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Telluric Correction of IRTF Spectra with Atmospheric Models

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1 Preamble

Accurate model spectra of the Earth's transmission will reduce the need for taking spectra of telluric standard stars at the IRTF. This document describes the program xtellcor_model, an adaptation of xtellcor (Vacca et al. 2003), that uses atmospheric models to divide out telluric absorption in iSHELL spectra. Other instruments are not addressed yet. The code is still under development, but a test version is available. In Section 2 we give a very brief summary of how to use the program. Section 5 gives detailed background information, and Sections 6 and onward give more detailed usage instructions, examples, and summaries of known issues and future work.

2 Cookbook

This is a brief summary of how to run xtellcor_model. For more detailed information, see Section 6.

I. reduce the iSHELL data using Spextool, including averaging of the spectra, but do not correct for telluric absorption and do not merge the orders

II. download the xtellcor_model package (http://irtfweb.ifa.hawaii.edu/research/dr_resources/) and unpack it in a directory that is in Spextool's IDL path (for a typical Spextool installation this is a called Spextool/ and contains subdirectories data/, helpfiles/, pro/, etc.)

III. start Spextool (the version for iSHELL)

IV. on IDL prompt, enter xtellcor_model

V. step 1: load reduced iSHELL spectrum and, if desired, a template blaze shape spectrum to correct for the order curvature. This template can be selected from a database that comes with the installation, and if not present, can be requested from the IRTF (aboogert@hawaii.edu).

VI. step 2: retrieve the atmospheric model.

   a. The molecules that contribute the most to a given mode are preceded by '*'. Scaling their column densities to the observations can be done automatically by entering -1 in the box. This is typically always needed for H_2O and CH_4.

   b. Click 'Retrieve Atmospheric Model'. The fitting and download typically takes 1-2 minutes.

VII. step 3: inspect the quality of the model spectrum. Different molecules can be plotted using the 'atmosphere' button. Apply small wavelength shifts and/or column density scaling corrections for optimal division.

VIII. step 4: this step is optional. Divide out the order blaze shape by using the template spectrum defined in step V above.

IX. step 5: plot and save the telluric and blaze function corrected spectra to fits file.

3 Do's and Don'ts

In its current state Xtellcor_model works well if these three conditions are true:

- flux calibration is not important (the program does not use standard stars and thus flux calibration cannot be done)
- there is continuum emission, not just line emission (the program uses telluric absorption lines to optimize the atmospheric model)
- the target spectrum is not densely packed with spectral features (i.e., if there are no isolated telluric lines to optimize the atmospheric model to)

In these particular, though fairly common, science cases the observer may consider not observing telluric standard stars.

Conversely, most likely Xtellcor_model is currently insufficient in the following science cases, and telluric standards must still be observed:

- if flux calibration is of science interest, i.e., if line-to-continuum ratio's are insufficient for the science goals
- targets with little 'line-free' continuum emission, e.g., late M-giants, or without a continuum at all

4 Sample Data

The xtellcor_model distribution includes a sample iSHELL observation ("extractedstandard.fits") in the K3 mode with the 0.375 arcsec slit. It has been reduced with Spextool version 5.0.1, but not divided over a standard star and not order-merged.

5 Background Information

A telluric absorption correction technique that uses weather models in combination with high spectral resolution transmission models was thoroughly tested on ESO/CRIRES (R=50,000-100,000) infrared spectra, yielding a correction accuracy of 2% or better, even near strong telluric lines (Seifahrt et al. 2010). The atmospheric radiative transfer code LBLRTM (Line-By-Line Radiative Transfer Model; Clough et al. 2005; http://rtweb.aer.com/lblrtm.html) was favored by Seifahrt et al. They recommend to use it with weather information (vertical profiles of pressure, temperature, and H_2O abundance) from

GDAS (Global Data Assimilation System) models, and with MIPAS (http://www-atm.physics.ox.ac.uk/RFM/atm/) model atmospheres for other molecules and at the highest altitudes. This method was subsequently adopted by a number of other groups:

- Molecfit: a C-based fitting code, developed by ESO for their UV, optical, and infrared spectrometers (Smette et al. 2015) and included in their Common Pipeline Library.
- Telfit: a Python-based fitting code tested on optical high resolution spectra (R=80,000; Gullikson et al. 2014). In contrast to the other codes, Telfit adjusts the vertical temperature and pressure profiles to measurements at the telescope at the time of the observations.
- Telrem: an IDL-based fitting code developed for the ESO instrument X-Shooter (Rudolf et al. 2016).

