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Atmosphere in a Test Tube

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Abstract. The ancestor philosophers' dream of thousand of new world is finally realised: more than 1800 extrasolar planets have been discovered in the neighborhood of our Sun. Most of them are very different from those we used to know in our Solar System. Others orbit the Habitable Zone (HZ) of their parent stars. Space missions, as JWST and the very recently proposed ARIEL, or ground based instruments, like SPHERE@VLT, GPI@GEMINI and EPICS@ELT, have been proposed and built to measure the atmospheric transmission, reflection and emission spectra over a wide wavelength range of these new worlds. In order to interpret the spectra coming out by this new instrumentation, it is important to know in detail the optical characteristics of gases in the typical physical conditions of the planetary atmospheres and how those characteristics could be affected by radiation driven photochemical and bio-chemical reaction. Insights in this direction can be achieved from laboratory studies of simulated planetary atmosphere of different pressure and temperature conditions under the effects of radiation sources, used as proxies of different bands of the stellar emission. "Atmosphere in a Test Tube" is a collaboration among several Italian astronomical, biological and engineering institutes in order to share their experiencece in performing laboratory experiments on several items concerning extrasolar planet atmospheres.

Key words. Extrasolar Planets – Laboratory Analogs

1. Introduction

The project "Atmosphere in a Test Tube" (ATM_ITT), started one year ago aims at preparing a background of data in order to interpret the results that are going to come out from both ground and space based new generation instruments. A short list of these instruments comprises SPHERE (Beuzit et al. 2014), the planet finder of VLT, that will be dedicated to study warm and young planets, GPI (Larkin et al. 2014) the same kind of instrument mounted to the Gemini Telescope, other future instruments like PCS, the evolution of SPHERE for E–ELT, and new space mission like JWST (Clampin et al. 2014a,b), CHEOPS (Former et al. 2014), PLATO and the very recently proposed ARIEL. The project associate several Italian structures of the ”Istituto Nazionale di Astrofisica” (INAF) and of the ”Istituto Nazionale di Fisica Nucleare” (INFN) leaded by the Astronomical Observatory of Padova (INAF- OAPD). The main aim of ATM_ITT is the study and the simulation of atmosphere of extrasolar planets both by means theoretical models and laboratory experiments in order to prepare a database of extrasolar planet atmosphere spectra. So, the activities of ATM_ITT are focalized in the followings:

- applications of Solar System Planetary Atmospheres studies to exoplanets
- planning of laboratory experiments to simulate planetary atmospheres with different thermodynamical parameters and star irradiation
- use of the Virtual Atomic and Molecular Data Centre (VAMDC) to get atomic and molecular data and other spectroscopic databases (HITRAN, CSDS etc.) for planetary atmosphere spectra simulations
- planning the development and use of codes in simulating ”ad hoc” planetary atmospheres
- exoplanets atmosphere formation simulations

With this aims our project is separated in three different paths. The first part concerns the laboratory measurements of the optical characteristics of Solar System planet and extrasolar planet atmospheres built or modified (see ahead) in laboratory. The second part would like to induce atmosphere alteration by biological non equilibrium phenomena induced by irradiation of biota with sources in order to simulate different spectral type stars. Finally the third concerns the study of modification of those atmospheres by photochemistry induced by different irradiation intensity and spectra in order to simulate the several host star spectral types. The bonanza of extrasolar planets found in so far (up to 1786 planets, Schneider et al. 2011) unveils a large diversity in the type of planets not known in our Solar System: hot Jupiters, hot Neptune, Jupiters and Saturns down to the smaller companion like Earth and super Earths. The result is that we have a huge parameter space to take into account in order to simulate the atmosphere of extrasolar planets. To try to simplify, assuming thermochemical equilibrium and don’t taking into account other modification process (like photochemistry and vertical transport etc.) or migration effects, we consider small temperate and cold (icy) planets those that have mass less than 10 Earth masses and a radius less than 2 Earth radius (see Figure 1). On the other hand, Jupiters and Neptunes, with masses greater than 10 Earth masses and with radius greater than 2 Earth radius, can be considered both as giant planets (atmospheric composition is independent by their masses).

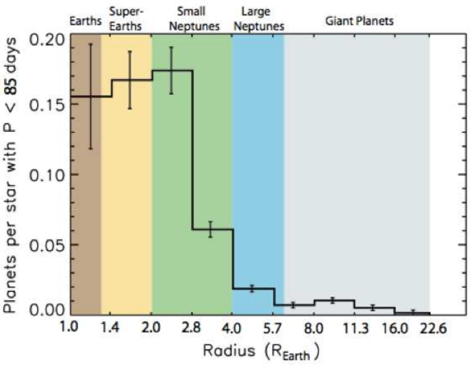

Fig. 1. Histogram of radii of Extrasolar planet candidates by Kepler (Fressin et al. 2013)

Following Tinetti et al. (2013) we use the normalized distance D_N to the star, as the distance of the planet from the Sun at which the planet itself receives the same flux at its distance D from the host star:

$$D = D_N (\frac{R_*}{R_\odot})(\frac{T_*}{5770})^2$$

Fig. 2. The cavity Ring Down (CRD) Cell

In this way we can associate values of interesting parameters to different planet (see Table 1) and use them for the simulation of atmospheres. The columns in the Table are the following:

1. The normalized stellar distance
2. The equilibrium temperature of the surface of the planet considering an albedo of 0.3 and rapid rotating planet
3. The mass limit of the planet
4. The radius of the planet (see Figure 1)
5. The type of the planet
6. The approximate value of the pressure evaluated by the Stevino Formula. This value should be multiplied by the mass of the atmosphere of the planet.
7. The main atmospheric components based on their mass and their equilibrium temperature (as already told in text, no complexity are take into account).

