COCCON open path measurements for ILS determination + updates in LFT 148

Presenter: F. Hase (work by Carlos Alberti and Lena Feld acknowledged)

Why open path measurements for ILS …

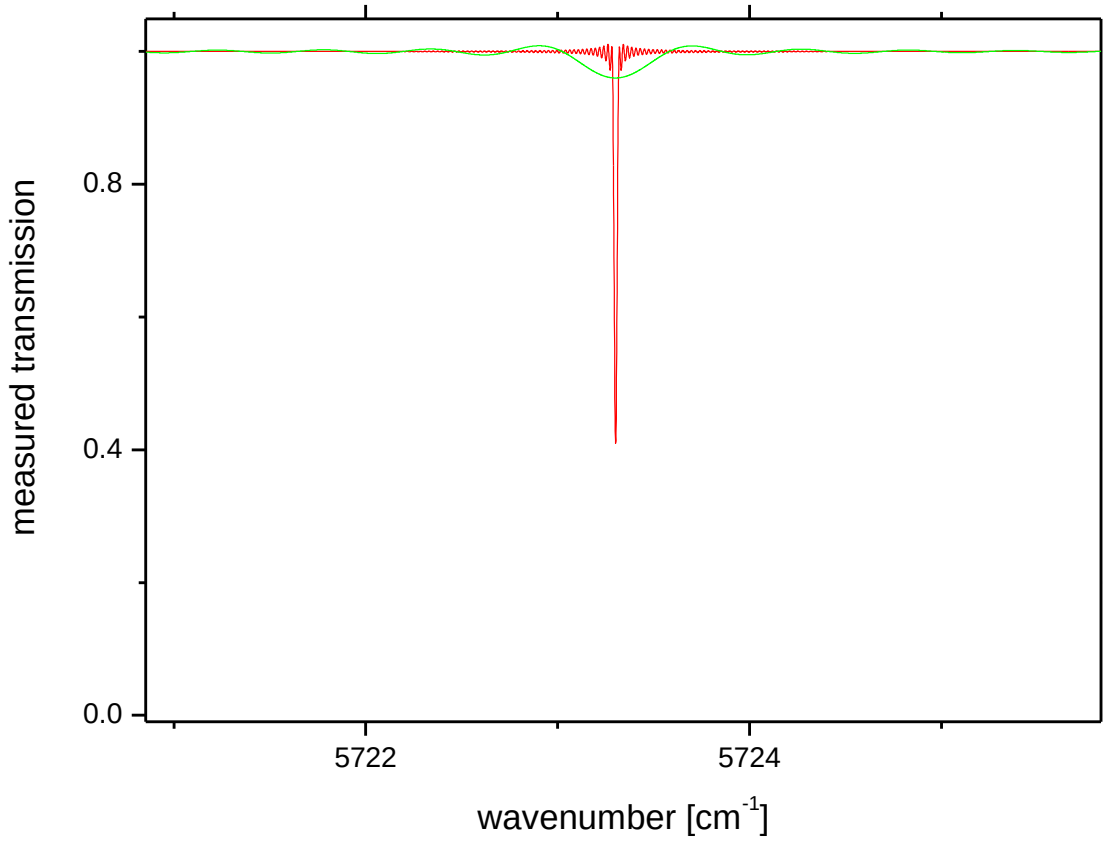
… is a cell not a better choice?

For a high-resolution spectrometer, use of a low-pressure gas cell (or a laser source) is mandatory. For a low-res spectrometer as the EM27/SUN, the open path measurement using strong H2O lines has some advantages:

- the method is portable (you just need lab air, a thermometer, and a barometer)
- so it does not require calibration and transport of cells.
- note that a low-pressure cell will not do: tiny line area of unresolved line.
- Working with a cell at higher pressure (e.g. target gas + N2) generates a reasonable spectral scene, but a T-error propagates into p_cell (and so linewidth), while p and T are independent variables in an open path measurement.

