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A new theoretical stellar library for stellar population applications

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Abstract. Theoretical libraries have been increasingly used to overcome limitations of empirical libraries, e.g. by exploring atmospheric parameter spaces not well represented in empirical libraries. This work presents a new synthetic library which covers $3000 \leq T_{\rm eff} \leq 25000$ K, $-0.5 \leq \log g \leq 5.5$, and 12 chemical mixtures covering $0.0017 \leq Z \leq 0.049$ at both scaled-solar and α-enhanced compositions. This library complements previous ones by providing: homogeneous computations of opacity distribution functions, models atmospheres, statistical surface fluxes and high spectral resolution spectra; high resolution spectra with continua slopes corrected by the effect of predicted lines, and; two families of α-enhanced mixtures for each scaled-solar iron abundance, to allow studies of the α-enhancement both at 'fixed iron' and 'fixed Z' cases. Comparisons to observed spectra were performed and confirm that the synthetic spectra reproduce well the observations, although there are wavelength regions which should be further improved. The atmospheric parameter scale of the model library was compared to one derived from a widely used empirical library, and no systematic deviation between the scales was found. This is particularly reassuring for methods which use synthetic spectra for deriving atmospheric parameters of stars in spectroscopic surveys.

Keywords : stars: atmosphere – stars: fundamental parameters – astronomical databases: miscellaneous

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1. Introduction

A stellar library is at the heart of accurate stellar population models, and should ideally provide complete coverage of the HR diagram, accurate atmospheric parameters (effective temperature $T_{\rm eff}$, surface gravities $\log g$ and abundances [Fe/H], [Mg/Fe], etc.), good compromise between wavelength coverage, spectral resolution and signal-to-noise (S/N). Both empirical and theoretical libraries can be used for this purpose, and which choice is "best" is a matter of on-going debate at related conferences and literature.

Model stellar spectra opened new important ways to study integrated light from stellar populations. Theoretical stellar libraries have been used to build fully theoretical stellar population models (e.g. Leitherer et al. 1999; Coelho et al. 2007; Percival et al. 2009), and were crucial for the development of methods which lead to the measuring of element abundances (beyond the global metal content) in integrated stellar populations (e.g. Trager et al. 1998). In recent years, model spectra are flourishing in extragalactic applications by allowing the spectral modelling of a variety of stellar histories via differential methods, i.e., combining empirical stellar libraries with model predictions (e.g. Cervantes et al. 2007; Prugniel et al. 2007; Walcher et al. 2009).

This work is the first of a series aiming at expanding our stellar population modelling (Coelho et al. 2005; Coelho et al. 2007; Walcher et al. 2009) towards larger coverage in ages, metallicities and wavelength range. A theoretical spectral stellar library is presented, tailored to the usage in stellar population models, though it is not limited to that application. It brings: *(a)* a homogeneous computation of opacity distribution functions, model atmospheres, emergent fluxes from 130 nm to 200 μm for low resolution studies, and high resolution spectra computed from 250 to 900 nm; *(b)* high resolution spectra with continuum slopes corrected for the effect of predicted lines, and; *(c)* two families of α-enhanced mixtures for each scaled-solar iron abundance, to allow differential studies of the α-enhancement both at 'fixed iron' and 'fixed Z' cases. Details are given in Coelho (2014) (http://adsabs.harvard.edu/abs/2014arXiv1406.0933P).

2. The theoretical library of model atmospheres, fluxes and spectra

The library consists of the homogeneous modelling of opacity distribution functions, model atmospheres, statistical samples of surface fluxes (SED models) and high resolution spectra (HIGHRES models). The whole library is available to the astronomical community upon request.

The target use of the present library, although not limited to that, is the spectral modelling of stellar populations and the measurement of ages, iron abundances and α over iron ratios in integrated light (Coelho et al. 2007; Walcher et al. 2009).

