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LIME: Semiautomated line measurement and identification from stellar spectra

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Abstract: We present LIME (Line Measurements from ECHELLE Spectra), an IDL-based code, as a powerful tool for semiautomated stellar line measurement and identification. Interactively selected line positions (i.e. wavelengths) are compared with a master line list of the user's selections. Each unknown line that the user interactively chooses is displayed with potential identifications provided by the code in the vicinity of the selected line. The best identification is evaluated on the basis of several criteria (e.g., atomic/molecular line information, wavelength displacement, and theoretical equivalent width for solar atmospheric values). We examined the identifications by LIME in the spectra of post-red supergiant star HD 179821 over a range of signal-to-noise values and wavelength ranges. We found that the results obtained by LIME show virtually complete agreement with the manual identifications for which the conventional and also tedious approach is to use a revised multiplet table as an initial guide and perform a systematic search that makes use of the lower excitation potential and gf-values. Comparison to previous identifications for HD 179821 in the literature revealed not only lines that were unmeasurable and/or blended but also misidentifications. While a manual identification process takes a relatively longer time to be accomplished by an experienced spectroscopist, LIME can provide a rapid extraction of line information in a few hours with moderate user interaction.

Key words: Spectroscopy, line identification, atomic data

1. Introduction

Identification of spectral lines is an essential and also time-consuming requirement in stellar spectroscopy, especially for obtaining chemical abundances. The classical approach to the task of line identification has been intensively described in the literature [1]. Web-accessible platforms that employ such approaches also exist as stellar spectral reference libraries for stellar line identification process (e.g., VALD (http://vald.astro.uu.se/∼vald/php/vald.php), NIST (http://physics.nist.gov/PhysRefData/ASD/lines_form.html), and SpectroWeb (http://spectra.freeshell.org/spectroweb.html)); however, since they provide a large number of nearby transitions that are mostly based on theoretical calculations for the unknown line, the identification process may turn into a complicated task. Furthermore, the listed (candidate) transitions in such platforms, most of the time from very large master lists, are only provided for individualized chemical compositions, which requires detailed knowledge of input physics and for certain spectral resolutions (i.e. low- or intermediate-resolution spectra for which lines may be blended). In addition, for those platforms providing theoretical spectra without instrumental broadening computation, no tool is available to ensure the reliability of the identifications. An instant visual assessment of those candidate identifications is thus desirable. In order to fulfill this requirement, we have developed a code to perform line identifications interactively. The code is also capable of measuring equivalent widths

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(EWs) in an interactive manner. Although there are many other programming language choices available for algorithm development, we preferred Interactive Data Language (IDL), which offers a great deal of options (e.g., continuum normalization via LIME-RADVEL, line identification via LIME-IDENT, EW measurement via LIME-EMS, creating input line lists with user supplied atomic and/or molecular data via LIME-GFS) for graphical utilization of the astronomical spectra. The code can be saved as a "save" file and run without having access to the IDL command line via the IDL Virtual Machine that can be used to execute an IDL save file.

This paper is organized as follows: Section 2 provides general features of the line identification code; general properties of the high-resolution optical spectra obtained at the McDonald Observatory (from 2008 to 2011) are briefly discussed in Section 3. Also provided are test results for line identifications from the ELODIE archive spectra as well as the spectra from the 10.0 m Hobby–Eberly Telescope; Section 4 presents concluding remarks.

2. Line measurement code: LIME

LIME is an in-house developed IDL code and the only required input to the code is a reduced standard (2D) FITS-format spectrum file (science frame). Prior to an interactive session by LIME for line measurement, the following standard steps should be followed: bias correction (step 1), cosmic-ray removal (step 2), flat fielding (step 3), scattering light subtraction (step 4), wavelength calibration (step 5), continuum normalization (step 6; blaze correction), concatenation of spectral orders to a single spectrum (for ECHELLE spectrum only; step 7), and correction for heliocentric velocity (step 8). The first five steps are essential in each spectroscopic analysis and are performed in a standard way, for instance in the same manner as in [2–5].

