

Recommendations concerning a common NDACC ILS analysis scheme based on HBr cell spectra

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The suggested reference input file for ILS retrieval from the NCAR HBr cell is found in “examples\ndacc\hbr\small-MWs-standard”. Alternatively, a broadband fit can be attempted, using the input file in “examples\ndacc\hbr\broadband+Tfit”, which includes a fit of the temperature of the gas cell contents (two T values from H79Br and H81Br lines, respectively, are retrieved. Both T values should agree within 0.5 K). The two retrieval recipes should generate compatible solutions when applied to the same spectrum, the ILS parameters should be nearly identical (as in the demo results). The spectral windows used as well as the OPDmax value of the demo input should not be modified. If the cell measurement has been taken with higher resolution, the resolution can be reduced using OPUS (FFT option “limit resolution”) before analysing the spectrum. Alternatively, the resampling option of LINEFIT can be used for limiting OPDmax. Note that a considerable zerofilling has been applied on the demo spectra. Although not required from the mathematical viewpoint, it is much easier to judge the fitting residuals of an ILS fit based on a densely oversampled spectrum, because the spectral lines are not fully resolved. Therefore, it is suggested to use a spectral sampling density similar to that of the demo spectrum. The background continuum level of the demo spectrum is approximately normalized to unity and care has been taken that the HBr lines are near the HITRAN predicted positions (within a fraction of their width) - a proper spectral calibration is very important for a successful fit. It is strongly recommended to visualize the fits achieved with LINEFIT at least on a sample basis in order to recognize unexpected problems of the measurement (e.g. the demo assumes that the spectrum is free of channeling, but it might be necessary to include one or several channeling frequencies in the fit)!

Only a few entries in the demo input file have to be modified:

- The name of the spectrum to be analysed
- The assumed cell pressure
- The global constraints for modulation efficiency amplitude and phase

Concerning the cell pressure, it is important to note that the amount of HBr differs between different cells. Because a calibration of effective pressure values for the sealed HBr cells has not yet been performed (as was recently done for the TCCON HCl cells), the best assumption concerning cell pressure is to request a self-consistent retrieval: the column amount retrieved by LINEFIT (the input column value times the resulting column scaling factor) has to be in agreement with the assumed temperature and the effective cell length of 20 mm. For achieving a final self-consistent solution, the ILS fit should be repeated while readjusting the pressure according to the relation mentioned before until a self-consistent solution is found (requires typically one or two iterations). If unrecognized traces of other gases are contained in the cell, the actual total pressure in the cell might be higher (and the HBr lines wider than we assume), but curing this problem requires empirical calibration wrt a reference cell. The pending calibration of all distributed HBr cells to a common reference is under

preparation and the topic will hopefully be closed in 2015 when the new batch of N2O cells is available.

Concerning the global constraints, there are two values in the input file:

Reg Modulation (dev+smooth), Reg Phase (dev+smooth), reg T(dev)
Reg column (dev+smooth, per species), reg spectral scale (mean, per species)

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1.0e4,2.0,0.0,2.0,0.0
....

The first value scales the smoothness constraint of the modulation efficiency (ME) amplitude (MEA), the second the smoothness constraint of the modulation efficiency phase (MEP). The required values are a function of the noise level in the measurement (so these values need to be adjusted only once for a given experimental setup and measurement procedure). Ideally, the noise level of your spectrum should achieve the noise level of the demo spectrum - at least, it should not be much poorer.

The values should be equal, so they should be changed by the same factor. An appropriate stepwidth for searching the optimum choice is to change the current values by a factor of 2 to 3. If the solution is underconstrained, the retrieved ME becomes noisy (as fitted spectral noise is mapped into the ILS solution), if the solution is overconstrained, the changes in ME as fct of OPD are underestimated (and the fit quality suffers). The alignment of a 125HR spectrometer can be nearly perfect, which results in MEA values close to unity and MEP values close to zero along the whole interferogram. Because this is in agreement with the constraints (zero slope), it is difficult to adjust the constraint in such a condition, because there is no "misalignment signal" which pushes the solution away from the a-priori. Therefore, it is useful to switch off the self apodisation in the definition of the ideal interferometer in the LINEFIT input or to insert an incorrect value for the internal semi FOV during this adjustment. Then the MEA will bend away from unity and the transition between over- and underconstrained solutions can be nicely seen when plotting the "modulat.dat" results for different strengths of constraints. (Certainly, after the adjustment, the input file should be restored for the actual determination of the ILS).

If you find it too difficult to adjust the input values or if other problems occur, please do not hesitate to contact me. In this situation, I usually request a spectrum from you and will send you back the tuned input file (which then can be used over and over again as long as your measurement procedure and the noise level in the spectrum is maintained) and a corrected spectrum, if the spectrum is the reason for the trouble (e.g. improper normalization of continuum level, spectral calibration).