EXO-PLANETARY HIGH-TEMPERATURE HYDROCARBONS BY EMISSION AND ABSORPTION SPECTROSCOPY (e-PYTHEAS PROJECT)

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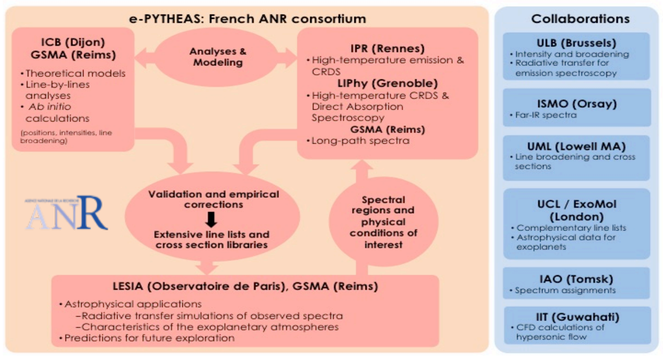
PROJET FINANCÉ PAR L'ANR - PROJECT FUNDED BY THE ANR

The project / Generalities

The e-PYTHEAS Project & Consortium

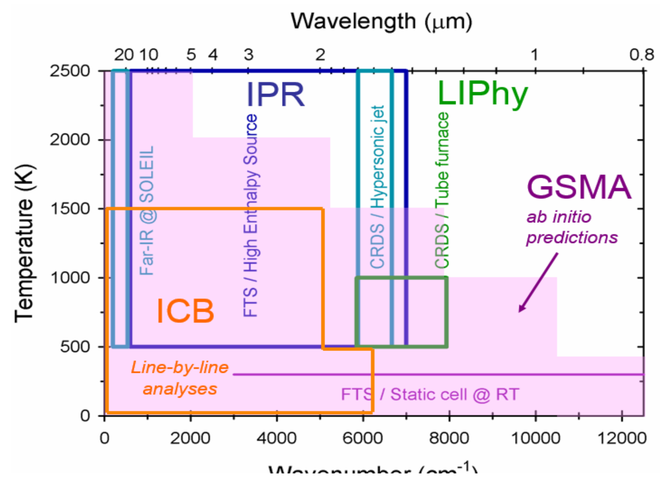
- Multidisciplinary between molecular physics, theoretical chemistry and astrophysics.
- Comprehend and model the radiative properties of hot gases.
- Allow for the analysis and interepretation of data pertaining to the atmospheres of exoplanets (like « hot Jupiters »)) from the ground and space.



Goals of the project

- $^{12}CH_4$, $^{13}CH_4$, CH_3D, C_2H_2, C_2H_4, C_2H_6
- Spectral region 0.8–17 µm and up to T=2500 K
- Update incomplete current databases
- Emission spectroscopy, CRDS technique
- High-level calculations and theoretical models
- Improve on current modeling with new parameters and input data to enhance exoplanetary spectral analyses (ARIEL)

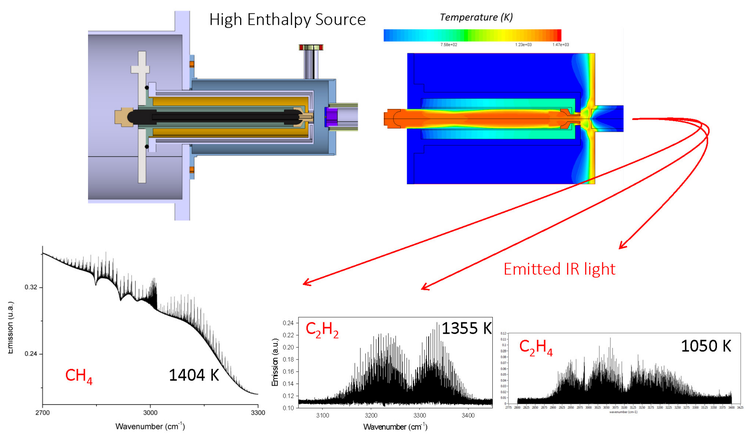
Spectral domains



IPR / Rennes

High-Resolution LTE Emission Spectroscopy

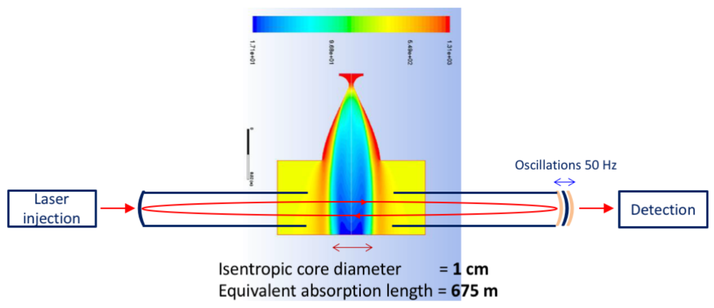
B. Amyay *et al* JCP 2016 ; B. Amyay *et al* JCP 2018
Collaboration: IPR, ICB, ULB