In our case, for those five steps, we used IRAF-CL scripts. Steps 6, 7, and 8 deserve special attention in stellar spectroscopic analysis, especially for line identification processes. Namely, in some certain cases, for the long slit spectra as well as the echelle spectra, continuum fitting via standard reduction packages (i.e. IRAF) may not give the best results for removal of blaze profiles from the spectra. Diffuse light in the spectrograph and inappropriate determination of dekker size are some common difficulties to mention causing problems in the continuum normalization process. (A dekker is a fork-shaped part of the slit assembly of a spectrograph and dekker size simply sets the length of the slit. The chosen dekker size limits the size of the light beam in the direction perpendicular to the spectrograph dispersion.) Moreover, for an echelle spectrum, overlapping regions should be carefully checked for an exact match. Thus, LIME is strengthened with a function that performs these three steps (steps 6, 7, and 8) at once with the help of a graphical display interface that makes visual inspection of all abovementioned intermediate stages of the reduction process possible. Steps 6 and 7 are carried out in an automated manner (Figure 1), without the need for user interaction, and the output merged spectrum is recorded as a two-column ASCII file, listing the flux at each wavelength. Then the continuum-normalized and merged spectrum is cross-correlated with a mask for radial velocity measurement via the LIME-RADVEL function (see Figure 2). The mask can be either a stellar (or observed sky) or a noise-free synthetic spectrum that ought to be degraded to the resolution of the input (stellar) spectrum (Figure 2). LIME outputs a separate log file for fitted polynomial coefficients, the computed cross-correlation function (CCF), and the peak value of the CCFs that provides the amount of correction in the velocity scale to be applied to the observed spectrum for further inspection and it is common to use the observed sky spectrum as a mask for solar-type stars as well as for sharp-lined F-type spectra. Although LIME was originally designed to process F-, G-, and K-type stellar spectra, the code is extended to include a synthetic spectrum as a template in the CCF computations to overcome unsatisfactory results for CCFs of rapidly rotating stars (a well-known problem).

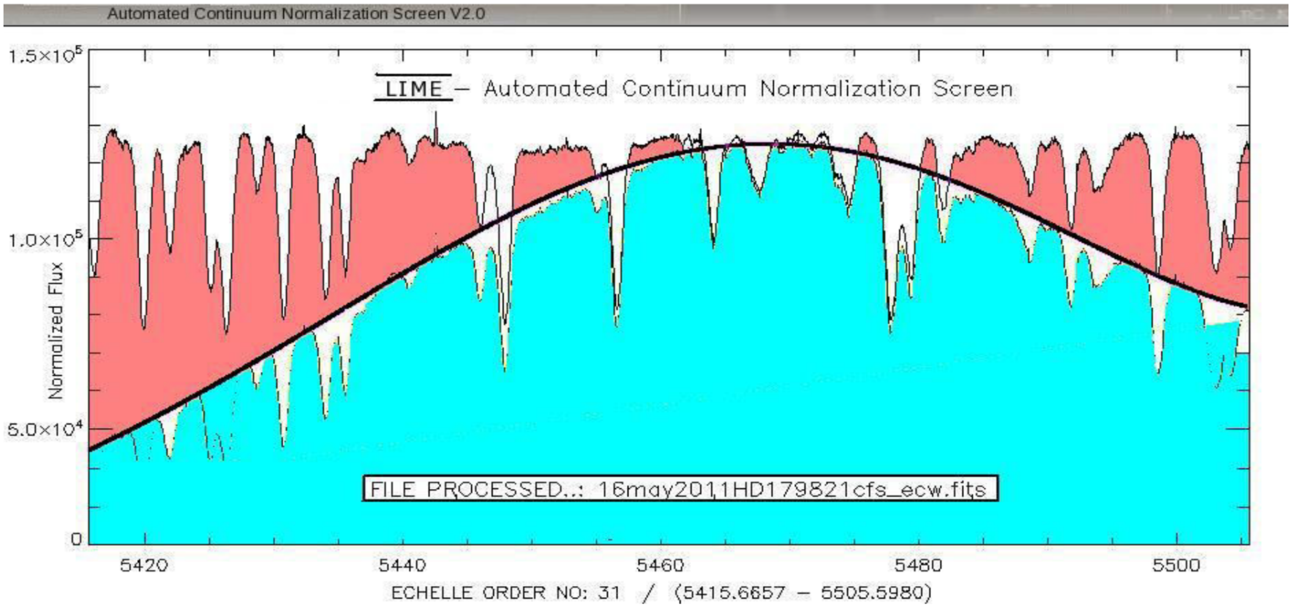

Figure 1. Screen copies of the LIME automated continuum normalization interface. Black drawn line shows the polynomial fit performed to a spectral order of the echelle spectrum of HD 179821 obtained on 16 May 2011 (S/N = 208, wavelength coverage: 3832–10,338 Å) for illustration.