All these fitting programs, Molecfit, Telfit, and Telrem require the LBLRTM atmospheric model code (FORTRAN) and the line list code LNLF (FORTRAN) along with the large LBLRTM-formatted line list (1.8 GB) to be installed by the users on their local machines. The same is true for the GDAS data files, which are ~0.5 GB in size for every week of data.

Installing the code and weather data would be big hurdles for many IRTF users, and therefore we decided to use an online server that generates these models. The Planetary Spectrum Generator (PSG; https://psg.gsfc.nasa.gov/; Villanueva et al. 2018) does mostly what is needed. We thus converted the much used Spextool program xtellcor (Vacca et al. 2003) to use PSG models rather than standard stars to correct for telluric lines in iSHELL spectra. We named it “xtellcor_model”. The rest of this document is about using the program “xtellcor_model” on iSHELL spectra. Its use on SpeX spectra has not been implemented yet. We note that in xtellcor, the telluric calibrators are also used to divide out the instrument’s strongly curved order blaze shapes. In the modeling approach we initially relied on flat fields for this, but the residual order curvature was fairly significant in some cases. Therefore, in this new (2024) release of “xtellcor_model” we use template spectra for the order blaze correction, which works much better. These template spectra are derived from standard star observations, but these observations may be obtained up to a year before or after the science observation, and they are derived by the IRTF staff and distributed along with the software or can be produced on request.

6 Using “xtellcor_model”

Xtellcor_model is not integrated in the Spextool distribution yet; it can be run by unpacking the tar file in a directory that’s in Spextool’s IDL path. Then on the IDL command enter xtellcor_model and the GUI (Figure 1) appears. The steps on the GUI labeled 1-5 are fairly self-explanatory but are further described below.

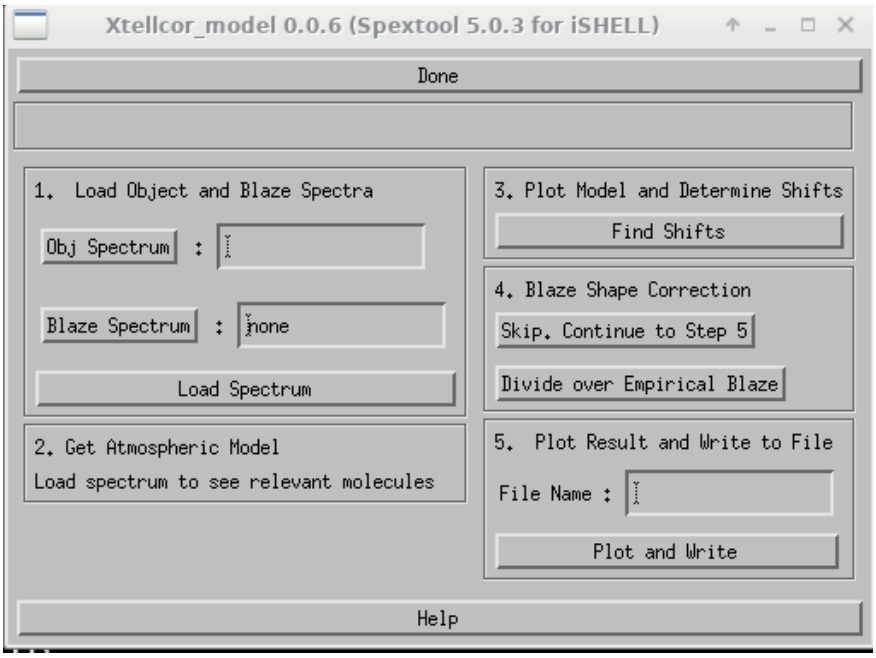

Figure 1: GUI for xtellcor_model.

Step 1: Load Spectrum

This loads a FITS file of an observation that has been fully reduced in Spextool, except for telluric line correction and order merging. The header keywords are used to determine essential parameters, such as the instrument configuration, slit width, date of observation, and airmass. In this step one can also specify a template blaze spectrum to be loaded. The user will then need to select a template from the database that is distributed along with the software, taking into account the iSHELL mode and the closest match to the data of the observations. If no suitable template is available one can be derived by the IRTF staff upon request. If no template is selected, xtellcor_model will work OK, but the final result will have strongly curved orders. This may be sufficient for some science cases (e.g., narrow isolated lines). After clicking ‘Load Spectrum’, the step 2 information is updated such that only the atmospheric molecules relevant for this configuration’s wavelength range are displayed (Figure 2).

