

FRM4GHG 2.0

Fiducial Reference Measurements for Greenhouse Gases



**Report: Characterisation of TCCON sites using the
FRM4GHG-II travel standard**

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Lead author(s):	Frank Hase (KIT)
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1 DOCUMENT CHANGE RECORD

Issue	Date	Item	Comment
V1.0	2025-Oct-08	-	Initial version

2 ACCESS LIST

This document is a deliverable “D3.2.2: Characterisation of TCCON sites using the FRM4GHG-II travel standard” – 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

The document describes the results achieved with the project’s travel standard (TS) EM27/SUN spectrometer. The TS visited globally distributed TCCON sites (specifically: Tsukuba in Japan, East Trout Lake in Canada, and Wollongong in Australia, the TCCON site Karlsruhe serves as reference site for the TS, therefore it also is implicitly part of the consistency check) and performed side-by-side measurements with each TCCON spectrometer operated on site. The purpose of the activity was to examine on which level different TCCON sites deliver globally consistent data and to quantify any potential residual biases between TCCON and COCCON.

4 DOCUMENT STRUCTURE

Please see Table of Contents.

5 RATIONALE AND DESCRIPTION OF THE TRAVEL STANDARD EM27/SUN

TCCON stations operate high-resolution FTIR spectrometers (typically of the type IFS125HR manufactured by the company Bruker), which are essentially immobile. On rare occasions, pairs of these spectrometers operated in laboratory containers were placed side-by-side and recorded solar observations in parallel for periods of weeks or months. While such activities revealed useful insights on instrumental problems, they cannot serve the purpose of verifying the consistency between different TCCON sites, as any transport event affects the instrumental characteristics of the spectrometer. Notably, the instrumental line shape, potentially also the optical coupling between solar tracker and spectrometer, and the signal level due to mechanical changes affecting the beam path are affected, and the delicate double-staged drive mechanism of the linear scanner also might require adjustments after a transport event. Thereby, even if the characteristics of a spectrometer were verified side-by-side with respect to a counterpart, these will inevitably be lost when the spectrometer reached the final operation site.

In contrast, the EM27/SUN spectrometer was developed as a field-deployable spectrometer and proved to maintain its instrumental characteristics due to use of a low-resolution very sturdy pendulum interferometer design, which is further supported by mechanical and optical solutions which help to ensure near-nominal and invariant instrumental characteristics. Explicit verifications of these claims have been performed in the course of various measurement campaigns using EM27/SUN spectrometers and involving transport of these between KIT and European and global overseas targets. By performing side-by-side measurements, which compare the campaign spectrometers before shipping and after back-receipt with (1) the COCCON reference EM27/SUN SN37 operated continuously in Karlsruhe and (2) with the TCCON station Karlsruhe the claim of invariant EM27/SUN characteristics can be tested explicitly.

These proven advantageous EM27/SUN stability characteristics suggest creation of a dedicated EM27/SUN travel standard (TS) for explicit testing of TCCON's internal consistency by performing side-by-side solar measurements with the visited TCCON spectrometer, thereby revealing potential station-to-station biases across TCCON. This highly desirable activity has been successfully realized in the framework of FRM4GHG. It consists of a remotely controllable EM27/SUN, which can be operated on various power grids. The TS EM27/SUN is integrated in a weather-sheltered housing, which offers a motorized dome, a rain sensor for automatically closing the dome in case of precipitation onset, a high-quality calibrated pressure sensor (Vaisala PTB-330), a ventilation / cooling system to keep the spectrometer temperature within operable limits, and an industrial PC, which controls the shelter functionalities, the spectrometer, and collects the raw data. The computer connects to the internet via Ethernet cable, WLAN, or LTE depending on local conditions of operation. An in-depth description of the TS setup and the calibration procedures applied for assuring the reference character of the TS has been provided in deliverable D3.2.1.

Figure 5.1 shows the results of the TS characterisation performed over a longer time frame (before, in-between, an after the campaign deployments), which indicates the excellent stability well within the TCCON accuracy requirements.

