Errata

Poster session E **Tuesday, 16:30**

E55 **Čermák P., Hovorka J., Veis P., Cacciani P., Cosleau J., Khelkal M., Foldes T., Auwera J. V.**
Analysis of NH3 absorption spectra in the 2.3 μm *atmospheric water window*

E56 **Garamov V., Rodin, Semenov, Spiridonov, Benderov**
Mid-IR heterodyne spectrometer concept for planetary science

Contributed Lectures G **Wednesday, 11:00**
lecture hall AII
chairperson: Tyuterev V.

Contributed Lectures I **Wednesday, 14:30**
lecture hall AI
chairperson: Coudert L.H.

I1 **Bunker P.R.,** 14:30
Ostojic B., Schwerdtfeger P., Jensen P.
An Ab Initio Study of SbH_2 and BiH_2: The Renner Effect, Spin-Orbit Coupling, Local Mode Vibrations and Rovibronic Energy Level Clustering in SbH_2

I2 **Špirko V.,** 14:48
Augustovičová L., Soldán P.
Effective Hyperfine-structure Functions of Ammonia

I3 **Tyuterev V.,** 15:06
Tashkun S.A., Kochanov R., Starikova E., Mikhailenko S., Barbe A., Kokoouline V., Lapierre D., Alijah A.
Recent Advances in the Theory of the Ozone Molecule: Ab Initio Calculations, Band Intensities and Highly Excited Ro-vibrational States

I4 **Domingos S.R.,** 15:24
Pérez C., Medcraft C., Pinacho P., Schnell M.
Conformational Flexibility of Acyclic Monoterpenes Revealed by Broadband Rotational Spectroscopy

I5 **Araki M.,** 15:43
Takano S., Sakai N., Yamamoto S., Oyama T., Kuze N., Tsukiyama K.
Detections of Long Carbon Chains CH_3CCCCH, C_6H, l-C_6H_2 and C_7H in the Low-Mass Star Forming Region L1527

Camber Concert Session **Friday, 19:30**

Martinů Quartet 19:55
W. A. Mozart: Divertimento D major, KV 136, Allegro, Andante, Presto
F. Mendelssohn-Bartholdy: Capriccio op. 81/3
A. Dvořák: The sting quartet F major, op. 96 American, Allegro ma non troppo, Lento, Molto vivace, Vivace ma non troppo

Analysis of NH_3 absorption spectra in the 2.3 µm atmospheric water window

Peter Čermák, Juraj Hovorka[1], Pavel Veis[1], Patrice Cacciani[2], Jean Cosléou[2], Mohamed Khelkal[2], Tomáš Földes[3], Jean Vander Auwera[3]

[1]Department of Experimental Physics, Faculty of Mathematics, Physics and Informatics, Comenius University, Bratislava, Slovakia, cermak@fmph.uniba.sk; [2]Univ. Lille, CNRS, UMR 8523 - PhLAM - Physique des Lasers, Atomes et Molecules, F-59000 Lille, France, Patrice.CACCIANI@univ-lille1.fr; [3]Service de Chimie Quantique et Photophysique, CP160/09, Université Libre de Bruxelles, 50 ave. Roosevelt, B-1050, Belgium, Tomas.Foldes@ulb.ac.be;

The laser absorption spectra of NH_3 ammonia isotopologues were analysed in the 4275-4355 cm^{-1} spectral range. The experimental conditions covered the temperature range from 180 to 296 K and pressures from 0.4 to 50 mbar in a 7 m path long Herriot cell probed by a Vertical External Cavity Surface Emitting Laser. A Fourier transform spectrum was recorded at 296 K with 28 m path length to complement the room temperature data. These spectra were used to continue our work [1] on NH_3 transitions characterisation (quantum state assignment and line shape parameter determination) in this important atmospheric window, suitable for trace gas measurements. Besides the spectroscopic description of this ammonia isotopologue, the goal of the presented work is to test the improved method for measurements of lower state energies of transitions [2] with datasets from completely independent sources (laser absorption and Fourier transform spectra in this case).

References

[1] P. Čermák, J. Hovorka, P. Veis, P. Cacciani, J. Cosléou,*et al*, J. Quant. Spectrosc. Radiat. Transfer **137**, 13-22 (2014)

[2] P. Cacciani, P. Čermák, J. Cosléou, J. El Romh, J. Hovorka, M. Khelkhal, Mol. Phys. **112,** 2476-2485 (2014)

Mid-IR heterodyne spectrometer concept for planetary science

Rodin[12], Semenov[1], Spiridonov[3], Garamov[1], Benderov[1]

[1]Moscow institute of physics and technology, Russia; [2]Space Research Institute, Russia; [3]Prokhorov General Physics Institute, Russia

We present a heterodyne spectrometer concept based on DFB QCL lasers operated in mid-IR region. The instrument will be tested at one of the Russian observatories characterized by environmental conditions suitable for astronomical observations in the infrared region. The core difference between existing instrument and introduced concept is utilizing of photonic integrated circuits and fiber optics in the optical scheme, precise local oscillator frequency stabilization with reference absorption line. This instrument is meant to supersede all existing analogues (Cologne University (Germany) and Tohoku University (Japan) instruments) in some parameters, including spectral resolution, spectral coverage in a single observation, and the working range shortwave boundary. New methods of reverse problems solving will be introduced for measured spectra treatment.