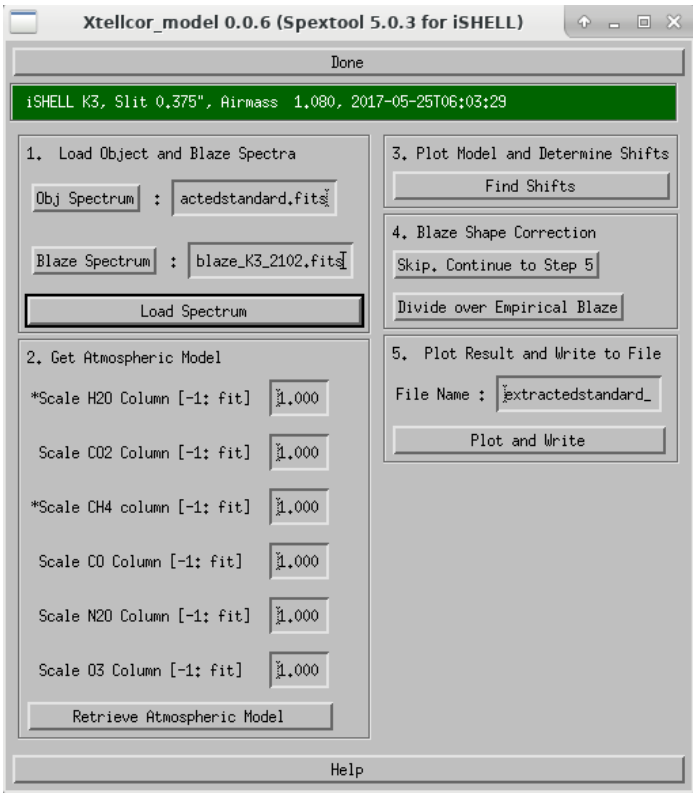

Figure 2: After loading the data, step 2 only displays molecules relevant to the atmospheric transmission in this iSHELL configuration. Species preceded by '' are most important: they have lines stronger than 10% absorption.*

Step 2: Retrieve Atmospheric Model

Clicking 'Retrieve Atmospheric Model' will get the model spectrum from the server using the weather conditions at the time of the observations. This usually takes 1-2 minutes. The IDL prompt shows the progress. This model is rarely good enough due to the local weather conditions being different from that assumed by the weather server. This will be obvious when plotting it in Step 3, and thus the column density scaling factors need to be adjusted. The program will do this automatically when one enters '-1' in the scaling boxes. For H_2O this is nearly always needed, and it is recommended for the species preceded with a '*' in the GUI. The fitting is done to a couple of individual telluric lines, defined in the file "teltool_lines.dat", and then the median across the best-fit scaling factors is taken. If one wants to inspect the fits, they are plotted in a postscript file ("xtellcor_model_fittedlines…..ps"; Figure 3). The fitting is done by χ^2 minimization to the line profile by varying the molecular column and peak wavelength. Experience so far has shown typical scaling factors of 0.1-2 for H_2O and up to 1.4 for other species, but for H_2O it is sometimes significantly lower or higher. Once the fitting is completed, the best-fit column of H_2O (PWV in units of mm) in the zenith is reported on the IDL

terminal. The wavelength shift is presently not applied to the data, however, because it is found to not be a constant across echelle orders and instead must be done ‘manually’ via inspection in step 3.

