

FRM4GHG 2.0

Fiducial Reference Measurements for Greenhouse Gases



Technical Note on LINEFIT update in support of
open path measurements for instrumental line shape
(ILS) characterisation

Deliverable:	D1.3.1
Date:	15/08/2024
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Subject:	ESA-Contract No. 4000136108/21/I-DT-lr
Category:	ESA Express Procurement (EXPRO)
Our ref.:	Proposal, FRM4GHG 2.0 – Expro, ESA RFP/3-17031/21/I-DT-lr, revision from 27 August 2021 and 7 September 2021

Table of contents

1 Document change record	3
2 Access list	3
3 Purpose	3
4 Document structure	3
5 Open path measurements for ILS characterisation	3
5.1 Open path spectral scene	4
5.2 Fit results using different linelists	4
5.3 Conclusions and perspectives	5
6 Applicable Documents	5
7 Reference Documents	5

1 DOCUMENT CHANGE RECORD

Issue	Date	Item	Comment
V1.0	2024-08-15	-	Initial version

2 ACCESS LIST

This document is a deliverable “D1.3.1: LINEFIT updates” – created for the project FRM4GHG 2.0 and will be submitted to ESA. The document can be downloaded from the project webpage <http://frm4ghg.aeronomie.be>.

3 PURPOSE

Here, we perform a comparison between this tailored line list included in LINEFIT (created in spring 2021) and the latest HITRAN H₂O line list (downloaded from HITRAN on Aug-15-2024), in order to decide whether migrating to the latest HITRAN data would offer an advantage for the analysis of open path laboratory air measurements in the 7000 to 7400 cm⁻¹ spectral region.

4 DOCUMENT STRUCTURE

See Table of Contents

5 OPEN PATH MEASUREMENTS FOR ILS CHARACTERISATION

The software LINEFIT has been developed and is made accessible to the scientific community for retrieving instrumental line shape (ILS) characteristics from gas cell, laser, or open path measurements. In the context of greenhouse gas measurements using portable FTIR spectrometers, the option of using LINEFIT for the analysis of open path laboratory air measurements is of special interest, as the resolution of the tested spectrometers is limited and this spectral scene is easily created and reproduced at any place on Earth - only a reliable measurement of pressure, temperature and distance between source and spectrometer are required for achieving comparable results. Effectively, using this method, the ILS is derived from the H₂O spectral lines forming in

lab air in the 7000 to 7400 cm^{-1} spectral region. The performance of spectroscopic parameters as provided in data bases unfortunately is still not fully satisfactory, therefore, open path measurements with the IFS125HR operated as TCCON station Karlsruhe have been conducted and the relevant H_2O line parameters (line positions, line intensities and air broadening parameters) have been empirically deduced from these spectra (starting from HITRAN 2008).

5.1 Open path spectral scene

Lab air spectra recorded with the EM27/SUN FTS as described by Alberti et al, 2022, have been used for this study. The EM27/SUN has a near nominal ILS, which is confirmed independently by C_2H_2 gas cell measurements (for further details, see Alberti et al., 2022).

Figure 1 shows the fit region used for the ILS determination.

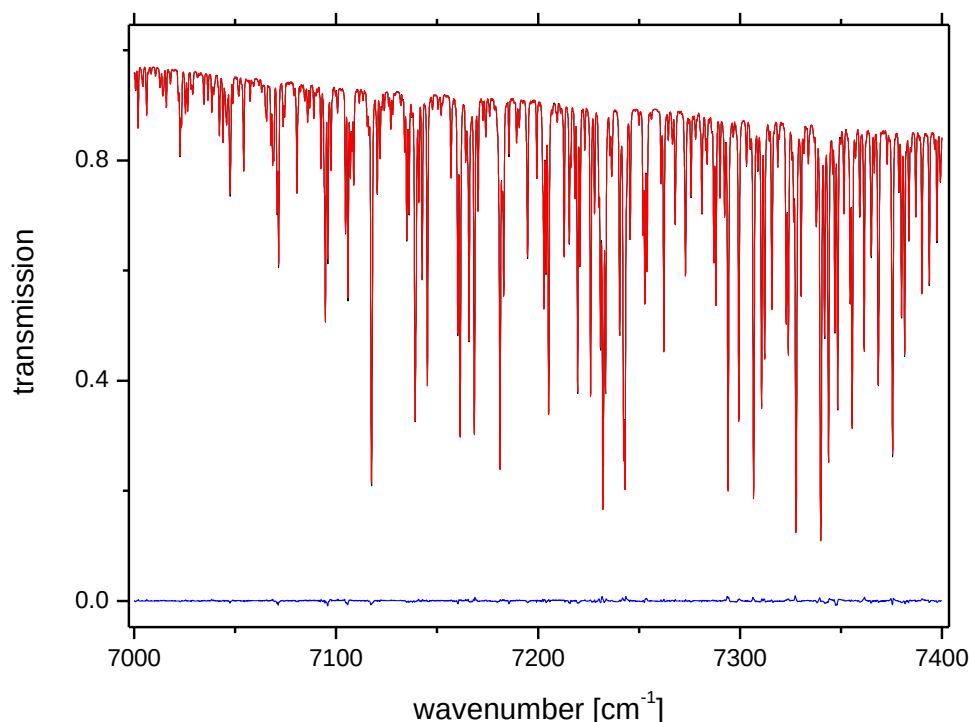


Figure 1: Typical laboratory air spectral scene used for ILS determination, spectral fit calculated with LINEFIT using the tailored linelist incorporated in LINEFIT. Distance between the spectrometer to the source is 4 meters.