Non-LTE absorption spectroscopy

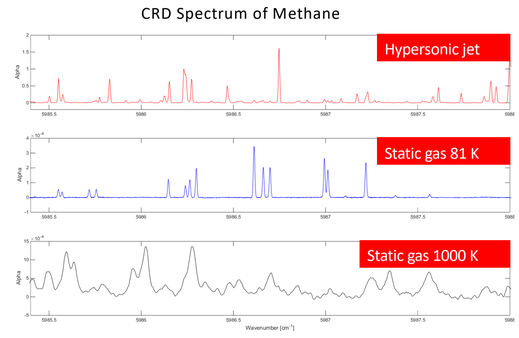
N. Suas-David *et al* CPL 2016
Cavity Ring-Down Spectroscopy coupled to a hypersonic de Laval nozzle

Collaboration: IPR, LiPhy, IIT Guwahati, ANU Canberra



Non-LTE absorption spectroscopy

Eszter Dudas *et al.* (first results)
Low translational temperature: reduced Doppler broadening
Low rotational temperature (10 < Trot < 100 K) : spectral simplification
High vibrational temperature (Tvib > 1000 K) : hot band contribution



LiPhy / Grenoble

High temperature (1000 K) Direct Absorption Spectroscopy

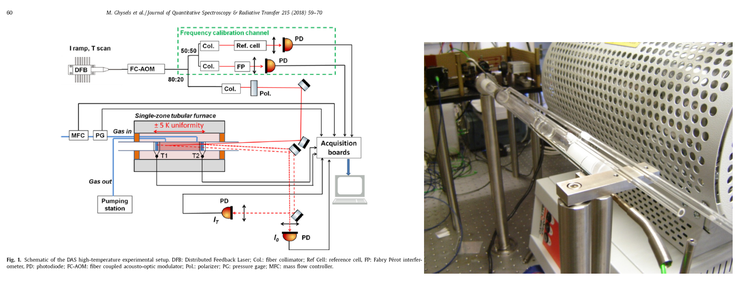
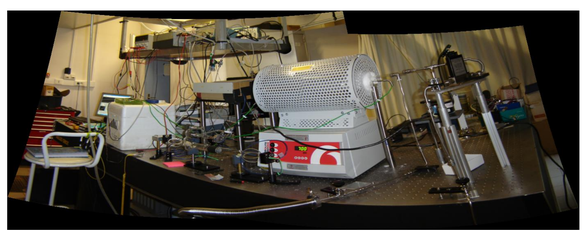


Fig. 1. Schematic of the DAS high-temperature experimental setup. DFB: Distributed-Feedback Laser; Col.: fiber collimator; Ref Cell: reference cell, FP: Fabry Pérot interferometer, PD: photodiode; FC-AOM: fiber coupled acousto-optic modulator; Pol.: polarizer; PG: pressure gage; MFC: mass flow controller.



The Tetradecad region

Derivation of the lower state energy level by the 2-Temperature method

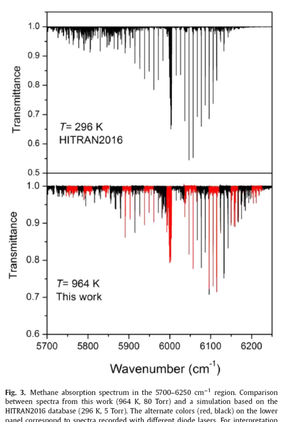


Fig. 3. Methane absorption spectrum in the 5700-6250 cm^{-1} region. Comparison between spectra from this work (964 K, 80 Torr) and a simulation based on the HITRAN2016 database (296 K, 5 Torr). The alternate colors (red, black) on the lower panel correspond to spectra recorded with different diode lasers. For interpretation

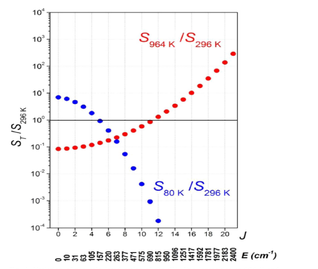


Fig. 4. Variation of the calculated ratios of the CH_4 line intensities at 964 K and 296 K (red dots) and at 80 K and 296 K (blue dots) versus the rotational quantum number of the lower state. The corresponding approximate lower state energies are given.