Why open path measurements for ILS …

HCl line from TCCON cell (100 mm , 5mbar) observed with TCCON (OPDmax = 45 cm, red) and EM27/SUN resolution (OPDmax = 1.8 cm, green).



Open path setup

Basic setup described in papers by Matthias Frey:

Frey, M. et al.: Calibration and instrumental line shape characterization of a set of portable FTIR spectrometers for detecting greenhouse gas emissions, Atmos. Meas. Tech., 8, 3047–3057, https://doi.org/10.5194/amt-8-3047-2015, 2015.

Frey, M., et al.: long-term stability and ensemble performance of the EM27/SUN Fourier transform spectrometer, Atmos. Meas. Tech., 12, 1513–1530, https://doi.org/10.5194/amt-12-1513-2019, 2019.

Picture: Carlos Alberti

Open path setup

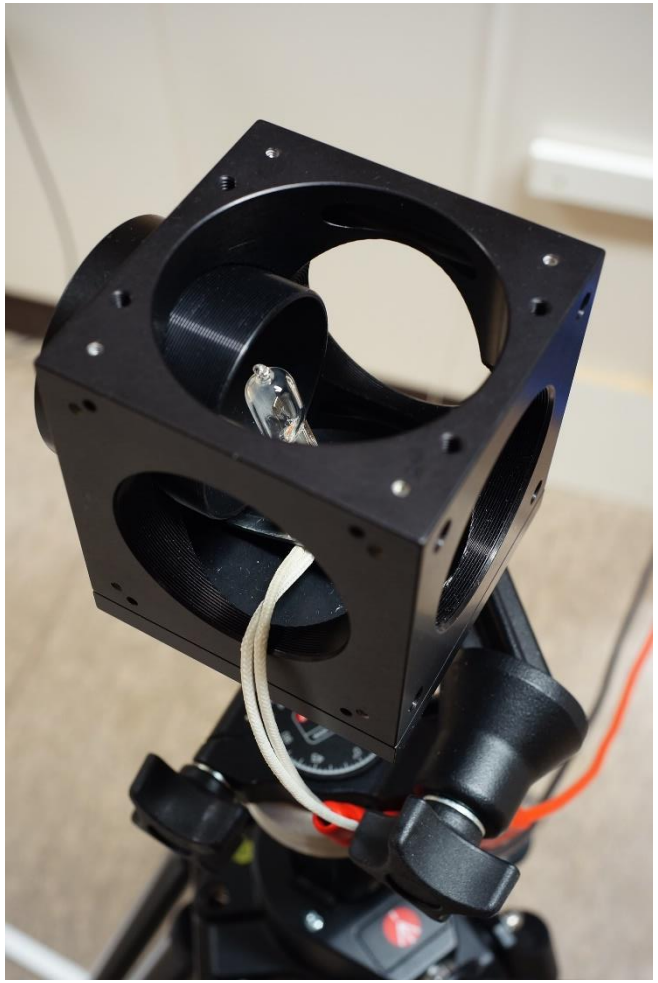
Important:

- Suitable lamp required (rectangular bulb filament, condensor, stable voltage supply)
- Avoid channeling from lamp bulb (tilt bulb, roughen with sand paper, operate at lower voltage 12 V -> ~ 10 V)
- Careful alignment: tracker mirror evenly illuminated (beam projected on white paper), condensor appears evenly illuminated when seen from tracker mirror – achieve even illumination on entrance field stop, use camtracker image for alignment (max gain + integration time).
- Use an open-path distance of several meters (~ 4 m).
- Vent the instrument (open top blind flange on cover and flange of cartridge with drying agent, remove cartridge).
- Allow for stable T conditions inside spectrometer (run for ~2 hours before collecting measurments, then record ~ 40x 1 min coadded spectra)
- Record temperature and pressure in the room.

