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EMRP
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1 Executive Summary

Introduction
This project developed the first European infrastructure for metrologically controlled measurements to derive highly accurate spectral reference data. Improved spectral reference data are needed to determine concentrations of pollutants or greenhouse gases in the atmosphere more accurately, both for remote and in-situ sensing. Ultimately, the project's results will contribute to improve the international efforts to track and model the progress of climate change, and to developing the government policies needed to mitigate future climate effects.

The Problem
Spectroscopy is a technique used in environmental and climate science to determine concentrations of pollutants and greenhouse gases in our atmosphere. Different molecules absorb and emit different wavelengths of electromagnetic radiation, called a spectral signature. The results of spectroscopic analyses are compared against reference data that describe these spectral signatures, allowing the molecules to be identified. More accurate reference data ensures more accurate analysis, which leads to more effective modelling. Ultimately, the higher the quality of the reference data, the more effectively European and global governments can monitor and mitigate atmospheric pollution and climate change.

With the large number of existing and planned global atmospheric monitoring networks and satellites dedicated to environmental monitoring, there is a global need for a long-term infrastructure to provide high-quality spectral reference data. Yet, despite considerable advances being made in the last decade in spectroscopic methods, the availability of high-accuracy reference data traceable to measurement standards is limited. There can be large deviations in the spectral data created by different research groups because multiple measurement methods are used, and there are no standardised procedures for establishing traceability and uncertainty. Additionally, environmental conditions such as temperature and pressure affect the properties of molecules, altering their spectral signature. Reference data are needed that have been produced under controlled conditions, to provide spectral signatures of molecules under the range of conditions experienced at different altitudes and temperatures in the atmosphere.

The Solution
The EUMETRISPEC project aimed to contribute to traceable line data with GUM-compliant uncertainty statements.

With regard to the identified problems, this project set out to solve this issue by

- establishing metrological structures for traceable line parameter measurements in Europe
- developing and validating laser and FTIR-based hardware for the determination of traceable line data,
- developing agreed procedures to measure and process raw data in spectral line data retrievals on NMI level, and
- providing and disseminating traceable spectral example data gathered under harmonized procedures for relevant molecular species.

At the end of the project, and based on the developed spectroscopy infrastructure traceability of line parameter is addressed: Pressure, temperature and cell lengths measurements are traceable to the SI. This is a major improvement to the situation before the beginning of the project. The software and line area determination are characterized, significant progress has been made. In the context of the project, a line-by-line data measurement system has been set up which represents the latest state of the art in terms of metrology. This system is open to the scientific community.

Impact
The project resulted into three classes of impact and improvement:

- new infrastructural and experimental capabilities at NMI level,

- measurement procedures, stated and documented to measure line parameters, and
- new measured line parameter sets with stated transparent uncertainty assessments which are compared to literature data, where available.

Line parameter retrievals can now be seen as a task on NMI level. At PTB, a metrology infrastructure is offered to the open scientific community for future collaboration and multiplication of work, and a persistent NMI commitment (e.g. at PTB) to continue this work.

The high-quality data, as obtained from this project became available to the scientific community through presentations, publications and two international workshops on traceable line parameter measurements organized by the project consortium.

The line data improvement by assessing measurement uncertainties has led to more accurate atmospheric monitoring. In networking, it will set the basis for analytical and theoretical studies on molecular line-by-line spectra.

The project data have been applied to other EMRP projects of later calls. In addition, the applications of line data have been brought to standardisation bodies targeting e.g. air quality measurement standards.

2 Project context, rationale and objectives

Climate change research and atmospheric monitoring programs are crucial to the protection of the earth's atmosphere and mitigation of global warming. Atmospheric monitoring as based on observed spectra relies on spectral line parameters which are measured in laboratories under well controlled conditions. The line parameters are subsequently used to process the observed atmospheric spectra in order to compute molecule specific concentration values. The quality of the input spectral line parameters directly impacts on the outcome of atmospheric monitoring. High quality laboratory studies of spectral line parameters serve as the foundation of reliable atmospheric monitoring.

The HITRAN and GEISA databases are two of the best-known and most extensive resources for spectral line parameters. They contain several million data sets that include molecular line strengths, pressure broadening and line shift coefficients, ground state energies etc. for tens of molecular species. Among them are the most relevant molecules for atmospheric monitoring and climate change research.

These databases allow atmospheric absorption spectra to be modelled. Such models are used to derive concentrations of relevant molecules like CO_2 in the atmosphere – the calculated spectra are matched to atmospheric spectral measurements from satellites, balloons, air planes and ground based measurement stations using LIDAR or FTIR instruments.

The quality of the input directly defines the quality of the output data.

Hence, the availability of highly accurate spectral data is essential as input for the accurate modelling of radiation transport in atmospheric sciences. Note that other scientific fields which rely on line measurements also need these data.

Whilst the databases have been put together in an impressive long-term effort, with great expertise from diverse sources and have served the community well, quantitative estimates of atmospheric molecular species based on these data are often inaccurate due to a number of metrological issues. These include a lack of information on the comparability of the retrieval algorithms or measurement conditions during the determination of spectral data as well as missing or incompletely stated uncertainty of the measured gas pressure, gas temperature, effective absorption path length, and path homogeneity or gas composition (including isotopic ratios). The consequences of missing information can result in large errors in atmospheric sciences, climate modelling and data retrieval, of which there are many examples in the literature.

Most severe are widely lacking or only rough uncertainty statements in these data bases. This is not the fault of these data bases. They only collect available data. Unfortunately one has to acknowledge that accurate uncertainty statements are still not state of the art in atmospheric sciences. Measurements without uncertainties are rather useless, and crude uncertainty statements are better than none, yet of only limited reliability.

For example, the most important anthropogenic greenhouse gas CO_2 has half a million entries in the latest version of the HITRAN data base (HITRAN 2012). None of the stated CO_2 line intensities has a stated uncertainty better than 1%. Only 0.3% of the CO_2 line intensities have a stated uncertainty between 1% and 10%. For the remaining 99.3% of the CO_2 lines in the HITRAN 2012 data base, the stated uncertainties of the CO_2 line intensities are worse than 10%, unreported or unavailable.

Comparing these uncertainty statements of the input data with the requirements in atmospheric sciences: The recently launched OCO2 satellite (Orbiting Carbon Observatory-2), is specialized in global CO_2 monitoring. Its main task is “to determine the concentration of atmospheric carbon dioxide to a precision of 0.3 to 0.5 percent” (source: NASA OCO2 fact sheet, http://www.jpl.nasa.gov/news/fact_sheets/oco2.pdf). It is clear that the absolute accuracy of these measurements is significantly worse if the uncertainties of the input data are larger than 1%.

CO_2 is one of the best-measured gases. For most other gases, the quality of the line data is even more inferior.

To put it in a nutshell: the limited quality of the input data often hampers an improvement in accuracy of atmospheric science.

Considering the impressive size of existing and planned global atmospheric monitoring networks and the large number of satellites dedicated to environmental monitoring, a global need for high quality spectral line parameters and for long-term infrastructures to precisely determine such parameters in lab experiments is imminent. Such high quality data is even more relevant as climate change detection or climate model validation requires an accurate quantification of small changes on large background signals over time spans of months, years and even decades.

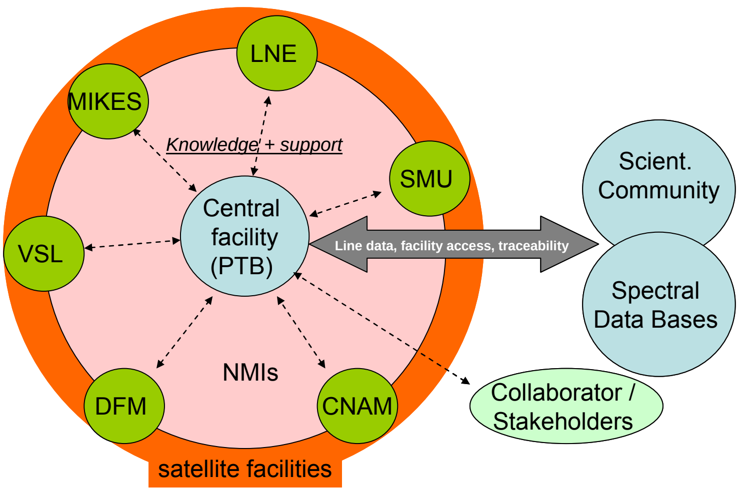
BIPM’s Resolution 11 of the 23rd CGPM (2007) directly emphasizes the need for SI traceable measurements to monitor climate change, a view supported by the World Meteorological Organisation.

The primary objective of this project was the establishment of a European spectroscopy infrastructure enabling measurements of traceable spectral line data under well controlled conditions.

This objective is implemented by setting up a central facility (CF) for high-quality spectroscopic measurements under metrological conditions.

The central spectroscopic facility (CF) has been

- based on a modified high-resolution VIS to MIR Fourier-Transform spectrometer (FTS) with a spectral resolution in the 10^{-3} cm^{-1} range,
- validated by means of high-resolution laser-based satellite facilities at the project partners (see diagram),
- used to determine accurate transition line data of atmospheric key molecular species,
- it will made available for the atmospheric community for user-driven determination of spectral data under tight metrological control of the measurement conditions in order to maintain high data quality,



and has been widely promoted to generate awareness that the CF is open for cooperation with the user community and that it is dedicated to disseminate the measured spectral data to the public.

The goal of the project was to develop a European measurement infrastructure for producing traceable spectral reference data for atmospheric monitoring. Three inter-related objectives were established to achieve this goal:

1. To set-up, test and validate a Central spectroscopic Facility (CF) for making traceable spectroscopic measurements under well controlled conditions.
2. To develop metrological procedures for spectral data determination and data handling.
3. To generate samples of high accuracy spectral line data and related metrological uncertainties for key greenhouse gases, including carbon dioxide (CO_2), methane (CH_4), nitrous oxide (N_20), water vapour (H_2O) suitable to demonstrate the CF capabilities and for reference gases like hydrogen chloride (HCl) or hydrogen bromide (HBr) used to test field FT-spectrometer performance.

3 Research results

3.1 Setting-up, testing and validation of a Central spectroscopic Facility (CF) for making traceable spectroscopic measurements under controlled conditions

Introduction

Spectroscopy is a technique broadly used in environmental and climate science to determine concentrations of pollutants and greenhouse gases in our atmosphere. With the large number of existing and planned global atmospheric monitoring networks and remote sensing satellites dedicated to environmental monitoring, there is a global need for a long-term infrastructure to provide high-quality spectral reference data of relevant atmospheric target molecules. Yet, despite considerable advances being made in the last decade in spectroscopic methods, the availability of high-accuracy metrologically validated reference data to measurement standards is limited. This is also caused by a lack of laboratory infrastructure dedicated to such measurements. In order to fill the gap of spectroscopic infrastructure suitable to measure line parameters in lab experiments as they are required for atmospheric monitoring, the EUMETRISPEC project aimed to set up a new spectroscopic facility at NMI level, addressing traceability of spectral line parameters.

Research undertaken

In order to have a highly versatile experimental approach within the EUMETRISPEC project and beyond, a central facility (CF) spectrometer was designed to be located at PTB and based on high-resolution Fourier-transform spectroscopy. The installed Fourier-transform (FT) spectrometer allows for a broad spectral coverage capable of targeting a broad range of atmospheric target molecules via their various absorption bands from the near to the mid infrared wavelength range by the same instrument. The idea was to have this flexible CF FT-spectrometer once in the project which is then validated and supported by other, specialized laser-based spectrometers located at the different project partners.

The central facility setup at PTB is based on a High-Resolution Fourier-Transform Infrared Spectrometer (Bruker IFS-125 HR). A photograph of the CF is shown in Fig. 1. The instrument has a maximum optical path-length difference (OPD) of 481 cm, resulting in a resolution of up to 0.002 cm^{-1}. The spectrometer has been installed in late 2011 and taken into operation at the beginning of 2012.

A major limitation of available HR FT-spectrometers used for spectral data generation is the background absorption inside the many meter long interferometer chamber, mainly by water or CO2. In order to completely suppress these background absorptions by atmospheric constituents particular care was taken to achieve an exceptionally good vacuum inside the spectrometer. For this purpose, the standard vacuum system has been extensively modified by using two specially tested, vibration-free, magnetically levitated turbo molecular pumps. The background pressure inside the spectrometer, and therefore the H_2O/CO_2 contamination, could be reduced by more than three orders of magnitude compared to the original manufacturer specifications. This fact combined with the small leakage rates, i.e. well below 0.03 mbar/day, provided excellent conditions for high-quality line parameter measurements.

Similar care was taken to improve the metrological control over the entire measurement process. The low interferometer chamber pressure allows to determine accurate line parameters of the target molecules. A specifically designed gas manifold was used to precisely handle reference gases and gas mixtures and to avoid modification or contamination. This gas manifold was capable to employ pressurized cylinder gases to the CF sample compartment where the new, specialized FT-absorption cells were mounted. The gas tubes and cells were evacuated, while the gas pressure in the manifold and the absorption cell were well controlled, monitored and recorded. The sample gas was then transferred into the absorption cells.

Fig. 1: Central facility Bruker IFS 125HR FTIR-spectrometer, gas manifold and continuous pressure and temperature monitoring setup.

