Second EUMETRISPEC newsletter

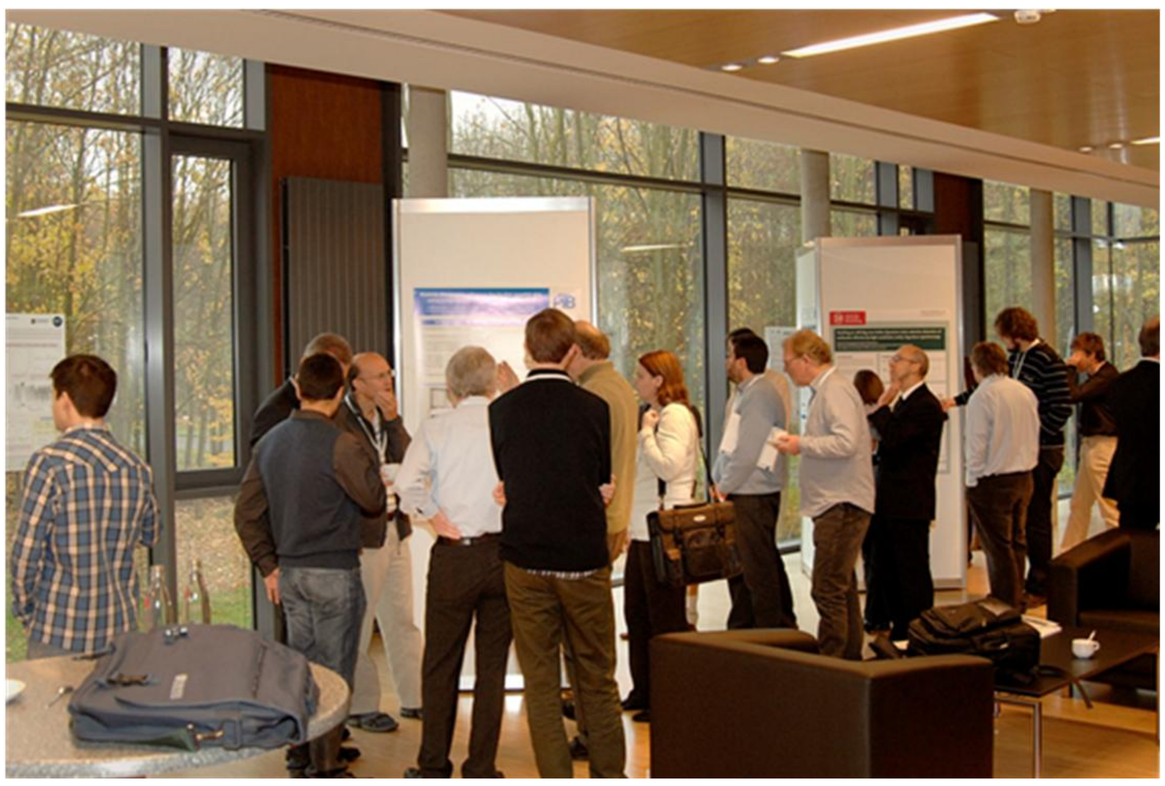
Introduction

This is the second newsletter of the EUMETRISPEC project, a joint metrology effort, which will 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 expanded uncertainties of one percent relative 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.

Recent activities

1st EUMETRISPEC Stakeholder Workshop



The very recent JRP period was highlighted by the 1st stakeholder workshop event that was organized by the JRP partners at Wolfenbüttel and Braunschweig, Germany, in November 2012. The workshop aimed to bring together the experience, wishes and needs of environmental monitoring community with metrological points of view and goals of the JRP (http://www.eumetrispec.org/emrp/workshop.html). Together with intensified presence of JRP partners on most important community conferences during the last six months, the workshop outcome will streamline the JRP's main focus with that of the stakeholders. Respective reports and projections on what the JRP finally will deliver can be given now. Some workshop details: 8 invited speakers, 49 attendees representing 31 institutions from 12 different nations were attending 15 plenary talks and 21 poster presentations for two days. A promising and partly agreed follow-on exchange of knowledge from stakeholders into the JRP as well as from the JRP into the stakeholder communities was achieved. Regarding standardization bodies the German mirror committee of the CEN/TC 264/Working Group 18 on FTIR standardization in remote sensing is to mention. By these means an

