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Exo-PlanetarY high-Temperature Hydrocarbons by Emission and Absorption Spectroscopy (the e-PYTHEAS project)

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Abstract

The e-PYTHEAS is a multidisciplinary project which combines theoretical and experimental work with exoplanet modelling applications. It sits on the frontier between molecular physics, theoretical chemistry and astrophysics. It aims at enhancing our understanding of the radiative properties of hot gaseous media to allow for improved analysis and interpretation of the large mass of data available on the thousands of exoplanets and exoplanetary systems known to date. Our approach is to use theoretical research validated by laboratory experiments and to then inject it into models of the atmospheres of the giant gaseous planets in the solar system and other planetary systems. This will help to analyse data and address essential questions on the formation and evolution of planetary systems.

1. Introduction

Most of the exoplanets are hot and therefore their spectra are very complex and contain numerous unassigned features [1]. The large number of exoplanetary observations acquired via a combination of new, larger telescopes and space missions will therefore only be exploitable if and only if the adequate laboratory and theoretical data are made available for their analysis, without the current limitations.

Our consortium of five French laboratories and multiple associated partners proposes to improve the existing high-temperature spectroscopy data for several molecular species detected in exoplanets. Our strategy consists in producing experimental and theoretical data that are then applied to observations.

The provision of infrared (IR) laboratory data of methane, acetylene, ethylene and ethane, between 500 and 2500 K will help to refine thermal profiles and provide information on the gaseous composition, the hazes and their temporal variability.

2. Present status

Currently available data are insufficient in several ways:

- All datasets are affected by large gaps below 1.65 μm, an important region in observations;
- High-temperature spectroscopic data cannot be extrapolated from low-T atmospheric databases such as HITRAN and GEISA. Such extrapolations fail to reproduce high *J* rovibrational transitions and hot band transitions involving highly excited

vibrational levels and thus opacity calculations at high temperatures present large uncertainties;

Accurate molecular models are still missing to generate complete high-T line lists for hydrocarbon absorbers which dominate the spectrum of brown dwarfs, exoplanets and Asymptotic Giant Branch stars and play a primary role in the physical chemistry of their outer atmospheres.

3. Methodology

Based on state-of-the-art theoretical calculations and new models, extensive line lists (including positions, intensities, profiles, *etc*.) will be generated and validated by laboratory experiments: (i) emission spectroscopy at thermal equilibrium above 500 K in the 1.4–17 µm region [2]; (ii) high sensitivity laser absorption spectroscopy by Cavity Ring Down Spectroscopy (CRDS) in non-thermal equilibrium and hypersonic relaxation in the 1.5–1.7 µm region [3]; (iii) direct absorption and CRDS at high sensibility from 500 to 1000 K in the 1.26–1.71 µm region for weak line measurements [4]; (iv) room temperature absorption down to 0.8 µm to reach highly excited vibrational states. These complementary interdisciplinary researches will permit a breakthrough towards interpretation of high-resolution exoplanetary observations (see Figure 1).

The feasibility of this challenging project is attested by our previous successful experience and established expertise in experiments, spectra analyses and theory: our low-T experimental data and *ab initio* predictions for methane, ethylene and their isotopologues are currently the most accurate available [5].

4. Expected results

The first CH_4 line lists produced already at 2000 K above 2 µm within this program show good agreement with observations [6], as well as C_2H_4 hot–T list up to 700 K [7].

At the end of our project, the scientific community will benefit from experimental and synthetic spectra in the 0.8–17µm region for hydrocarbons and their isotopologues ($^{12}CH_4$, $^{13}CH_4$, CH_3D, C_2H_2, C_2H_4 and C_2H_6) in large temperature ranges (up to 2500 K). For each of these species, we will provide rovibrational assignments, broadening coefficients (by H_2) and cross-sections, directly usable in radiative transfer codes.

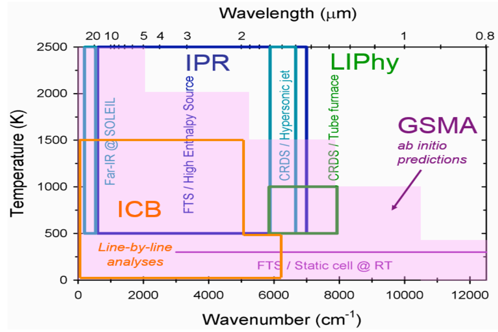

Figure 1: Schematic of the project's experimental and theoretical set up, available means and proposed contributions per team involved. The spectral zones indicated in pink and orange correspond to the theoretical work in the case of methane.

Our consortium seeks to establish the framework for a large international collaboration, which will benefit from the sharing of unique access to observations, special facilities, manpower, software and experimental means.

For more information, see the e-PYTHEAS Web site:

http://e-pytheas.cnrs.fr

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