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### 1.1. Validation of the ILS with C<sub>2</sub>H<sub>4</sub> gas cell measurements

The Instrument Line Shape (ILS) is an inherent property of the LHR, and determined by the radio-frequency (RF) filter characteristics used to limit the detection bandwidth and hence the spectral resolution of the instrument. The ILS can easily be measured experimentally (Fig. 1.1), using a spectrum analyser in the RF domain, and mirroring the response curve about 0 Hz. If a band-pass filter is used with a certain cut-on frequency, this results in the characteristic gap in the middle of the ILS, which is responsible for the distinctive molecular transition doublet appearance, when convolving the ILS with a narrow and single lineshape.

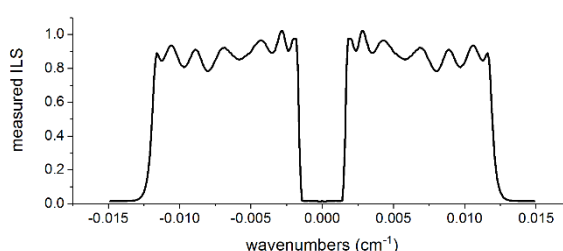




Figure 1.1. LHR normalized instrument lineshape (ILS), measured in the RFM domain using a spectrum analyser. The ILS corresponds to the Lorch 7BP8-200/300-SM/S (30 – 350 MHz) filter used for the campaign.

Whilst it is straightforward to measure the ILS, which remains constant and unaffected by other instrument settings, it is conversely less straightforward to retrieve it experimentally from measured spectra. Here, we validate our measured ILS, used routinely during retrieval processing, by comparing a simulated spectrum to a measured one from a reference gas cell with known contents. More specifically, rather than solely comparing the spectra, a full Optimal Estimation Method-based retrieval (fitting) is run over the measured spectra to retrieve the cell content, and to compare it against the expected value. If the retrieved value converges towards the ‘known’ value, and if the residuals do not suggest systematic differences between measured and modelled molecular lineshapes, we assume that the ILS used for convolution is indeed appropriate and can be deemed ‘validated’.

Since the LHR measures over a very narrow spectral microwindow, identifying an appropriate gas to use in the reference gas cell is not straightforward. Ideally, the gas should have a few well-characterized transitions with clear lineshapes that produce a large-enough signal without saturating in a cell of limited size, and should be easy to handle. The lines should ideally also be sufficiently spaced to enable a reliable extraction of the instrument baseline power variation. An extensive modelling exercise was undertaken within the context of a different project (LHR spectral emission measurements demonstration, 2016) to identify suitable gases, concentrations and cell dimensions. Ethylene (C<sub>2</sub>H<sub>4</sub>) had been retained as the best-suited option. However, it was found that the HITRAN 2012 database used for the forward modelling most probably does not include all the transitions within the microwindow scanned, and the lines are relatively densely spaced, such that instrument baseline fitting and determination is not quite as reliable as it should be. These limitations need to be borne in mind when analysing the results.

Using the LHR instrument in its final configuration but with pre-operational settings and before shipment to the field, C<sub>2</sub>H<sub>4</sub> cell measurements were performed, using a 10-cm glass cell with 15 torr (20 mbar) of pure gas at ambient lab temperature (assumed to be ~293 K), and a small IR source. The same

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Lorch 200/300 band-pass RF filter was used as for the atmospheric measurements in the field, for consistency.

Over 1h worth of gas cell measurements<sup>1</sup> were collected, with a 1 minute spectral acquisition time (83 spectra, SNR of ~10-40 across the microwindow per individual spectrum, measured as the mean signal divided by the standard deviation over the successive measurements). These were analysed with a purpose-built piece of code<sup>2</sup> serving as wrapper to a newly-built generic cell fitting (OEM-retrieval) algorithm<sup>3</sup>.