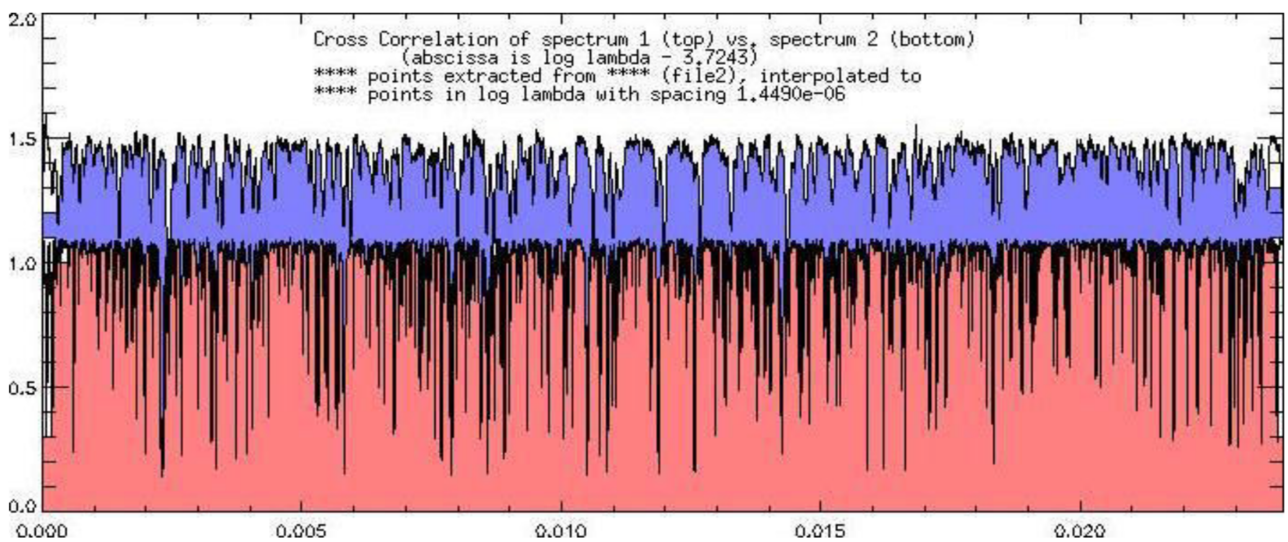

Figure 2. Screen view of the LIME-RADVEL function. The cross-correlation process is depicted for an example object spectrum (upper plot). The synthetic (mask) spectrum is presented at the bottom. The x-axis shows the logarithm of wavelength displacement. The y-axis gives relative intensity and added 0.5 for the merged object spectrum.

The code, in principle, allows the user to compare the continuum-normalized (and merged) object spectrum, for instance to a day sky spectrum, and/or the user's choice of spectrum for the line identification process, especially for testing continuum normalization (i.e. problems in interorder gaps for an echelle spectrum due to problematic continuum normalization and/or incorrect wavelength calibration), and also to visualize possible secondary contributors (i.e. blending) to a given stellar line. Each spectral line indicated by the user via a mouse cursor in a 10–20 Å wide (user selected) spectral region of interest is generated on the screen that awaits user confirmation in an interactive session of LIME (Figure 3). As soon as candidate identification is marked on the graphical display, an indexing number to be typed by the user for a positive identification is returned. The indexing number represents tabulated candidate stellar lines(s) from the revised multiplet table [6]. Each processed region of spectra saved in PNG file format allows the user to generate a (digital) spectroscopic atlas.

```
CLICK ON THE ACTIVE WINDOW to SELECT a LINE to IDENTIFY >> FILE CREATED: linelist_5000_5050.dat
-----------------------------------------------------------------------------------------------

WAV-MEAS  WAV-ROW   EW-SUN  dl/l  IDENT   LowEP RMT   loggf
--------  -------   -----   ----  ------  ----- ---   -----
5040.0065 5039.964    66.    14    TI1    0.02  5     0.042609469    4990
5040.0065 5040.122     7.     1    C1     7.94       -0.11559366     4991

Please type the index = 4990
Would you like to add -- comment --(y/n)?n
```

Figure 3. Line identification display on a Linux terminal. WAV-MEAS and WAV-ROW columns show LIME-IDENT measured line positions and laboratory measurements from Rowlands preliminary table of solar spectrum wavelengths, respectively. The third column presents measured EWs of the candidate lines in the solar spectrum [6] and the fourth shows laboratory intensities of the lines. The rest are self-explanatory.

The measured wavelength of the line is matched with all laboratory wavelengths of candidate identifications, each with a given indexing number, from the master list within a specified tolerance. The value of this tolerance should be chosen to be appropriate to the spectroscopic data (i.e. spectral resolution), i.e. 0.20 Å for HD 179821 (see Section 3 for details). Prior to determination of this tolerance window and its limit, a day sky spectrum obtained with the same configuration and via the same instrument is used. LIME also returns a flag to be input on the command line in the output file for each coincidence (mouse hit) to allow the user to note any probable misidentification and/or contamination. The current version of LIME (ver. 4.0.), via the LIME-IDENT function, lists the related atomic information (e.g., lower excitation potential (LEP), log gf) for a reliable determination of blend features in the spectra. It should be noted that the details for blend features in the spectral line identification process are generally sidestepped by web-accessible platforms. In fact, the blends are mostly identifiable via synthetic spectrum matching that requires input physics based on local thermodynamic equilibrium (LTE) or non-LTE schemes.

