

First EUMETRISPEC newsletter

Introduction

This is the first newsletter of the EUMETRISPEC project, a joint metrology effort, which aims to establish a European FT-IR based spectroscopy infrastructure targeted towards traceable measurements of spectral line data under well controlled conditions. While a vast amount of spectral data is available in numerous line by line databases (e.g. HITRAN and GEISA) or in the scientific literature the uncertainty of such data is – in a metrological sense - often only insufficiently specified, estimated or even unknown which frequently limits the accuracy and thus the strict interpretation of measurements of atmospheric molecular species. EUMETRISPEC aims to develop hardware (instruments), software and data protocols and disseminate this knowledge to enable traceable line data measurements. In order to demonstrate the capabilities of the developed or studied hard/software/ and protocols we will also determine within the project first traceable sample line data sets for the major greenhouse gases and other molecules of atmospheric relevance. Typical relative expanded uncertainties of one percent or better for line strength and better than 0.1 % for pressure broadening coefficients and down to 0.01% for line positions will be targeted.

Every 6 months a newsletter will be distributed containing highlights of the latest achievements, information on available documentation like good practice guides or measurement protocols, and opportunities for training and measurements at a central facility established at the Physikalisch-Technische Bundesanstalt (PTB) in Germany.

Upcoming activities

1st EUMETRISPEC Stakeholder Workshop

The project consortium organises a 1½-day ad-hoc workshop for stakeholders to inform them about the project activities and the possibilities for participation. In an informal atmosphere there will be presentations and discussions on the work of the consortium and the stakeholders. Possible subjects include:

- Spectroscopic techniques
- Traceability in gas analysis
- Gas mixtures for line strength measurements
- Radiation transport modelling
- Satellite and ground based FTIR monitoring

When: 15 November 2012

Location: PTB, Braunschweig

More information on the workshop will be made available through www.EUMETRISPEC.org. You can also register by mail (anne.rausch@ptb.de) in order to get updated details on the planned stake holder workshop

Research highlights

Setting up of the central facility core infrastructure (PTB)

The core of the central facility is a High-Resolution Fourier-Transform Infrared Spectrometer (Bruker IFS-125 HR). It has a maximum optical path-length difference (OPD) of 481 cm, resulting in a resolution of up to 0.002 cm^{-1} . Our new spectrometer has been installed in late 2011 and taken into operation at the beginning of 2012. Particular care is taken to reach an excellent vacuum inside spectrometer in order to completely suppress the



background absorptions by atmospheric constituents like water vapour or CO_2 . This low inside pressure and thus minimized contamination by the air inside the interferometer chamber is, e.g., key to determine accurate line strengths of the target molecules but in particular for CO_2 and water. For this purpose, the standard vacuum system has been upgraded by two turbo molecular pumps. The background pressure inside the spectrometer and therefore the H_2O contamination could be reduced by three orders of magnitude to typical manufacturer values. Combined with the small leakage rates well below 0.7 mbar/day this forms a good starting condition for high-quality H_2O and CO_2 line parameters measurements, which are one of the primary goals of the project.

Comparisons (VSL)

During the project three comparisons will be organized, which are aiming to critically evaluate the project partners' capabilities, and to identify the extent of robustness of the experimental data analysis methods. The three comparisons cover line strength measurements, mole fraction retrievals, and bilateral validations of the central facility. The protocols for these comparisons are available from the project partners which can be found on the [EUMETRISPEC website](#). Interested spectroscopy groups from outside the project might be attracted to join-in one of those comparisons. In this case they may simply contact the project's coordinator or one of the partners' representatives. Results of the comparisons will be published on the website (first report scheduled in September 2013).

Permeation facility for nitric acid (VSL)

While the focus of the EUMETRISPEC project is on the main greenhouse gases, also other compounds of atmospheric relevance are taken into account such as nitric acid (HNO_3). Nitric acid plays a crucial role in atmospheric chemistry and about one-fourth of the acidity of rain is accounted for by nitric acid. Therefore, nitric acid along with a host of other species is continuously monitored in the atmosphere mostly using infrared spectroscopic techniques. However, line strength data for HNO_3 are scarce and highly variable due to the high reactivity of nitric acid. For the strong fundamental ν_1 -band around 3550 cm^{-1} no line strength data are available at all. At VSL, one of the partners in the project, a permeation set-up is currently under construction to generate nitric acid at low amount of substance levels (typically $<1\text{ }\mu\text{mol/mol}$) and cavity ring-down spectroscopy will be used to determine line strengths.

Protocols and harmonized measurement procedures (DFM, PTB)

In order to harmonize measurements and their respective outcomes, the EUMETRISPEC project relies on certain standard approaches, documented measurement procedures and technical protocols. This strategy shall further be used as an input to future standardization efforts within scientific and technical communities referring to spectroscopic methods and application fields. DFM and PTB have brought their expertises on this topic to the EUMETRISPEC project resuming their impact on previous iMERA-plus and EURAMET projects (http://www.euramet.org/fileadmin/docs/projects/934_METCHEM_Interim_Report.pdf). First EUMETRISPEC-internal standardized procedure descriptions have been set up, enabling all project partners to work on the same harmonized basis. The approved EUMETRISPEC procedures will be made public available through the project's website.

Consortium-Publications with relevance to Eumetrispec

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

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 presentation, NDACC-IRWG/TCCON Meeting, Wengen, Switzerland, June 11-15, 2012.

V. Ebert, "EUMETRISPEC: a project on Spectral Reference Line Data for environmental monitoring", oral presentation, NDACC-IRWG/TCCON Meeting, Wengen, Switzerland, June 11-15, 2012

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 June, 2012.

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.

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", oral presentation and poster, 22nd Int. Conference on High Resolution Molecular Spectroscopy, Prague, Czech Republic, September 4-8, 2012.

Klaus-Dieter Sommer, Petra Spitzer, Volker Ebert, "New Challenges in environmental metrology", oral presentation, accepted for publication in proceedings of the XX IMEKO World Congress Metrology for Green Growth, Busan, Republic of Korea, September 9-14, 2012

J. Brunzendorf, A. Serdyukov, O. Werhahn, V. Werwein, A. Rausch, V. Ebert, "Towards SI-traceable reference line-by-line spectral data using a modified Bruker IFS125HR spectrometer", poster, Annual Meeting of the Astronomische Gesellschaft 2012, Hamburg, Germany, September 24-28, 2012.

Meet us

In the coming period you can meet us at the following events:

Event	When	Location	Whom	Presentation
Praha2012	4-8 September 2012	Prague, Czech Republic	PTB	poster+talk
ICAMData	30 September-4 October 2012	Gaithersburg, USA		
Annual Meeting of the Astronomische Gesellschaft 2012	24-28 September 2012	Hamburg, Germany	PTB	poster
MACPoll WS on Zero Gas	4 June 2013	Rotterdam, the Netherlands	PTB	talk/poster
GAS2013	5-7 June 2013	Rotterdam, the Netherlands	VSL/PTB	poster

Contact and further information

This is a newsletter about on-going work and development of the EUMETRISPEC project, which is carried out by the following partners / institutions:

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

Additional information on EUMETRISPEC and the partners can be found on the project homepage www.EUMETRISPEC.org, where our contact details and a registration access are available to get access to the stakeholder area. Additional information will be made available.

Please forward this newsletter to your colleagues. They can send an email to any of the project's representatives with subject 'register EUMETRISPEC newsletter' to register for this 6-monthly newsletter.