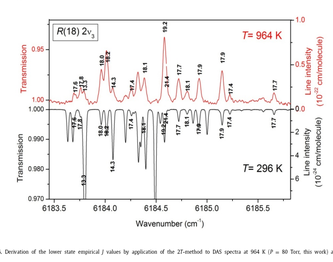


Fig. 6. Derivation of the lower state empirical J values by application of the 2T-method to DAS spectra at 964 K (P = 80 Torr, this work) and at 297 K

Comparison to the CH_4 calculated databases

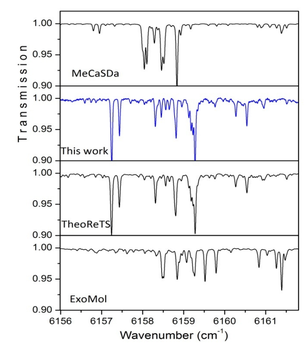


Fig. 9. Comparison of the high temperature methane absorption spectrum in the region of the $R(15)$ transitions of the $2\nu_3$ band (T = 964 K, P = 80 Torr, l = 40 cm).

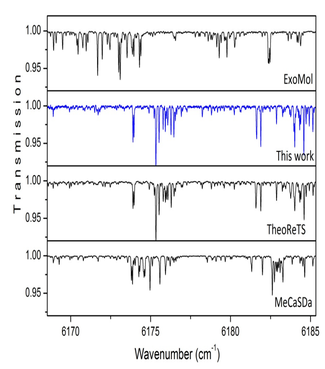


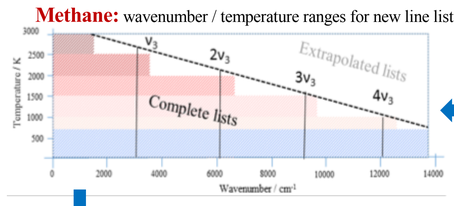
Fig. 11. Comparison of the high temperature methane absorption spectra in the region of the $R(17)$ transitions of the $2\nu_3$ band.

GSMA / Reims

Reims & Tomsk Universities: Theoretical line lists for astrophysical applications

Aim: Global *ab initio* predictions of IR high-temperature spectra PH3, CH4, C2H4 – available

Methane: wavenumber / temperature ranges for new line lists: C2H2, GeH4, SiH4, CH3X, C2H6 … – in progress



Completeness: 150 billion lines (T=3000K)

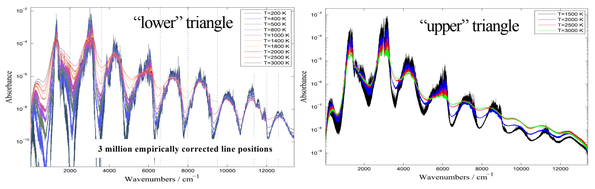
data compression via "*super-lines*"approach: *Rey et al , JMS,327,138(2016)*

Few million strong lines + quasi-continuum ➔

Reims-Tomsk TheoReTS database

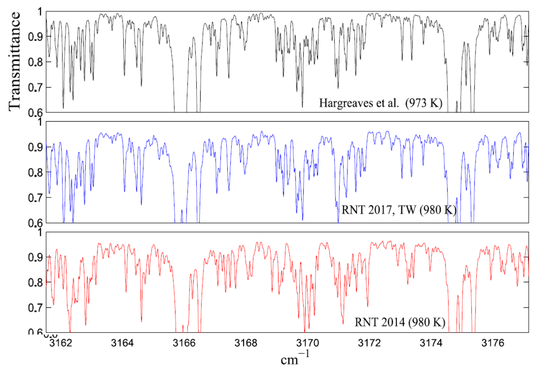
http://theorets.univ-reims.fr

High-T methane absorbance simulations



Rey, Nikitin, Tyuterev, APJ 847, 105 (2017)

High-T validations: comparisons theory – experiment (methane)