During an interactive LIME session, supplementary annotations containing the type of the atomic species, multiplet designations (as in the revised multiplet table [6]), laboratory line intensity information (for instance, for solar spectrum as a comparison), and the displacements from the laboratory positions of the stellar lines are also printed on the active terminal screen (Figure 4). The final ASCII output file (see Figure 5) by LIME-IDENT is suitable for direct input into the LTE line analysis code MOOG, a widely used 1D LTE stellar atmosphere code in stellar spectroscopy for chemical abundance analysis [7], for further chemical abundance calculations as the line identification process is completed. For calculation of abundances, measurements of EWs are needed. LIME is also capable of measuring EWs with the LIME-EMS function embedded in the code (Figure 6). A Gaussian/Voigt profile is fitted to determine the EWs.

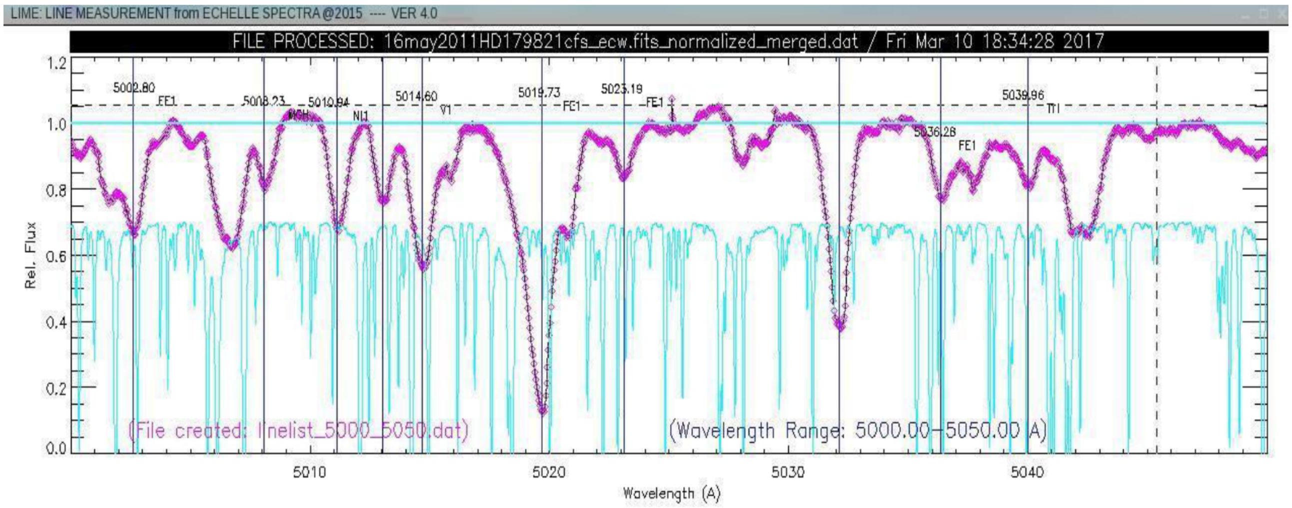

Figure 4. Example display for an interactive session in LIME. Measured spectrum is presented in purple and the solar spectrum for comparison/illustration purposes is in aqua. Vertical lines show user-identified features via mouse hits. The continuous line in aqua is to guide the eye for continuum level. The intersection of the dotted vertical and dotted horizontal lines shows the current position of the mouse in this interactive session.

```
LIME - Line Measurement from Echelle Spectra
- VER 4.0 -
File created: linelist_5000_5050.dat
Data file    : HD179821cfs_ecw.fits_normalized_merged.dat
Date         : Fri Mar 10 18:34:28 2017
Directory    : /home/sahin/
Created by   : test
- HRSS -
WAV-MEAS   WAV-ROW   EW-SUN  dl/l  IDENT    LowEP RMT   loggf
--------   -------   ----    ----  ------   ----- ---   -----
5011.1239 5010.943    46.      9    NI1     3.63  144
5013.0324 4000.257    66.     17    FE1     3.26  556   -1.58
5023.1265 5023.189    35.      7    FE1     4.28  1095  -1.58
5002.5991 5002.798    85.     16    FE1     3.40  687   -1.53
LIME - Line Measurement from Echelle Spectra
```

Figure 5. Example content of the output file by the LIME subroutine of line identification. Explanations for columns are as in Figure 3.