New, custom-designed gas absorption cells were developed and employed in the CF. Several measurement systems on gas conditioning, monitoring and handling completed the spectroscopic infrastructure, as shown in **Error! Reference source not found.** Fig. 2. The CF comes with

- Optical path lengths of gas absorption cells: from 0.02 m to 42 m.
- Gas pressures: from a few 10^{-5} mbar to 1.4 bars
- Gas temperatures: from room temperature down to 220 K

The CF development thus enabled high-accuracy measurements of pressure, temperature and matrix composition dependent molecular spectra. Hence, the CF can used to derive line parameters for the entire pressure-temperature combination scale relevant to tropospheric and stratospheric studies. Installation and validation procedures allowed the investigation of:

- Pressure-independent transmission of the gas absorption cells
- Reproducible filling and preparation
- Reproducible mounting
- Well-defined traceable path lengths.

Traceable optical path length calibrations in specialized absorption cells with respect to metrological length standards have been developed and performed by PTB and DFM in a joint effort.

Continuous, automated pressure and temperature monitoring was developed and installed to all gas absorption cells. The gas pressure and temperature sensors were calibrated traceable to the SI.

One example of the gas cells used in the CF is a custom-made 20-cm-single pass cell, consisting of a massive copper cell body. An active fluid heat exchange structure inside the cell walls generated a spatially homogenous gas temperature inside the cell. Cell windows were designed as follows: 5 mm thick sapphire disks, 50 mm in diameter, 6 mrad wedge angle. The excellent thermal conductivity of sapphire prevented temperature gradients across the windows and assured homogenous temperature distributions along the entire gas column in the absorption cell.

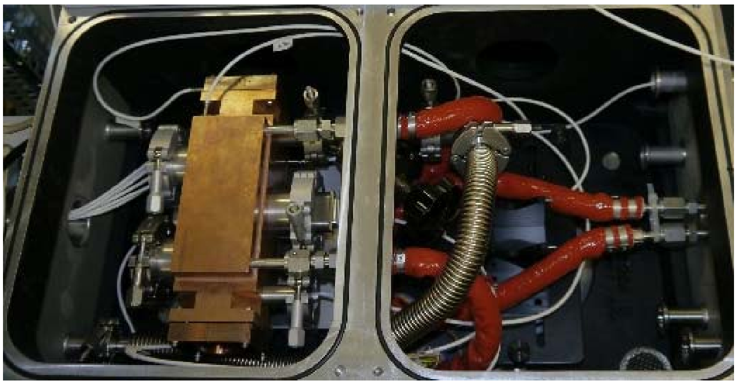


Fig. 2: Temperature-stabilized, 20-cm-single pass cell installed in the CF for measurements at gas sample temperatures from 300 K down to 220 K.

Traceable target gas temperature measurements were realized using six precision class 1/10 B (referring to European standard EN 60751) platinum resistant thermometers of the PT-100 type distributed across the cell. Five of them were inserted into different points of the cell body (referred to as cell sensors) and one PT100 was fed through a flange inside the gas sample to measure the gas temperature directly (referred to as the gas sensor). The accuracy of the gas sensor was verified in a comparison to a PTB PT100 thermometer, which was calibrated for SI-traceable measurements. Temperature regulation of the cell was realized using a high-stability fluid cryostat with a temperature fluid stability of 0.01 K (inside the cryostat). For example, with ethanol as heat-exchange medium a temperature regulation range of 220-300 K was achieved. LNE has brought its support to temperature sensor calibrations for the CF.

For pressure measurements, a set of high-accuracy capacitance diaphragm gauges (full scale of 1000 Torr / 100 Torr / 10 Torr and 1 Torr) were connected to the gas manifold, next to the sample compartment of the spectrometer. The sensors are regularly traced back to PTB's national primary pressure standards. During the measurements the gas sample pressure and temperature were continuously recorded.

The CF is operated and controlled by means of a dedicated combination of the manufacturer's operating system matched to the desired measurement procedures, an own proprietary control software for gas pressure and temperature measurement data and finally a raw spectra and data storage and transfer protocol developed at PTB.

For line data retrieval processing multiple tools were developed in order to retrieve various molecular spectral parameters via a non-linear recursive fitting processes, which adapted different line shape models to the measured CF spectra. For fitting entire absorption bands, an open state-of-the-art multi-line multi-spectrum fitting approach has been implemented to the CF processing software. The most relevant line shape profiles, including Voigt and higher order line shape functions can be applied to derive line-shape-dependent spectral parameters. The suite of line shape profile includes the IUPAC reference line shape profile called the Hartmann-Tran profile (HTP), which was implemented via the original numerical codes in cooperation with the French developers (Tran/Hartman).

A subsequent validation of the CF spectrometer has been achieved by comparisons to available literature or certificated dataas well as results of the partner NMIs inside EUMETRISPEC.

Line parameters, including line positions, line strengths, pressure induced line shift and line broadening coefficients, were compared to the HITRAN database entries (as well as other literature data) before initiating measurements. The gas purity has been checked against certificated specs by means of measured broad band spectra. Amount-of-substance fractions were retrieved from the measured spectra.

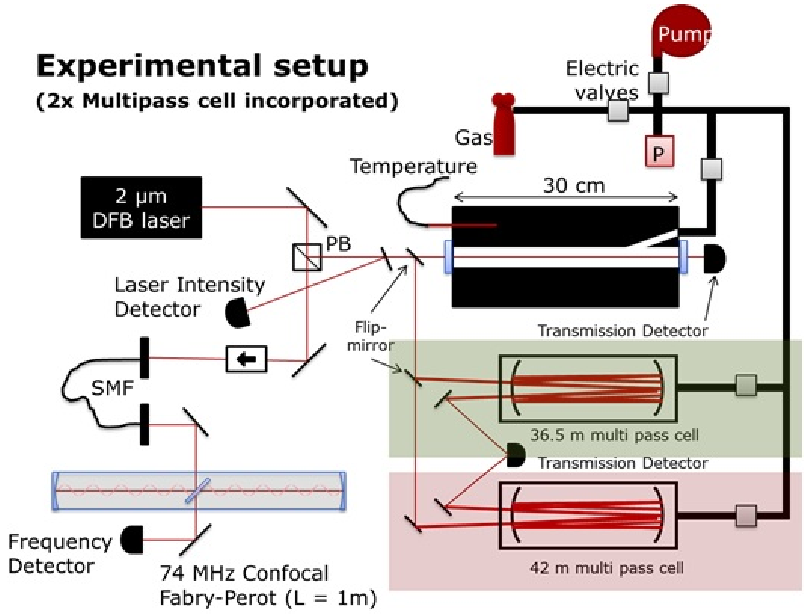


Fig. 3: Satellite spectral Facility (SF) at DFM based on a traceable DFB-TDLAS setup.

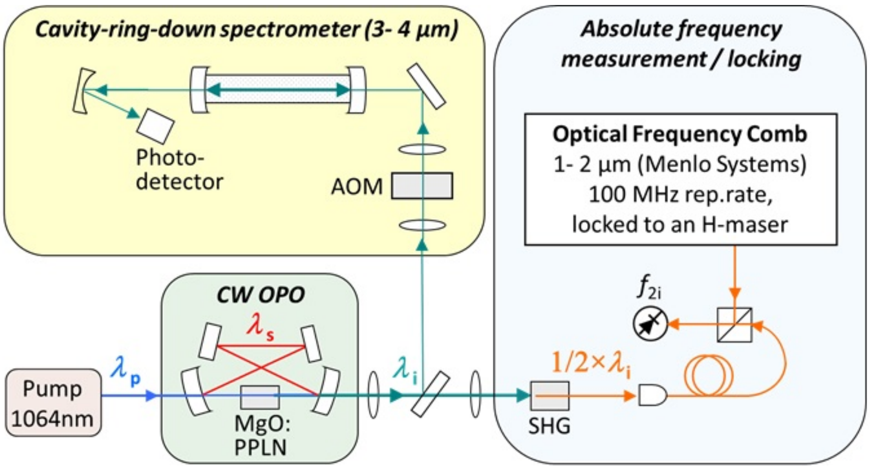


Fig. 4: SF at VTT-MIKES based on a new, very high resolution OPO-CRDS setup.

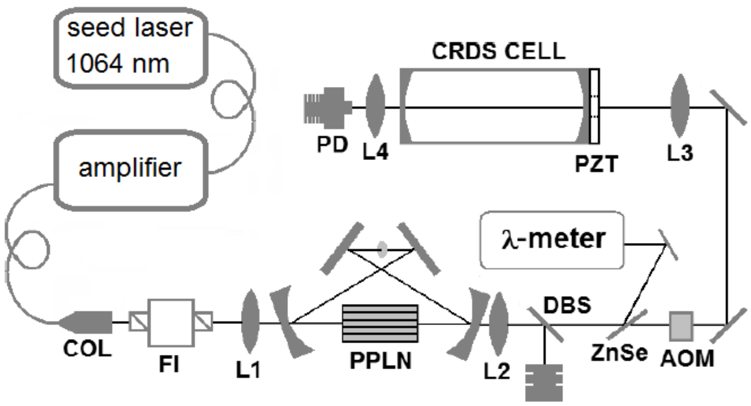


Fig. 5: SF developed at VSL employing a novel CRDS-setup.

According to the basic idea of the project a joint effort was initiated and executed to validate the CF performance by using specific line parameters, i.e. line positions and line strengths in the stakeholder community and in particular at the partner NMIs inside EUMETRISPEC. These measurements were performed in laser-based spectrometers at partner sites by setups as shown in Figures 3, 4 and 5. In addition the project partners SMU and VSL prepared specially designed reference gas standards, e.g. of N_2O or CH_4 in "air" for these validation processes. Here, "air" means gravimetrically prepared N_2/O_2 mixtures, with traceably certified composition prepared by VSL.

The overall performance of the spectroscopic measurements capabilities across all project partners, including the CF, was studied. In order to do so, dedicated gas mixtures were gravimetrically prepared and validated according to ISO 6142 and ISO 6143, respectively, by the project partner SMU, matching the individual measurement range of each project partner's instrumentation. The participants of this final comparison were required to use line parameters from the project (where available) to assign an N_2O amount of substance fraction to the provided gas mixture using their own spectrometers without previous knowledge of its N_2O content. Based on this comparison, the project line parameters were cross validated, in addition to the validation of the CF performance. The CF performance in this comparison is presented in Fig. 6 and was found to be excellent. This confirmed that:

- the CF was successfully validated,
- the established and employed measurement procedures are fit for purpose
- the line strengths parameters for N_2O band are cross-validated.

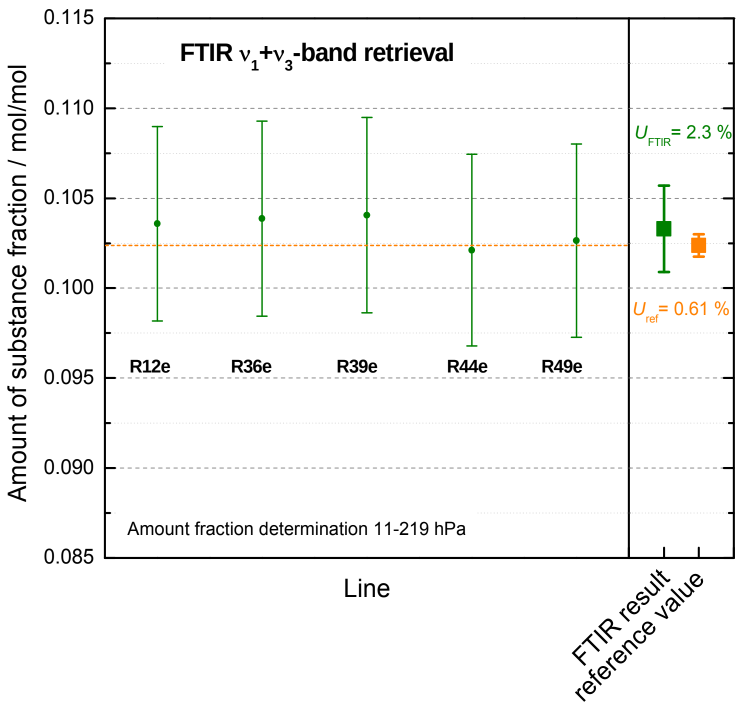


Fig. 6: Typical FTIR-based results of amount fractions from the CF assigned to a gravimetric N_2O in air gas standard. The retrieved N_2O amount of substance fractions based on evaluation of five different absorption lines and the combined value assigned to the unknown gas mixture by PTB are compared to the comparison reference value for FTIR analysis provided by SMU.

Key research outputs and conclusion

A novel, highly versatile, metrological Central spectroscopic Facility (CF) was established, characterised and validated at PTB, including the necessary gas handling hardware, FT-IR control software, as well as metrological measurement and spectral data evaluation software to derive spectral data. The CF is based on an ultra-high resolution, visible to mid-infrared (VIS to MIR FT-IR) Fourier transform spectrometer. Specialized absorption cells and metrological control infrastructure was developed to provide highly stable and accurate measurement conditions, but still allow precise variation of gas pressure and temperature over the relevant atmospheric range. Several Satellite facilities (SFs) were also developed or adapted at partner institutes - France (CNAM and LNE), DFM (Denmark), VTT-MIKES (Finland) and VSL (the Netherlands) - using high-resolution laser-based spectrometers to validate CF results and provide traceability. The SFs at MIKES, DFM and VSL were operational by the end of the project, and those at LNE/CNAM soon after.