Species	Date	$K_{\text{SN37}}^{\text{SN39}}$	$\Delta K_{\text{SN37}}^{\text{SN39}} (\%)$	$\Delta \overline{X}_{\text{Gas}}$	$\Delta(\Delta \overline{X}_{\text{Gas}})$	Estimated TCCON accuracy
XCO ₂	January 2022	0.99886 ± 0.00004	—	−0.4684 ppm	—	0.2 %
	June 2022	0.99949 ± 0.00005	0.06307 %	−0.2575 ppm	0.21096 ppm (0.053 %)	
	October 2022	0.99961 ± 0.00003	0.01201 %	−0.1626 ppm	0.09484 ppm (0.024 %)	
	March 2023	1.00032 ± 0.00004	0.07103 %	0.1444 ppm	0.30700 ppm (0.077 %)	
XCH ₄	January 2022	1.00035 ± 0.00004	—	0.0007 ppm	—	0.43 %
	June 2022	0.99968 ± 0.00005	−0.06698 %	−0.0006 ppm	−0.00129 ppm (−0.072 %)	
	October 2022	1.00067 ± 0.00002	0.09903 %	0.0013 ppm	0.00188 ppm (0.104 %)	
	March 2023	0.99996 ± 0.00004	−0.07097 %	−0.0001 ppm	−0.00135 ppm (−0.075 %)	
XCO	January 2022	1.00161 ± 0.00030	—	0.1608 ppb	—	5.4 %
	June 2022	1.00107 ± 0.00078	−0.05391 %	0.0831 ppb	−0.07767 ppb (−0.078 %)	
	October 2022	1.00060 ± 0.00022	−0.04695 %	0.0403 ppb	−0.04282 ppb (−0.043 %)	
	March 2023	0.99472 ± 0.00053	−0.58765 %	−0.4636 ppb	−0.50394 ppb (−0.504 %)	
XCH ₄ ^{S5P}	January 2022	1.00035 ± 0.00003	—	0.0006 ppm	—	n/a
	June 2022	0.99836 ± 0.00007	−0.19893 %	−0.0032 ppm	−0.00384 ppm (−0.213 %)	
	October 2022	0.99962 ± 0.00002	0.12621 %	−0.0008 ppm	0.00246 ppm (0.137 %)	
	March 2023	0.99866 ± 0.00011	−0.09604 %	−0.0023 ppm	−0.00154 ppm (−0.086 %)	

Figure 5.1: overview of TS XGAS characterisation, as presented in Herkommer et al., 2024. The results are provided for column-averaged abundances of CO₂, CH₄, and CO. The XCH₄-S5P is an additional data product provided by COCCON. This uses the same spectral band as TROPOMI

instead of the standard band used by TCCON (located in the $\sim 5800 \text{ cm}^{-1}$ region). There is no TCCON equivalent for this data product, thereby the “n/a” entry in the last column. In case of CO, an airmass-dependent bias from the COCCON reference unit SN37 was found and empirically corrected for (for details, see Herkommer et al., 2024).

6 CAMPAIGN DETAILS

This chapter and the following chapter present the execution of the campaigns and the results achieved. The chapters are based on the publication “Using a portable FTIR spectrometer to evaluate the consistency of Total Carbon Column Observing Network (TCCON) measurements on a global scale: the Collaborative Carbon Column Observing Network (COCCON) travel standard” by B. Herkommer et al., published in 2024 in AMT. Table 6.1 gives a summary of the campaign activities.

Table 6.1: Overview of campaign activities

Station, country, short name	Coordinates [°]	Altitude [km]	Campaign duration
Tsukuba, JP (TK)	36.052N 140.122E	0.030	2022-03-24 to 2022-04-25
East Trout Lake, CN (ETL)	54.354N 104.987W	0.502	2022-08-16 to 2022-08-21
Wollongong, AU (WG)	34.406S 150.879E	0.030	2022-12-06 to 2023-01-26

The following figures 6.1 to 6.3 show the XGAS time series recorded during the campaigns. The COCCON analysis was applied both to the TS and the IFS125HR / TCCON measurements. The truncation of the TCCON interferograms to the maximum optical path difference of the EM27/SUN (MPD = 1.8 cm) removes the smoothing error from the comparison, as the vertical sensitivities of the observations become identical. The official data as provided by TCCON (derived from the full-resolution interferograms recorded with the IFS125HR and analysed with GGG2020) are also shown. From these data, an upper threshold of the residual systematic bias between TCCON and COCCON can be estimated.