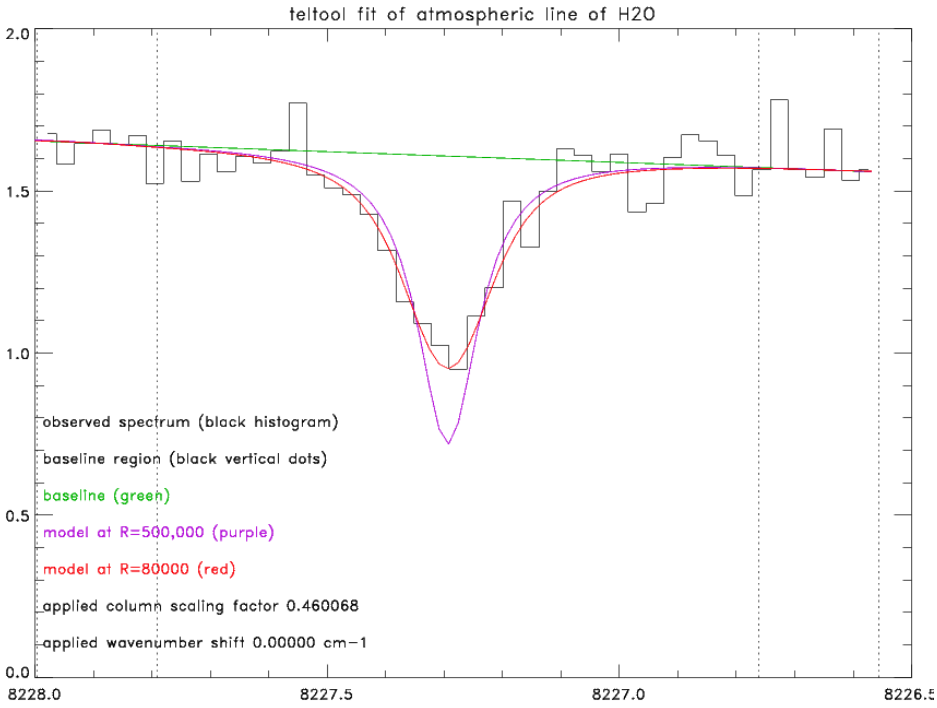

Figure 3: Example fit to an individual atmospheric line to get the best column scaling factor. These plots are saved in files named "xtellcor_model_fittedlines....ps".

Step 3: Plot and Fine-Tune the Model

This is an important step to inspect the fitting result and manually fine-tune it. Under the button ‘Atmosphere’ (Figure 4) one can overplot (in yellow) the total transmission model or that for individual molecules. The fine-tuning consists of applying small (sub-pixel) wavelength calibration corrections to the data and of changing the column density scaling factors for each of the molecules included in the model. This is done on a per-order basis, so first select the order to be worked on.

Wavelength shifts: As is also the case when using standard stars to remove telluric lines, the telluric residuals can be greatly reduced by applying sub-pixel shifts. We find that currently, shifts can vary within and across echelle orders, and the user needs to decide what’s best. To help with that, one can do an automated determination by clicking ‘s’ on the command line and then define a line to fit to with the left mouse button. The ‘Apply to All’ button will apply this shift to all orders, if desired.

Column density scaling factors: The atmospheric model fitted to the data in Step 2 is rarely perfect and small adjustments can be made using the ‘Column Scaling’ box in this GUI. This adjustment is

independent for each molecule. If ‘All’ is selected under ‘Atmosphere’ the same scaling factor is applied to all molecules. Once a satisfactory scaling factor is found for the selected order, it can be applied to all echelle orders for that specific molecule using the right most ‘Apply to All’ buton.

When satisfactory wavelength shifts and column density scaling factors are determined for the complete observation, click ‘Done’ to exit this particular order and then click the ‘Accept’ button at the bottom of the GUI.