Laboratory experiment
Hargreaves, Bernath et al. APJ 2015

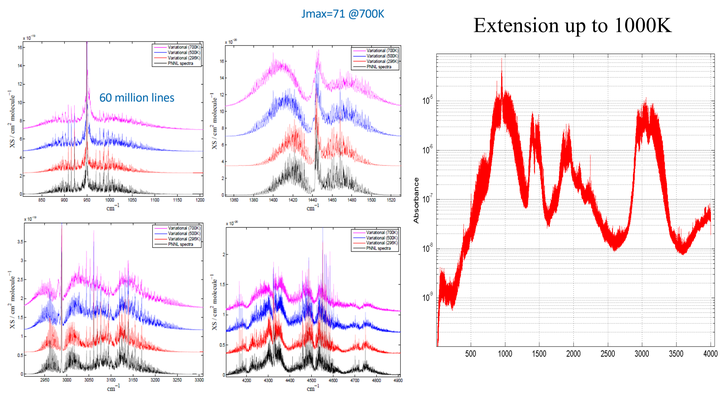
NEW LISTS
Reims-Tomsk 2017
Rey, Nikitin, Tyuterev APJ 847, 105 (2017)
http://theorets.univ-reims.fr
Reims-Tomsk 2014
Rey, Nikitin, Tyuterev, APJ , 789,1 (2014)

Complete lists up to 3000 K (all hot band included) for high-resolution astrophysical applications:

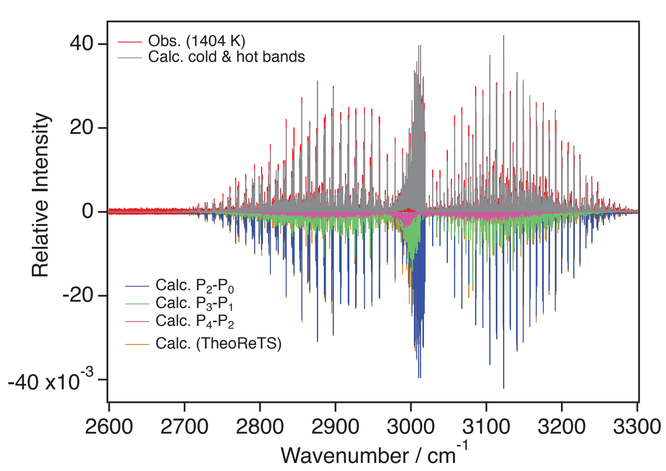
Designed for resolving power: R = 10^5–10^6 in the range up to 3500 cm^{-1}, R= 10^5 up to 6200 cm^{-1}, R= 10^4 up to 7800 cm^{-1} , R = 10^3 around 10000 cm^{-1}.

