Non-LTE line-formation for CNO

Norbert Przybilla, Rolf-Peter Kudritzki

Institute for Astronomy, 2680 Woodlawn Drive, Honolulu, HI 96822, USA

Keith Butler, Sylvia R. Becker

Institut für Astronomie und Astrophysik, Universitätsternwarte, Scheinerstr. 1, D-81679 München, Germany

Abstract. Accurate atomic data have become available in the recent past due to the demands of astrophysics and fusion research. We report on the impact of such data on non-LTE line-formation calculations for CNO in early-type stars. Considerable improvement is achieved by the derivation of consistent results from practically all available spectroscopic indicators, regardless of ionization stage or spin system, and the uncertainties in the analyses are drastically reduced. Moreover, systematic trends are revealed, e.g., an increase of the N\textsubscript{i} abundances from previous studies of BA-type supergiants by a factor of two is indicated. The present work promises stringent observational constraints on chemical mixing in the course of massive star evolution. First results on BA-type supergiants in the Galaxy and the Magellanic Clouds are discussed.

1. Introduction

Carbon, nitrogen and oxygen represent the body of the heavy elements in the universe. Knowledge of their abundances is a key ingredient for understanding the evolution of stars, galaxies and the universe. However, reliable and accurate information on CNO abundances is scarce. In the late-type stars it is primarily the convective nature of the atmospheres that introduces systematic uncertainty, such that even the solar CNO abundances are under debate still (e.g. M. Asplund, these proceedings). On the other hand, non-LTE effects prevail in the earlier spectral types. Besides efficient numerical techniques, accurate atomic data are required for solving the non-LTE radiative transfer problem. Vast amounts of radiative and collisional data from quantum-mechanical \textit{ab-initio} calculations have been provided by the Opacity Project (Seaton et al. 1994) and the IRON Project (Hummer et al. 1993) in the recent years, supplemented by contributions from fusion research and state-of-the-art experiments. 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 discuss the impact of such data on non-LTE abundance determinations for CNO in early-type stars and report on first applications.
Comprehensive model atoms for C\textsubscript{i/ii}, N\textsubscript{i/ii} and O\textsubscript{i} are implemented (Przybilla, Butler, & Kudritzki 2001; Przybilla & Butler 2001; Przybilla et al. 2000; Przybilla 2002) for the non-LTE line-formation programs DETAIL and SURFACE (Giddings 1981, with substantial modifications by K. Butler). For the first time also detailed excitation cross-sections for electron collisions are accounted for in hundreds of transitions, besides accurate radiative data, adopted from sophisticated quantum-mechanical computations.

Testing of the models is performed on high-resolution and high-S/N Echelle spectra of several bright galactic main sequence stars and supergiants of spectral types B and A, using line-blanketed ATLAS9 model atmospheres (Kurucz 1993). 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 (the model atom of Becker & Butler (1988) is adopted for O\textsubscript{ii}). A comparison of non-LTE and LTE abundances for individual lines in a sub-sample of the test objects is made in Fig. 1. In the main-sequence star Vega departures from LTE hardly affect the weaker C\textsubscript{i} and O\textsubscript{i} lines, whereas the strong lines of these species and the N\textsubscript{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. In particular, the new models indicate much higher nitrogen abundances from the analysis of N\textsubscript{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 terms of chemical mixing in the course of massive star evolution, see below and Venn & Przybilla (VP, these proceedings).

To conclude, the new model calculations reduce the random scatter in the spectral line analyses and largely remove systematic error. They indicate that absolute abundances with 1\(\sigma\)-uncertainties of 0.05 to 0.10 dex (random) and \(\sim 0.10\) dex (systematic error) can be derived in main sequence to supergiant stars alike. In addition, the presence of lines from two ionic species of the elements allows to exploit the ionization equilibria for the stellar parameter determination.
Figure 1. 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 (circles) and singly-ionized species (boxes) are displayed as a function of equivalent width. The grey band spans the uncertainty range associated with the mean abundances (±1σ random errors). Note that for the derivation of the mean abundances a few additional blended lines have also been accounted for by means of spectrum synthesis.
A few issues remain to be solved. The comparatively large uncertainty in the carbon abundances is interpreted as an indication for the need of further improvement of the atomic data. Discrepant abundances from the C\textsc{ii} $\lambda\lambda 6578$–$82$ doublet, formed in the wing of H$\alpha$, result from the neglect of sphericity and mass-loss effects on the H$\alpha$ feature, leading to inappropriate line-formation depths for the C\textsc{ii} lines in the current modelling. Sphericity and mass-loss are also affecting the oxygen triplet $\lambda\lambda 7771$–$5$ and O\textsc{i} $\lambda 8446$, which belong to the strongest lines in luminous supergiants, sampling the body of the stellar atmosphere. The N\textsc{i} $\lambda\lambda 8184$–$8242$ multiplet analysis currently suffers from problems with realistically modelling the line merging and level dissolution of hydrogen near the Paschen series limit, again leading to inappropriate line-formation depths for the N\textsc{i} features. Finally, the strongest line in the doublet spin system, N\textsc{i} $\lambda 8629$, turns out to indicate too low abundances still, despite significant improvement compared to previous studies. This line is extremely sensitive to inaccuracies in the atomic data and the atmospheric structure.