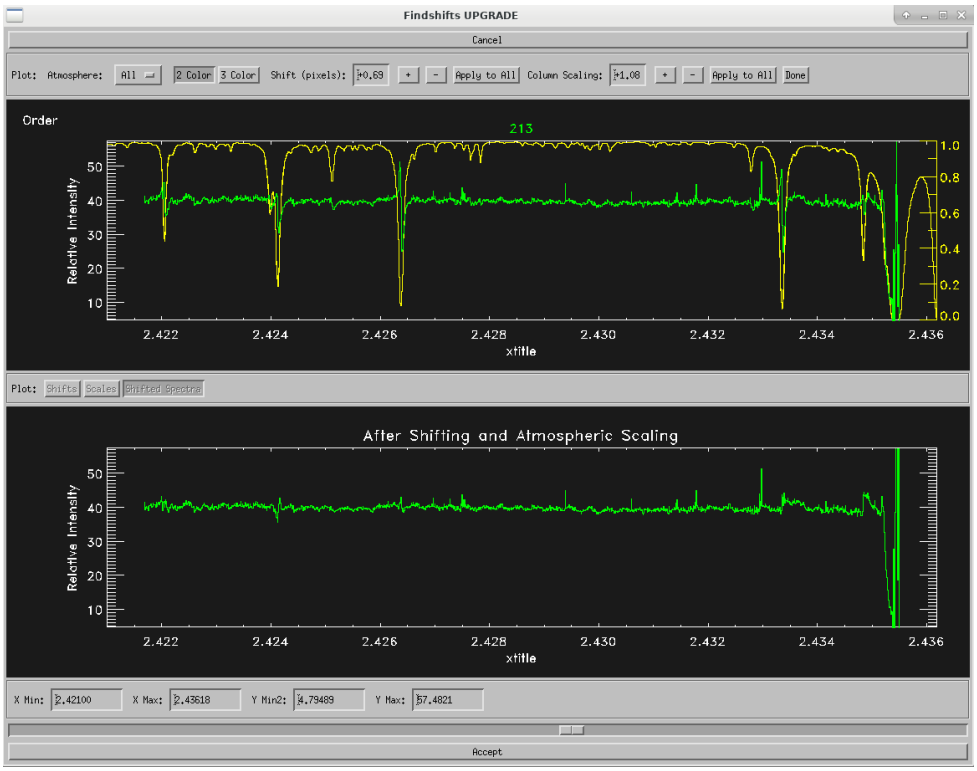

Figure 4: tool to inspect the telluric correction, fine-tune the column density scaling factors, and apply sub-pixel wavelength shifts. The top panel shows the division before the shift and column density scaling factor adjustment are applied.

Step 4: Correct for Order Blaze Shape

If the user selected a blaze shape spectral template in Step 1, it was already applied when clicking ‘Load Spectrum’ in Step 1. However, if small wavelength corrections were applied in Step 3, this division needs to be re-done with the improved wavelength scale. The user may also opt to not correct for the blaze shape by clicking the ‘Skip’ button, but then the final telluric-corrected spectral orders will be strongly curved.

Step 5: Plot Result and Write to File

Finally, the atmospheric absorption-corrected spectra can be written to FITS file. Two files are written to disk: ‘inputfile_xtm.fits’ and ‘inputfile_xtm_tellspec.fits’, where ‘inpufile’ is the name of the file entered in Step 1. These filenames can be modified by the user. The second file contains both the complete atmospheric model and the transmission for each molecule. At the same time the spectrum is plotted, which is particularly useful to see how well the blaze shapes were corrected for (Figure 5). Note that in this case, the plotted atmospheric transmission spectrum is a generic ATRAN model, not the one optimized to the observations.