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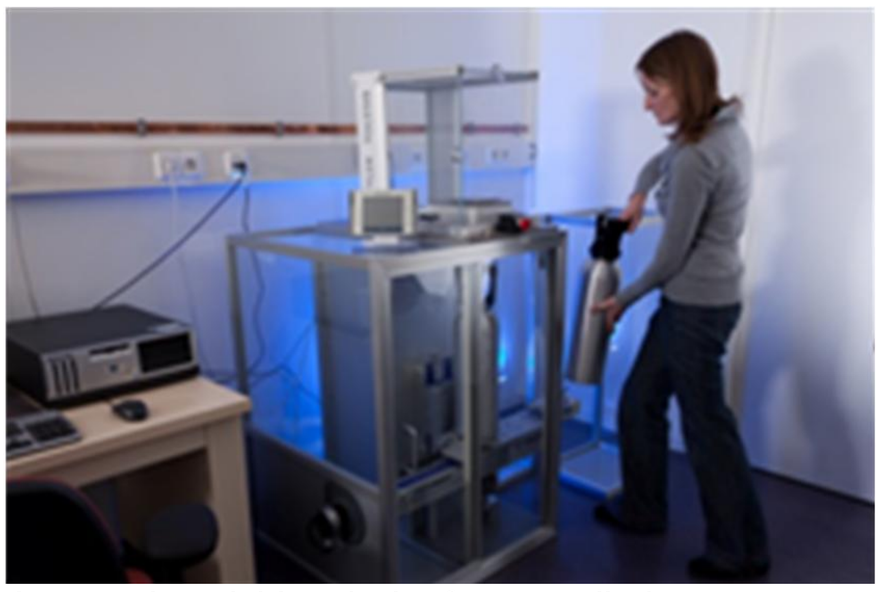
uptake of JRP results will be favoured and the interplay of expertise from inside and outside the JRP is assured. The workshop presentations and posters will be publicly available via an issued report PTB-CP-x, which is to be published under ISSN 1614-953X (http://www.ptb.de/cms/de/publikationen/reihen/ptb-berichte.html). The next workshop, which is scheduled for the 2nd period of the JRP, will be announced through the JRP's web site.

Research highlights

Preparation of reference gas mixtures (SMU, VSL)

Within the EUMETRISPEC project SMU (Slovakia) and VSL (The Netherlands) are responsible for preparation of reference gas mixtures. These mixtures are provided to the other project partners and the Central Facility located at PTB. The gas mixtures are prepared in cylinders via gravimetric methods (ISO 6142) and validated by comparison with standard gas mixtures. Typical uncertainties in the amount of substance are in the range of 0.1-1%. Mixtures are being prepared for amongst others CO_2, N_2O, and CH_4 with synthetic air as matrix gas. The amount of substance levels prepared range from 300 nmol/mol up to the % level as different spectroscopic techniques are used to study line strengths that differ up to 8 orders of magnitude. Besides these static mixtures, dynamical methods based on permeation are used to generate low amount of substance levels of the reactive compound nitric acid (HNO_3).



Automatic weighing device for gas cylinders

Measurement of the absolute frequencies of absorption line centers (LNE-CNAM, MIKES)

The frequencies and pressure shifts of absorption line centers are among the spectral line parameters whose traceable measurements are being developed within the EUMETRISPEC project. While the actual measurements of these parameters are done using a High-Resolution Fourier-Transform Infrared Spectrometer at the central facility (PTB), the accuracy of the measurements will be validated using laser spectroscopy. At LNE-CNAM (France) and MIKES (Finland), new laser based methods for mid-infrared absolute frequency spectroscopy are being developed. The core of these methods is a high-power, narrow-linewidth continuous-wave optical parametric oscillator (cw OPO), which is ideal for high-resolution (sub-Doppler) measurements. These OPOs have wide tuning range in the mid-infrared region, around 3 to 4 μm. In addition, the OPO frequency can be referenced to an optical frequency comb for absolute frequency scale, which makes it possible to determine the positions of molecular absorption lines with high accuracy.

One of the recent highlights of this part of the EUMETRISPEC project is the development of a new method for fast and continuous scanning of the OPO frequency. The figure on the next page shows spectra of wide portions of the the ν_3 fundamental absorption band of methane (CH_4) in the 3.31 μm range that have been recorded by rapid (4.5 THz/s) mode-hop-free electronic tuning of the 1064 nm pump laser (an extended-cavity diode laser, ECDL) of the OPO. These measurements demonstrate the widest idler-wave continuous tuning range (up to 72 cm^{-1} at 3.3 μm) ever obtained from a cw singly-resonant OPO spectrometer which, in this case, behaves as a fast Fourier transform spectrometer with a sub-MHz (<3×10^{-5} cm^{-1}) resolution (to be published in *Optics Letters*).