As such, the coverage of the HR diagram was fine-tuned to encompass evolutionary stages relevant to the integrated light of populations with ages between 30 Myr and 14 Gyr, from lower main sequence to the early Asymptotic Giant Branch. The library encompasses 12 chemical mixtures, both scaled-solar ([Fe/H] = -1.0, -0.5, 0.0, 0.2) and α-enhanced ([α/Fe] = 0.4)

ODFs were computed with the Linux port of the code DFSYNTHE (Kurucz 2005; Castelli 2005). Model atmospheres were computed using a linux port of the code ATLAS9 (Kurucz 1970; Sbordone et al. 2004) for stars with $T_{\rm eff} \geq 4000$ K. Atmosphere models were calculated under the assumption of plane-parallel geometry, using the turbulent velocity $\xi = 2$ km/s and mixing length parameter $\alpha_{ML} = 1.25$. For stars below $T_{\rm eff} = 4000$ K, pre-computed MARCS models were adopted (Gustafsson et al. 2008), as these models are computed with a larger set of molecular opacities important to the atmosphere structure of cool stars (in particular VO and ZrO). Model surface fluxes for the present library were computed with the code ATLAS9v, made available by F. Castelli at her website (`http://wwwuser.oat.ts.astro.it/castelli/sources/atlas9codes.html`). High spectral resolution (HIGHRES) synthetic spectra were computed from 250 to 900 nm with the spectral synthesis code SYNTHE (Kurucz & Avrett 1981) in its public Linux port by Sbordone, Bonifacio, Castelli & Kurucz (2004), at a wavelength resolution $R_\lambda = 300000$. The models were then broadened to a gaussian line spread function of R = 20000 and resampled to a constant wavelength sampling of 0.02 Å.

The atomic line list adopted is based on the compilations by Coelho, Barbuy, Melendez, Schiavon & Castilho (2005) and Castelli & Hubrig (2004). Lines for the molecules C_2, CH, CN, CO, H_2, MgH, NH, OH, SiO and SiH (published online at `http://kurucz.harvard.edu/`) were included for all stars, and TiO lines (Schwenke 1998) were included for stars cooler than $T_{\rm eff} = 4500$ K.

3. Effect of predicted lines in the fluxes

The effect of the atomic lines with predicted energy levels (or more shortly '*predicted lines*', PLs, Kurucz 1992) on high and low spectral resolution models has been discussed and shown in e.g. Bell, Paltoglou & Tripicco (1994); Short & Lester (1996); Castelli & Kurucz (2004); Munari et al. (2005). Typically, libraries which are aimed at high resolution studies do not include PLs, while libraries which aim at photometric predictions include them. In the case of stellar population applications, where both regimes are of interest, some combined solution has to be achieved.

In the present work, the photometric effect of the PL was quantified by the comparison between the SED and HIGHRES libraries. Fig. 1 shows comparisons for four combinations of atmospheric parameters, selected to illustrate the dependence of the PL blanketing with temperature. A quantitative criteria was used to identify which stars are affected by the PLs in a non-negligible way: the fluxes in HIGHRES and SED

