#### **INTERNATIONAL WORKSHOP**

# Spectroscopy of methane and derived molecules for atmospheric and planetary applications

Dole, France, 26-28 November, 2012

#### FIRST ANNOUNCEMENT

Dear colleague,

We are very happy to invite you to participate and contribute to the Workshop "Spectroscopy of methane and derived molecules for atmospheric and planetary applications", to be held in Dole, France, from 26 to 28 November 2012. The goal of this meeting is to bring together the experts working in this field and to provide the communities of spectroscopists, astrophysicists and astronomers with the most recent results and the most advanced methods of analysis for various kinds of applications. The workshop will also aim to summarize the current needs in the domain and to engage a large coordination of research projects on the methane and derived molecules.

**Methane** (CH<sub>4</sub>) is a key molecule for many research domains in fundamental and applied sciences. In the Earth's atmosphere, it is present as a pollutant of both natural and anthropogenic origin and is the second greenhouse gas (after carbon dioxide) whose emission should be strongly reduced, according to the Kyoto protocol. It is present in significant quantities in the atmospheres of many Solar System bodies, such as the giant planets, Titan, Triton, Pluto and other Kuiper-Belt objects. In particular, the Cassini-Huygens mission, exploring Saturn's system, and especially Titan, since 2004, has greatly revived the interest in modeling the methane absorption spectrum. Moreover, CH<sub>4</sub> has been detected in some hot astrophysical objects such as brown dwarfs and exoplanets. From the fundamental point of view, methane, as the simplest saturated hydrocarbon molecule, is a prototype for quantum chemistry calculations.

Despite all the scientific interest and applications, until recently, the absorption spectrum of methane was insufficiently explored and modeled, mainly due to the huge complexity of the molecule's excited vibrational polyads, featuring numerous strong rovibrational interactions. The present status of the models makes them still insufficiently complete to meet the goals of most applications. Astrophysical objects with large atmospheres including important methane concentrations (Titan) or hot bodies (brown dwarfs, hot Jupiters, etc.) clearly necessitate the study of highly excited rovibrational levels, which are not presently understood. The interpretation of Earth-observing satellite data now requires high precision laboratory measurements and models for line intensities and collisional broadening coefficients.

On the other hand, the increasing need of precise knowledge of absorption spectra concerns some **methane-derived molecules** (CF<sub>4</sub>, CH<sub>3</sub>Cl, CH<sub>3</sub>Br, CH<sub>3</sub>CN,...) which are known as important atmospheric pollutants. In addition, current (Cassini-Huygens, Hubble Space Telescope) and future (DARWIN) space missions focus an important part of their programs on the identification and spectroscopic characteristics of these molecules. Besides the usual detection in the infrared region, a novel spectroscopic technique operating with terahertz frequencies progresses very rapidly: a HIFI heterodyne reception system is envisaged on the next generation of the IR

observatory Hershel, and three from ten instruments of the Stratospheric Observatory for Infrared Astronomy (SOFIA) use the terahertz region.

The knowledge of spectroscopic parameters of methane and methane-derived molecules is constantly improved due to the development, on the one hand, of new highly sensitive spectroscopic techniques and, on the other hand, of new and powerful theoretical approaches. From the observational point of view, numerous data are constantly flowing from space probes satellites and telescopes observing methane-rich environments and await detailed interpretation. This research is supported, in particular, by the National Research Agency (Agence Nationale de la Recherche – ANR), e.g. via the project CH4@Titan involving four French laboratories.

All papers focusing on experimental spectroscopy of methane and methane-derived molecules, on theoretical calculations (effective Hamiltonians and transition moments, *ab initio* calculations, line positions and intensities, collisional broadening coefficients, etc.), analyses and simulations as well as applications to planetary atmospheres (radiative transfer, concentration measurements, atmospheric chemistry, etc.) are welcome. Main session topics will cover:

- Experimental developments and new experimental results
- Theoretical spectra modeling (line intensities and positions)
- Line shape studies (both experimental and theoretical)
- Reactivity of methane
- Applications to the terrestrial atmosphere and remote sensing of pollutants
- Applications to planetary and stellar atmospheres

You will find hereafter some practical information.

Please send us (<u>Vincent.Boudon@u-bourgogne.fr</u>) an indication of interest for attending and/or presenting your work at this workshop as soon as possible and, in any case, before October 15, 2012.