Spectra were frequency-calibrated in 2 steps for relative and absolute frequency calibration. For the relative frequency calibration, the free spectral range of the well-characterized etalon is assigned between 2 successive peaks of the continuously-measured etalon channel trace, followed by higher-order polynomial fitting to the measured data points (Fig. 1.2, LHS). The absolute frequency adjustment is done using a line matching procedure, identifying the peak centroid of a user-chosen control reference transition, situated here at 953.012319 cm<sup>-1</sup>. The centroid is found after fitting a Lorentzian or Gaussian lineshape with an undefined baseline to a sub-region of the spectrum. Note here that the densely-spaced lines make it difficult to reliably estimate a baseline, and that the fact that the measured lineshape is already broadened by the ILS (giving the characteristic central dip) may introduce some bias to the fitting. In practice, though, the method works well on the C<sub>2</sub>H<sub>4</sub> spectra, and the centroid fitting converges consistently towards a relatively stable point (Fig. 1.2, RHS).

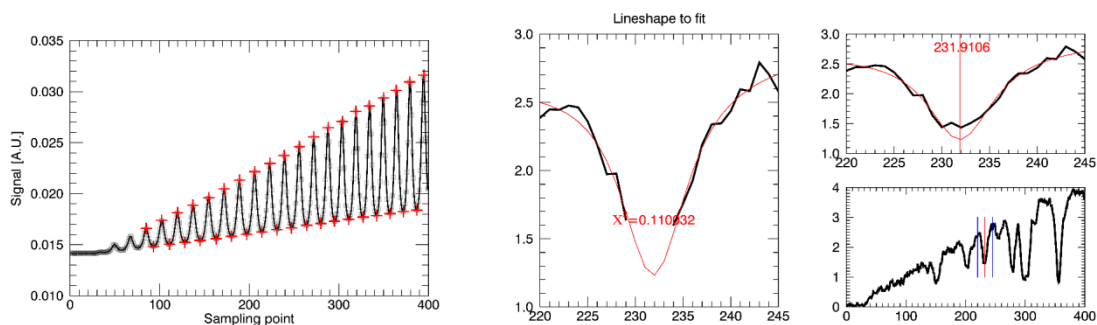




Figure 1.2. Intermediate diagnostics output from the frequency calibration routines, plotted for the first measurement in the sequence. LHS, etalon trace with peak identification. RHS, lineshape fitting associated with centroid identification for absolute frequency adjustment.

The instrument has been configured to measure an etalon trace for every second acquisition. Where no etalon trace is available, the absolute frequency calibration from the preceding measurement with a trace is used. Within the stable frequency calibration range, frequency vectors produced remain very stable, mostly to within an average difference of less than 1 sampling point (<0.003 cm<sup>-1</sup>). Two outliers, corresponding to one etalon trace, were removed, along with the associated spectra. The first 100 samples are trimmed from all the measurements because unreliable (unreliable frequency calibration

<sup>1</sup> file: RAL60LHR.a0.20170404.114423.nc

<sup>2</sup> ils\_validation.pro, git-commit 9e9927b4c2606225efe8f32701a7e5c52936f5de

<sup>3</sup> fct\_cell\_fit.pro, git-commit 9f9442b87254ab411d72942322d448f62da9091d

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and excessively weak signal), and all frequency-calibrated spectra are interpolated onto the absolute wavenumber axis of the first measurement. From these interpolated spectra, the noise is estimated as the standard deviation across the set, and the SNR as the mean divided by the noise across the microwindow.

These spectra are individually fitted using the OEM-cell retrieval algorithm, taking into account the convolution by the ILS. Only the cell pressure and a frequency-shift parameter (accounting for inaccuracies in the absolute wavenumber calibration) are fitted. The first guess of the pressure was set to 25 mbar (to avoid starting at the expected solution) with a  $\pm 5$  mbar prior error range. Fitting the 2<sup>nd</sup> order polynomial baseline parameters did not produce good fits, most likely because of insufficient baseline within the spectrum. The baseline was therefore introduced as a fixed parameter set into the retrieval, for each spectrum, as estimated from 4 small anchor sub-regions (Fig. 1.3).