A key advantage of high spectral resolution in the analysis of the outgoing radiation spectra of planets is concerned with the capability to retrieve detailed information about composition, structure, and photochemical kinetics of their atmospheres. Ultra-high spectral resolution provided by a heterodyne detection of the infrared radiation, allows for Doppler wind measurements at different altitudes. The most valuable problems to be solved are vertical temperature and wind profiles on Mars and Venus, integral and vertical concentration measurements of minor constituents on Mars and Venus, wind and temperature on Titan.

Cavity Ring-Down Spectroscopy around 2.3 µm

P. Čermák[1,2,4], S. Vasilchenko[1,2,3], D. Mondelain[1,2], S. Kassi[1,2], A. Campargue[1,2]

[1]Univ. Grenoble Alpes, LIPhy, France, alain.campargue@univ-grenoble-alpes.fr; [2]CNRS, LIPhy, France, alain.campargue@univ-grenoble-alpes.fr; [3]Laboratory of Molecular Spectroscopy, V.E. Zuev Institute of Atmospheric Optics, SB, Russian Academy of Science, Russia, vss544@gmail.com; [4]Department of Experimental Physics, Faculty of Mathematics, Physics and Informatics, Comenius University, Slovakia, cermak@fmph.uniba.sk;

The first application of continuous wave Cavity Ring Down Spectroscopy (CRDS) around 2.3 µm is presented. The instrument operates in the important atmospheric transparency window and provides a high sensitivity (minimum detectable absorption down to the 10^{-11} cm^{-1}). The system uses a two types of tunable sources to operate a Distributed Feedback Diode (DFB)[1] and a Vertical External Cavity Surface emitting laser (VECSEL)[2,3].

The VECSEL performances combine a large continuous tunability in the range 4295-4380 cm^{-1} together with a powerful (~5 mW) TEM_{00} diffraction limited beam and linewidth below MHz level (for 1 ms of integration time). With much narrower operational range (~15 cm^{-1}) and wider linewidth (>1 MHz), the main advantage of the DFB diode is its frequency stability due to the fact that whole laser is built on a single semiconductor element (compared to the open space design of the VECSEL).

The performance of the CRDS instrument will be discussed comparing recordings of different spectra of absorbing molecules in the region.

References

[1] D. Mondelain, S. Vasilchenko, P. Čermák, S. Kassi, A. Campargue, Phys. Chem. Chem. Phys. **17**, 17762-1777, 2015.

[2] S. Vasilchenko, D. Mondelain, S. Kassi, P. Čermák, P., B. Chomet, B., *et al*, J. Mol. Spectrosc. **326**, 9-16, 2016.

[3] P. Čermák, B. Chomet, L. Ferrieres, S. Vasilchenko, D. Mondelain, *et al*, Rev. Sci. Instrum. **87**, 083109, 2016.

Contributed Lectures P **Saturday, 9:00**
lecture hall AII

chairperson: McNaughton D.

P1 **Urbanczyk T.,** 9:00
Koperski J.
Diatomic Molecules in Supersonic Expansion Beam Experiment from Separation of Overlapped Profiles to Determination of Interatomic Potential

P2 **Bielska K.,** 9:18
Domysawska J., Wójtewicz S., Cygan A., Masłowski P., Trawiński R.S., Morzyński P., Bober M., Zawada M., Ciuryło R., Lisak D.
Precise Determination of Line Shapes and Positions of Self-perturbed Oxygen B-band Transitions

P3 **Ganpathi N.P.,** 9:36
Sen S.
Unifying Hydrogen Bonding with Vibrational Stark Effect

P4 **Lisak D.,** 9:54
Cygan A., Wójtewicz S., Wcisło P., Zaborowski M., Kowzan G., Masłowski P., Ciuryło R.
Cavity-enhanced Absorption and Dispersion Spectroscopy for Molecular Line-shape Investigations

Contributed Lectures R **Saturday, 11:00**
lecture hall AII

chairperson: Lessari A.

R1 **Gatti D.,** 11:00
Gotti R., Gambetta A., Belmonte M., Galzerano G., Laporta P., Marangoni M.
Comb-assisted Cavity-enhanced Lamb Dip spectroscopy

R2 **Wachsmuth D.,** 11:18
Lesarri A., Herbers S., Grabow J.-U.
A Broad View at High Resolution the Versatile Conformational Landscape of Cyanocycloheptane Unravelled

R3 **Čermák P.,** 11:36
Vasilchenko S., Mondelain D., Kassi S., Campargue A.
Cavity Ring-Down Spectroscopy around 2.3 μm

R4 **Hougen J.T.** 11:54
An Effective-Hamiltonian Approach to Large-amplitude Motions in PF_5, with Potential Application to CH_5^+