Participants who are interested could submit their manuscripts in a special Journal of Molecular Spectroscopy issue (V. Boudon, A. Coustenis, Eds) planned to be published in mid-2013.

Hoping to have the pleasure to see you soon in France, With kind regards The Organizers

### **PRACTICAL INFORMATION**

The workshop will be held at "Maison Ramel" (see <u>http://www.maisonramel.com/</u>) in Dole, France.

We can accommodate a maximum of 50 participants.

It will start on Monday, November 26<sup>th</sup>, 2012 at 12:00 am (before lunch) and will end on Wednesday, November 28<sup>th</sup>, 2012 at 2:00 pm (after lunch).

It will feature 10 to 12 invited talks (30', including questions) and 24 to 26 contributed talks (15', including questions), and possibly, some poster presentations, according to the number of participants.

Dole is easily accessible by train from Paris, either by direct TGV (one per day),

- Direct TGV from Paris Gare de Lyon to Dole Ville at 7:57 am,
- Direct TGV from *Dole Ville* to *Paris Gare de Lyon* at 2:00 pm,

or via Dijon (TGV plus TER, several times a day).

A detailed map and list of nearby hotels will be sent to all participants.

All lunches (Monday, Tuesday and Wednesday), coffee breaks, and the Workshop dinner (Tuesday evening) will be offered to all participants. Hotel and travel fees will have to be paid by participants.

More information about Dole and its region: http://www.tourisme-paysdedole.fr/welcome-to-dole.htm

## **SPONSORS**

This workshop is organized with the help of:

- Pôle de Recherche et d'Enseignement Supérieur (PRES) de Bourgogne Franche-Comté.
- Région de Franche-Comté
- Agence Nationale de la Recherche
- CNRS
- EuroPlaNet European Network
- Laboratoire Interdisciplinaire Carnot de Bourgogne
- Institut UTINAM

# Special issue of *Journal of Molecular Spectroscopy* focusing on methane spectroscopy and its applications to planetary atmospheres, including the Earth's

Methane (CH<sub>4</sub>) is a key molecule for many research domains in fundamental and applied sciences. In the Earth's atmosphere, it is present as a pollutant of both natural and anthropogenic origin and is the second greenhouse gas (after carbon dioxide) whose emission should be strongly reduced, according to the Kyoto protocol. It is present in significant quantities in the atmospheres of many Solar System bodies, such as the giant planets, Titan, Triton, Pluto and other Kuiper-Belt objects. In particular, the Cassini-Huygens mission, exploring Saturn's system, and especially Titan, since 2004, has greatly revived the interest in modeling the methane absorption spectrum. Moreover,  $CH_4$  has been detected in some hot astrophysical objects such as brown dwarfs and exoplanets. From the fundamental point of view, methane, as the simplest saturated hydrocarbon molecule, is a prototype for quantum chemistry calculations.

Despite all the scientific interest and applications, until recently, the absorption spectrum of methane was insufficiently explored and modeled, mainly due to the huge complexity of the molecule's excited vibrational polyads, featuring numerous strong rovibrational interactions. The present status of the models makes them still insufficiently complete to meet the goals of most applications. Astrophysical objects with large atmospheres including important methane concentrations (Titan) or hot bodies (brown dwarfs, hot jupiters, etc.) clearly necessitate the study of highly excited rovibrational levels, which are not presently understood. The interpretation of Earth-observing satellite data now requires high precision laboratory measurements and models for line intensities and collisional broadening coefficients.

The situation has recently improved, however, due to the development, on the one hand, of new highsensitivity spectroscopic techniques and, on the other hand, of new and powerful theoretical approaches. From the observational point of view, numerous data are constantly flowing from space probes satellites and telescopes observing methane-rich environments and await detailed interpretation. The aim of this special issue is to gather papers covering all the fields of methane spectroscopy and its applications.

All papers focusing on experimental aspects of methane spectroscopy, on theoretical calculations (effective Hamiltonians and transitions moments, *ab initio* calculations, etc.), analyses and simulations (line positions and intensities, collisional broadening coefficients, etc.), as well as applications to planetary atmospheres (radiative transfer, concentration measurements, atmospheric chemistry, etc.) that meet the publication standards of the *Journal of Molecular Spectroscopy* will be considered. All papers will be subject to the normal submittal (<u>http://ees.elsevier.com/jms/</u>) and refereeing process.

Deadline for submission of manuscript: January 31, 2013.

Expected publication date: August 2013.

Guest editors:

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