Open path setup

Opened spectrometer + lamp housing

(pictures: Carlos Alberti)



Data analysis

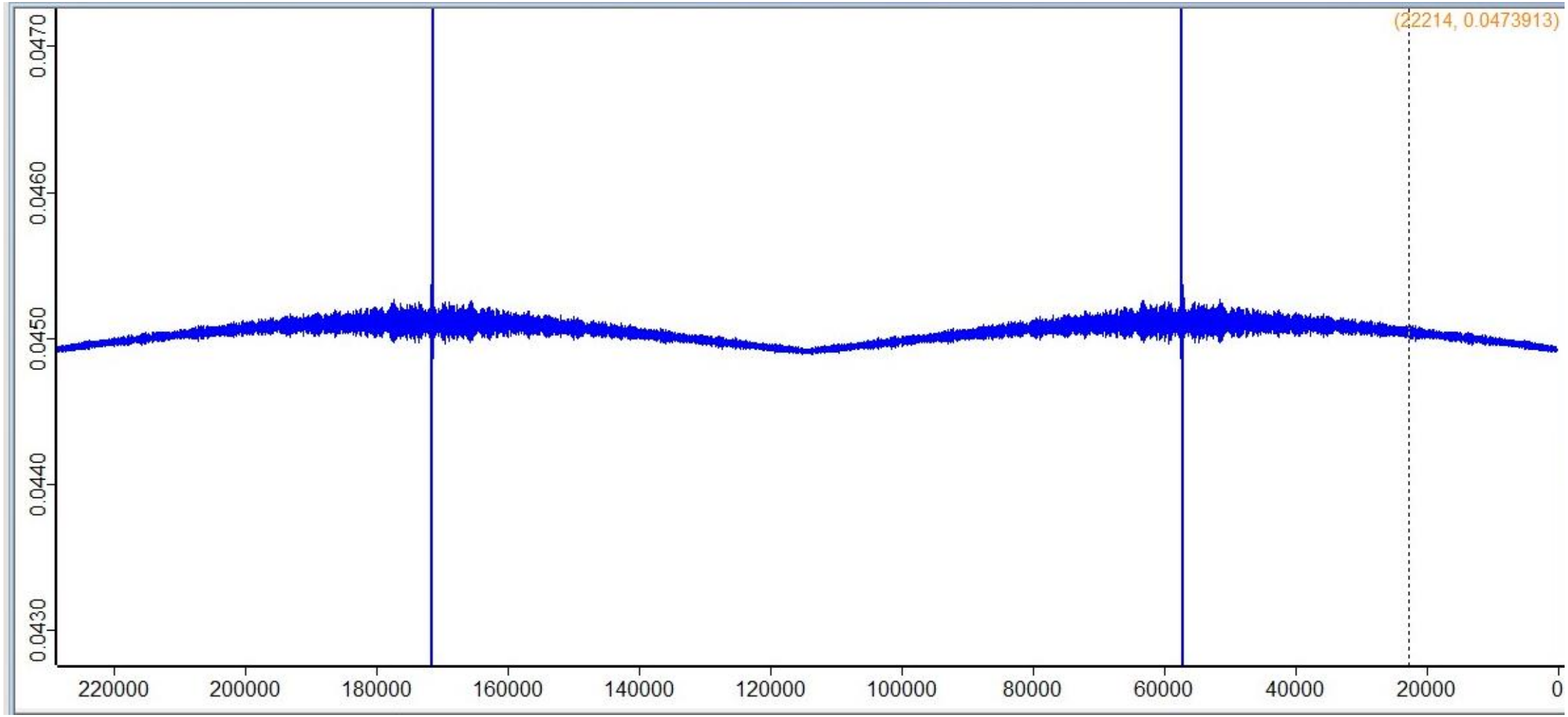
Before the LINEFIT analysis can be started, we need to coadd the recorded interferograms and then calculate a spectrum. The OPUS software can be used for this purpose.