3. Observational data for testing the code: McDonald, ELODIE, and Hobby–Eberly spectra

For illustration of the code, it was tested for high dispersion ($\lambda/\Delta\lambda \approx$ 60,000) and high signal-to-noise ratio (S/N) spectra that were obtained between 2008 and 2011 at the McDonald Observatory with the 2.7 m Harlan J. Smith reflector and the Tull Coudé echelle spectrograph [8] for the spectroscopic investigation of HD 179821 (see [5] for details). HD 179821 is a massive star evolving to become a red supergiant and finally a type II supernova. Its spectra show line profile variations (see Figure 7): the shapes of the line profiles vary with their strengths. Hence, for testing the code and to highlight the effect of blending (Figure 8), we used 10 spectra

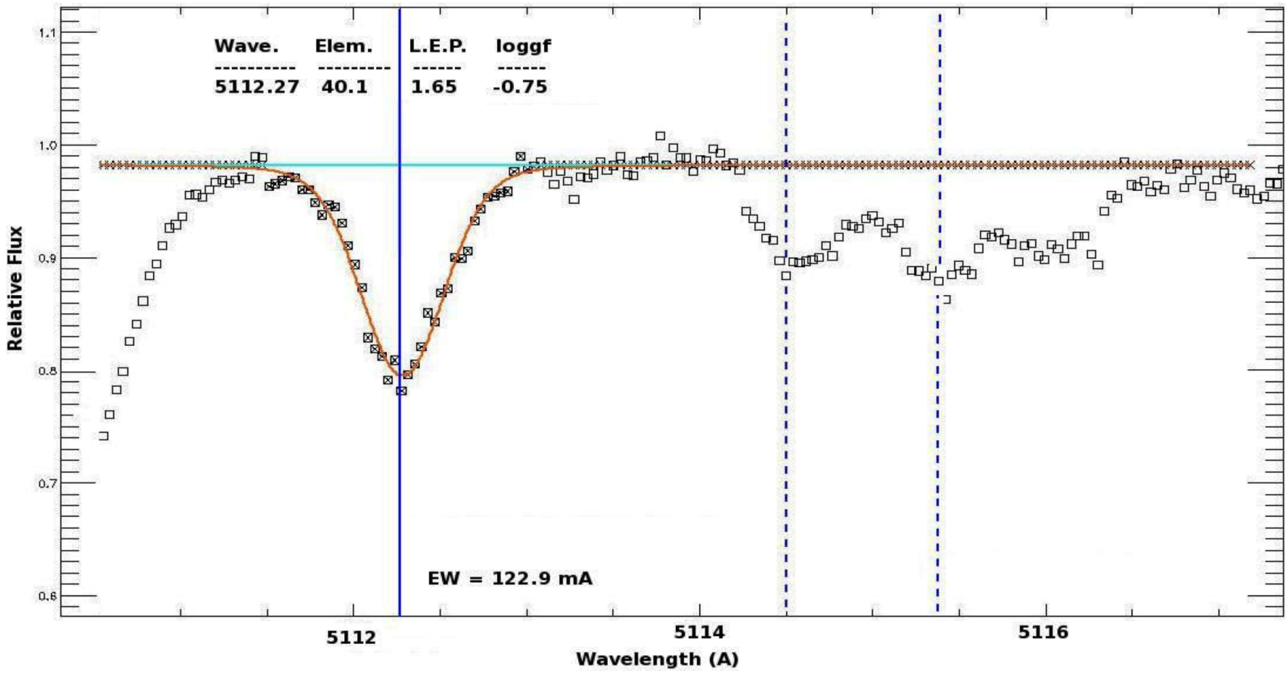

Figure 6. Example screen view for the LIME-EMS function. The horizontal line in aqua shows the fitted continuum. The continuum fitting width can be adjusted by the user. The user-selected line via a mouse hit is fitted a Gaussian and/or a Voigt profile and indicated by blue vertical line at the line center. The EW of the fitted line is reported on the plot screen. The dashed vertical lines show two neighboring identifications in the line list that is created with the LIME-IDENT function and provided to LIME-EMS for EW measurements.

obtained at different epochs rather than using a single combined spectrum, generally the usual case. The reader is referred to [5] for a log of observations and general features of the spectra.

A single exposure covered the wavelength range from about 3800 Å to 10,500 Å with an incomplete spectral coverage from about 5800 Å to longer wavelengths. The 20 and 30 min exposure times provided a satisfactory S/N ratio (ranging from 123 to 208). Observations were reduced using the software package in IRAF, distributed by the National Optical Astronomy Observatories, which is operated by the Association of Universities for Research in Astronomy (AURA), Inc., under cooperative agreement with the National Science Foundation. The bias level in the overscan area was modeled with a polynomial and subtracted. The scattered light was modeled and removed from the spectrum. Pixel-to-pixel sensitivity variations were corrected via flat field exposures from a halogen lamp. Echelle orders were cosmic-ray cleaned and wavelength was calibrated. The internal accuracy of the wavelength calibration via the Th-Ar lamp spectra was always better than 0.003 Å rms. Then rectification and merging of the individual orders into one spectrum were performed within IDL with the LIME-BLAZE function. The final spectrum was processed further using the LIME-IDENT function to accomplish the line identification process.