3.2 Developing metrological procedures for spectral data determination and data handling

Introduction

In many cases spectral line parameters published in scientific literature have shown a substantial quality spread among different publications. Possible deviations between spectral absorption data from different research groups around the world, in particular in combination with often ill-stated uncertainties significantly hamper atmospheric research. The variation in data quality is due to the broad and diverse set of instrumental setups, as well as multiple measurement and spectral data retrieval methods being used to collect data as well as the various data handling approaches by the involved research groups. Collection of data is generally made without use of standardised methods and without common procedures for establishing data quality, traceability or derivation of standardised measurement uncertainties.

Research undertaken

The project set out to generate project-wide homogeneous measurement procedures finally used for research work with the project's instruments measuring traceable line parameters. Using these procedures the goal was to seek a more homogenous data quality and comparability between the different project partner labs and in particular between the generated results.

These written documents are based on the methods used and techniques developed, adapted or optimized during the project. The documents are written in such a way that they should easily be adaptable to other approaches. During the project and thereafter the documentation was regularly updated based on experiences from practical use in order to ensure their robustness and practicality. The documents include the concept of traceable measurement of spectral data and uncertainty estimation principles. They include the measurement methods of FTIR, TDLAS and CRDS (as implemented by the project partners) for the collection of traceable spectral absorption data, collection of environmental condition parameters including temperature and pressure of gases within spectral absorption cells, purity of test gases, mathematical data analysis techniques for the correction of absorption spectra, including correction for instrumental spectral broadening (instrumental line shape), wavelength non-linearity correction, thermal and pressure correction, calculating the required spectroscopic reference data, including line fitting to establish peak positions, line widths and line areas. Finally, the documents also deals with the estimation of uncertainties from the obtained spectra according to the GUM.

A procedure has been established describing the general boundary conditions and measurement data required to generate traceable molecular line reference data. It includes guidance about generating spectral absorption data, gathering related environmental data (required to establish the uncertainty budget), and an overview of the equations and models that can be used for data correction, data processing, and data retrieval. The requirements for the recording of spectral absorption data (wavelength range, instrumental bandwidth etc.) also have to include information about the spectral instrumentation used. In addition, environmental requirements and boundary conditions of the molecular species under test (temperature, pressure, gas purity and cell parameters) needs to be determined and recorded. The procedure also includes the use of equations and models for spectral data correction, establishing peak positions, line widths and line areas from the spectral absorption data and deriving their dependence on pressure, temperature and the gas matrix, methods for calculating uncertainties.

Procedures for collecting spectra and for the determination of spectral line data at the CF and at the partners' setups (SFs) were generated. Three procedures have been written; a procedure describing the use of the high-resolution FTIR spectrometer; a procedure describing the use of Cavity Ring-Down Spectrometers (CRDS) with various laser sources and one describing continuously Tunable Laser Absorption Spectrometers (TDLAS) with various laser sources. The latter two procedures contain information that describes the specific influences of the individually used laser sources. The procedures are based on the work of the partners on recording spectral absorption data and have been updated during the project. Over the course of the project and thereafter the ultimate, up-date information shifted from the more general documentation (like good practice guides) to the specialized, peer-reviewed publications from within EUMETRISPEC dealing with the most recent development of spectrometer hardware and line parameter retrievals

Inter-comparison protocols for comparing measurements of molecular reference data from the CF and the project partner spectrometers for a few selected molecular species have been produced. Two types of inter-comparisons were performed, one dealing with molecular line data and one with determination of mole fractions via the use of spectral data. Both comparisons were based on metrological gas samples prepared using standard reference techniques by VSL and/or SMU and then circulated amongst the comparison participants. Each satellite facility participated in at least one inter-comparison. The molecular species chosen for the intercomparison were CO_2, CH_4, and N_2O.

Finally, a comparison of mole fractions was conducted with the aim to demonstrate that established molecular line data enables an accurate determination of molecular gas concentrations. The result of this exercise is presented in Fig.7 **Error! Reference source not found.** in terms of relative degrees of equivalence $D = (x_i - x_{crv})/x_{crv}$ for the participants' values x_i with respect to the comparison reference value x_{crv}.

The reported results of VSL and MIKES showed good agreement with the reference value for low concentration nitrous monoxide mixtures. For the high concentration N2O mixtures, PTB is within 1 % in agreement with the reference value, whereas DFM's result did not agree with the reference value and needed further revisions. By means of this finding, an initial bias caused by DFM's data acquisition approach could be identified and later on overcome, now producing the results shown in Fig 7 which demonstrate an agreement within 3 % between the project partners.

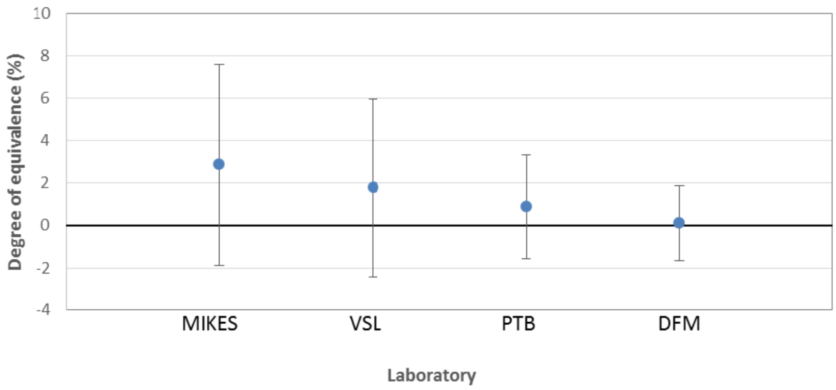


Fig. 7: Results of the EUMETRISPEC intercomparison on N_2O amount fraction measurements using CF and SF.

Based on comparison results like in Fig. 6 and **Error! Reference source not found.**7, the project succeeded to anchor and validate the FTIR-based central facility by means of different, independent laser-based instruments. This also nicely demonstrated the usefulness of spectral intercomparisons to cross validate general lab performances, as well as the applicability and accuracy of the measurement procedures and the retrieval codes.

Key research outputs and conclusion

Standardised procedures are needed to generate high-quality data, and to ensure that data from different sources/techniques can be analysed and compared within defined uncertainties. Data evaluation and analysis procedures were successfully developed for spectroscopic measurements at the CF and the SFs. Technical procedures on general requirements for line parameter measurements were developed, agreed and adopted by each partner institute. Specific procedures were defined and documented to enhance the comparability of data from the most common spectroscopic techniques. For this, the consortium developed and optimised the procedures and documentation through practical use during the work carried out in objectives 1 and 3. The most recent procedures, which are molecule-specific and spectrometer technique specific, were disseminated via publications on the spectral data derived from the CF and the SFs.

3.3 Samples generation of metrological line data and related uncertainties for key greenhouse gases

Introduction

To demonstrate the applicability of the developed hardware and the developed procedures to substantially reduce (in the future) the lack of traceable spectral line parameters, the EUMETRISPEC project set out to employ the developed instruments and spectroscopy infrastructure in combination with the measurement procedures.

For key greenhouse gases in selected spectral regions spectral line parameters were measured to realize first example-type sets of traceable spectral line data using the new metrological hardware (CF and SFs) and the procedures developed within this project. For the generation of line data within the project, data quality objectives (DQOs) had been set and updated right from the initial phase of the project up to the very end of the project in view of 1) available data in literature, 2) documented requirements from stakeholders, 3) established project contacts to stakeholder groups, and 4) finally technical realities at project partner's instrumentation. Intensified stakeholder contacts, however, revealed that the new metrology approach for line parameter retrievals realized in this project and the targeted traceability and thus improved comparability of spectral line parameters derived from this project attracted a very interested reception at the stakeholder side. A high demand for traceable line parameters with improved comparability was expressed at various occasions, e.g. at the two well-visited stakeholder workshops organized by EUMETRISPEC.

High resolution spectra and spectral parameters were measured for the following analytes, which are all key species for the understanding of atmospheric processes and therefore relevant for atmospheric monitoring:

- Carbon dioxide, CO_2,
- Nitrous oxide, N_2O,
- Methane, CH_4, and
- Water, H_2O as well as
- Carbon monoxide, CO, and Hydrogen Chloride, HCl

Research undertaken

With the instrumentation developed for objective 1, the CF at PTB and the SFs at the partner sites have measured spectra targeting the following line parameters:

- the line position $\tilde{\nu}_0$,
- the line strength S_0 at T_0 = 296 K and its temperature dependence,
- the pressure (air) induced line shifts δ_{self}, δ_{air},
- the pressure broadening coefficients γ_{self} and γ_{air} at 296 K, and
- the temperature exponent of pressure broadening n_{air}.

A typical spectrum measured at the CF is shown in Fig 7b **Error! Reference source not found.**. Whereas the CF tackled most of the parameters and combined it to molecule specific line data sets on multiple lines, the SFs were typically concentrating on very high resolution measurements of a specific line parameter for low number of individual lines. Obviously this is related to the limited spectral coverage of most laser-based SF spectrometers.

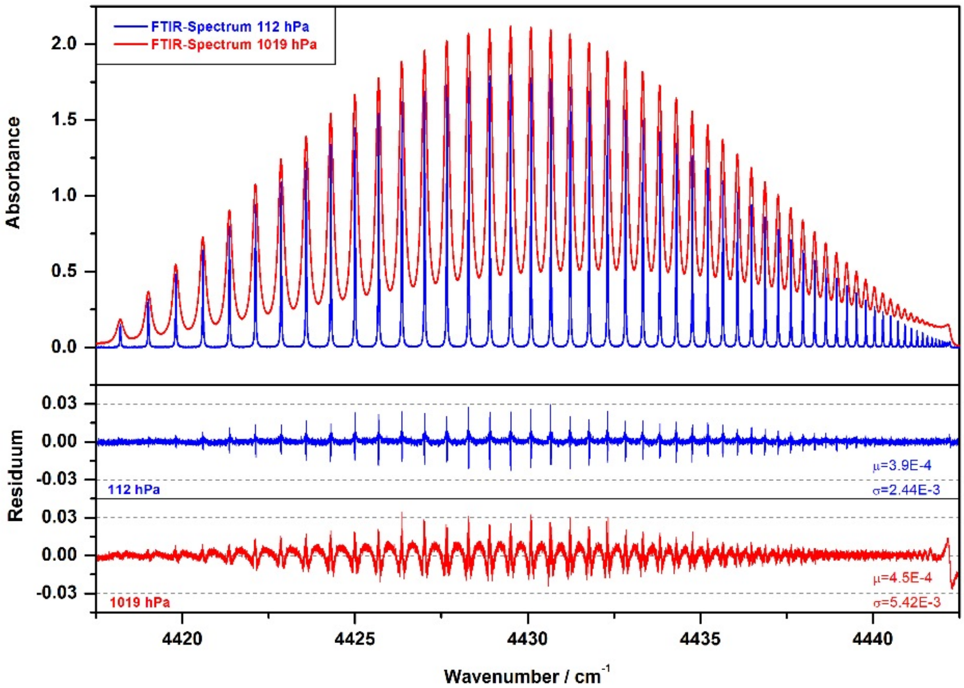


Fig. 7b: Measured Fourier-Transform spectra of N_2O in the 2.26 µm wavelength range. Shown are spectra for N_2O pressures of 112 mbar and 1019 mbar, respectively. The bottom panels show the residuals between the measured data points and respective points of a multi-line Voigt profile fitted to the experimental data.

Examples on parameter-specific data from different partners are shown in Fig. 8, Fig. 9, Fig. 10, and Fig. 11.

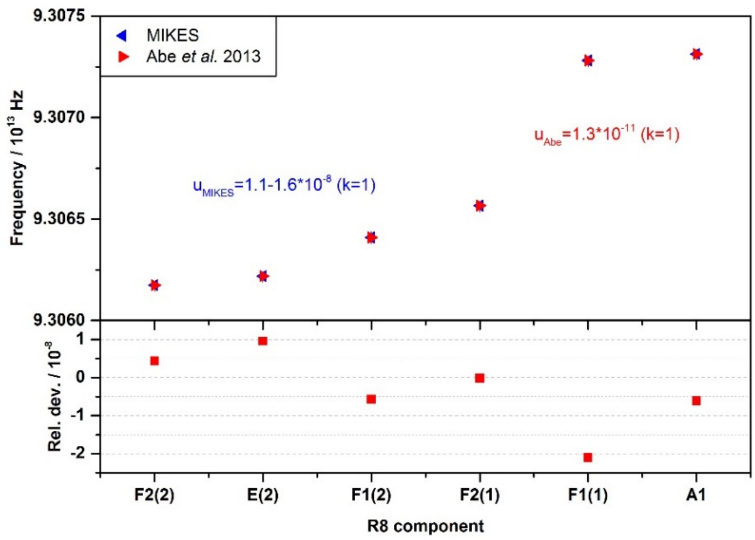


Fig. 8: Typical traceable line position measurements for CH_4 (R8 multiplett at 3.2 µm) from VTT-MIKES compared to literature data (for full details see the relevant publications).