IMPORTANT:

- The EM27/SUN records DC-coupled interferograms. The interferogram DC of the EM27/SUN is slightly variable (due to OPD dependent vignetting effects). A DC correction needs to be applied before the spectrum is calculated from the resulting AC interferogram. Otherwise, the deduced ILS parameters are incompatible with those for solar observations (as here a DC correction is included)
- The “limit resolution“ option needs to be activated in the OPUS FFT menue, otherwise the software will deliver a spectrum with slightly higher resolution than the desired nominal 0.5 cm^{-1} (equivalent to 1.8 cm OPD, Bruker uses OPDmax = 0.9 / RES). LINEFIT expects a NBM apodized spectrum.

Data analysis

OPD-dependent DC of an EM27/SUN (note : strong ordinate zoom, vertical blue lines are FWD and BWD centerbursts).



Data analysis

- There are two beam sections: outside and inside the spectrometer (different T, same total pressure, same H2O VMR (same partial H2O pressure)).
- Geometry: measure the distance D between lamp and first tracker mirror, note that there is an additional 33 cm path length up to the entrance filter (so d_out = D + 33 cm). The path length inside the spectrometer amounts ~ 74 cm.
- Due to the higher T inside the spectrometer, LINEFIT models two absorption contributions: the H2O outside the spectrometer (d_out, T_out, p_tot, ppart_h2o) and inside the spectrometer (d_in, T_in, p_tot, ppart_h2o).
- Note that the self-broadening of H2O is not negligible and depends on the amount of H2O.
- The inversion is an iterative procedure: only col_out is adjusted by LINEFIT, the user has to redistribute the adjusted column into both H2O contributions (respecting geometry and temperatures) and update the partial pressure (respecting geometry, total pressure and T_out).
- Note that the self-broadening of H2O lines is not negligible, so we need to determine the H2O partial pressure reasonably well.

Data analysis

(0) total pressure is the same in and out, value is set according to measured value (and kept constant during the iteration described below)
(1) a reasonable starting H2O column value for the outside column is chosen, col_out.
(2) ratio of columns in and outside is calculated: col_in / col_out = (d_in / d_out) * (T_out / T_in), so we can init col_in also.
(3) the starting partial pressure of H2O is calculated from this choice (using col_out and measured values T_out, ptot, d_out)
(4) the H2O partial pressures inside and outside are chosen equal (and so remain equal during iterative LFT calls - they are both updated to the same new value), so ppart_h2o_in = ppart_h2o_out.

Now initialization is ready, we can iterate ...
(5) fitted column scaling factor is applied to both col_in and col_out during repeated LFT calls
(6) H2O partial pressures values are updated during the iteration together with col_in and col_out, also applying the column scaling factor (so H2O col_in and col_out both change but preserve ppart_h2o_in = ppart_h2o_out).