The line measurement and identification tests for the McDonald spectra in this study provided the same lines reported in tables 3 and 4 of [5]. Thus, the manual identifications in [5] by us using the revised multiplet table as an initial guide and carrying out a systematic search that made use of LEP and gf-values were confirmed and proved to be accurate. The difference in measured line positions by LIME-IDENT was in the order of 0.01 Å. However, comparison to the line lists belonging to previous analyses in [9] and [10] for the star provided

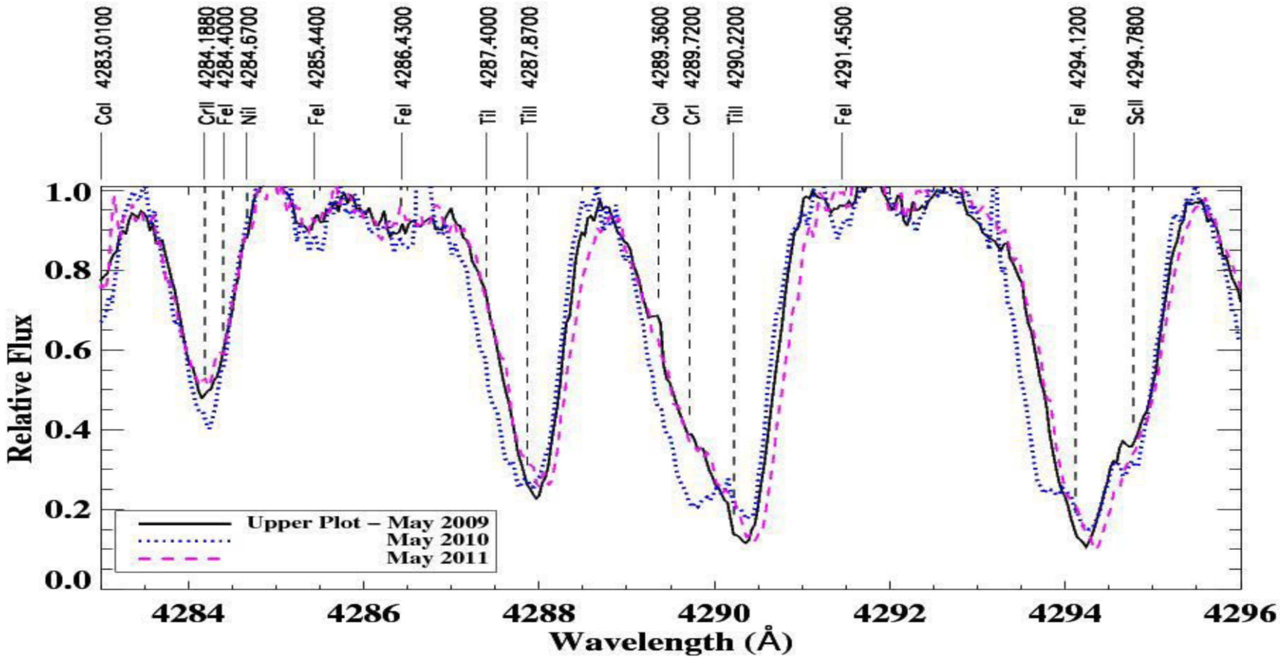

Figure 7. The McDonald spectra (9 May 2009 with S/N = 172; 22 May 2010 with S/N = 123; and 16 May 2011 with S/N = 208) of HD 179821 show line profile variations and splits.

