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Spectral synthesis in the near UV (3000-4500 Å)

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Abstract. In this work we review the details, with emphasis on the near UV (3000-4500 Å), of the molecular database and the continuous opacity sources as implemented in the spectrum synthesis code used to calculate the spectral library presented in Coelho *et al.* (2005). We discuss our recent and future efforts towards the improvement of the calculation in this spectral range.

Keywords. atomic data, molecular data, ultraviolet: stars

1. Introduction

Recently, Coelho *et al.* (2005) made available a high resolution, high coverage ($\Delta\lambda =$ 0.02 Å, $\lambda\lambda$ 3000 Å - 1.8 μm) synthetic stellar spectra library to be used in the analysis of stellar populations. The library relies in a reliable database of atomic and molecular lines built and tested over the years (see Coelho *et al.* for details and references) in abundance analyses of high resolution and high S/N spectra stellar spectra.

The spectra were calculated with PFANT; a revised and improved version of the code presented in Cayrel *et al.* (1991) and Barbuy *et al.* (2003). It is based on the FANTOM code of Spite (1967) and includes the calculation of molecular lines (Barbuy 1982) and of the first 10 Balmer lines of H using a revised version of the code of Praderie (1967).

Here, we restrict ourselves to the 3000-4500 Å region. A region of difficult analysis for its large number of atomic and molecular lines. Nevertheless, interesting features for the study of stellar populations lie in this region. As an example of the wealth of information that can be derived from this region we refer for example to Rose (1985) and Schiavon (2006). We also recall that this region may be optimal to the analysis of galaxies with z $\sim$ 0.8, since it is red-shifted to the most sensitive spectral domain of the CCDs.

In this work, we review the continuous opacity sources and molecular systems important for the spectra in the near UV region. We list the features included in our code, point out what is still lacking, and discuss the steps that will be taken towards its improvement.

2. Continuous Opacity

The continuous opacity sources included in the PFANT code are: Electron scattering, Rayleigh scattering of H and H_2, bound-free (*bf*) and free-free (*ff*) absorptions of H^-, H_2^+, neutral H, neutral He, He^+, and H_2^- *ff* absorption.

These sources were implemented in the first versions of the code and since then were not updated. Important changes, however, are not expected. Nevertheless, we intend to search the literature for more recent results, and update the calculations if necessary.

Among additional sources still lacking in the calculations are, for example, the Rayleigh scattering of He and the *bf* opacities from metals. At least Mg I, Al I, Si I, and Fe I, have photo-ionization edges in the 3000-4500Å region.

It is important here to note that the flux calibrated spectra presented in Coelho *et al.* (2005) were divided by the continuum obtained with PFANT and multiplied by the continuum computed using the same ATLAS9 model atmosphere.

Theoretical photo-ionization cross-sections for these elements are available thanks to the Opacity Project (Seaton *et al.* 1994) and the Iron Project (Hummer *et al.* 1993). They may be included in the calculations through the polynomial fittings of the smoothed cross-sections (Bautista *et al.* 1998, Allende Prieto *et al.* 2003).

Whereas the relative importance of the Fe I photo-ionization cross sections seem to be large, that of Al I, Si I, and Mg I in 3000-4500 Å, is expected to be small, even for solar metallicity (Bell *et al.* 2001). The importance should also decrease with metallicity. On the other side, for α enhanced metal rich stars, the importance of Si I and Mg I should increase. Thus, the effort to include these opacities sources seem to be worthwhile.

3. Molecular Database

Transitions for MgH, C_2, CN, CH, OH, NH, and TiO affecting the region between 3000 and 4500 Å were included in the database by the time the spectral library was calculated. The blue systems of CN, OH, NH, and CH are of particular importance.

The OH ($A^2\Sigma$-$X^2\Pi$), NH ($A^3\Pi$-$X^3\Sigma$), and CN ($B^2\Pi$-$X^2\Sigma$) bands were implemented by Castilho *et al.* (1999) while the CH band systems ($A^2\Delta$-$X^2\Pi$), ($B^2\Sigma$-$X^2\Pi$), and ($C^2\Sigma$-$X^2\Pi$) were implemented by Melendez *et al.* (2003). While the NH and CH bands are adequately fitted to the Sun and Arcturus, the CN bands are not.

In an effort towards the improvement of the CN bands we have recently implemented the line lists of B. Plez (2005, private communication) for the CN blue system including four different isotopic variations, $^{12}C^{14}N$, $^{12}C^{15}N$, $^{13}C^{14}N$, $^{13}C^{15}N$.

A comparison with the previous $^{12}C^{14}N$ line list show the wavelengths and molecular gfs to be slightly different. Both set of lines yielded the same results in a preliminary analysis of low resolution spectra of main sequence stars in 47 Tuc. A more detailed evaluation is still under way but the new set of lines still seems not to be fully adequate.

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