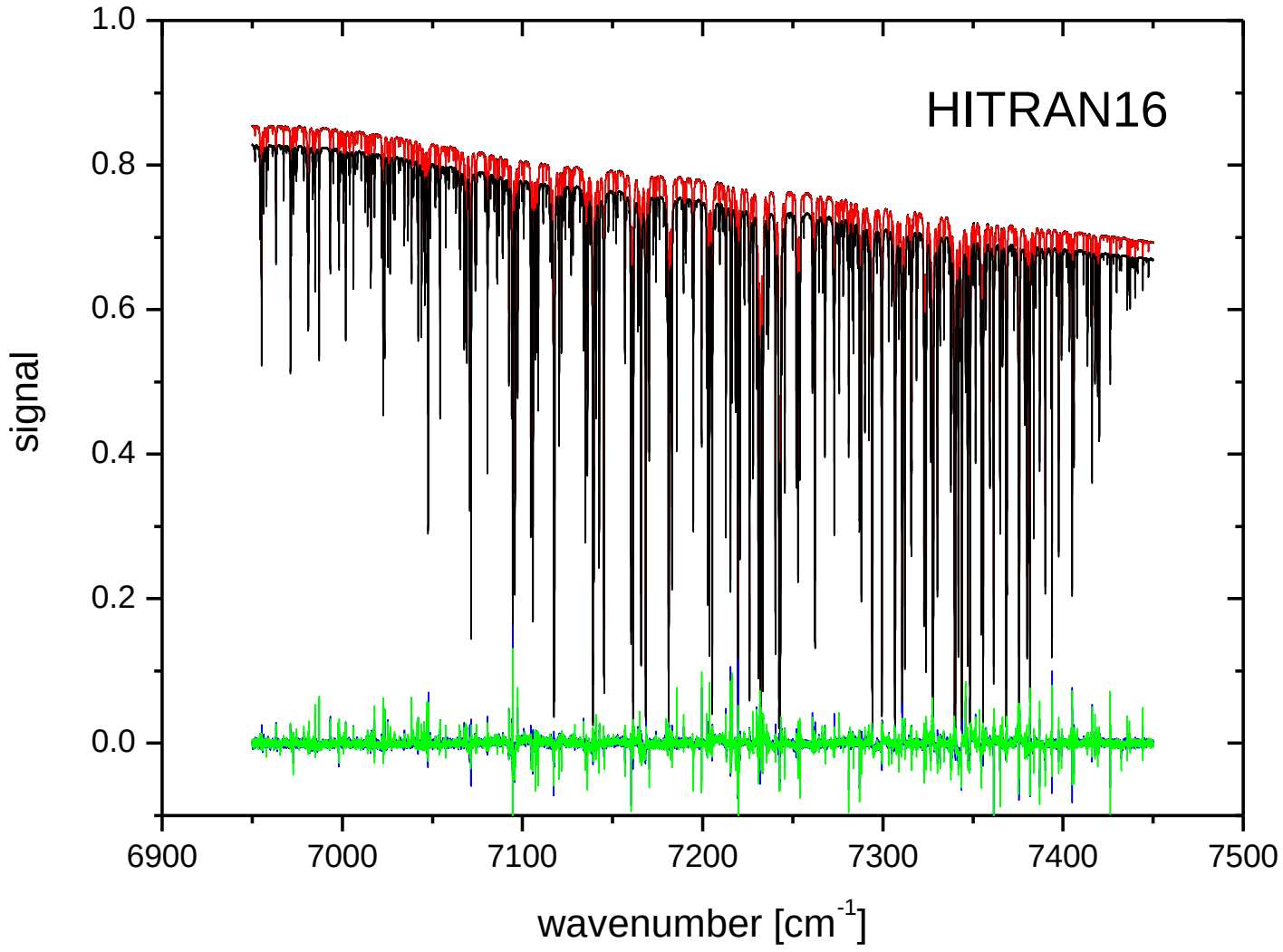
LINEFIT 14.8: empirical H2O line lists for open path ILS measurements

The upcoming ESA project foresees a revision of the H2O spectroscopy for the open path measurements. In agreement with ESA, this work has been pulled forward (the line list is included in the LFT148 distribution).