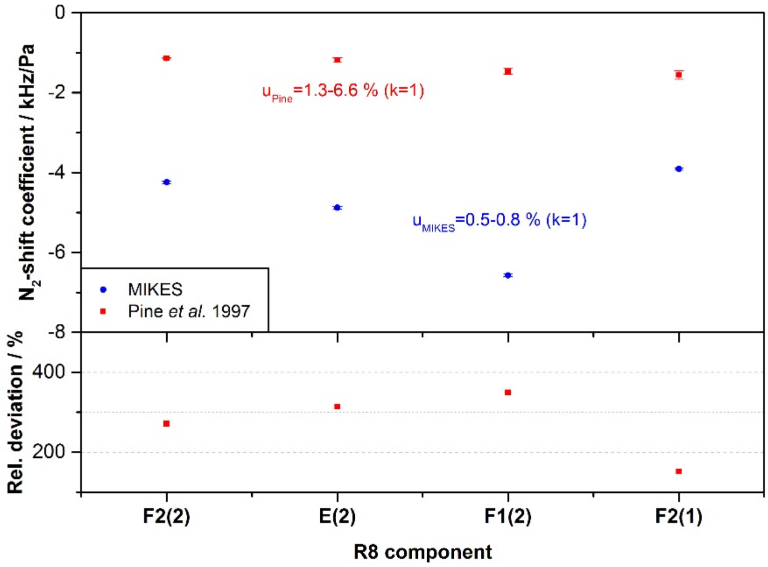


Fig. 9: Exemplary pressure induced line shifts for CH_4 (R8 multiplett at 3.2 μm) in N_2 realized by VTT-MIKES and compared to literature data (for full details see the relevant publications). As in some other EUMETRISPEC measurements large systematic deviations with respect to previous literature was found.

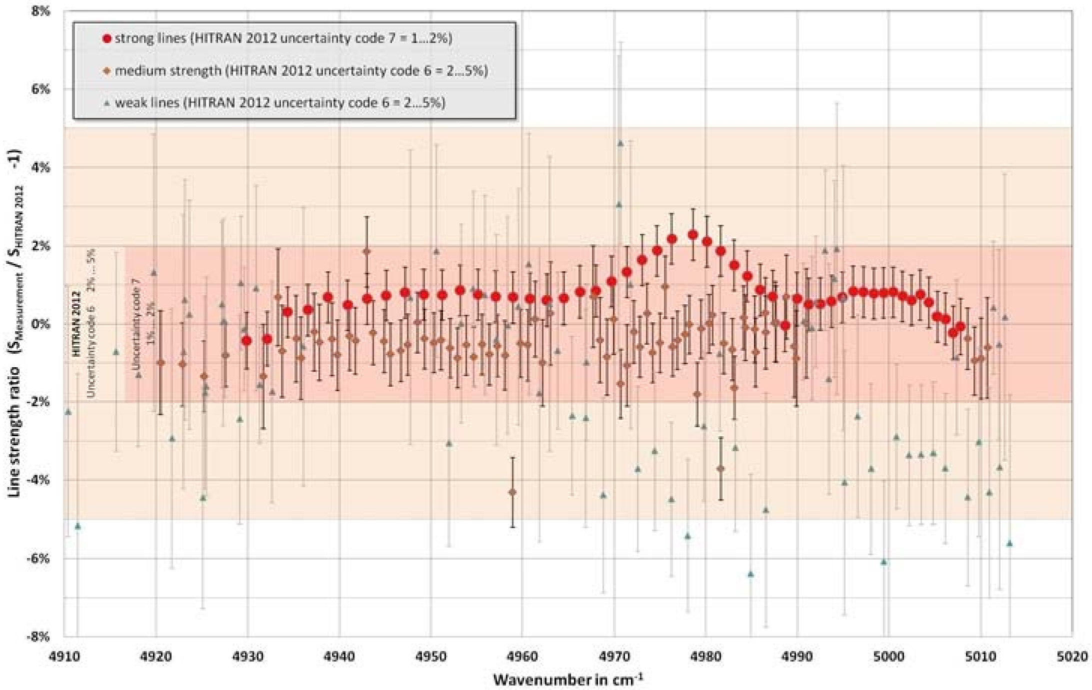


Fig. 10: Retrieved line strengths of CO_2 in the 2 μm wavelength range measured at the CF at PTB compared to existing data base entries in HITRAN2012.

The project generated spectral parameter-specific data sets across most of the targeted analytes. Tables 1 to 3 summarize targeted spectral parameters and for which analyte they were inferred. Compilations on line parameter-specific data reductions have been generated that were summarizing the results from partners with laser-based instrumentation.

For the targeted molecular species listed above, data sets have been created which combine the results on different line parameters. All but one analyte-line parameter combinations were provided by more than one research group and by both, laser and FTIR-based measurements..

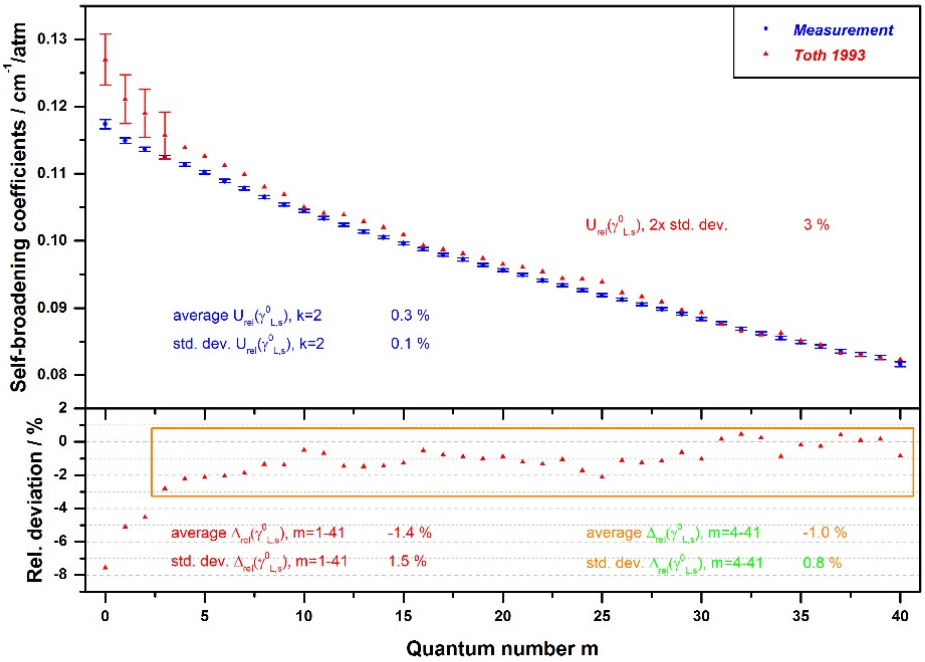


Fig. 11: First, high resolution measurements of N_2O self-broadening coefficients retrieved from PTB-FTIR measurements at the CF compared to interpolated literature data by Toth et al. (for full details see the relevant publications).

Measurements on H_2O were provided by PTB on the basis of raw spectra and a first processed data set by means of TDLAS.

Tables 1 to 3 list the molecules, spectral ranges, spectral parameters and physico-chemical parameter ranges covered in this project. The measured spectra, experimental boundary conditions, spectral data and other results were integrated in the available data structure of the project and will be further evaluated over the end of the research funding period if new background data e.g. like line shape models or retrieval algorithms become available.

Table 1: Data sets on nitrous oxide (N_2O).

Institution	Molecule	Spectral band	Wavenumber range /cm^{-1}	Lines	Matrix gas	S/N ratio	Temperature range / K	Pressure range / hPa	Target parameters
PTB	N_2O	$\nu_1+\nu_3$	3250 - 3550	5	SMU N_2O-air mixture	> 1000	296	10 - 200	Amount fraction comparison
MIKES	N_2O	$\nu_1+\nu_3$	3500	~ 10	Air	Dep. on mix. ratio	296	1 - 100	ν_0, δ_{air}
VSL	N_2O	$\nu_1+\nu_3$	3506 - 3508	4	N_2 + Air	100	296	35 - 1000	S
PTB	N_2O	$2\nu_3$, ν_3	4350 - 4445	~ 40	Pure N_2O + Air	50-2000	216-296	100 - 1300	ν_0, S, δ_{self}, δ_{air}, γ_{self}, γ_{air}, n_{self}, n_{air}
DFM	N_2O	$3\nu_3$	6563	P18e	Air	> 1000	296	5 - 120	S, γ_{self}

Table 2: Data sets on methane (CH_4).

Institution	Molecule	Spectral band	Wavenumber range /cm^{-1}	Lines currently analyzed	Matrix gas	S/N ratio	Temperature range / K	Pressure range / hPa	Target parameters
PTB	$^{12}CH_4$	Tetradecad	2000 - 10000	6	Pure CH_4 + Air	10 - 200	219 - 307	20 - 1300	γ_{self}, γ_{air}
VSL	$^{12}CH4$	ν_3	2945 - 2948	~10	N_2 + Air	1000	296	50 - 100	S
CNAM-LNE	$^{12}CH4$	ν_3	2947 - 2949	4	Pure CH_4	200	296	< 150	ν_0
VSL	$^{12}CH4$	ν_3	3008 - 3010	~10	N_2 + Air	200	296	20 - 1000	S
CNAM-LNE	$^{12}CH4$	ν_3	3009 - 3039	3	Pure CH_4 + N_2	150	296	< 0.75 - 570	S, δ_{N2}, γ_{N2}
MIKES	$^{12}CH4$	ν_3	3095 - 3105	12	N_2	Dep. on mix. ratio	296	1 - 100	ν_0, δ_{N2}
VSL	$^{12}CH4$	ν_3	3479 - 3482	~10	N_2	200	296	100 - 1000	S
PTB	$^{12}CH_4$	Octad	4560 - 4700	10	Pure CH_4	50 - 2000	296	30 - 1300	S, δ_{self}, γ_{self}, n_{self}
RU	$^{13}CH_4$	$2\nu_3$	5998 - 6009	2	Air		296	20 - 100	S
RU	$^{12}CH_4$	$2\nu_2 + \nu_3$	6009 - 6046	10	Air		296	20 - 100	S

Table 3: Data sets on carbon dioxide (CO_2), carbon monoxide (CO) as well as hydrogen chloride (HCl) and water vapor (H_2O).

Institution	Molecule	Spectral band	Wavenumber range /cm^{-1}	Lines	Matrix gas	S/N ratio	Temperature range / K	Pressure range / hPa	Target parameters
PTB	CO_2	$\nu_1 + 2\nu_2 + \nu_3$	4700 - 5200	> 100	Pure CO_2 + Air	> 1000	210 - 303	1-1300	ν_0, S, δ_{self}, δ_{air}, γ_{self}, γ_{air}, n_{self}, n_{air}
DFM	CO_2	$\nu_1 + 2\nu_2 + \nu_3$	4984 - 4992	8	Pure CO_2 + Air	> 500	296	5 - 150	S, γ_{self}
PTB	CO	2-0	4050 - 4345	> 100	Pure CO + Air	10 - 2000	210 - 296	5-1000	ν_0, S, δ_{self}, δ_{air}, γ_{self}, γ_{air}, n_{self}, n_{air}
PTB	HCl	2-0	5400-5850	21	Pure HCl	200	296	50-1100	S, δ_{self}, γ_{self}
PTB	H_2O	n.n.	3800-9000	> 100	Pure H_2O	n.n.	296	20	S, γ_{self}

Due to the large number of line parameters, molecules, and physical parameter ranges studied in the project, we refer to the publications at the end of this report for a more detailed view of the data generated. For the sake of clarity and conciseness of this report we thus do not further elaborate on the full detail of the data quality achieved or detail it on the level of uncertainty assessments for each of the analytes and for each of the boundary conditions studied. Uncertainty data like this have to be analyzed in case studies as the “final” accuracy depends very sensitively on the boundary conditions chosen for the measurements but also on the quantum number of the transition studied. Thus, we refrain to the exemplary data as shown above. More detailed case studies are delivered within the EUMETRISPEC project reports and in particular with the suite of scientific papers following this project in order make the complete data set for all molecules studied available to the science community.

Where ever possible cross references among project partners have been made, to validate the CF but also to compare the retrieved line parameters. For example, Fig. 12, and 13 show line strengths of CO_2 comparing DFM and PTB results and of CH_4 comparing VSL, CNAM-LNE and PTB results.