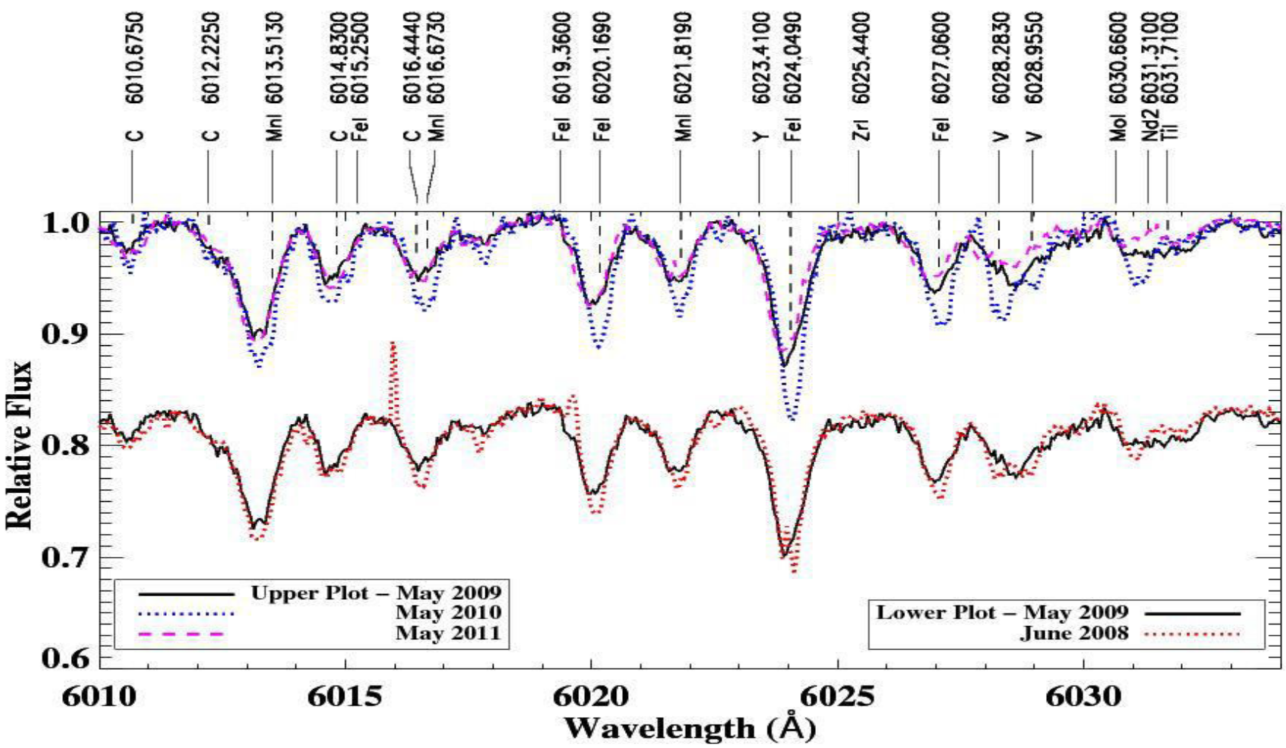

Figure 8. The spectra of HD 179821. The Fe I line at 6016.66 Å is found to be a blend with the Mn I 6016.73 Å (multiplet no. 127) line; however, it was identified and included as an Fe I line in the analysis of [8] (see their table 2). Similarly, the Mn I blend at 6016.67 Å line was reported as an Fe I line at 6016.66 Å in [8] (see their table 2).

important findings. On examination of the line lists in those studies, identifications for some lines could not be verified (see Figure 8).

Reddy and Hrivnak [9] used the 15–16 October 1997 McDonald spectra of the star. We obtained this spectra (EB Reddy, 2016, private communication) and examined the line lists from [9]. We found that 9 of 23 Fe I lines and 3 of 9 Fe II lines did not meet our criteria of a measurable and unblended line. Similar findings were also seen for other atomic species; for instance, the line reported as an Ni I line at 6086.29 Å in [9] was, in fact, a C I blend. Furthermore, our analysis of their spectra with a LIME measured line list provided 400 K hotter temperature and 0.3 dex greater metallicity ([Fe/H]) for the star (see [5] for details). Our suggestion is that the differences in model parameters likely emanate from imperfectness of the line list for Fe lines reported by [9].

We also extracted the ELODIE spectra (September 2000) of HD 179821 from the archive [11]. These ELODIE spectra were used by Kipper [10] in his analysis and not continuum-normalized. The LIME-BLAZE function was used to normalize the spectrum. Then the spectrum was merged and radial velocity corrected in LIME by using the LIME-RADVEL function.

Examination of reported lines in table 5 of [10] and comparison to the identifications by LIME in the ELODIE spectra showed that the Na I line as listed in [10] at 6154.23 Å was a blend. Also, the line misidentified in [9] as an Fe I line at 6016.65 Å was seen to be reported as a neutral manganese line in [10].

One additional test was performed by using the spectrum of HD 179821 (E Luck, 2016, private communication) from 21 July 2010 obtained at the 10 m Hobby–Eberly Telescope (HET [12]) to test the line identification and to compare EW measurements by LIME. Given the estimated uncertainties in abundances, the LIME-EMS measured EWs for LIME-IDENT identified lines in the Hobby–Eberly spectrum of the star led to a fair agreement in abundances by [13] for HD 179821 (see table 9 of [5]). It should equally be noted that in the process of comparing abundances to those reported in the literature, atomic data compilation for the analysis constitutes a very important and crucial stage of abundance analysis. At this stage, LIME, via a separate function called LIME-GFS, allows the user to add atomic data to the master line list, for instance from the Kurucz compendium, for the transition of Fe-group as well as neutron-capture elements.