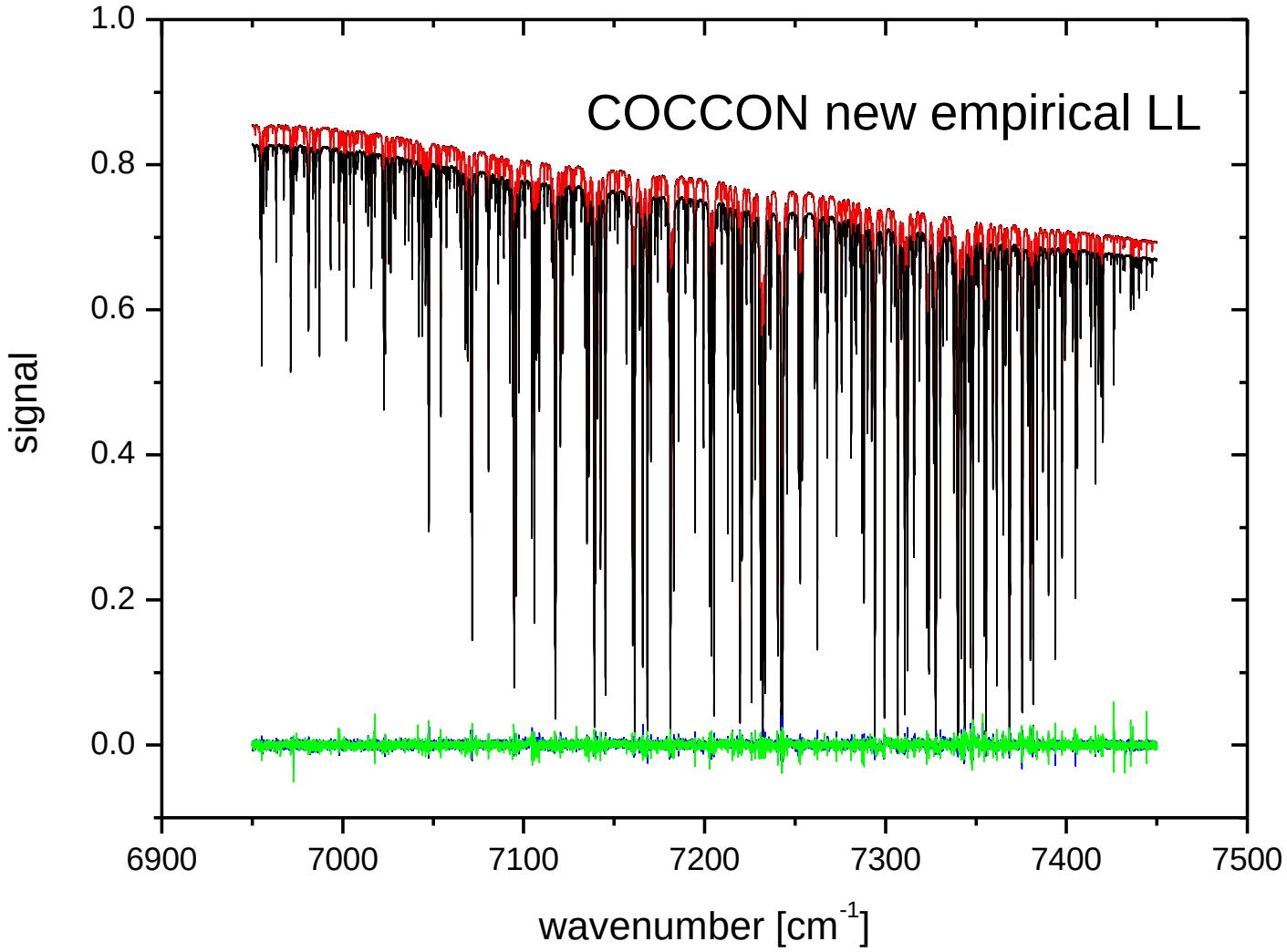
The H2O line parameters have been adjusted empirically using open path measurements recorded with a 125HR at higher spectral resolution. Two measurements at relevant temperatures were used (15 deg C and 30 deg C). A multi-spectrum fit of line parameters has been performed using LINEFIT and a wrapper. NOTE: this is just an empirical line list for the purpose of analyzing the open-path spectral scenes.

A new spectral region (5275.0,5400.0) in addition to the standard region (7000.0,7400.0) was included. The new spectral region is covered by both detectors, so allows a sensitive comparison between ILS of the main channel and the CO channel.