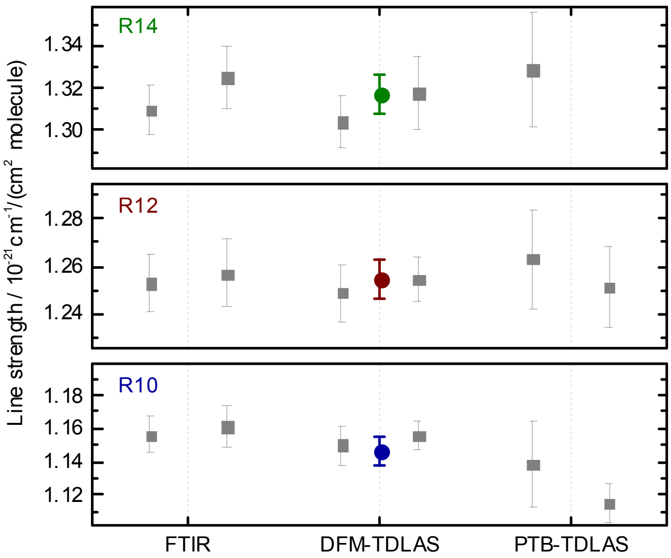


Fig. 12: Comparison of CO_2 line strengths in the $\nu_1+2\nu_2+\nu_3$ combination band at 2 µm. Results of the R10, R12, and R14 lines from measurements at DFM by TDLAS and PTB by TDLAS and the CF (FTIR) in grey. The coloured data are the combined results from this study.

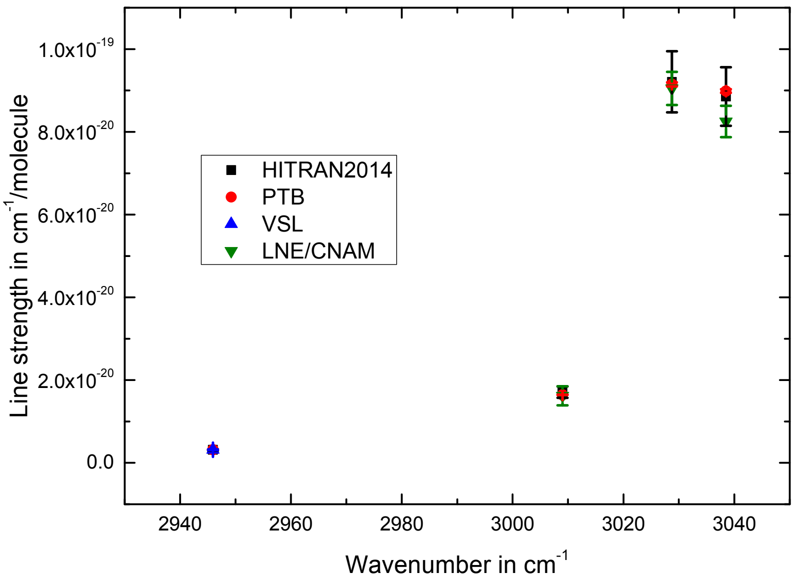


Fig. 13: Comparison of CH_4 line strengths measured by PTB (CF), VSL, and CNAM-LNE. Project partner results agree with each other. HITRAN data are also shown and in agreement with EUMETRISPEC data.

From such comparisons within the project an increased confidence level on the experimental results was achieved, i.e. for anchoring the CF by means of the other laser-based partner instruments.

One exemplary molecule-specific data set derived from the CF is a new, complete, high-accuracy line data set comprising all spectral N_2O parameters needed for atmospheric remote sensing e.g. in the TCCON network. The N2O data set for TCCON comprises line strength (Fig. 15), line broadening (Fig. 11, Fig. 17), line shift (Fig. 16), and vacuum line positions (Fig. 14)). This novel data set is uniquely coherent as it completely originates for the first time from a single spectroscopic setup and a single set of metrologically defined data evaluation and retrieval procedures. The entire data set was submitted to HITRAN, GEISA and TCCON directly and is currently under evaluation for the resulting improvements.

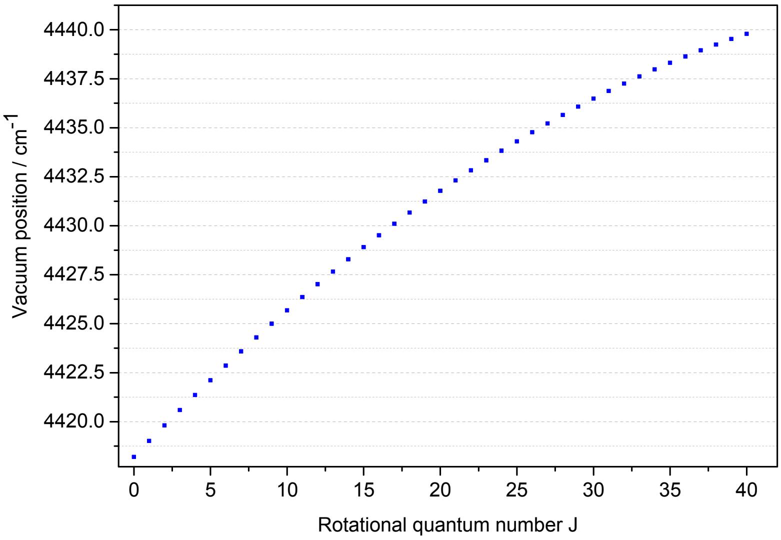


Fig. 14: Line positions in the R-branch of the $2\nu_3$ band of N_2O at 2.26 µm as measured by the CF.

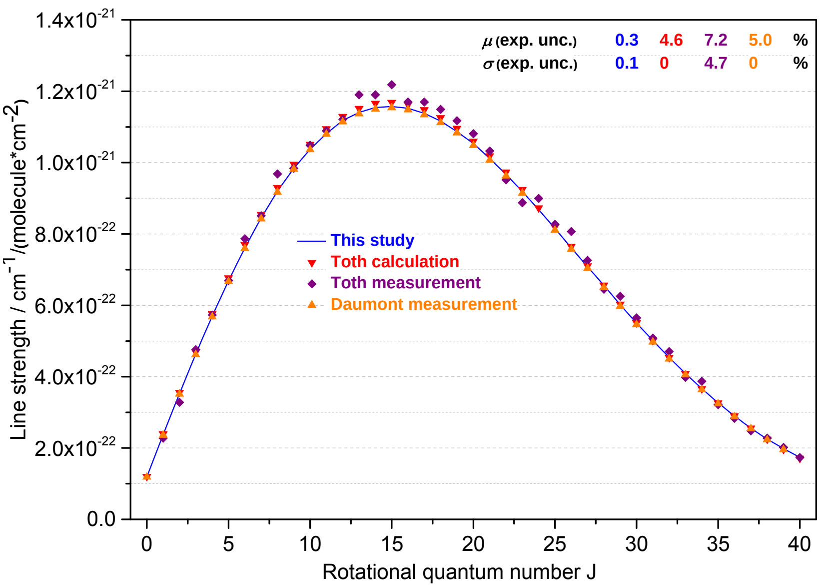


Fig. 15: Line strengths of N_2O in the R-branch of the $2\nu_3$ band at 2.26 µm as measured by the CF compared to literature data, R. A. Toth, "Linelist of N2O parameters from 500 to 7500 cm-1," http://mark4sun.jpl.nasa.gov/n2o.html as down triangles, R. A. Toth, Journal of Molecular Spectroscopy **197**, 158–187 (1999) as diamonds, L. Daumont et al., Journal of Molecular Spectroscopy 208, 281–291 (2001) as up-triangles.

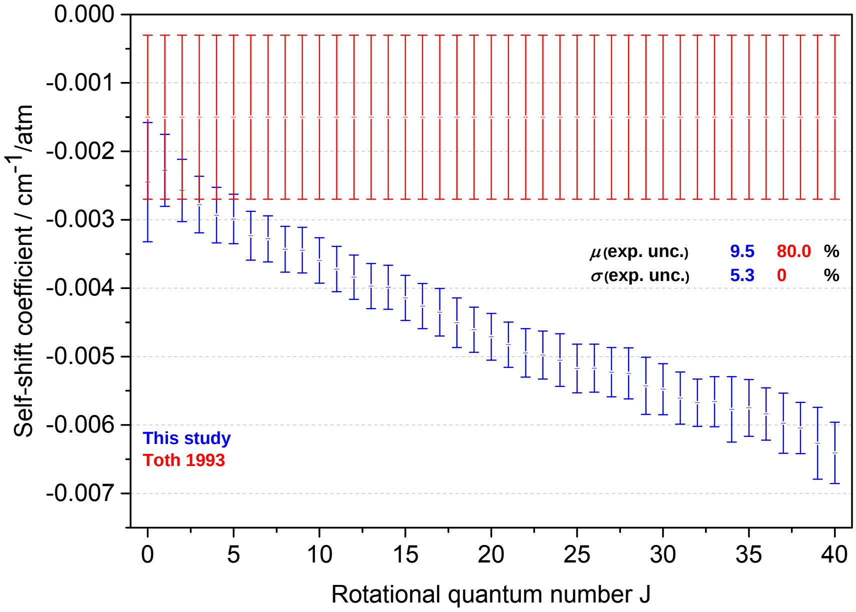


Fig. 16: Self-shift coefficients of N_2O in the R-branch of the $2\nu_3$ band at 2.26 µm as measured by the CF compared to literature data from R. A. Toth, Appl. Opt. 32, 7326-7365, 1993.

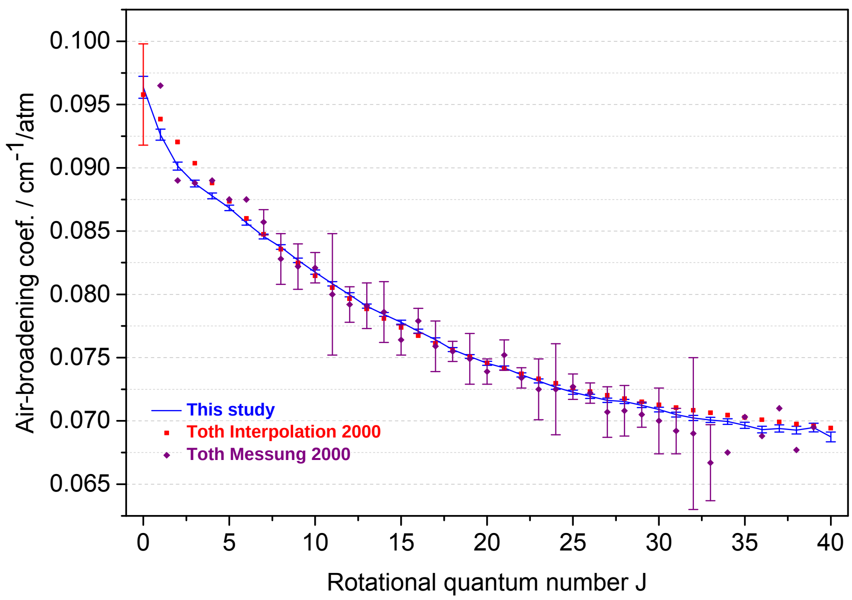


Fig. 17: Air broadening coefficients for N_2O lines in the R-branch of the $2\nu_3$ band at 2.26 µm as measured by the CF compared to literature data, R. A. Toth, Journal of Quantitative Spectroscopy and Radiative Transfer 66 (2000) 285-304.

Figures shown here on N_2O from the CF are example data, based on measured spectra using different experimental configuration of the CF FTIR spectrometer. It is beyond the scope of this report to go into the full details, as these are discussed extensively in the relevant peer-reviewed papers. The spectra have been processed to yield the different line parameters. Respective results have been compared to literature information and to HTRAN. Those studies have been detailed in papers submitted to peer reviewed journals, they were also discussed and in if relevant shared with specific key persons of the atmospheric monitoring community by personal communication (e.g. Geoff toon from the TCCON network. They mostly agree with the large, often ill-posed uncertainty ranges of the existing literature data, e.g. present in HITRAN. All EUMETRISPEC data sets significantly, in some cases drastically improve the accuracy of the spectral data.

Improvements of up to 1-2 orders of magnitude could be realized in some cases. For the case e.g. of pressure induced line shifts and self-broadening of N2O the new data revealed some distinct systematic differences to existing data. Generally the data quality in terms of uncertainties and traceability statements for this studied N_2O branch is significantly improved by EUMETRISPEC.

Key research outputs and conclusion

Large sets of pressure-dependent spectra were recorded at the CF and SFs for greenhouse gases (incl. N_2O, CO_2, CO, CH_4). Spectra of HCl, the TCCON reference molecule, have been processed at the CF based on developed retrieval strategies. Novel, highly stable absorption cells specifically designed for the CF also enabled the recording of gas spectra over a pressure/temperature range of -70°C to 70°C / 0.01 to 1200 mbar, which allowed to study the effects of variable atmospheric temperature and pressure on the gas spectra. The data were generated using the CF and SFs created in objective 1, and in accordance with the measurement and traceability protocols developed in objective 2. Metrological line data, including line strength, pressure broadening, pressure line position shifts as well as absolute positions were derived from the measured spectra. Due to the vast amount of spectra and the need for multiple evaluation cycles with different evaluation approaches but also with different line shape models, the evaluation of the measured spectra will be ongoing far beyond the project duration. This situation offers interesting possibilities to include the stakeholder communities in the data retrieval and to derive from this valuable comparison data to further evaluate the comparability of the different retrieval approaches. One exemplary data set derived from the CF is a new, complete, high-accuracy line data set comprising all spectral N_2O parameters needed for atmospheric remote sensing (strength, broadening, shift, and positions). This set is uniquely coherent as it originates for the first time entirely from a single spectroscopic setup. It includes the first high-resolution, self-broadening measurements for N_2O (previously this data was based on interpolation not measurement). The new N_2O-results are for large fraction of spectral parameters and lines in good agreement within the large uncertainties in the HITRAN database. But, those data are now available with up to 80x improved uncertainties. Strong systematic deviations were found for certain regions of the N_2O band particular for pressure induced line shifts and self-broadening of low J lines. The project also generated a set of new or improved accuracy HCl self-broadening, self-shift and line strength data. HCL is used for cross referencing of TCCON/NDACC instruments and for remote sensing purposes. The new HCL data set thus helps to significantly improve the internal quality control of the TCCON network via the HCL reference cells. Further data sets on spectral line positions and data retrievals were also achieved for CH_4 and N_2O at MIKES and CNAM/LNE, for CO_2 at DFM and H2O at PTB using laser-based instruments. Results were broadly disseminated accompanied by meta-data, traceability statements, and measures of uncertainty. Data sets have been submitted to the HITRAN and GEISA databases – online, open-access databases of atmospheric spectral data – as well as to important focus points of the atmospheric and the spectral sciences communities, and to peer reviewed journals. Social networks like *Linkedin* were used to trigger the communities for cooperation.