Unfortunately, the reference laser of the IFS125HR operated at East Trout Lake broke down immediately before the arrival of the TS. Therefore, no direct comparison of XGAS data was possible. However, the qualitative comparison of the data recorded at the station immediately before arrival of the TS and the TS data recorded during the campaign do not indicate a significant systematic bias (see Fig. 6.2).

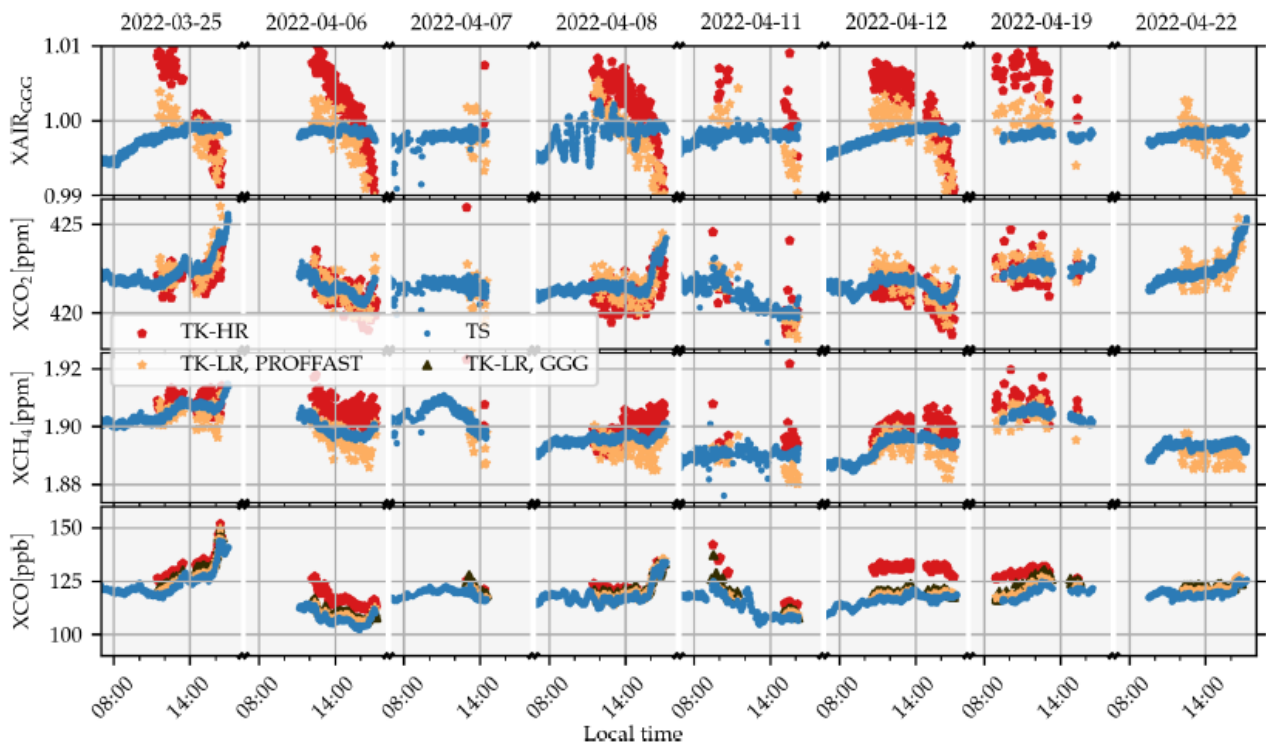


Figure 6.1: Time series of solar measurements recorded in Tsukuba with the TS and the IFS125HR operated for TCCON.