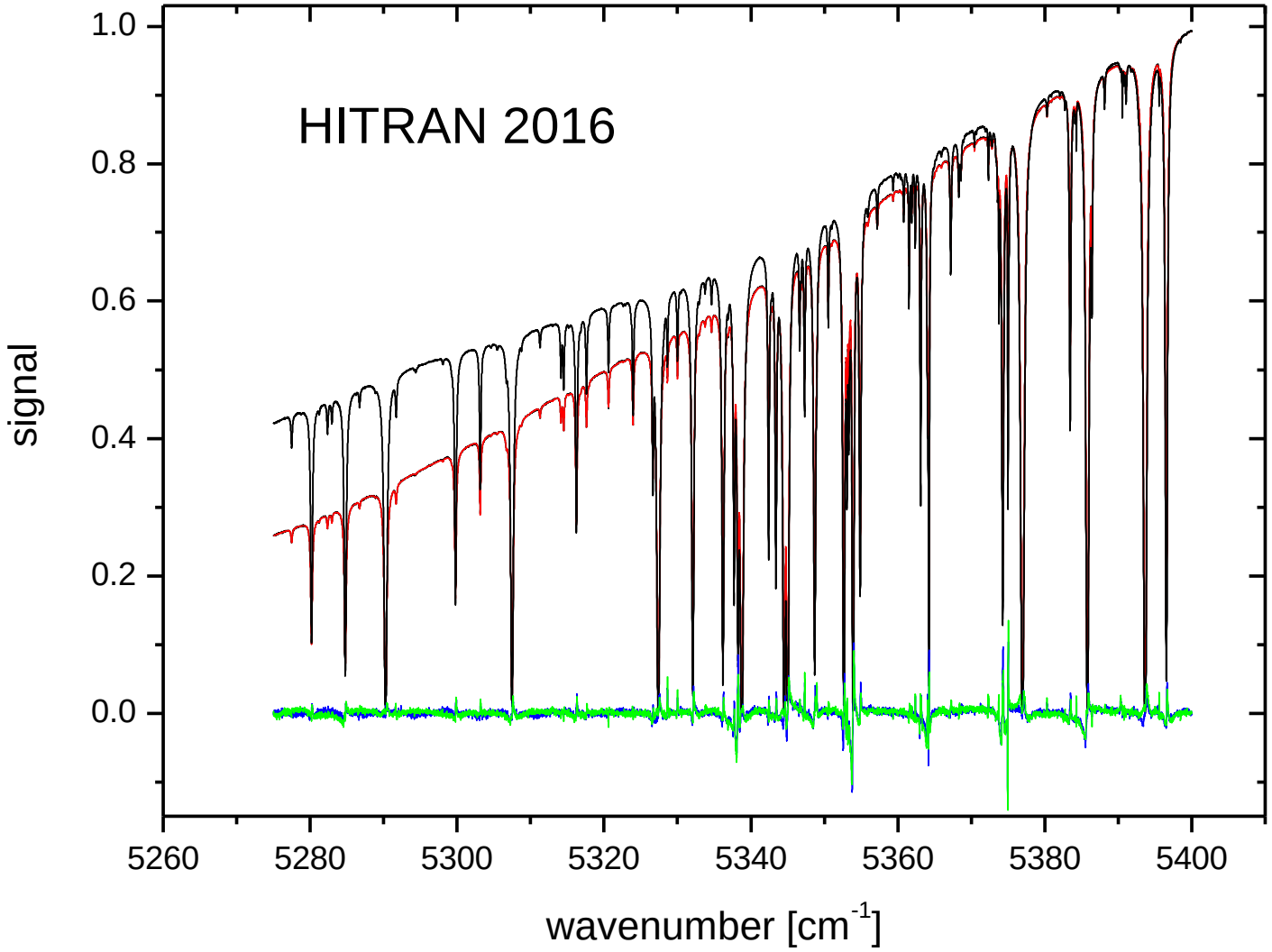
Empirical line lists



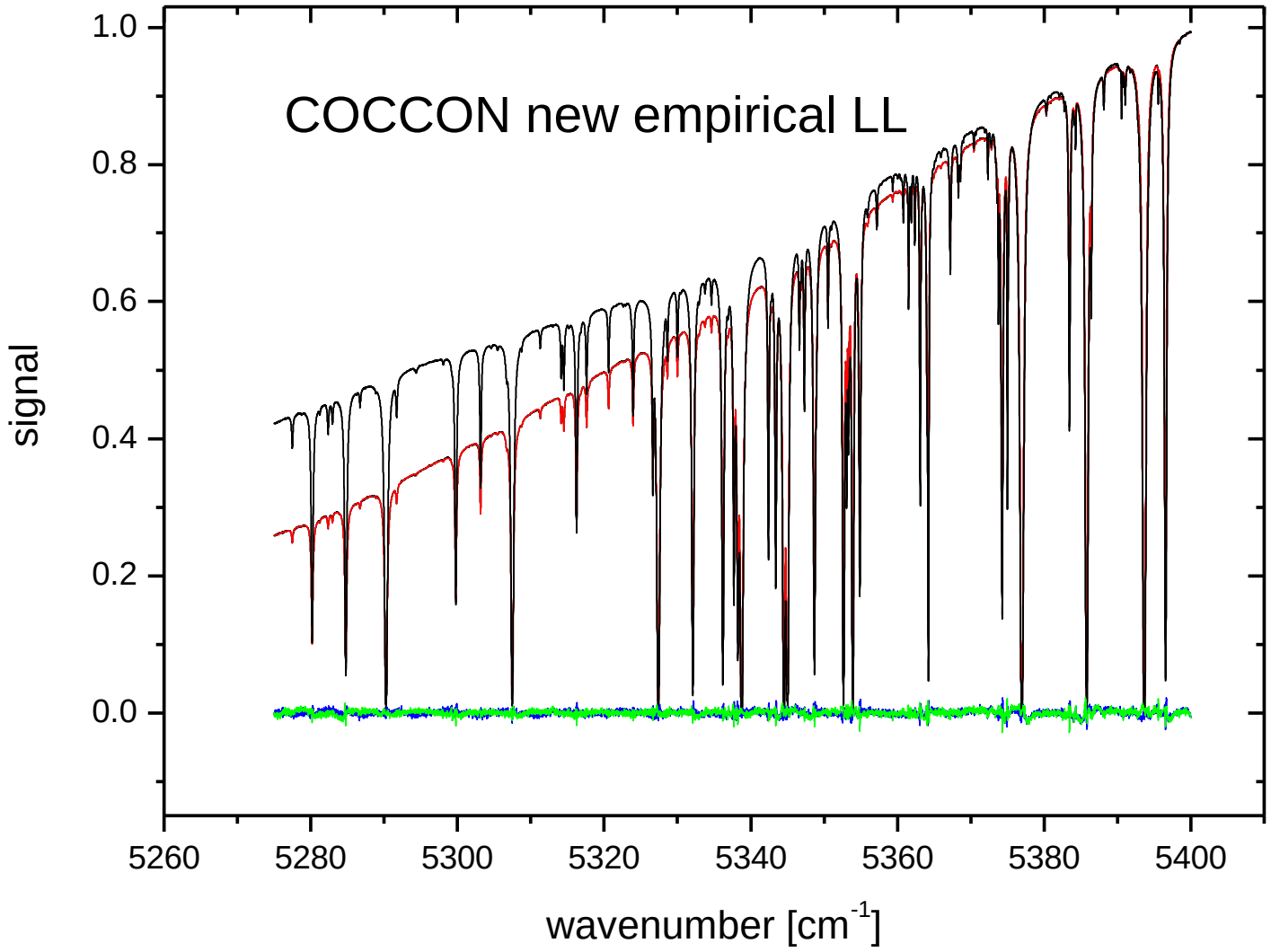
Empirical line lists



Empirical line lists



Empirical line lists



LINEFIT 14.8: empirical H2O line lists for open path ILS measurements

The pressure broadening parameters of the new line list have been adjusted in a way to reproduce previous results (connected with AICFs and ADCFs), although the general tendency of a low bias in EM27/SUN seems largely created by an underestimation of H2O pressure broadening parameters.

CA prepares a follow-up paper with revised ILS results (and results for many new spectrometers).

LF contributed a comparison Win-Linux of the LINEFIT examples (successful!).

New LFT148 version will be made available within 1 … 2 weeks.