5.2 Fit results using different linelists

Figure 2 compares the fit residuals between the latest HITRAN and the tailored linelist incorporated in LINEFIT (this linelist has been created in spring 2021. The work was based HITRAN2016, incorporating empirical changes of line parameters). Overall RMS is significantly worse when using

the latest HITRAN linelist (0.00174 to 0.00081).

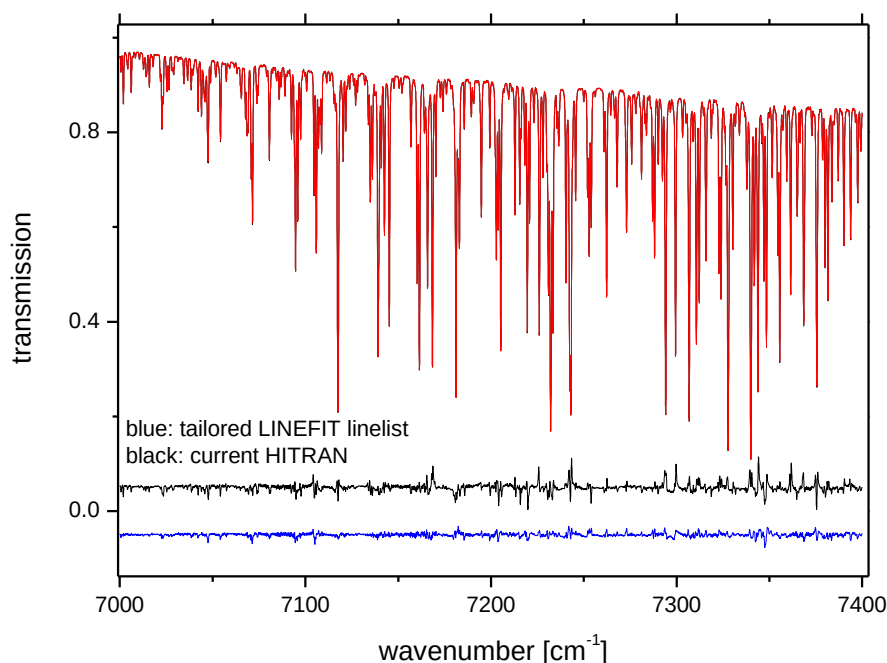


Figure 2: Fit results using either the tailored or the current HITRAN H₂O line lists. Residuals are vertically shifted for clarity and stretched by a factor of 5. HITRAN residuals are significantly poorer.

5.3 Conclusions and perspectives

The current HITRAN H₂O linelist does not prove an improvement of fit quality over the tailored linelist included in LINEFIT to open path spectra in the 7000 – 7400 cm⁻¹ region. Therefore, we recommend to continue use of the tailored linelist incorporated in LINEFIT which was deduced in spring 2021 using open path spectra recorded with the IFS125HR operated as TCCON Karlsruhe site.

6 APPLICABLE DOCUMENTS

Statement of Work: Fiducial Reference Measurements for Ground-Based IR Greenhouse Gas Observations (FRM4GHG 2.0)
Prepared by: EOP-GMQ, Reference: ESA-EOPG-EOPGMQ-SOW-21

7 REFERENCE DOCUMENTS

Alberti, C., Hase, F., Frey, M., Dubravica, D., Blumenstock, T., Dehn, A., Castracane, P., Surawicz, G., Harig, R., Baier, B. C., Bès, C., Bi, J., Boesch, H., Butz, A., Cai, Z., Chen, J.,

Crowell, S. M., Deutscher, N. M., Ene, D., Franklin, J. E., García, O., Griffith, D., Grouiez, B., Grutter, M., Hamdouni, A., Houweling, S., Humpage, N., Jacobs, N., Jeong, S., Joly, L., Jones, N. B., Jouglet, D., Kivi, R., Kleinschek, R., Lopez, M., Medeiros, D. J., Morino, I., Mostafavipak, N., Müller, A., Ohyama, H., Palmer, P. I., Pathakoti, M., Pollard, D. F., Raffalski, U., Ramonet, M., Ramsay, R., Sha, M. K., Shiomi, K., Simpson, W., Stremme, W., Sun, Y., Tanimoto, H., Té, Y., Tsidu, G. M., Velazco, V. A., Vogel, F., Watanabe, M., Wei, C., Wunch, D., Yamasoe, M., Zhang, L., and Orphal, J.: Improved calibration procedures for the EM27/SUN spectrometers of the Collaborative Carbon Column Observing Network (COCCON), *Atmos. Meas. Tech.*, 15, 2433–2463, <https://doi.org/10.5194/amt-15-2433-2022>, 2022.

Frank Hase, Thomas Blumenstock, and Clare Paton-Walsh, "Analysis of the instrumental line shape of high-resolution Fourier transform IR spectrometers with gas cell measurements and new retrieval software," *Appl. Opt.* **38**, 3417-3422, 1999.