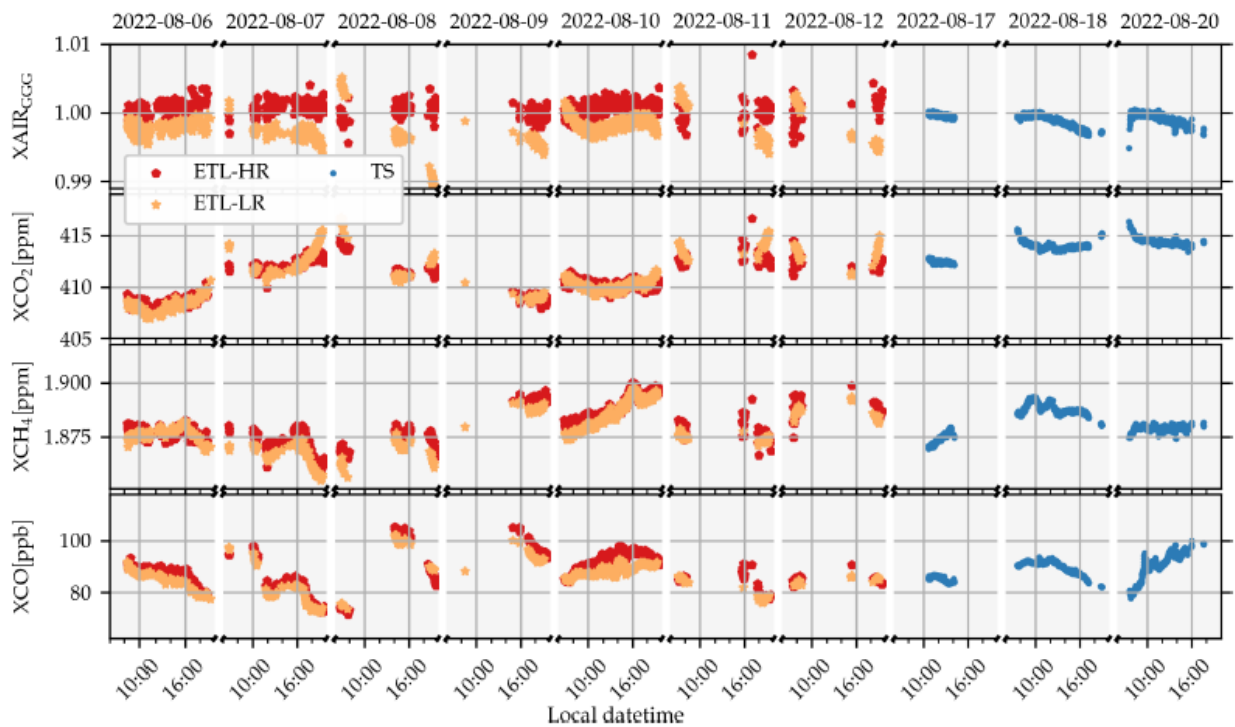


Figure 6.2: Time series of solar measurements recorded in East Trout Lake with the TS and the IFS125HR operated for TCCON.



Figure 6.3: Time series of solar measurements recorded in Wollongong with the TS and the IFS125HR operated for TCCON.

7 CONSISTENCY OF TCCON STATIONS AND OF COCCON VERSUS TCCON

Table 7.1 and Figure 7.1 present a summary of the findings for Tsukuba and Wollongong. Due to the laser failure of the TCCON spectrometer operated at East Trout Lake, a direct XGAS comparison was not possible. The expected level of station-to-station consistency assumed by TCCON seems compatible with the campaign results (TCCON assumptions see table 5.1, last column, 1σ -level uncertainties).

Table 7.1: Statistics of XGAS comparisons between the Tsukuba (TK) and Wollongong (WG) stations and the TS. Results are shown for full resolution (HR) and low-resolution (LR) spectra derived from the IFS125HR.

Site	Species	$\Delta_{XX-LR}^{SN37} (\%)$	$\Delta_{XX-HR}^{SN37} (\%)$
TK	XCO ₂	$0.11289 \pm 0.00826 - 0.06314$	$0.02760 \pm 0.00839 - 0.06309$
	XCH ₄	$-0.18871 \pm 0.00869 + 0.06685$	$0.19398 \pm 0.00906 + 0.06711$
	XCO	$1.18157 \pm 0.04809 + 0.05455$	$7.11865 \pm 0.04916 + 0.05775$
TK t-corr -44 s	XCO ₂	$0.11387 \pm 0.00829 - 0.06314$	—
	XCH ₄	$-0.18343 \pm 0.00871 + 0.06685$	—
	XCO	$1.16653 \pm 0.04870 + 0.05454$	—
WG	XCO ₂	$0.01264 \pm 0.00744 - 0.07104$	$0.00163 \pm 0.01023 - 0.07103$
	XCH ₄	$-0.09253 \pm 0.00840 + 0.07089$	$0.06115 \pm 0.00956 + 0.07100$
	XCO	$-5.57937 \pm 0.23080 + 0.55486$	$1.82105 \pm 0.11168 + 0.59835$