The idea of EUMETRISPEC was based on the following pillars, namely to come up with

1. harmonized formalisms to define the line data and their uncertainties
2. standardized and harmonized data processing approaches,
3. transparent and harmonized uncertainty assessments according to the GUM and by
4. aiming at traceability for the retrieved line parameters

throughout the whole project and with the aim to continue as metrology institutes in the same direction beyond the project duration. This holds in particular for the FTIR-CF where this has been achieved in most cases.

At present, almost all instruments used for remote sensing purposes use existing non-metrological line parameters from managed line collections like HITRAN or GEISA. These comprise paramount information on millions of lines for many different molecular species.

It is worthwhile to mention here explicitly that, it was not the intention of the EUMETRISPEC project to either compete or replace large fractions of any existing database like HITRAN or GEISA, or to deliver huge amounts of line data within a 3-year project duration. Instead, right from the beginning the EUMETRISPEC project aimed to deliver a profound impact on which requirements the spectroscopic hardware has to fulfill to deliver traceable line data, and *how* line data can be gathered in a metrological perspective by laboratory spectroscopy including data reduction and uncertainty assessment. Here, the EUMETRISPEC project aimed to establish the respective hardware, procedural and measurement infrastructure at the NMI level. To achieve the full impact of the metrological approach to line data retrieval it is important to generate open access to the metrological infrastructure for spectral line data retrieval, which is achieved by running the CF FTIR on a long-term basis as an open infrastructure which invites and allows community groups to participate. In addition, to significantly improve the amount of traceable line data available, it is desirable to develop a managed multi-instrument hardware infrastructure consisting e.g of a larger number of CF-copies across Europe to ensure the required throughput and to spread the metrological spectroscopy know-how ideveloped at the NMIs to as many community institution as possible. By setting up the CF, and by ensuring a long-term availability, EUMETRISPEC has set a first cornerstone to achieve this.

EUMETRISPEC was only possible in a collaborative approach of all partners involved. This is in particularly based on the need to combine expertise on gas metrology and gas spectroscopy, the need to combine different spectroscopic techniques and thereby validating each other, and the need to harmonize measurement approaches and procedures. No partner would have been able to cover all aspects of gas metrology, gas spectroscopy and metrological traceability of input quantities by himself. The project generated a large added value as compared to the sum of individual efforts as the collaboration formed a spectroscopic metrology community and infrastructure among partners. This has been exploited already for addressing further needs in subsequent projects and for the commitment of partners to continue the work of EUMETRISPEC on traceable line parameters.

To summarize, the EUMETRISPEC project concluded with the following results:

- lab spectroscopy infrastructure for measurements of traceable line parameters in the wavelength range from 0.8 µm to 10 µm
  - High resolution Fourier-transform infrared spectrometer based measurement system
  - path lengths 0.2 m up to 42 m
  - gas pressures from 10^{-5} to 1400 mbar
  - gas temperatures from room temperature down to 200 K
- measurement procedures for traceable line parameters using the developed spectroscopic infrastructure
- line parameter results on key atmospheric molecules as there are N_2O, CO_2, CO, CH_4, H_2O and HCl at different spectral regions

4 Actual and potential impact

To promote the uptake of the project's results, outputs were shared broadly with end-user communities, including spectral data community, climate and environmental researchers, industrial process control communities, and international standards organisations. In 2012 a stakeholder workshop in Germany brought the environmental monitoring, spectral data and metrology community together to explain measurement science perspectives and to describe the aims of the project. The workshop was attended by representatives from 31 institutions from 12 different nations. A second stakeholder workshop was then held in 2014 to update the community on the project's results. The 53 participants represented 28 institutions from 12 countries in Europe, Russia and the US, ensuring a broad awareness and uptake of results by the stakeholder communi-ty. A more immediate and wide spread dissemination was realized via publication in peer reviewed journals like JQSRT, J Mol Spec, Appl. Opt. or by active participation in conferences. 17 papers were published in international journals (listed in the next section), and a large number of presentations were given at confer-ences and workshops. Web based activities further enhanced the dissemination via a dedicated project website and by active distribution via ResearchGate, LinkedIn, or GoogleScholar. Individual high impact members were also directly contacted, to ensure immediate use and evaluation of the project spectral data (e.g. members of TCCON data evaluation group, and other members of the spectral sciences community).

To further enhance the dissemination of the results it is planned to also offer metrological raw spectra from the CF incl. meta data to allow comparisons of data evaluation procedures from the different communities, to further develop and support comparability between communities and to foster cooperation with the spec-tral data community by coordinated data retrievals.

Crucially, the project's data have been submitted to the global HITRAN and GEISA databases – the most widely used open-access spectral databases – to allow a wide range of users to access the project's re-sults. A sub data set has been passed-on, for example, to the Total Carbon Column Observing Network (TCCON), a global network of 23 ground-based spectrometers that monitor atmospheric greenhouse gas-ses: TCCON is a key user of the HITRAN database, and is currently testing the new spectral data set. The project's contribution of highly accurate and traceable spectral data will reduce TCCON's reliance on the practice of side-by-side validation and calibration, which is difficult to achieve and expensive to perform. This high-quality reference data provided to TCCON will enhance the data the network provides to its users, such as climate modellers. Other users of the project's reference data include the Atomic, Molecular, Optical and Positron Physics group at the University College London, UCL, UK, or the combustions diagnostics group (RSM) at the Technical University of Darmstadt, TUDa, Germany. UCL is currently modelling spectral lines for environmental, climate and planetary research and uses the project's spectral results as an inde-pendent and experimental corroboration of their theoretical quantum-chemical models, providing validation and weight to their own and related environmental and climate research. TUDa, on the other hand is using e.g. the HCl and H2O data set, to further develop absolute laser spectrometric in-situ analysers to better monitor e.g. pollutant formation or temperature in oxyfuel coal combustion in a large integrated research cluster called SFB129.

The project will enable users of spectral reference data to derive increasingly accurate and traceable spec-troscopic results, with higher-resolution modelling. Reducing uncertainties in environmental and climate anal-yses, as well as in industrial spectrometric applications, will aid effective monitoring and prediction of cli-mate change, allowing European and global governments to mitigate and adapt. Furthermore, industrial process monitoring will also be advanced by the development of absolute species monitors using high accuracy spectral data. Finally, metrological quality spectral data will also serve metrological key services like the development and dissemination of gas standards. High accuracy spectral data are a prerequisite to foster the development of spectroscopy-based optical gas standards, which serve as absolute analytical transfer standards in cases where high adsorptivity or reactivity of the target gas, prohibits or hinders the development of classical reference gas mixtures due to a lack of chemical stability.

4.1 Metrology achievements

From the metrology point of view the project marked a new set point for the field of *spectroscopic gas analysis*. It refined the European NMI capabilities and views on the possibility to enable spectroscopy to derive traceable results in terms of substance fraction measurements relying on line parameter-based spectra processing. Line parameters measured in the project will strongly benefit the future development of optical transfer standards for gases based on infrared spectrometry.

Additionally, this project opened a possibility to define a new kind of NMI service to customers ranging from remote sensing environmental sciences to industrial stakeholder developing or applying spectroscopy-based process diagnostics. It provided them with accurate, comparable and traceable molecular line parameters for specific applications.

All partner NMIs became part of this new idea which complements existing gas metrology based on CRM-based gas mixture standards, with the fundamental science for a new absolute spectros-analytical approach which relies on traceable molecular line parameters. This opens a new field of service to the metrology community.

The project developed new long-term measurement facilities to the metrology community, including the central facility FTIR spectroscopy located at PTB

The project focused on standardization of procedures which will positively affect:

- future research and service at national metrology institute level
- standardization in industrial or air quality applications supported by metrological principles.

The delivered technical protocols and the refined procedures documented in the peer-reviewed publications are available for use in future metrology projects.

Spectroscopy is already one of the most important tools for environmental monitoring using airborne or ground-based instruments and in particular for remote sensing using space-based sensors on satellites. The metrology community has an impact on this field of application not only by means of the reference materials provision, i.e. gas mixture standards, but also by means of traceable line parameters based on the results of this project. These results will benefit analytical methods based on techniques like TDLAS or CRDS which depend on the availability of traceable spectral line parameters and spectroscopic retrieval principles.

4.2 Dissemination activities

4.2.1 Scientific presentations and publications

A large number of scientific presentations (both oral and poster) were held at a broad range of scientific meetings including the biannual HITRAN and GEISA meetings, numerous molecular spectroscopy conferences such as *HRMS* and applied spectroscopy meetings like *FLAIR*. All stakeholder communities relevant to UEMETRISPEC were thus closely and timely informed about the project status, the recent output and the potential cooperation options. Scientific results as well as project strategies were further published in both renowned peer-reviewed scientific journals as well as popular/trade journals. An overview of the large number of presentations and publications can be found in section 6.

4.2.1 Project presentations and stakeholder engagement on conferences and standardization meetings

The project was presented in several standardization meetings and also distributed via press releases. Examples of conference presentations include the well-known *SPIE remote sensing* as well as the *CLEO conference*. Two well visited, specialized EUMETRICSPEC workshops were organized by the project-partners, which are the first workshops/conference meetings exclusively devoted to the field of traceable spectral parameters. The stakeholders participated strongly in both workshops. They expressed the need and great interest to maintain the EUMETRISPEC workshop/conference and develop a special biannual conference series for the scientific topic of traceability in spectral diagnostics and spectral data.

A large group of stakeholders were engaged in this project, including:

- Contributors and managers of the two largest spectral databases (GEISA, HITRAN),
- Environmental measurement network representatives, e.g. from the two largest ground-based spectral remote sensing networks (NDACC and TCCON), which are based on FTIR instruments
- university groups on spectro-analytics, molecular spectroscopy and spectral data retrieval
- instrument companies such as Bruker, Los Gatos, ThermoScientific or Picarro
- other NMIs engaged in spectroscopic topics outside the project including NPL and NIST.

The stakeholders provided input and received output from the project on required spectral data, database requirements, information on the experimental set-ups (including reference cells) and the provision of software tools among others. They have also given overview presentations on the state of the art and current strategies at both stakeholder workshops. Agreements were made on future inclusion of line data from the project and subsequent metrology initiatives with links to metrological data quality flags, such as GUM-compatible uncertainties and traceability statements into HITRAN and GEISA. Standardization committees have been updated on the project results as well as on the long-term plans. This included meetings of German mirror committee of the CEN/TC 264/Working Group 18 on FTIR standardization in remote sensing. In addition project results had an impact on the drafting process of a new guideline (“VDI-Richtlinie 4211”) related to remote sensing methods operated by FTIR instrumentation. It will be issued by the KRdL im VDI und DIN, NA 134-04-02-16 UA. Finally, EUMETRISPEC experts provided input to the certification protocol for zero gases (developed within ENV01 MACPoll). This protocol will form the basis of a NWIP for the future ISO 19229 (prepared by ISO/TC 158, *Analysis of gases).*

A list of project presentations on conferences is provided in Sect. 6 (oral and poster presentations)

4.2.3 Workshops

Two successful international, well-visited workshops were organized. These brought together leading experts (Figures 18 and 19) of various fields related to spectral reference data topics including:

- atmospheric spectroscopy

- atmospheric environmental monitoring
- lab spectroscopists for spectral line data
- quantum chemistry groups devoted to the ab initio computation of molecular spectral data.

These workshops took place in 2012 and 2014.The talks and posters of each workshop are published in two books (see Sect. 6, books), but were also made available online

Fig. 18: EUMETRISPEC stakeholder workshop 1 participants. The workshop 'Traceable spectral reference line data for atmospheric monitoring' was held at the 15th of November 2012 in the Palace of Wolfenbuettel, Wolfenbuettel, Germany and at the 16th of November 2012 at PTB, Braunschweig, Germany.

Fig. 19: Photograph of the participants of the 2nd EUMETRISPEC stakeholder workshops held at PTB in Braunschweig, 2014, October 9/10.