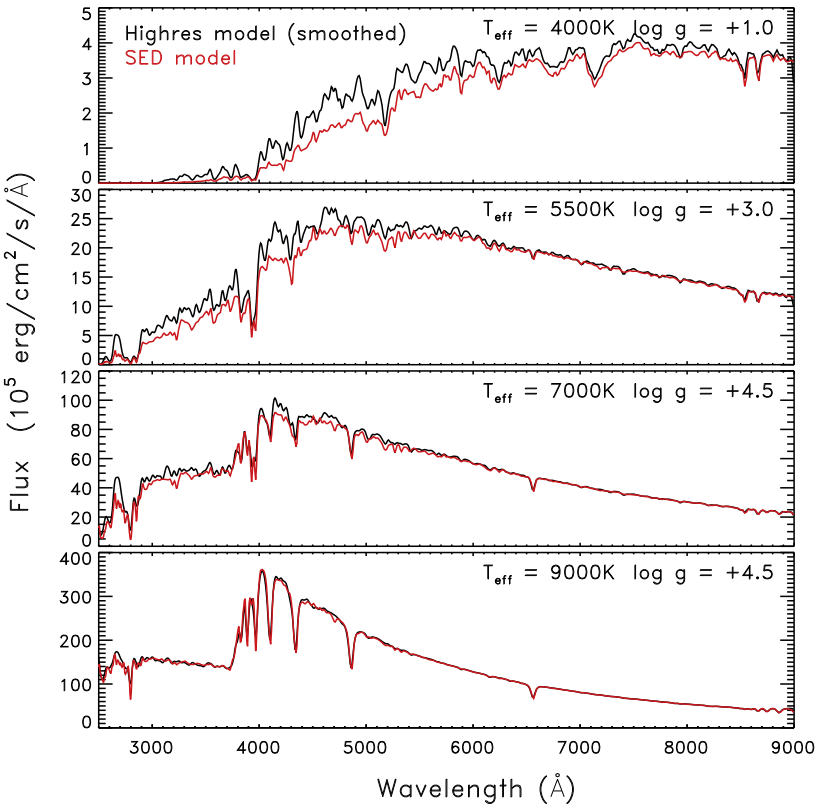

Figure 1. SED (red curves) and HIGHRES models (black curves) are compared for four combinations of stellar parameters, indicated in each panel. All models have solar abundance mixtures (p00p00). All models are smoothed to a resolution of FWHM ∼ 30 Å for easier visualization. The blanketing due to the inclusion of PLs is easily noticed in the coolest star and diminishes as temperature increases.

models were integrated from 2500 to 6000 Å for the whole library. The stars with differences between SED and HIGHRES models larger than or equal to 0.05 mag were flagged. In those cases, flux ratios $F_{ratio} = F_{SED} / F_{HIGHRES}$ were computed, after convolving both fluxes to a common spectral resolution of FWHM = 30 Å at 4000 Å. To each flux ratio, a function of the form: $y = \tanh[(x - a)/b] + c$, was fitted, where y is the flux ratio, x is the wavelength in Å, a, b and c are fitting constants. This functional form was chosen because it provides a smooth tracing of the continua ratio, being less sensitive to the residual lines/bands than a polynomial or a spline function. As a final step, the fitted functions were multiplied by the HIGRHES models, resulting in models which kept the high spectral resolution features unhampered by the PLs, but flux distributions similar to the SED models. This is a compromise solution given current

atomic data, as it does not replace a necessary improvement on the quality of the PL list (see the promising work being done by Peterson & Kurucz, ApJ submitted).

After these corrections were applied, colours in the Johnson-Morgan system measured on the HIGHRES models reproduce the values measured on the SEDs within the 0.02 mag level (they reached 0.17 mag in the U-B colour before the correction).

4. Comparisons between model predictions and observations

The HIGHRES models were compared to observed spectra from the empirical stellar library MILES (Sánchez-Blázquez et al. 2006; Cenarro, et al. 2007). For each pair $[T_{\rm eff}, \log g]$ existing in solar mixture from the model library, MILES library (adopting parameters from Prugniel, Vauglin & Koleva 2011) was searched for stars with parameters within intervals given by the $[T_{\rm eff}, \log g]$ pair of the model and corresponding adopted uncertainties (see Coelho 2014). To compare each model spectrum to a number of empirical spectra serve two purposes: to take into account how uncertainties in the atmospheric parameters affect the fluxes, and to smooth out individual chemical peculiarities in stars. Taking intervals of empirical stars to be used as reference helps establishing confidence limits for evaluating the quality of the model.

Relatively few intervals (35) were found containing at least three empirical stellar spectra. Above $T_{\rm eff}$ = 12000 K, at most two stellar spectra are found in a given interval. The average absolute deviation $\overline{\Delta}$ between each model spectrum and the corresponding averaged empirical stellar flux were computed ($\overline{\Delta} = \frac{1}{N_\lambda} \sum_\lambda \left| \frac{[f_{\rm model}(\lambda) - f_{\rm obs}(\lambda)]}{f_{\rm obs}(\lambda)} \right|$ where N_λ is the number of pixels in each spectrum, $f_{\rm model}$ is the model flux and $f_{\rm obs}$ is the average empirical flux). Model stars with $T_{\rm eff} \geq 4750$ reproduce observed fluxes within $\sim$ 5%. The model spectra systematically deviates from empirical fluxes as $T_{\rm eff}$ drops below this limit, reaching $\sim$ 50% at the coolest interval. Hotter stars, in particular for $T_{\rm eff} \geq 6250$, are typically reproduced within 2%.