Comparison of measured EWs by LIME-EMS to [9] and [10] (see columns for 15Oct97 and 13Sep00 in table A1 of [5]) indicates significant differences in measured EWs in previous analyses (Figures 9a and 9b). For instance, the EWs measured in [9] in the McDonald spectrum (15 October 1997) appear to be systematically lower when compared to LIME-EMS measurements. Scrutiny of the 1997 McDonald spectrum showed continuum normalization problems (under normalization). The normalization problem was treated by the LIME-BLAZE function. Again, a similar comparison with EWs measured in [10] also gave systematically higher EWs due to continuum normalization problems.

One can certainly conclude that these differences in EWs will lead to uncertainty in the determination of model atmosphere parameters of the star and hence will result in determining the physical nature of the star incorrectly.

4. Concluding remarks

The line identification code LIME is presented and has been applied to spectra of HD 179821. The star was identified as a low-mass post-AGB star in the literature by several earlier spectroscopic analyses. However, recent analysis of the star by us [5] provided an alternative identification for the star as a massive red supergiant star.

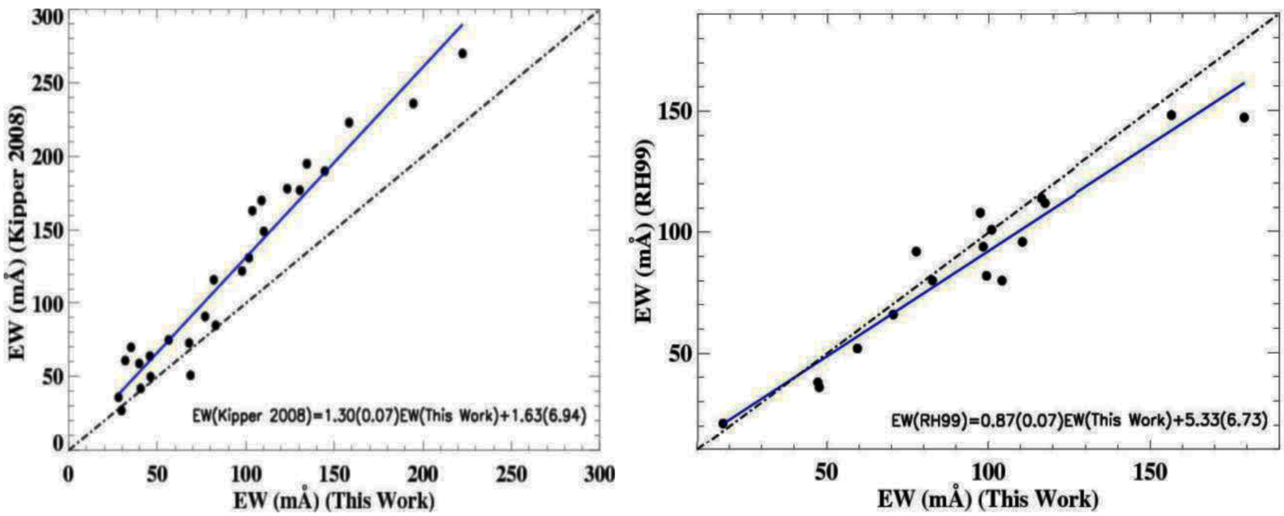

Figure 9. a) Equivalent widths for ELODIE spectrum by [9] versus the EWs of the same lines via LIME-EMS function. The equation for least-square fit is provided. b) Equivalent widths for McD spectrum (15 October 1997) by [8] versus the EWs of the same lines via LIME-EMS function. The equation for least-square fit is given on the plot.

The spectra used for testing the code, in the framework of this paper, were obtained over several epochs and also included the McDonald spectra used in [5]. Comparison to previous spectroscopic studies of the star in [9], [10], and [13] provided important findings: some of the identified lines could not be verified, and blend features were determined. Comparison of measured EWs and reported lines in those analyses suggest an imperfect line list and hence uncertain model parameter determination for the photosphere of HD 179821. LIME proved to be useful in demonstrating the star's ρ Cas and HR 8752 like characteristics as a galactic supergiant star, and hence identification of the star as a post-AGB star, as earlier spectroscopic analyses [14,15] stated, can be excluded.

The code is planned to be improved to allow for stellar parameter determination in an automatic procedure based on equivalent width analysis. We also plan to include a derivative test (e.g., second and third) to identify splits and blend features better. The code can be obtained by contacting the author.

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