### 3. First applications

Stellar evolution models accounting for the effects of mass-loss and rotation have become available recently (Meynet & Maeder 2000; Heger & Langer 2000). These reproduce many of the observational constraints (e.g. A. Herrero, these proceedings; VP) on massive star evolution at least qualitatively, in particular the surface contamination with CN-cycle products. In addition to convective mixing during the red-supergiant stage (first dredge-up) a second channel opens, rotationally induced mixing. This can account for abundance anomalies of the light elemental species already on the main sequence.

We compare the predictions from the new stellar evolution models with the findings from our test sample and preliminary results on the visually brightest, i.e. the most massive, A-type supergiants in both Magellanic Clouds in Fig. 2. Non-LTE abundances for the fusion product helium have been determined in addition to data on CNO. The objects are assumed to be single stars, as binary evolution will alter the interpretation of the results significantly. To summarise, good agreement is found in terms of helium enrichment and N/C ratios. For the least-massive galactic object a blue-loop scenario with first dredge-up abundances is indicated and the more massive objects have most likely evolved directly from the main sequence, allowing for variations in the initial rotational velocities. Far stronger mixing acts in the SMC supergiant, which is well understood if metallicity effects on stellar evolution are accounted for, that affect mass-loss and angular-momentum transport (Maeder & Meynet 2001). In addition, good agreement between the combined CNO abundances and stellar metallicity (relative to the solar standard, Grevesse & Sauval 1998) is found, as can be expected for the catalysts of the main fusion cycle.

However, the consistent picture is shattered when the N/O ratios are considered. These deviate from the predictions, as oxygen remains practically undepleted. The reason for this has to be investigated. Moreover, a CNO overabundance relative to the heavier metals is indicated, if the solar abundances from 3D hydrodynamical simulations (M. Asplund, these proceedings) are preferred over the results from classical 1D model atmospheres.
How do our conclusions compare with those of previous investigations? Until recently, CNO abundances in galactic and SMC AF-type supergiants in the mass-range $\sim5$–$20$ $M_\odot$ (Venn 1995, 1999) seemed to indicate a direct evolution from the main sequence, with no necessity to invoke blue-loop scenarios. In view of the improved non-LTE abundance analysis – in particular with respect to nitrogen – the situation has to be reinvestigated, with an important first step taken by VP. Blue-loop evolution can no longer be ruled out, and large efforts will be required to disentangle the different alternatives for explaining the observational findings, see VP for details. An extension of the sample size is mandatory, including many more objects of masses above $\sim20$ $M_\odot$, where the signatures of rotationally induced mixing are supposed to get more pronounced.

A related field of application is the analysis of unevolved B-type main-sequence stars. Here, Korn et al. (2002) use the new model atoms to derive pristine stellar CNO abundances in the LMC, based on VLT/UVES observations. These compare well with results from H II region analyses and confirm the extraordinary low present-day nitrogen abundance of this galactic environment.

4. Perspective

The future certainly belongs to extensive applications of the new CNO model atoms for quantitative spectroscopy. Efficient multi-object spectrographs like FLAMES on the VLT will provide the plethora of observations needed to systematically investigate massive star evolution throughout the HRD. On the theoretical side, the model atoms will see occasional updates with improved atomic data, whenever it becomes available. Furthermore, an implementation of the model atoms for non-LTE computations of line-blanketed, spherically extended stellar atmospheres accounting for mass-loss is aspired, in order to solve the remaining few problems with the current approach. Finally, an extension of the applications towards later-type stars should also be considered. This will however require major efforts from theoretical atomic physics to generate reliable data on hydrogen collisions, which can presently be treated in a highly approximative manner only.

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Figure 2. Indicators for mixing of nuclear-processed matter into atmospheric layers: (a) surface He abundance (by mass), (b) N/C and (c) N/O mass ratio. The light-grey and dark-grey bands denote predictions from stellar evolution models (Meynet & Maeder 2000) for objects crossing the HRD for the first time and in the blue-loop phase, respectively (at $T_{\text{eff}} = 10^4$ K, for solar metallicity and $v_{\text{rot}} = 300$ km s$^{-1}$). Results from the abundance analyses of four galactic BSG and the visually brightest stars in both Magellanic Clouds are indicated by dots. A comparison of the sum of CNO abundances with the stellar metallicity (as defined by the heavier elements, grey bands) is made in (d), the values are given relative to the solar standard (Grevesse & Sauval 1998). The width and the breadth of the bands in (d) indicates the $\pm 1\sigma$ uncertainties in metallicity and ZAMS mass, respectively. Horizontal lines mark the expected metallicities in the three galactic environments.