The second workshop was held at PTB in Braunschweig, 2014, October 9/10. In total, 53 participants gave 55 presentations (6 invited talks, 13 regular talks and 36 posters). The workshop was accompanied by guided tours through PTB labs including primary standards and spectroscopic facilities set up during the project. Ot this occasion spectroscopy infrastructure and procedures developed in EUMETRISPEC was efficiently disseminated to most relevant representatives of a broad range of stakeholder communities

The second workshop e.g. has seen the following invited talks:

Speed-dependent effects and Dicke narrowing in spectral line shapes
by Roman Ciurylo, Uniwersytet Mikolaja Kopernika
Precision laser spectroscopy of water isotopologues in the near-IR
by Livio Gianfrani, Seconda Università di Napoli
SI-traceable line parameters of greenhouse gases measured using cavity ring-down spectroscopy
by Joseph Hodges, NIST
GEISA-2014 spectroscopic data base: context, contents, quality requirements, evolution
by Nicole Jaquinet, Ecole Polytechnique
Accurate and Precise FT Spectroscopy and the Complete Eigenenergy List of HCN
by Georg Mellau, Justus-Liebig-Universität
High accuracy intensity calculations of H_2O, CO and CO_2
by Oleg Polyanski, University College of London

The workshop book of abstracts is available online at www.eumetrispec.eu, and the conference proceedings book on the workshop contents, will include all posters and presentations. (PTB-report ISSN 1614-953X). Furthermore pdfs are also announced and made aviable via downloads at the coordinators research gate profile as well as special EUMETRISPEC related user group in sociel science networks like Researchgate as well as LinkedIn.

4.2.4 Good Practice Guides

The project generated Good Practce Guides (GPG) in order to document practices found to be helpful in order to work on traceable line parameters. GPGs on "Assessing uncertainty budgets", on "How to retrieve molecular line data ...", and on "Ensuring comparability of spectral data using FTS and HRLS spectrometric techniques" have been documented. They were available on request from the web site. The advices in the GPG were updated and further developed. The most updated application and spectral parameter specific procedures can be found in the latest published papers on the measured line parameters on individual molecules as they were released after the actual funding period.

4.2.5 Exploitation of Intellectual Properties

The central Fourier-transform spectroscopic facility at PTB generated through the project will be offered to external researchers for collaboration based on the procedures defined by the EUMETRISPEC project to measure line parameters. The concept of an "open facility" will be continued, discussed and promoted in scientific communities. The concept will be advertised through the web (including the project website), personal contacts and conference presentations. Plans to amend the capabilities of the facility will be followed and new collaborations on metrology research will be seeked.

4.3 Networking NMI activities on spectral line data, cooperation between project partners

Work on the line data measurements has been discussed on many official (e.g., conferences, standardization meetings, and workshops) and informal to personal occasions with spectroscopy experts and users of the spectral data. Furthermore, stakeholder groups at LinkedIn as well as on Researchgate e.g. (www.linkedin.com/groups?home=&gid=7472859&trk=anet_ug_hm&goback=%2Egmp_7472859) were established. The project was presented and actively discussed with stakeholders.

Strong interaction amongst the project partners has taken place during the course of the project via various means such as e-mail, telephone, research visits and Skype. Examples of the research visits between the project partners include:

- LNE researchers visited MIKES for work related to the frequency comb based measurements
- PTB researchers visited DFM to discuss the protocols and fitting software
- DFM researchers visited PTB to assist them with the cell length measurements.
- SMU visited DFM and PTB to discuss the structure of the molecular line database and to assist in FTIR-based spectra recording.

Part of all project meetings was a lab tour in which the set-ups and current issues which were faced with the measurements were discussed between the partners.

Finally, the REG-researcher has visited DFM (to discuss the fitting software developed DFM), PTB and VSL. VSL also visited the REG-researcher to discuss the experimental set-up.

4.4 Example of early impact

To allow a wide range of users to access the project's results, the project's data have been submitted to the global HITRAN and GEISA databases – the most widely used open-access spectral databases –. There also is an agreement between database manager and EUMETRISPEC to cross link the spectral datasets in each database structure as soon as they appear on both sides. This means e.g. as soon as EUMETRISPEC spectral data are accepted for HITRAN, HITRAN will include a link to the EUMETRISPEC website to indicate where a more detailed uncertainty information for the EUMETRISPEC originated data can be found. On the other side EUMETRISPEC will show a link the HITRAN data base to indicate the existence of a much data set with a much larger spectral coverage but reduced uncertainty information in the HITRAN data base.

Furthermore e.g. the unique N_2O data set has been directly passed-on, for example, to the Total Carbon Column Observing Network (TCCON), a global network of 23 ground-based spectrometers that monitor atmospheric greenhouse gasses for direct testing of the implementation impact. TCCON is a key user of the HITRAN database, and is currently testing the new spectral data set. The project's contribution of highly accurate and traceable spectral data will reduce TCCON's reliance on the practice of side-by-side validation and calibration, which is difficult to achieve and expensive to perform. This high-quality reference data provided to TCCON will enhance the data the network provides to its users, such as climate modellers. The N2O data set e.g. has also been forwarded to the managers of a specialized N2O spectral data base at the Tomsk University, Russia, from where it will also be made available.

Other users of the project's reference data are e.g. the Atomic, Molecular, Optical and Positron Physics group at the University College London, UCL, UK, the Laboratoire de Météorologie Dynamique, IPSL, CNRS, Sorbonne Universités, Paris, France, the Laboratoire de Météorologie Dynamique, LMD/IPSL, CNRS, Ecole polytechnique, Université Paris-Saclay, France or the combustions diagnostics group (RSM) at the Technical University of Darmstadt, TUDa, Germany. **UCL** is currently modelling spectral lines for environmental, climate and planetary research and uses the project's spectral results as an independent and experimental corroboration of their theoretical quantum-chemical models, providing validation and weight to their own and related environmental and climate research. Univ. Sorbonne is taking advantage of the EUMETRISPEC HCl broadening data to test and further optimize advanced line shape models as well as to optimize the description of line mixing behaviour. Université Paris-Saclay on the other hand is developing collisional simulation models to derive broadening coefficients from simulations and intermolecular potentials instead of extensive measurements. These models are currently compared to components of the EUMETRISPEC HCL (and lateron CO2) broadening data set. TUDa, on the other hand is using e.g. the HCl and H_2O data set, to further develop absolute laser spectrometric in-situ analysers to better monitor e.g. pollutant formation or temperature in oxyfuel coal combustion in a large integrated research cluster called SFB129.

A new collaboration on the national German level with two different standardization committees (both ongoing over the nominal duration of the project) has been realized, which relies on the expertise built within the project. PTB became member of the subcommittee for remote sensing techniques of the commission for clean air (NA-134-04-02-16_UA der KRdL im VDI und DIN) and for gas analysis and gas quality of the DIN (NA 062-05-73 AA).

In addition, a liaison was recently formed between the International Atomic Energy Agency (IAEA) and the BIPM on isotope ratio measurements. The BIPM is reporting to the Consultative Committee for Amount of Substance (CCQM) of the International Committee for Weights and Measures (CIPM) and within the CCQM to the Gas Analysis Working Group (GAWG) on this collaboration with the IAEA. For this topic isotope-specific line parameters were and will be addressed in the future based on the expertise developed in EUMETRISPEC.

The stakeholder workshops organized by the project in 2012 and 2014 led to strong feedback from participating stakeholders for further activities development and facilities maintenance. The capabilities in traceable spectroscopy and spectral line data retrieval were the only European activities devoted to the metrological aspects of traceable spectral data for remote sensing or relevant industrial applications. The stakeholder present at the workshops encouraged the intentions of the project partners to start further initiatives continuing the work in future research programmes, like in the EMPIR environmental call in 2016.

Furthermore, numerous later EMRP and EMPIR projects have made use of the substantial EUMETRISPEC output and EUMETRISPEC methodologies or are based on information from the EUMETRISPEC consortium partners. This in particular concerns the availability, measurement capabilities and options to measure traceable line parameters. Such projects included ENGGAS, MACPoll, MetAMC, HIGHGAS, METEOMET1, METEOMET2, IMPRESS, BIOGAS, HIT, or MetNH3. Even in the third environmental call several new spectroscopy projects (SIRS, IMPRESS2, BIOGAS2, and METNO2) are funded and will be starting in 2017 which are taking great advantage of the EUMETRISPEC capabilities and infrastructure. IN Each of this projects involves a broad range and large number of NMIs and non-NMI stakeholders learns about the EUMETRISPEC concept and its output and implications so that the projects impact is steadily growing and has been multiplied many times.

Finally EUMETRISPEC is also active on a global scale and in the meantime lead to negotiations to formulate a memorandum of understanding between PTB and KRISS, the Korean NMI, which is one of the world leaders in metrological gas analysis. Close contacts also have been established to the NIST spectral data group.

4.5 Potential impact

One key impact of EUMETRISPEC is the uptake of line parameters, as well as the follow up spectroscopic analytical principles, such as optically based gas standards and traceable laser spectroscopic or FTIR diagnostics. This information is useful to the relevant committees oriented towards atmospheric measurement networks including GAW and World Metereological Organisation (WMO). Efficient communication has already been set up with representatives from TCCON and NDACC on data products, as well as HITRAN, GEISA and other spectral data bases. Scientific collaboration is currently being discussed which shall exceed the project's duration with research groups - partners of the WMO - throughout Europe. This is demonstrated by the list of attendees at the two EUMETRISPEC stakeholder workshops in 2012 and 2014 (see section 4.2.3 above). First discussions have also taken place with the European space agency on spectral diagnostics for atmospheric as well as planetary missions,, e.g. via project funding application for such topics.

Potential impact is also present in improvements and complementation of existing line data bases. Based on presentations of project results, personal communications and close discussions during the 2nd stakeholder workshop in October 2014, a scientific exchange on standardized line data representation is envisaged based on future publications beyond the project duration. Examples of successful inclusion of stake holder knowledge and strengthening of the communication is the integration of a previous member of the HITRAN working group in the FT-spectroscopy working group at PTB.

The project will enable users of spectral reference data to derive increasingly accurate and traceable spectroscopic results with higher-resolution modelling. Reducing uncertainties in environmental and climate analyses will aid effective monitoring and prediction of climate change, allowing European and global governments to mitigate effects and adapt measures. Furthermore, industrial process monitoring will also be advanced by the development of absolute species monitors by using high accuracy spectral data. Finally, metrological quality spectral data will also serve metrological key services like the development and dissemination of optical gas standards or the improved validation of classical gas standards via absolute optical techniques. High accuracy spectral data are a prerequisite to foster the development of spectroscopy-based optical gas standards, which serve as absolute analytical transfer standards in cases where high adsorptivity or reactivity of the target gas, prohibits or hinders the development of classical reference gas mixtures due to a lack of chemical stability. Such topics are in particular for strongly adsorbing or even reactive gas species like H2O, NH3, HCl, HF, or NO2.

5 EUMETRISPEC Website address and contact details

The project summary, documents and citations can be found on the project website maintained under the URL:

http://www.eumetrispec.eu/emrp/eumetrispec.html as well as www.ptb.de

Some contact details of all project partner representatives are as follows:

- Physikalisch-Technische Bundesanstalt (**PTB**), Germany / Contact: volker.ebert@ptb.de
- Conservatoire National des Arts et Metiers (**CNAM**), France / Contact: malo.cadoret@cnam.fr
- Dansk Fundamental Metrologi (**DFM**), Denmark / Contact: jcp@dfm.dtu.dk
- Laboratoire national de métrologie et d'essais (**LNE**), France / Contact: jean-jacques.zondy@cnam.fr
- Mittatekniikan Keskus (**MIKES**), Finland / Contact: Mikko.Merimaa@vtt.fi
- Slovenský Metrologický Ustav (**SMU**), Slovakia / Contact: valkova@smu.gov.sk
- VSL B.V. (**VSL**), Netherlands / Contact: spersijn@vsl.nl
- Radboud University Nijmegen (**RU**), Netherlands / Contact: F.Harren@science.ru.nl

6 List of EUMETRISPEC publications

Books

[1] V. Ebert, J. Brunzendorf, V. Werwein (eds.), “Spectral reference line data for atmospheric monitoring”, Proceedings of the EUMETRISPEC workshop held at Wolfenbüttel castle and PTB Braunschweig, November 15-16, 2012, PTB Bericht CP-8, 361 p., ISBN 978-3-95606-034-2, http://www.ptb.de/cms/publikationen/reihen/ptb-berichte/verzeichnis-der-ptb-berichte/ptb-berichte-chemische-physik-ptb-cp.html?tx_sevenpack_pi1%5bshow_uid%5d=5653&cHash=ab37bf74e1a6c5b78ae5d8b1a7e2dc7b%20-%20c5653.

[2] V. Ebert, O. Werhahn, J. Brunzendorf (eds.), “Traceability of Spectral Reference Line Data – Proceedings of the 2nd EUMETRISPEC Workshop, PTB Braunschweig, October 9-10, 2014”, PTB-Report CP, ISSN 1614-953X, approved, awaiting publication.

Peer-reviewed articles

[1] O. Werhahn, A. Pogány, J.A. Nwaboh, V. Werwein, V. Ebert, “Spectral reference data of molecules relevant to earth's atmosphere: Impact of European metrology research on atmospheric remote sensing”, Remote Sensing of Clouds and the Atmosphere XVIII, Proceedings of SPIE 8890, 889007, 2013. DOI: 10.1117/12.2028761.