For the intervals with at least 8 MILES stars, root mean squared r.m.s. observed spectrum were computed, besides the averaged empirical spectra. The difference between averaged observed spectrum and model spectrum is shown in Fig. 2 as black curves, for seven intervals of atmospheric parameters. The orange areas correspond to ± r.m.s limits, derived from the observed stars. At first approximation, residuals below the r.m.s. area correspond to missing opacities in the model, while residuals above the r.m.s. area correspond to lines excessively strong. Some prominent regions, seen in more than one interval, are: features below 4200 Å corresponding to missing opacities, noted in $T_{\rm eff}$ up to 4750 K; evidence for excessive opacity near 4300, 4700 and 5200 Å (seen in particular in $T_{\rm eff}$ = 4000 and 4750 K), potentially related to bands of CH, C_2 and MgH respectively, and; too strong core of H lines, in $T_{\rm eff}$ = 6500 K and above, related to the fact that core of very strong lines are formed in N-LTE in the chromosphere layers. It has been discussed during the conference that some of the

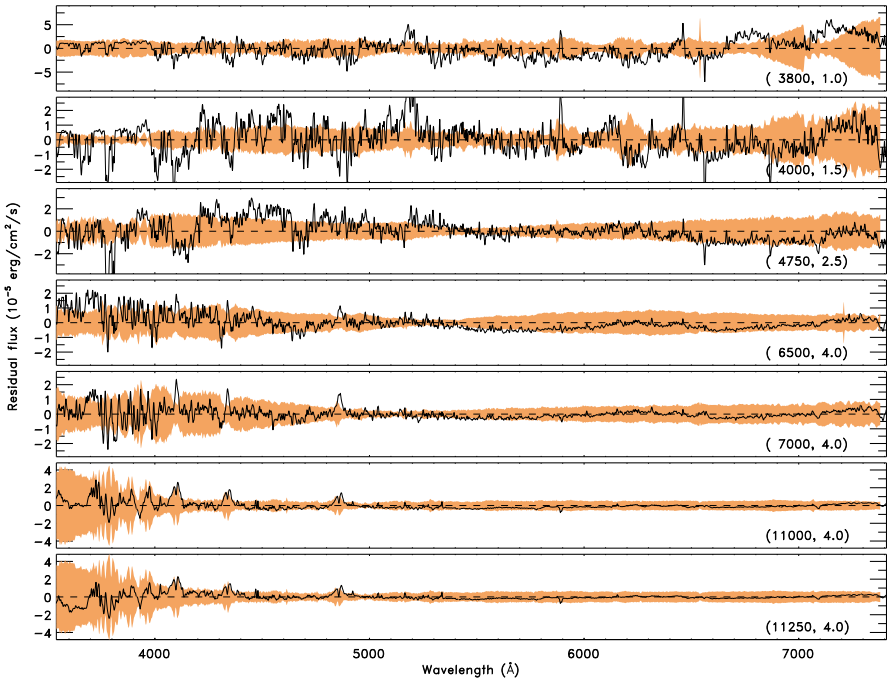

Figure 2. Black curves show the flux difference between the average MILES star in a given interval of atmospheric parameters minus the correspondent HIGHRES model (with atmospheric parameters indicated in each panel). The orange area in each panel indicate the correspondent r.m.s. of the observed stars fluxes.

missing opacity might be due to PLs, and R. Peterson kindly offered help to further study this question.

Models were also compared directly in the space of the atmospheric parameters. The spectral interpolator based on MILES published by Prugniel et al. (2011) was used with the code ULySS (Koleva et al. 2009) to "derive" atmospheric parameters for the models. The comparison between the fitted parameters and the nominal ones allow the comparison between the model parameter scale and a scale which was built for an empirical library. All stars in the library which follow the [α/Fe] vs. [Fe/H] relation obtained in Milone, Sansom & Sánchez-Blázquez (2011) were fitted. The model stars which do not have a neighbouring MILES star in the HR diagram (regions poorly sampled by MILES) were flagged for further identification ($\Delta T_{\rm eff} \geq 5\%$, $\Delta \log g \geq 0.3$ dex, Δ[Fe/H] ≥ 0.15 dex). The remaining model stars (those which have neighbouring empirical stars) were considered *safe fits*. These *safe fits* correspond to 29% of the total number of comparisons performed (459 out of 1585).