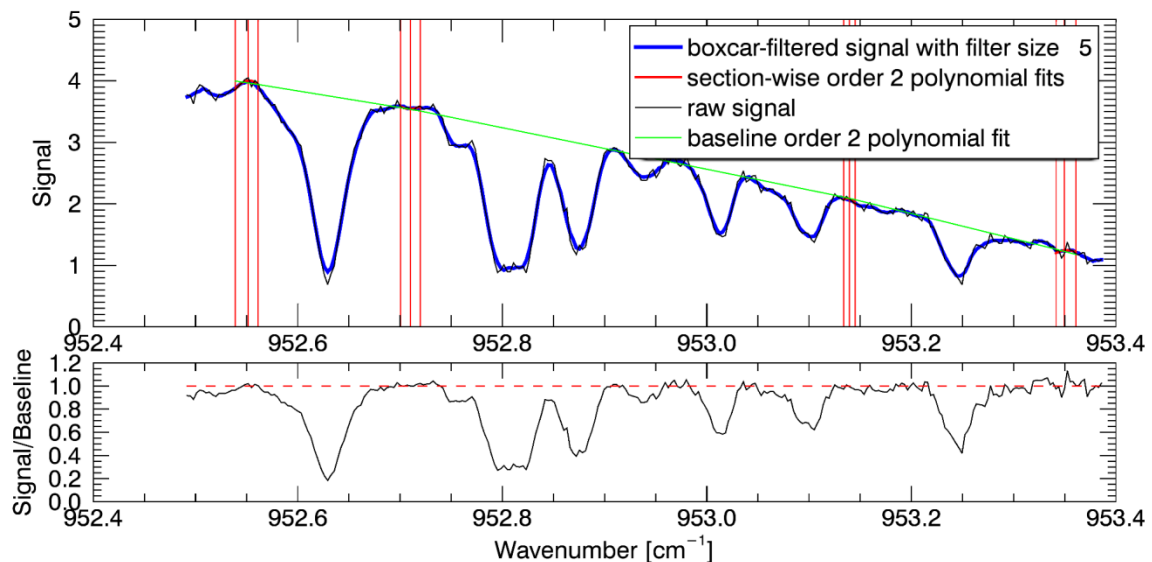


Figure 1.3. Anchor regions used for baseline estimation prior to cell fitting

An example output from the 81 fits is shown in Fig. 1.4, the remaining fits look roughly similar, within the underlying noise variations. Visually, the measured signal and the fit look very similar, in particular in terms of the lineshape and line broadening, and no obvious systematic differences are apparent from the residuals. Some inconsistencies are obvious (e.g. around 952.575, 952.75, 952.95), but these are most likely due to missing lines in the database (this was more obvious from direct laser absorption measurements done previously).