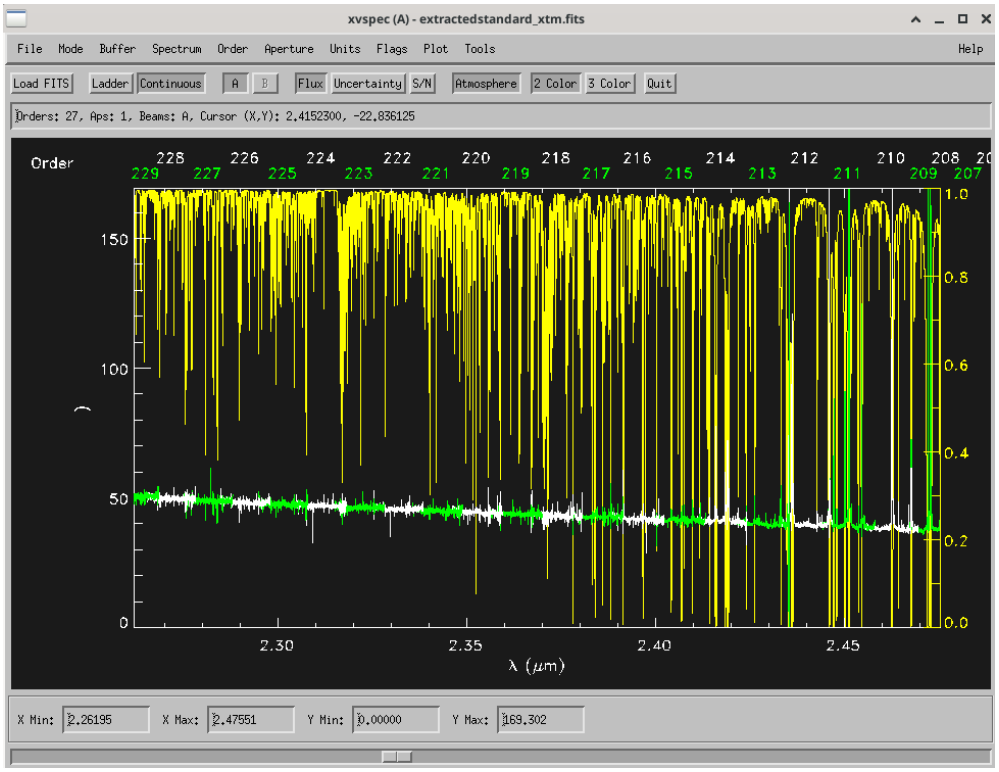

Figure 5: Fully atmosphere and (optional) blaze-shape corrected spectrum produced at Step 5. Yellow is an atmospheric transmission model (a generic ATRAN model, not the one optimized to the observation) and white and green the echelle orders.

7 Known Issues and Troubleshooting

The use of xtellcor_model is limited depending on the target being observed, the science being done, or yet unresolved calibration or software issues. Many of these issues will be addressed in future releases. Here we provide a summary.

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Unable to Retrieve Atmospheric Model

Occasionally, the retrieval of the model in Step 2 fails. This may be because of a poor internet connection, either for uploading to or downloading data from the PSG server. Standard high speed internet connections usually are sufficient, but sometimes the upload band width is too small. The PSG website may also be down. Please access https://psg.gsfc.nasa.gov/ in your browser to check this. Also, the PSG server has set a limit for the number of times a particular IP address may download spectra. If this limit is encountered, then continue after 24 hours. Please contact us (aboogert@hawaii.edu) if you encounter PSG download problems.

Residual Telluric Features

The automatic determination of the molecular scaling factors in Step 2 not seldomly leaves atmospheric residuals that the user will have to improve on by manually adjusting the scaling factors in Step 3. This is because one scaling factor per molecule is determined from the median of the factors across just a few pre-defined lines (in the file 'teltool_lines.dat'). Simultaneous fitting over many lines or entire or multiple orders would give better results, but is currently not done as it requires baseline fitting that is difficult to generalize for the many different kinds of targets that iSHELL observers study (e.g., targets with many or few lines, with emission or absorption lines, with weak or strong continua, with broad dust emission or absorption lines).

In addition, poor fits to the telluric spectrum may occur for data obtained less than 2 months ago. This is because the database with weather information that PSG uses (MERRA2) is updated only after 2 months. For more recent data, atmospheric conditions of exactly one year earlier are used by PSG.

Unavailable Order Blaze Shape Templates

The database of blaze shape templates, stored in the directory 'Empirical_blaze_functions' is currently rather small due to the effort it takes to produces them. Please let us (aboogert@hawaii.edu) know if a template is needed for a particular iSHELL mode or date, and we will make it available. It would be useful if the observer observed one standard star in their runs so that this can be used to derived the template. Templates based on data observed up to a year before or after the run are OK.

Wavelength Shift Solution Not Robust

We find that when selecting different wavelength regions to determine the wavelength shift in Step 3, different values for the shift are found. It works better when narrow regions on single telluric lines are selected and if a blaze shape template is selected in Step 1.

Incorrect Header Information

If the FITS header contains wrong header information (e.g., date or slit width), one can override it by replacing the entry 'header' with the correct entry in the parameter file teltool_ishell.param. This is very rarely needed, probably only for data obtained during instrument commissioning.

8 Change Log

- 09/12/24: major upgrade to Beta release 0.0.6. Blaze shape correction is now done using spectral templates instead of flat fields. The number of times the the PSG server is accessed is strongly reduced. Manual adjustment of column density scaling factors is implemented.
- 12/05/18: updated Beta release (v 0.0.2) on IRTF web page. Includes line profile fitting instead of peak depth fitting and correction of several small bugs.
- 10/18/18: updated Beta release (v 0.0.1) on IRTF web page. Includes items below.
- 10/18/18: output telluric spectrum (.._tellspec.fits) at final step also written in Spextool 5.0.2
- 10/17/18: teltool.pro: take into account gaps in wavelength coverage (such as for iSHELL M-band) when checking if absorption line can be fitted to for column determination
- 10/15/18: Beta release (version 0.0) on IRTF web page

9 References

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