The results are shown in Fig. 3 for a fitting performed in the wavelength range

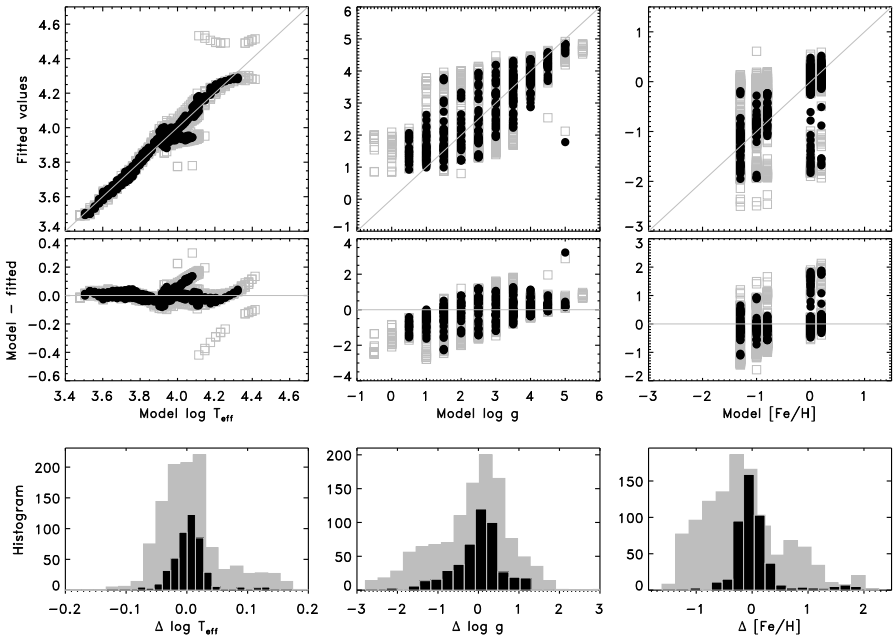

Figure 3. Comparisons between atmospheric parameters fitted by ULySS vs. the input parameters for model stars. The black symbols indicate the model stars whose parameters are well covered in MILES. The grey symbols indicate poorly sampled regions in MILES coverage (where fitted values were either extrapolated or interpolated in regions devoid of stars). The left-hand, middle and right-hand columns show results for $T_{\rm eff}$, $\log g$ and [Fe/H] respectively. Input vs. fitted values are shown in the top panels, with residuals shown in the middle row panels. The bottom panels show the histogram distributions of the residuals, computed with bins of 300 K, 0.25 dex and 0,15 dex for $T_{\rm eff}$, $\log g$ and [Fe/H] respectively.

4828 – 5364 Å (see Walcher et al. 2009). The figures show the model versus fitted parameters and corresponding residuals (first and second rows, respectively). The third row shows the histogram distributions of the residuals. The columns, from left to right, shows results for $T_{\rm eff}$, $\log g$ and [Fe/H] respectively. In all panels, black symbols correspond to *safe fits*, i.e., within close coverage of MILES library, as defined above. Grey symbols are the stars in regions not well covered by MILES (they were either extrapolated by the spectral interpolator or interpolated in the region devoid of stars).

One notices that the distribution of residuals between safe and unsafe fits (black and grey symbols) can be notably different. This raises a warning of caution over using spectral interpolator beyond the close coverage of the library where it was derived from. Secondly, the histograms of residuals are centred close to 0 (zero-points below the uncertainties). Gaussian fits to these distributions in Fig. 3 (only *safe fits* considered) yield: $\Delta T_{\rm eff}$ = 73 ± 216; $\Delta \log g$ = 0.06 ± 0.45; Δ[Fe/H] = -0.05 ± 0.2.

This is reassuring for methods which employ model libraries to automatically derive atmospheric parameters of stars in spectroscopic surveys, and highlight the advantage of model libraries in terms of covering the HR diagram.

5. Conclusions

A library of model stellar spectra is presented. This library consists of newly computed ODFs, ATLAS9 model atmospheres, low spectral resolution fluxes from UV to far–IR (SED) and high resolution spectra from 2500 to 9000 Å (HIGHRES). The library comprises 12 chemical abundance mixtures, four of those being scaled-solar and the remaining being enhanced in α-elements by 0.4 dex. The intended main use of this library is as an ingredient to fully theoretical and differential stellar population models, therefore the coverage in the $T_{\rm eff}$ vs. $\log g$ parameters space was fine-tuned to the requirements of stellar evolutionary tracks for populations between 30 Myr and 14 Gyr and Z between 0.0017 and 0.049.

Through the comparison between SED and HIGHRES models, a study on the spectrophotometric effect of lines with predicted energy levels was performed. It is demonstrated that these lines affect the spectrophotometric predictions for stars below $T_{\rm eff} \sim 7000$ K only. Ad-hoc correction functions were derived on a star-by-star basis to bring the spectrophotometric predictions of the HIGHRES models (which do not include lines with predicted energy levels) into better agreement with those of the SED models (which include them).