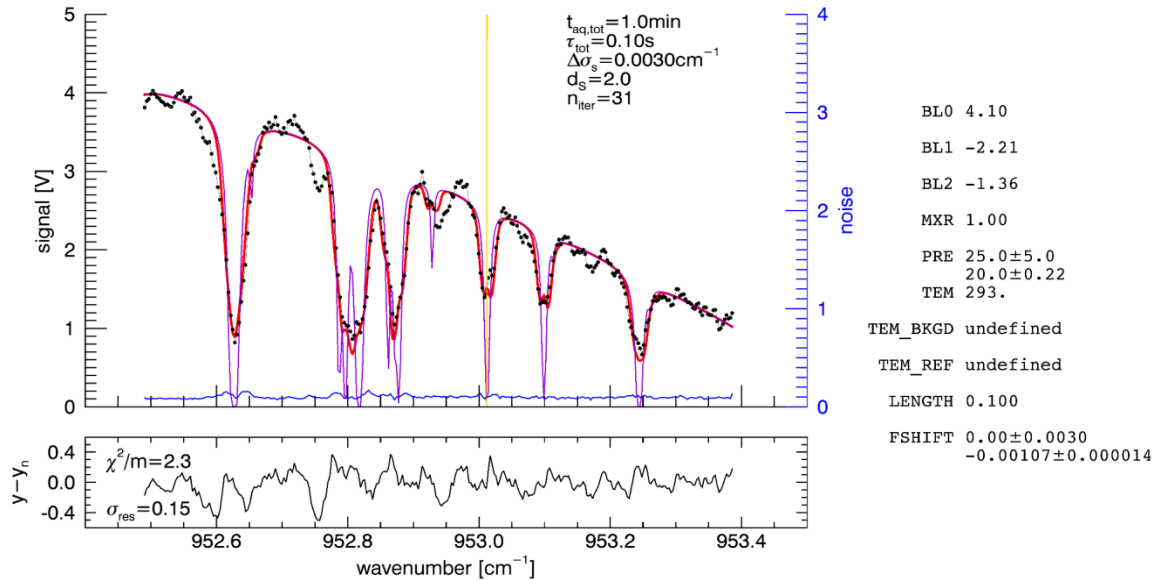


Figure 1.4. Example output from the OEM-based retrieval for data from a  $C_2H_4$  gas cell. Only pressure (PRE) and a frequency-shift parameter (FSHIFT) are fitted; the baseline parameters (BL0/1/2) remain fixed. The standard deviation of the residuals ( $\sigma_{res}=0.15$  V) is only slightly higher than the mean noise level introduced with the spectra (0.10 V). The yellow line marks the transition used as an absolute frequency calibration reference. The purple spectrum is a forward model run with the same parameters but without ILS convolution. Two full degrees of freedom for signal were retrieved for both parameters.

Most importantly, the retrieved pressure ( $20.0\pm 0.22$  mbar) is spot on the expected value (20 mbar). Fig. 1.5 shows the retrieved cell pressure across the entire series of 81 measurements. The average across the series is 20.08 mbar, with a standard deviation of 0.81 mbar; and there is no systematic drift in the retrieval.

The visual similarity between measured and modelled spectra, the systematic convergence of the retrieved pressure to the expected value, and experience from past atmospheric measurements is deemed proof enough to consider the ILS of the instrument as validated.

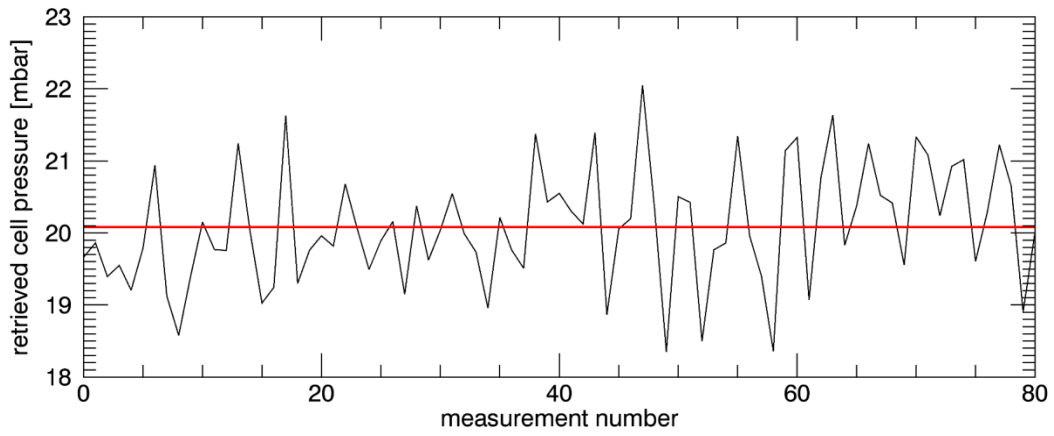


Figure 1.5. Series of retrieved pressure from gas cell retrievals across all spectra. The red line is the average across the series.