Complete ethylene (C_2H_4) line lists up to 700K

Rey, Nikitin, Delahaye,Tyuterev, A&A, 594 (2016) → TheoReTS database

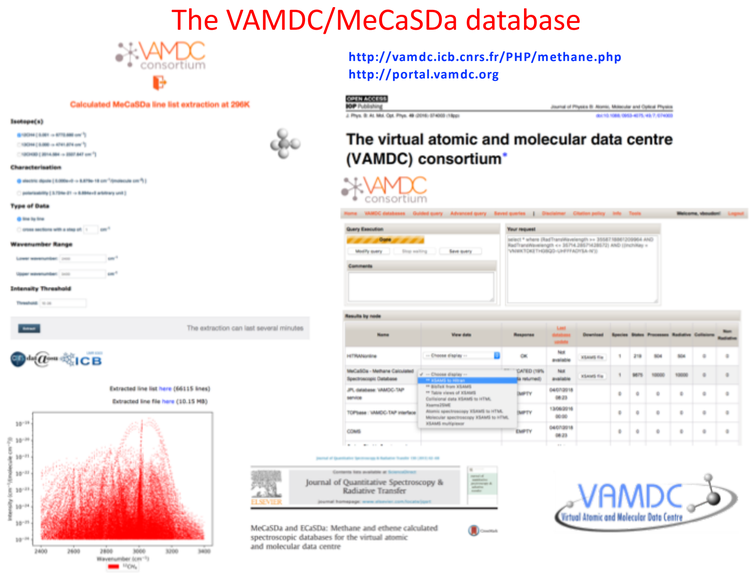


Pentad region: simulation with "all" hot bands

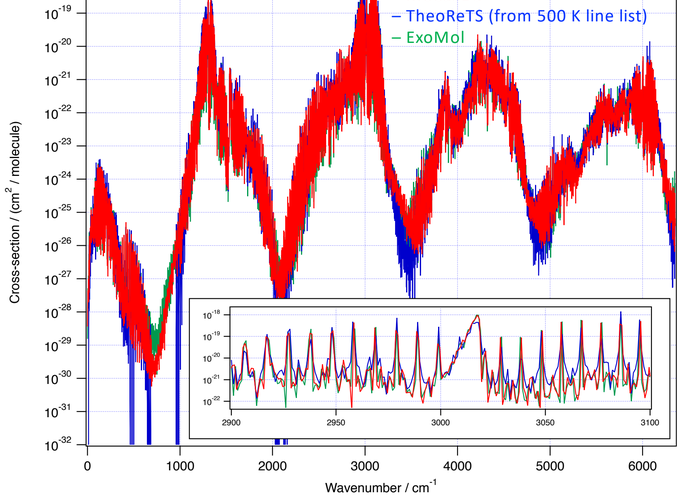


The VAMDC/MeCaSDa database

http://vamdc.icb.cnrs.fr/PHP/methane.php
http://portal.vamdc.org



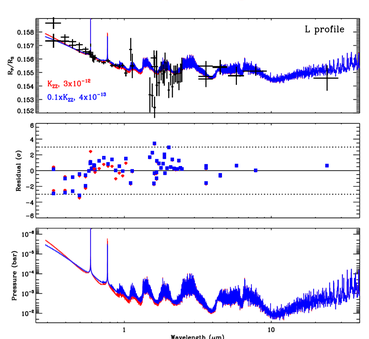
Comparison with other databases



ICB / Dijon

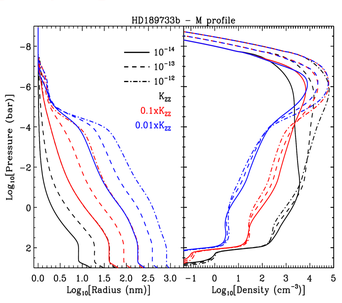
LESIA / Meudon & GSMA / Reims

Examples of modeling in progress, GSMA



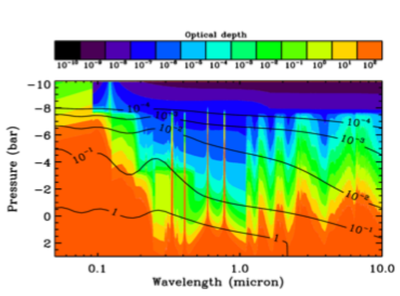
Simulated and observed transit depth for the atmosphere of **HD189733b** including photochemical aerosols.

Lavvas & Koskinen 2017.



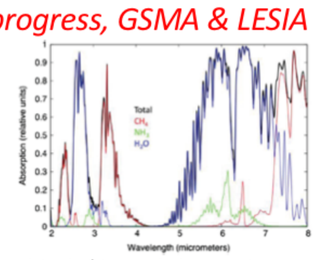
Average size and density of photochemical aerosols in the atmosphere of **HD 189733 b.** Lines and colors present sensitivity on aerosol mass flux and atmospheric mixing

Examples of modeling in progress, GSMA & LESIA



Comparison of gas (color contour) and aerosol (black lines) opacities for the atmosphere of **HD 189733 b**.

Lavvas & Koskinen 2017.

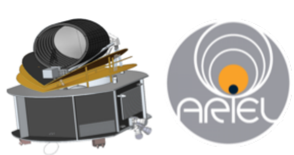


A typical transmission spectrum, observed in primary transit, for a temperate Jupiter (T = 350 K). Jupiter-like relative abundances are assumed for the molecules in the troposphere below the clouds, and no condensation is assumed for H_2O: H_2O:CH_4:NH_3 = 2.0:1.0:0.1. The full scale is equal to the amplitude of the calculated absorption signal.

Encrenaz, Tinetti & Coustenis 2017.

Perspectives / Expected impact

For exoplanets and other research fields



- ARIEL selected as ESA's M4 (medium class) mission to fly in 2028!
- Produce experimental and theoretical data directly applicable to the observations.
- Study and understand in detail the characteristics of exoplanets.
- Understand their origin and evolution processes.
- Impact on other fields: combustions, …