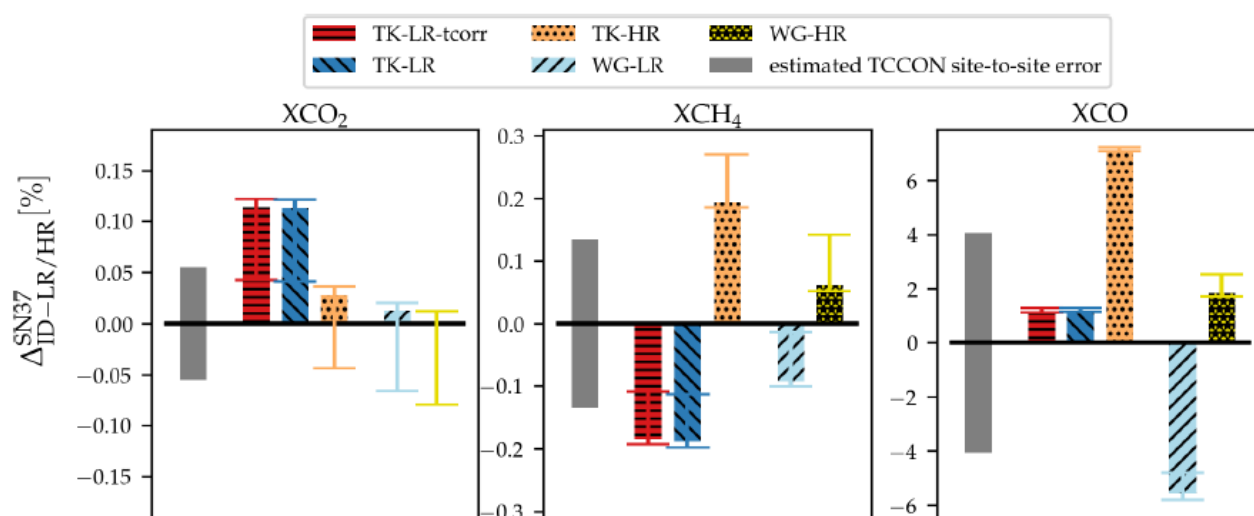


Figure 7.1: Graphical summary of XGAS comparisons between the Tsukuba (TK) and Wollongong (WG) stations and the TS. Results are shown for full resolution (HR) and low-resolution (LR) spectra derived from the IFS125HR. The grey bars indicate the level of station-to-station consistency assumed by TCCON (1σ -level) for CO_2 , CH_4 , and CO , so on station average these claims seems realistic.

8 SPECTRAL NOISE STUDY FOR TCCON INSPIRED BY TS CAMPAIGNS

The TS campaign showed a further useful side effect in addition to the primary task of testing TCCON's station-to-station consistency. Despite the fact, that TCCON is a network, the operation of individual, well-separated sites by different local operators unsurprisingly favours a local perspective. The direct station-to-station cross-linking perspective induced by the TS visits revealed station-specific problems which previously remained unnoticed. In case of Tsukuba, a time offset error was recognized (which was corrected for in the comparisons shown here), and in case of Wollongong, an erroneous assumption concerning the altitude difference between the station's pressure sensor and the TCCON spectrometer was revealed (via an observed inconsistency of the pressure records with those collected by the TS). Moreover, an enhanced noise level of all XGAS products (in comparison to other TCCON sites) was found in the comparison. As underlying reason, the strong spectral slope of the InGaAs detector used in the Wollongong IFS125HR was identified. The resulting decrease to higher wavenumbers degrades the oxygen retrieval, which in turn affects all XGAS products (as the retrieved oxygen column appears in the denominator of all XGAS calculations). Once uncovered, it is possible to compare the instrumental performance of nearly all TCCON stations from in this respect, including all stations which deliver the required diagnostics to the TCCON archive in the framework of their operational data processing.

Figure 8.1 shows the results derived by B. Herkommer for the TCCON as a whole (Herkommer, 2024). Several sites with significantly below-average noise level were identified. The comparison with TS spectra performed in Wollongong suggests that an exchange of the InGaAs detector element (selecting for flatter spectral response) could significantly reduce the noise level of XGAS data products at several TCCON stations.