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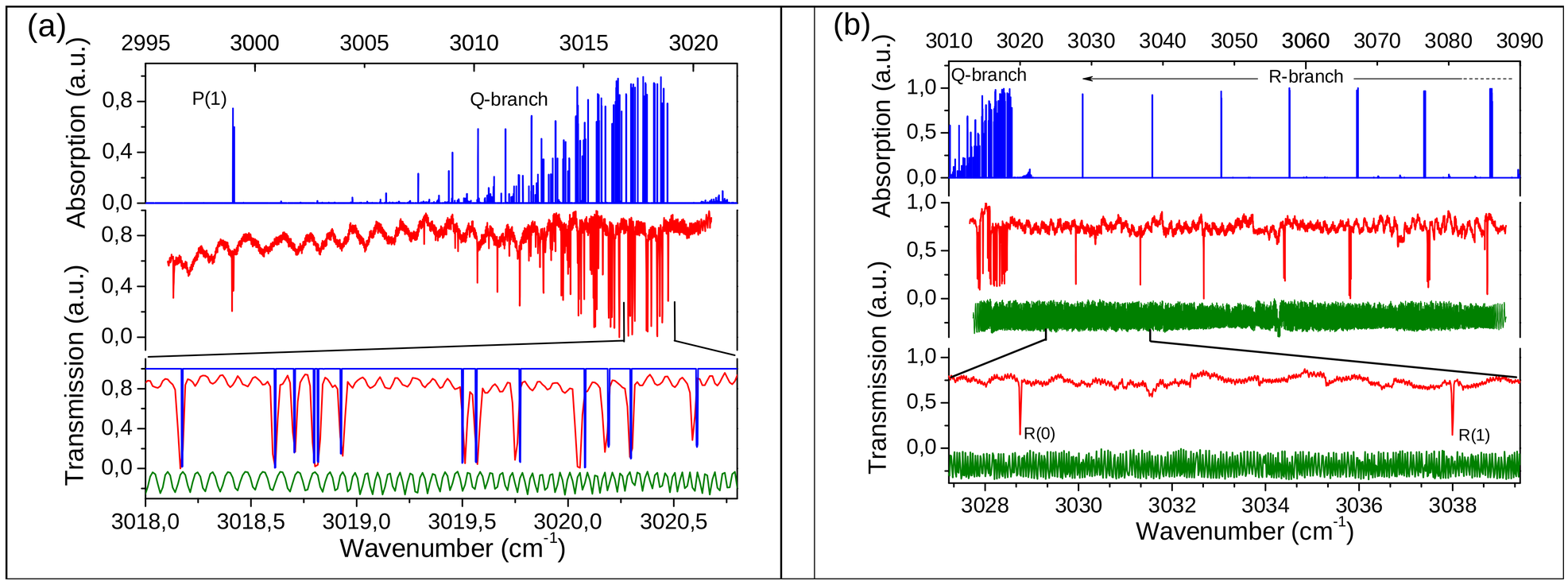

(a) Single-scan spectrum of the P(1) and entire Q-branch of the ν_3 band of methane near λ_i = 3.31 μm, recorded in 0.5 s (pump scan speed 4.5 THz/s, spectral span ~30 cm^{-1}. Top: HITRAN simulation; Middle: experimental mode-hop-free recorded spectrum. Bottom: zoomed portion of the Q-branch with the sinusoidal fringes of the Ge etalon used as a relative frequency marker in the measurements. (b): Single-scan spectrum of part of the Q and R-branches, with a spectral span of ~72 cm^{-1}. The CH_4 pressure is 0.5 mbar.

New Consortium Publications with relevance to Eumetrispec

J. Courtois, R. Bouchendira, M. Cadoret, J.-J. Zondy, I. Ricciardi, S. Mosca, M. De Rosa, P. De Natale, "High-Resolution Spectroscopy of the Methane ν3 Band in the 3.3 μm Range using Widely Tunable Single-Frequency Optical Parametric Oscillators", Oral presentation (paper Ctu3H.5), CLEO 2013, San Jose CA, USA (Session: Novel Trace Gas Sensing, 11 June 2013, Room A8, San Jose Convention Center).

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-fre tunable mid-IR laser spectrometer", Opt. Lett., Apr 2013 (accepted).

V. Werwein, A. Serdyukov, J. Brunzendorf, O. Ott, A. Rausch, O. Werhahn, V. Ebert , "Bestimmung von N2O-Selbstverbreiterungskoeffizienten im 0001-0000-Band bei 2150-2275 cm^{-1} mittels hochauflösender FTIR-Spektroskopie,", DPG-Frühjahrstagung 2013, Jena, Germany, February 2013 .

J.-J. Zondy (invited), "Widely tunable, narrow linewidth cw single-frequency optical parametric oscillators for mid-IR molecular spectroscopy and trace molecular detection", 2012 International Breath Analysis Meeting, Sonoma (CA), USA, 28 oct – 1st nov, 2012.

J.A. Nwaboh, O. Werhahn, P. Ortwein, D. Schiel, V. Ebert, "Laser-spectrometric gas analysis: CO2-TDLAS at 2 μm", Measurement Science and Technology, 24, 015202, doi:10.1088/0957-0233/24/1/015202 available as open-access paper.

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.

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.

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Meet us

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

Event	When	Location	Whom	Presentation
CLEO 2013	9-14 June 2013	San Jose, USA	LNE-CNAM	Oral (CTu3H.5)
GAS2013	5-7 June 2013	Rotterdam, the Netherlands	VSL	Poster
DGaO	21-25 May	Braunschweig, Germany	PTB	Poster
HRMS 2013	25-30 August	Budabest, Hungary	PTB	Oral

Contact and further information

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

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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 is available to get access to the stakeholder area where 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.

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