical uncertainties of the heavier element abundances are slightly higher than those discussed previously for CNO, reflecting a decrease of accuracy in the atomic data, as theory is confronted with a problem of much higher complexity. Accurate atomic data turns out to be the key for improving the standards also in this case.

The discussion so far shows that we have succeeded in performing comprehensive non-LTE line-formation calculations for the most important chemical species of astrophysical relevance, allowing us to reproduce the better part of the spectra of BA-type stars in the visual and near-IR with high accuracy. By accounting for the remainder in LTE, practically the entire observed line spectra can be synthesized. Such comprehensive spectrum synthesis is the only way to perform stellar analyses even at low spectral resolution. The most exciting applications will comprise studies of galaxies beyond the Local Group, based on quantitative spectroscopy of individual stars within these systems. First results on analyses of BA-type supergiants (typically the visually brightest normal stars in star-forming galaxies) in NGC 3621 and NGC 300, at distances of 6.6 and 2.0 Mpc, respectively, show the large potential of the present work for the field of extragalactic stellar astronomy (Bresolin et al. 2001, 2002). Detailed high-resolution studies of such objects within the Local Group, in different galactic environments, will also be crucial for improving our understanding of stellar and galactochemical evolution, see e.g. Venn (1999) and Venn et al. (2000, 2001) for results on the Small Magellanic Cloud, M 31 and NGC 6822, and also Venn's contribution in these proceedings for more recent work.

1.7 Conclusions

Significant improvement can be achieved in stellar parameter and elemental abundance studies when the ubiquitous non-LTE effects are addressed thoroughly with *accurate* atomic data. The non-LTE approach is certainly more time-consuming than the widely used LTE techniques, but it is highly rewarding: all fields of stellar astrophysics do benefit from reduced statistical and systematic uncertainties. It is therefore of essential interest to us astronomers to support the field of atomic physics, as many of the crucial data are still missing. In order to improve the status of the atomic databases further work is required in particular on particle collision data. Only with a comprehensive set of accurate atomic data we can exploit the potential offered by the new generation of large telescopes to full extent.

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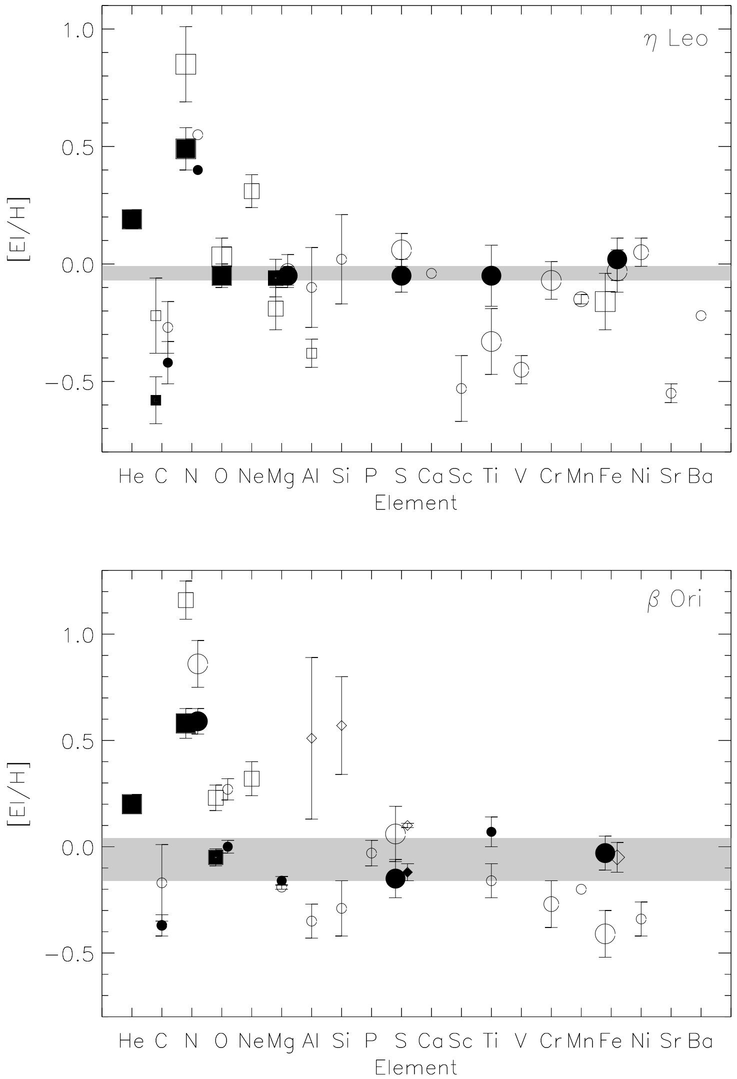

Fig. 1.6. Abundance pattern determined for the two Milky Way supergiants η Leo and β Ori, relative to the solar standard (Grevesse & Sauval 1998) on a logarithmic scale. Non-LTE (filled symbols) and LTE abundances (open symbols) for neutral (boxes), single-ionized (circles) and double-ionized (diamonds) species. The symbol size codes the number of spectral lines analyzed. Error bars represent 1σ-uncertainties from the line-to-line scatter. The gray shaded area marks the deduced stellar metallicity within 1σ-errors. The non-LTE computations reveal a striking similarity to the solar abundance distribution, except for the light elements which have been affected by mixing with nuclear-processed matter.