

FRM4GHG 2.0

Fiducial Reference Measurements for Greenhouse Gases



Reanalysis of ILS of COCCON and low-resolution spectrometers: report

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1 DOCUMENT CHANGE RECORD

Issue	Date	Item	Comment
V1.0	2025-10-08	-	Initial version
V1.1	2025-10-10		Comments from DG

2 ACCESS LIST

This document is a deliverable “D1.3.2: Report on ILS reanalysis” – 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 extend the comparison between the tailored line list included in LINEFIT (created in spring 2021) and the latest HITRAN 2020 H₂O line list (downloaded from HITRAN on Aug-15-2024), to the IRCube and test if the same outcome as reported for the EM27/SUN (detailed in deliverable D1.3.1) is realised. Deliverable D1.3.1 investigated 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. The lab path open laboratory measurements are not used for the Vertex70 (HCl cells) or the LHR (different technology) so are not included in this report.

4 DOCUMENT STRUCTURE

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5 OPEN PATH MEASUREMENTS FOR ILS CHARACTERISATION

As reported earlier in deliverable D1.3.1, 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. It was concluded that the HITRAN 2020 H₂O linelist does not provide an improvement of fit quality over the tailored linelist included in LINEFIT to open path spectra in the 7000 – 7400 cm⁻¹ region. To fully test this outcome, the same methodology was applied to the IRCube, that is, use the COCCON method via water lines in a

controlled lab setting to see if there is any benefit in adopting the HITRAN2020 water lines rather than the current HITRAN2016 lines currently being used.

5.1 Open path spectral scene

Lab air spectra have been recorded with the IRCube using the method as described by Hase et al, 2019 and Alberti et al, 2022 over the course of the FRM4GHG campaign. Unlike the EM27/SUN, the IRCube's ILS is not quite nominal, but has been measured to be between 0.94 and 0.97 in its standard configuration. This range is due to various optical configurations and improvements to the IRCube over the course of the FRM4GHG campaign. The IRCube was rebuilt in 2023 with an internal optical setup very similar to the EM27/SUN which is now under testing. The ILS for that EM27/SUN "like" optical configuration has an ILS near nominal. For the purposes of this deliverable, this new configuration will not be described but will be reported on in terms of its ME and Phase for this exercise.

5.2 Fit results using different linelists

Table 1 lists the fit residuals, ME and phase for both the EM27/SUN (for comparison), the standard IRCube, and the modified IRCube in an EM27/SUN like configuration. The EM27/SUN result is reported here to simply confirm the method is the same as that used in deliverable D1.3.1.

The RMS fit residuals for the IRCube, either modified or standard, shows that the RMS is worse using the HITRAN linelist (labelled HIT2020) compared with the HITRAN2016 (labelled HIT2016) list that incorporate empirical changes to the water line parameters. The ME reduces slightly but not significantly (less than 0.01) and the phase is worse using the HITRAN2016 list.

Table 1. The LINEFIT results for the EM27/SUN and IRCube confirming that the new HITRAN water lines are worse in terms of the RMS residual fits.

Instrument/Date	rms	ME	Phase
EM27/SUN			
01/12/2014			
HIT2016	7.97e-4	0.9995	-2.92e-3
HIT2020	1.74e-3	1.013	-2.0e-4
IRCube			
22/08/2022			
HIT2016	9.42e-6	0.958	-7.3e-3
HIT2020	1.91e-5	0.967	-3.5e-3
02/10/2025			
HIT2016	4.4e-5	0.989	-7.76e-3
HIT2020	8.1e-5	0.999	-4.77e-3

5.3 Conclusions and perspectives

The extension of the ILS testing to include the IRCube on the current HITRAN H₂O linelist does not improve fit quality over the tailored linelist that is incorporated in LINEFIT for open path spectra in the 7000 – 7400 cm⁻¹ region, consistent with the result found for the EM2/SUN. The recommendation from deliverable D1.3.1 to continue to use the tailored linelist in LINEFIT does not change.

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

Deliverable D1.3.1: Technical Note on LINEFIT update in support of open path measurements for instrumental line shape (ILS) characterisation

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.