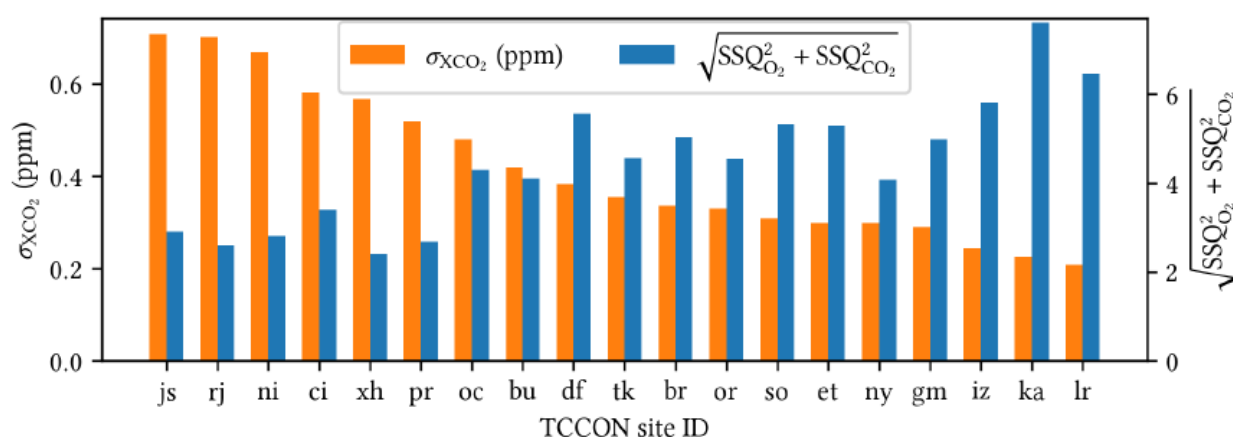


Figure 8.1: result of noise study performed across the TCCON by Herkommer et al., 2024, as triggered by the TS deployments. Orange: Noise level in XCO₂ product Blue: effective signal-to-noise ratio derived from the TCCON engineering data. A clear anti-correlation is found, the sites with high noise level appear on the left of the plot.

9 SUMMARY AND CONCLUSIONS

The site deployments performed in the framework of FRM4GHG shows the feasibility and usefulness of the TS approach. The sites tested so far are compatible with the accuracy claims of TCCON, but indications for different kinds of potential improvements, which would further enhance the network performance, have been identified.

Therefore, the operational perpetuation of these exploring activities carried out by KIT has been suggested as an important item to the European infrastructure ICOS. Unfortunately, despite ongoing discussions about the integration of GHG remote sensing components into ICOS since many years, no perceivable support has ever been realized up to the date of this writing.

10 ACKNOWLEDGEMENTS

The cover of the travel standard acquired by KIT during the first phase of FRM4GHG and the software for remote access have been developed by TUM (Jia Chen et al.). TUM moreover significantly supported this work by continuing the development of the software and supporting Benedikt Herkommer in case of problems with the remote operation.

The TS deployments and the associated studies would not have been possible without strong involvement and support of the local TCCON groups. We thank the TCCON teams operating the Tsukuba site (PI: Isamu Morino), the East Trout Lake site (PI: Debra Wunch), and the Wollongong site (PI: David Griffith).

11 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

12 REFERENCE DOCUMENTS

B. Herkommer et al.: “Travelling standard EM27/SUN & calibration procedure”, deliverable D3.2.1 of the FRM4GHGII project, January 2023.

B. Herkommer, Alberti, C., Castracane, P., Chen, J., Dehn, A., Dietrich, F., Deutscher, N. M., Frey, M. M., Groß, J., Gillespie, L., Hase, F., Morino, I., Pak, N. M., Walker, B., and Wunch, D.: Using a portable FTIR spectrometer to evaluate the consistency of Total Carbon Column Observing Network (TCCON) measurements on a global scale: the Collaborative Carbon Column Observing Network (COCCON) travel standard, *Atmos. Meas. Tech.*, 17, 3467–3494, <https://doi.org/10.5194/amt-17-3467-2024>, 2024.

B. Herkommer, dissertation “Improving the consistency of greenhouse gas measurements from ground-based remote sensing instruments using a portable FTIR spectrometer”, DOI: 10.5445/IR/100016872, 2024, accessible at <https://publikationen.bibliothek.kit.edu/1000168723>.