[2] O. Werhahn, J. Brunzendorf, J.A. Nwaboh, A. Serdyukov, V. Werwein, V. Ebert, “Spectral reference line data relevant to remote sensing applications – A review and outline of the EUMETRISPEC project”, Remote Sensing of Clouds and the Atmosphere XIX, Proceedings of SPIE 9242, 92420D, 2014. DOI:10.1117/12.2067358.

[3] A. Pogány, O. Ott, O. Werhahn, V. Ebert, “Towards traceability in CO2 line strength measurements by TDLAS at 2.7µm”, Journal of Quantitative Spectroscopy and Radiative Transfer 130, 147-157, 2013. DOI: 10.1016/j.jqsrt.2013.07.011.

[4] J.A. Nwaboh, O. Werhahn, V. Ebert, “Line strength and collisional broadening coefficients of H2O at 2.7 µm for natural gas quality assurance applications”, Molecular Physics 112, 2451-2461, 2014. DOI: 10.1080/00268976.2014.916823.

[5] J.A. Nwaboh, O. Witzel, A. Pogány, O. Werhahn, V. Ebert, "Optical path length calibration: a standard approach for use in absorption cell-based IR-spectrometric gas analysis", International Journal of Spectroscopy, 132607, 2014. DOI: 10.1155/2014/132607.
[6] V. Werwein, J. Brunzendorf, A. Serdyukov, O. Werhahn, V. Ebert, "First measurements of nitrous oxide self-broadening and self-shift coefficients in the 0002-0000 band at 2.26 µm using high resolution Fourier transform spectroscopy", Journal of Molecular Spectroscopy 323, 28-42, 2016. DOI: 10.1016/j.jms.2016.01.010.
[7] M.P. Moreno, M. Cadoret, M. Jahjah, L. Nguyen, F.C. Cruz, J.-J. Zondy, "Application of a continuous-wave singly resonant optical parametric oscillator to spectral line intensity measurements in the ν_3 band of methane", Applied Physics B: Lasers and Optics 117, 681-687, 2014. DOI: 10.1007/s00340-014-5883-1.
[8] M. Jahjah, M.P. Moreno, M. Cadoret, L. Nguyen, J.-J. Zondy, "Measurements of N2-induced pressure broadening and shifts of some nu_3 band singlets lines of methane by use of a cw mid-IR OPO spectrometer near 3,3 microns", Journal of Quantitative Spectroscopy and Radiative Transfer 151, 251-259, 2015. DOI: 10.1016/j.jqsrt.2014.10.006.
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[10] I. Ricciardi, E. De Tommasi, P. Maddaloni, S. Mosca, A. Rocco, J.-J. Zondy, M. De Rosa, P. De Natale, "Frequency-comb-referenced singly-resonant OPO for sub-Doppler spectroscopy", Optics Express 20, 9178-9186, 2012. DOI: 10.1364/OE.20.009178.
[11] J. Courtois, R. Bouchendira, M. Cadoret, I, Ricciardi, S, Mosca, M, De Rosa, P. De Natale, J.-J. Zondy, "High-speed multi-THz-range mode-hop-free mid-IR laser spectrometer", Optics Letters 38, 1972-1974, 2013. DOI: 10.1364/OL.38.001972.
[12] G. Li, A. Serdyukov, M. Gisi, O. Werhahn, V. Ebert, "FTIR based measurements of the self-broadening and self-shift coefficients as well as line strength in the first overtone band of HCl at 1.76 µm", Journal of Quantitative Spectroscopy and Radiative Transfer 165, 76-87, 2015. DOI: 10.1016/j.jqsrt.2015.06.021.
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[14] V. Werwein, J. Brunzendorf, G. Li, A. Serdyukov, O. Werhahn, V. Ebert, "High-resolution Fourier transform measurements of line strengths in the 0002-0000 main isotopologue band of nitrous oxide", Applied Optics 56, E99-E105, 2017. DOI: 10.1364/AO.56.000E99.
[15] A. Pogány, A. Klein, V. Ebert, "Measurement of water vapor line strengths in the 1.4–2.7 µm range by tunable diode laser absorption spectroscopy", Journal of Quantitative Spectroscopy and Radiative Transfer 165, 108-122, 2015. DOI: 10.1016/j.jqsrt.2015.06.023.

Conference papers

[1] V. Ebert, J. Brunzendorf, G. Li, A. Serdyukov, O. Werhahn, V. Werwein, "EUMETRISPEC: A Versatile, Metrological, High-resolution Fouriertransform-spectrometer- Infrastructure to Determine Accurate Spectral Data", Laser Applications to Chemical, Security and Environmental Analysis 2016, Imaging and Applied Optics 2016, LM3G.1. DOI: 10.1364/LACSEA.2016.LM3G.1.
[2] V. Werwein, G. Li, J. Brunzendorf, A. Serdyukov, O. Werhahn, V. Ebert, "Nitrous oxide line positions in the 0002-0000 band at 2.26 µm as test case for high-resolution FTIR-spectrometer stability", Laser Applications to Chemical, Security and Environmental Analysis 2016, Imaging and Applied Optics 2016, JT3A.14. DOI: 10.1364/3D.2016.JT3A.14.

Trade/Popular journals

[1] PTB, "Lob für europäische Metrologie", announcement of EUMETRISPEC within a German press release, May 8, 2012.

Oral and poster presentations

[1] V. Ebert, J. Brunzendorf, O. Ott, A. Rausch, A. Serdyukov, V. Werwein, O. Werhahn, M. Cadoret, J.C. Petersen, J.-J. Zondy, M. Vainio, M. Valkova, S. Persijn, M. Kiseleva, "Introduction of a new project on Traceable Reference Spectral Line Data for environmental monitoring", presentation and poster, 22nd International Conference on High Resolution Molecular Spectroscopy, Prague, Czech Republic, September 4-8, 2012.
[2] V. Werwein, A. Serdyukov, J. Brunzendorf, O. Ott, A. Rausch, O. Werhahn, V. Ebert , "Bestimmung von N_2O-Selbstverbreiterungskoeffizienten im 0001-0000-Band bei 2150-2275 cm-1 mittels hochauflösender FTIR-Spektroskopie", presentation, DPG-Frühjahrstagung 2013, Jena, Germany, February 25-March 1, 2013.

[3] V. Ebert, J. Brunzendorf, O. Werhahn, A. Serdyukov, A. Rausch, V. Werwein, "EUMETRISPEC: European metrology infrastructure for traceable spectral reference data", 11th ASA conference and 12th International HITRAN Conference, Université de Reims, France, August 29-31, 2012.
[4] A. Simonsen, J. Hald, J. Lyngsø, J.C. Petersen, "Hollow Core Photonic Crystal Fibers for Quantitative Measurements of Fractional Amounts of Gases", oral presentation, Imaging and Applied Optics Congress, Monterey, USA, June 24-28, 2012.
[5] M. Vainio, J. Peltola, M. Merimaa, L. Halonen, "High-accuracy molecular spectroscopy in the mid-infrared region", CLEO Europe 2013, Munich, Germany, May 12-16, 2013.
[6] V. Werwein, A. Serdyukov, J. Brunzendorf, A. Rausch, O. Werhahn, V. Ebert, „EUMETRISPEC: Traceable reference line data for spectroscopic sensors", poster, 5th IPM Gassensor-Workshop, Freiburg, Germany, March 13-14, 2013.
[7] V. Werwein, A. Serdyukov, A. Rausch, J. Brunzendorf, O. Werhahn, V. Ebert, „Self-broadening coefficients of N2O and CO as reference data for atmospheric measurements or industrial gas sensors", poster, Innovationsforum Photonik 2013, Goslar, Germany, May 28, 2013.
[8] S. Persijn et al., „Traceable spectral reference data for gas analysis", poster, GAS 2013, Rotterdam, June 5 -7, 2013.
[9] A. Rausch, O. Werhahn, A. Serdyukov, V. Werwein, J. Brunzendorf, V. Ebert, „Einfluss der Reihenfolge von Mittelung und FFT auf spektroskopische FTIR Messungen", poster, DGaO-Proceedings 2013, Braunschweig, Germany, May 21-25, 2013.
[10] V. Werwein, J. Brunzendorf, A. Rausch, A. Serdyukov, O. Werhahn, V. Ebert, "First measurements of N2O-self-broadening coefficients in the 0001-0000- and 0002-0000-bands", poster, 24th Colloquium on High Resolution Molecular Spectroscopy (HRMS) 2013, Budapest, Hungary, August 25-30, 2013.
[11] O. Werhahn, A. Pogány, J.A. Nwaboh, V. Werwein, V. Ebert, "Spectral reference data of molecules relevant to Earth's atmosphere: Impact of European metrology research on atmospheric remote sensing", presentation, SPIE Remote Sensing conference, Dresden, Germany, September 23 -26, 2013.
[12] J. Peltola, M. Vainio, T. Fordell, M. Merimaa, L. Halonen, "High-Accuracy Molecular Spectroscopy with Frequency Comb-Linked Mid-Infrared Continuous-Wave Optical Parametric Oscillator", poster, 24th Colloquium on High Resolution Molecular Spectroscopy (HRMS) 2013, Budapest, Hungary, August 25-30, 2013.
[13] J. Peltola, M. Vainio, T. Fordell, M. Merimaa, L. Halonen, "High-Accuracy Molecular Spectroscopy with Frequency Comb-Linked Mid-Infrared Continuous-Wave Optical Parametric Oscillator", presentation, Mid-Infrared Coherent Sources (MICS) 2013, Paris, France, October 27 - November 1, 2013.
[14] J.-J. Zondy, J. Courtois, R. Bouchendira, M. Cadoret, I. Ricciardi, S. Mosca, M. De Rosa, P. De Natale, "High-Resolution Spectroscopy of the Methane nu3 Band using widely tunable single-frequency optical parametric oscillators", presentation, Conference on lasers & Electroptics (CLEO) 2013, San Jose, USA, June 11-18, 2013.
[15] M. Lopez, R. Bouchendira, J. Courtois, M. Cadoret et J.-J. Zondy, "Développement d'un oscillateur paramétrique optique monofréquence et rapidement accordable sur 2,25 THz dans le MIR: Application à la spectroscopie d'absorption du méthane", poster, Colloque sur les Lasers et l'Optique Quantique (COLOQ'13), Paris, France, July 8-11, 2013.
[16] I. Ricciardi, S. Mosca, V. Di Sarno, P. Maddaloni, M. Parisi, L. Santamaria, M. De Rosa, J.-J. Zondy, P. De Natale, "Absolute frequency measurements of CH3I and CH4 rovibrational transitions by a frequency-comb-referenced optical parametric oscillator", poster, 24th Colloquium on High Resolution Molecular Spectroscopy (HRMS) 2013, Budapest, Hungary, August 25-30, 2013.
[17] M. Cadoret, R. Bouchendira, J. Courtois, M. Lopez, I. Ricciardi, S. Mosca, M. De Rosa, P. De Natale, J.-J. Zondy, "High-Speed, Multi-THz-Range Mode-Hop-Free Tunable Mid-IR OPO Spectrometer", poster, OSA Optics &Photonic Congress 2013: Advanced Solid State Lasers (ASSL)/MidInfrared Coherent sources (MICS) & Laser Sensing & Communications (LS&C), Paris, France, October 27- November 1, 2013.
[18] V. Ebert, "EUMETRISPEC: a project on Spectral Reference Line Data for environmental monitoring", presentation, NDACC-IRWG/TCCON Meeting, Wengen, Switzerland, June 11-15, 2012.
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[20] A. Pogány, A. Klein, B. Buchholz, V. Ebert, "Measurement and validation of water vapor line strengths in the 1.4-2.7 µm range by high sensitivity TDLAS", presentation, 23rd Conference on High Resolution Molecular Spectroscopy 2014, Bologna, Italy, September 2-7, 2014.
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[22] J. Brunzendorf, A. Serdyukov, V. Werwein, O. Werhahn, V. Ebert, "FTIR-based CO_2 line strength measurements in the 20012 – 00001 band near 2 µm", poster, 23rd Conference on High Resolution Molecular Spectroscopy 2014, Bologna, Italy, September 2-7, 2014.

[23] O. Werhahn, D. Balslev-Clausen, J. Brunzendorf, J.A. Nwaboh, A. Rausch, A. Serdyukov, V. Werwein, J.C. Petersen, V. Ebert "Intercomparison of laser- and FITR-based CO_2 line data in the 2 µm combination band", poster, 23rd Conference on High Resolution Molecular Spectroscopy 2014, Bologna, Italy, September 2-7, 2014.

[24] V. Werwein, D. Balslev-Clausen, J. Peltola, M. Valkova, J. Brunzendorf, T. Fordell, T. Hieta, A. Rausch, A. Serdyukov, M. Vainio, J.C. Petersen, O. Werhahn, V. Ebert, "Validation of the EUMETRISPEC central FTIR-spectroscopy facility: a metrological intercomparison on N_2O spectroscopy, 23rd Conference on High Resolution Molecular Spectroscopy 2014, Bologna, Italy, September 2-7, 2014.

[25] V. Ebert [on behalf of the consortium partners], "Spectral reference data for atmospheric monitoring: EUMETRISPEC a European metrology infrastructure for traceable spectral reference data", poster, NDACC-IRWG/TCCON Meeting, Wengen, Switzerland, June 11-15, 2012.

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