

## *Questions, Comments and Answers following the presentation*

### *Molecfit* Alain Smette

*Ballester: Comment: Molecfit is one tool in a suite of tools delivered by the Austrian in-kind contribution. The suite includes a model for both the emission and absorption of the atmosphere and is used in both exposure time calculator, instrument modelling for ELT and VLT instruments and correction tools.*

#### Goto:

- 1. Why is a fast rotator dwarf a better spectroscopic standard?*
  - 2. One can use molecfit to correct water [lines] and most standard?*
  - 3. Atmospheric profile input parameters? Or determined by iterations?*
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1. Lines that are formed in the atmosphere of a fast rotator are broad and therefore can be easily distinguished from telluric lines. A B type star in addition show few intrinsic lines. Of course, these characteristics become a problem if the interesting lines in the science object appear in the spectral regions affected by the lines intrinsic to such stars. In this case, observation of a sun-like star is usually recommended, leading to even less time dedicated to the science target.
  2. Yes. Since they are the ones that usually change fastest, molecfit is particularly appropriate to correct water vapor lines. Various strategies involving standard stars can also take place if the spectrum of the science target does not show enough or show too many intrinsic lines.
  3. Molecfit reads the date, time, and location for the FITS header given in the parameter file, or provided explicitly in the parameter file if not available in the FITS header. Then, it retrieves the relevant atmospheric profile from a NOAA GDAS server, which provides information for altitude, temperature and humidity as a function of pressure; for other molecules, the profile is given by a typical equatorial profile. During the fitting process, Molecfit slightly changes only one parameter for each molecule: its total content above the observatory.

#### Modigliani:

- 1. Should we propose MPE the use of Molecfit?*
  - 2. We are implementing a general algorithm to determine the instrument response. This includes a step of telluric correction based on a catalog of 72 spectra. Should we rather use molecfit to perform telluric correction?*
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1. Yes. With the instrument scientists of SINFONI, we are already looking at using Molecfit. For this instrument, the line profile is particularly complicated: but its determination is a major first step to simplify the use of molecfit.

2. The instrument response is used to convert measured counts to flux above the atmosphere. Molecfit can be used to identify the spectral regions affected by telluric lines, but not for the spectrophotometric calibration.

Janssen:

1. *Does the comparison between molecfit synthetic spectra and high resolution observation allow for the identification of spectral regions or molecules where current molecular data are not sufficient?*
  2. *Which molecular line profile model is used in the molecfit software?*
1. In principle, yes. Indeed, Villanueva (private communication) reported problems with Ethane lines, whose parameters were then corrected in a subsequent version of HITRAN. Usually, such work requires a systematic comparison which – to my knowledge – has only been done once so far: in the spectrum of 10 Leo as part of the CRIRES-POP project ([Nicholls, C.P. et al, 2017 A&A 589, 79](#)).
  2. The one used by LBLRTM for the radiative transfer one, which is a Voigt profile, modified as needed (see, e.g., [LBLRTM Description](#)). This profile is then convolved by the kernel(s) chosen or provided by the user

Roth: *Comment: Beyond the objective of molecfit proper, you have shown an example of how to use telluric lines for wavelength calibration (CRIRES). This has also been shown to be very useful for low resolution in the case of MUSE, essentially providing radial velocity accuracies of 1 km/s for globular cluster stars.*

Altavilla: *If I understood correctly, I first check the correction in a few wavelength regions and then apply it to the whole spectrum. Is there an automatic procedure to look for the best parameters to obtain the best result in these testing regions?*

Yes, Molecfit uses MPFIT (Markwardt, 2009), an implementation of the Levenberg-Marquardt algorithm to find the best fit in the inclusion regions.