EUMETRISPEC Newsletter 5

Highlights

To conclude the project, a 2nd stakeholder workshop on

Traceability of spectral reference line data

was organized and held at PTB, 9 – 10 October 2014.

During the workshop the current outcome of the project was presented to the international community. To this end, measurement results regarding the traceability of spectral data as well as metrological approaches for data acquisition and analysis were shown. Furthermore the workshop served to link metrological aspects of spectroscopy to stakeholder interests. Interesting presentations and poster contributions from stakeholders and participants were discussed.

Fig. 1: Workshop participants (photo: PTB 2014).

Some numbers: 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.

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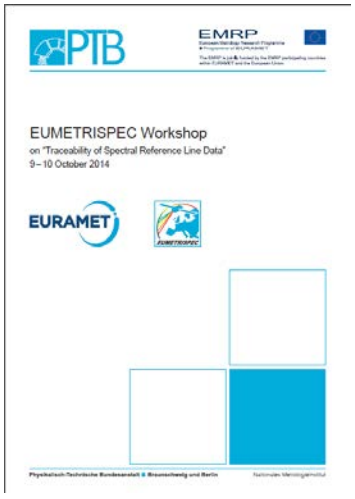
The workshop organizers are grateful to the presenters of the following invited talks:

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

The workshop book of abstracts is available online at www.eumetrispec.eu.



Proceedings of the workshop, which will include all posters and presentations, is currently in preparation. It will be released as PTB-report (ISSN 1614-953X).

The proceedings of the 1st stakeholder workshop 2012 have been released as PTB-report CP-8 in 2013 and is available for download at PTB website. *Spectral reference line data for atmospheric monitoring : proceedings of the EUMETRISPEC workshop held at Wolfenbüttel castle and PTB Braunschweig, Nov. 15 - 16, 2012:*

http://www.ptb.de/cms/publikationen/reihen/ptb-berichte/verzeichnis-der-ptb-berichte/ptb-berichte-chemische-physik-ptb-cp.html.

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Comparison on N_2O amount of substance fractions assigned by IR spectroscopy relying on spectral line parameters

As an important metrological validation procedure a blind comparison on N_2O amount of substance fraction measurements was organized within the project. The task for participants was to measure isolated, rovibrationally resolved, spectral features of N_2O in a mixture with air and to process the measured spectra by means of spectral line parameters. By this a N_2O amount of substance fraction value was to assign to the gas mixture. Two types of samples were distributed to the partners, depending on the sensitivity of the spectroscopic techniques used: Cavity ring-down spectroscopy instruments (CRDS) were supplied with a mixture with a nominal concentration of 10 µmol/mol, whereas tunable diode laser absorption (TDLAS) and Fourier-transform infrared (FTIR) spectroscopy users analyzed mixtures with nominal concentrations of 100 mmol/mol. The mixtures for this comparison were prepared gravimetrically by SMU.

Measurements were performed by FTIR at PTB, by TDLAS at DFM, and by CRDS at MIKES and VSL. The data were analysed by individual evaluation procedures fitting Voigt profiles (multi line at PTB) to the measured spectra. Amount fractions were computed using measured spectral line area and line-strength values from the project and the HITRAN2012 database. The results of the participants referring to the different measurement methods are summarized in the Fig.

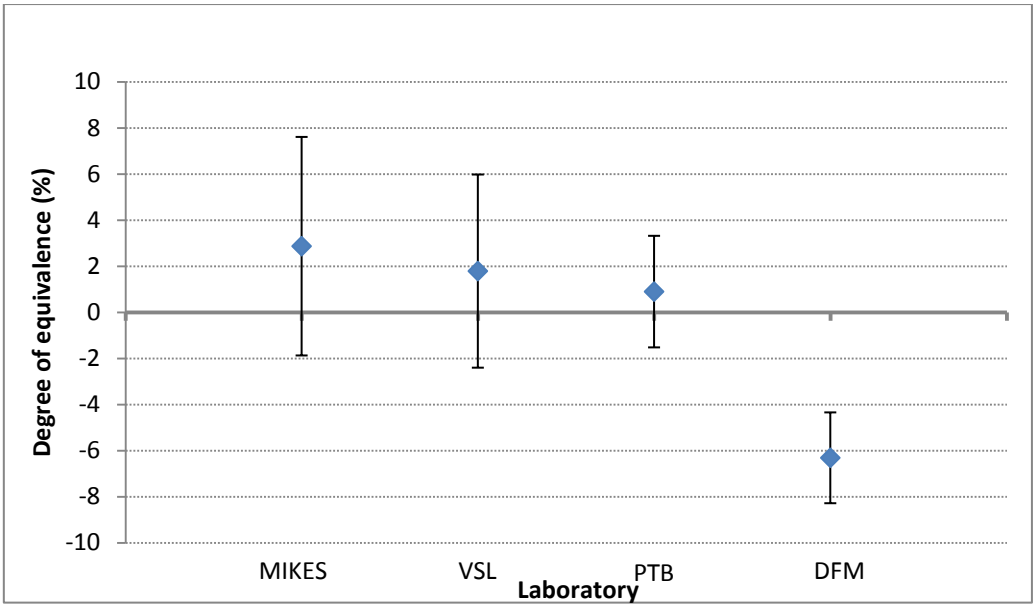

Fig. 2: Results of the N_2O comparison presented as degrees of equivalence between the results reported by the different institutions and their individual comparison reference values.

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The reported results of VSL and MIKES show an excellent agreement with the comparison reference values (CRVs) for low concentration nitrous monoxide mixtures, i.e. the computed participant's amount fraction value agrees within the reported uncertainty with the CRV. For high concentration nitrous monoxide mixtures, PTB is within 1 % in agreement with the CRV. By means of the DFM result, which does not coincide with the CRV, a technical issue with DFM's data acquisition procedure could have been identified. This fact will lead to a further amendment of the respective comparison report. The report shall also be submitted to a peer reviewed journal.

Selected consortium publications

O. Werhahn; J. Brunzendorf; J. Nwaboh; A. Serdyukov; V. Werwein; V. Ebert, „Spectral reference line data relevant to remote sensing applications: a review and outline of the EUMETRISPEC project", Proc. SPIE 9242, Remote Sensing of Clouds and the Atmosphere XIX; and Optics in Atmospheric Propagation and Adaptive Systems XVII, 92420D (17 October 2014); doi: 10.1117/12.2067358

Javis A. Nwaboh, Olav Werhahn, Volker Ebert, „Line strength and collisional broadening coefficients of H_2O at 2.7 µm for natural gas quality assurance applications", Molecular Physics (Taylor & Francis), vol. 112, 18, 2451-2461 (2014), dx.doi.org/10.1080/00268976.2014.916823.

Javis A. Nwaboh, Oliver Witzel, Andrea Pogány, Olav Werhahn, Volker Ebert, "Optical path length calibration: a standard approach for use in absorption cell-based IR-spectrometric gas analysis", Int. J. Spectroscopy, vol. 2014, 132607, dx.doi.org/10.1155/2014/132607.

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, Vol. 117 (2014), pp 681-687, DOI: 10,1007/s00340-014-5883-1.

J. Peltola, M. Vainio, T. Fordell, T. Hieta, M. Merimaa, L. Halonen, "Frequency-Comb-Referenced Mid-Infrared Source for High-Precision Spectroscopy", Opt. Express, submitted.

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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:

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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 are 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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