Model spectra were compared to empirical spectra in two ways: by the statistical comparison of the fluxes and by comparing their atmospheric parameters scales. Regarding the first comparison, it was shown that at medium spectral resolution used nowadays at stellar population studies, the model spectra reproduce the observations for a large range of temperatures and wavelength intervals (typically within 3% in flux above $T_{\rm eff} = 6000$ K, raising to 10% at $T_{\rm eff} = 4000$ K), even though there are wavelength regions which deviate and should be further investigate in terms of atomic and/or molecular opacities. Regarding the second comparison, the parameter scales of the model and empirical library agree within the uncertainties.

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References

Bell R. A., Paltoglou G., Tripicco M. J., 1994, MNRAS, 268, 771
Castelli F., 2005, Memorie della Societa Astronomica Italiana Supplement, 8, 34

Castelli F., Hubrig S., 2004, A&A, 425, 263
Castelli F., Kurucz R. L., 2004, A&A, 419, 725
Cenarro A. J., Peletier R. F., Sánchez-Blázquez P., Selam S. O., Toloba E., Cardiel N., Falcón-Barroso J., Gorgas J., Jiménez-Vicente J., Vazdekis A., 2007, MNRAS, 374, 664
Cervantes J. L., Coelho P., Barbuy B., Vazdekis A., 2007, in Vazdekis A., Peletier R. F., eds, Stellar Populations as Building Blocks of Galaxies Vol. 241 of IAU Symp, A new approach to derive [α/Fe] for integrated stellar populations. Cambridge University Press, pp 167–168
Coelho P., Barbuy B., Melendez J., Schiavon R., Castilho B., 2005, A&A, 443, 735
Coelho P., Bruzual G., Charlot S., Weiss A., Barbuy B., Ferguson J. W., 2007, MNRAS, 382, 498
Coelho P., 2014, MNRAS, 440, 1027
Gustafsson B., Edvardsson B., Eriksson K., Jorgensen U. G., Nordlund Å., Plez B., 2008, A&A, 486, 951
Koleva M., Prugniel P., Bouchard A., Wu Y., 2009, A&A, 501, 1269
Kurucz R. L., 1970, SAO Special Report, 309
Kurucz R. L., 1992, Revista Mexicana de Astronomia y Astrofisica, vol. 23, 23, 45
Kurucz R. L., 2005, Memorie della Societa Astronomica Italiana Supplement, 8, 14
Kurucz R. L., Avrett E. H., 1981, SAO Special Report, 391
Leitherer C., Schaerer D., Goldader J. D., Delgado R. M. G., Robert C., Kune D. F., de Mello D. F., Devost D., Heckman T. M., 1999, ApJS, 123, 3
Milone A. D. C., Sansom A. E., Sánchez-Blázquez P., 2011, MNRAS, 414, 1227
Munari U., Sordo R., Castelli F., Zwitter T., 2005, A&A, 442, 1127
Percival S. M., Salaris M., Cassisi S., Pietrinferni A., 2009, ApJ, 690, 427
Prugniel P., Koleva M., Ocvirk P., Le Borgne D., Soubiran C., 2007, in Vazdekis A., Peletier R. F., eds, Stellar Populations as Building Blocks of Galaxies Vol. 241 of IAU Symp, Analysis of stellar populations with large empirical libraries at high spectral resolution. pp 68–72
Prugniel P., Vauglin I., Koleva M., 2011, A&A, 531, A165
Sánchez-Blázquez P., Peletier R. F., Jiménez-Vicente J., Cardiel N., Cenarro A. J., Falcón-Barroso J., Gorgas J., Selam S., Vazdekis A., 2006, MNRAS, 371, 703
Sbordone L., Bonifacio P., Castelli F., Kurucz R. L., 2004, Memorie della Societa Astronomica Italiana Supplement, 5, 93
Schwenke D. W., 1998, Chemistry and Physics of Molecules and Grains in Space. Faraday Discussions No. 109. The Faraday Division of the Royal Society of Chemistry, London, 1998., p. 321, 109, 321
Short C. I., Lester J. B., 1996, ApJ, 469, 898
Trager S. C., Worthey G., Faber S. M., Burstein D., Gonzalez J. J., 1998, ApJS, 116, 1
Walcher C. J., Coelho P., Gallazzi A., Charlot S., 2009, MNRAS, 398, L44