2. Giant planet atmospheres

The simulation of a planetary atmosphere has been planned to be conducted in the laboratory with chemical composition, temperature and variable density in order to measure their optical characteristics. The preliminary laboratory measurements have been performed on the absorbance of mainly CO_2 and SF_6, by using the FTIR spectrometer and Cavity Ring Down (CRD) cell (see Figure 2).

This is a really sensitive technique able to measure absorption coefficient up to about 10-8 cm^{-1} in the spectral range of $1 - 12\mu m$. The Cavity Ring Down (CRD) technique is able to reproduce an optical path of some tens of km into a cell of 50 cm of length. In order to reproduce the different condition of a real atmosphere, it is possible to vary the temperature of the cell in both direction and insert gasses with pressure in the range between 0 and 50 bar. The CRD cell will be mounted inside a vacuum chamber and it will operate with cooling or warming system and illuminated by a tunable laser with appropriate optics and detectors. To evaluate the sensibility of the experimental, just before to simulate complex giant planet atmosphere, we try to simulate the Venus atmosphere. The experiment investigated the optical properties of a CO_2 atmosphere with traces of other gasses like water vapor, CO, O_2 and other gasses. We found that with this technique, exploiting a tunable laser at $1.18\mu m$, it is possible to detect 50 ppm of water vapor in a CO_2 atmosphere at 40 bar of pressure.

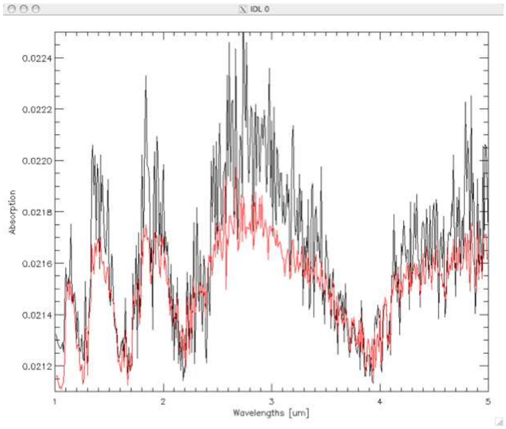

Fig. 3. Absorption spectra obtained with TAU CODE. In these spectra the only absorber is H_2O.

In the mean time some radiative transport codes (LibRadTran Mayer et al. (2005), SASKTRAN Bourassa et al. (2008), TAU-CODEHollis et al. (2013) just to mention some) have been analyzed and compared in order to reproduce Hot Jupiter atmospheres. These codes require absorption coefficients as input that it is possible to evaluate by some ”line by line” numerical codes (e.g. RFM: www.atm.ox.uk/RFM) starting from data available in atomic and molecular database like HITRAN (Rothman et al. 2013) (HITEMP for higher temperature Rothman et al. 2010), GEISA (Jacquinet-Hussan et al. 2011) and EXOMOL (Hill et al. 2014). Some simulations have been performed

Table 1. Grid of parameters for atmosphere simulation

DN (AU) (AU)	Teq (K) (K)	Mass ($M_\oplus$)	Radius ($R_\oplus$)	Kind	P0 (kPa)	Atm. Comp. (Tinetti et al. 2013)
[-6pt] 0.05	1221	≤ 10	≤ 2	Hot Rocky	$10^{-3} - 10^{-2}$	Si/Mg gas/liquid?
0.1	870	≤ 10	≤ 2	Warm Rocky	$10^{-3} - 10^{-2}$	CO_2,N_2, CO, H_2O, O_2
1.0	273	≤ 10	≤ 2	Temp. Rocky	$10^{-3} - 10^{-2}$	
5.0	122	≤ 10	≤ 2	Icy Planets	$10^{-3} - 10^{-2}$	N_2, CH_4, CO
20.0	61.0	≤ 10	≤ 2	Icy Planets	$10^{-3} - 10^{-2}$	
0.05	1221	≥ 10	≥ 2	Hot Giants	$\geq 10^{-3}$	H_2, H_2O, CO, N_2
0.1	870	≥ 10	≥ 2	Warm Giants	$\geq 10^{-3}$	CH_4, N_2
1.0	273	≥ 10	≥ 2	Warm Giants	$\geq 10^{-3}$	H_2, CH_4, NH_3, H_2O
5.0	122	≥ 10	≥ 2	Cold Gaseous Giants	$\geq 10^{-3}$	H_2, CH_4, NH_3, H_2O
20.0	61.0	≥ 10	≥ 2	Icy Giants	$\geq 10^{2}$	H_2, CH_4

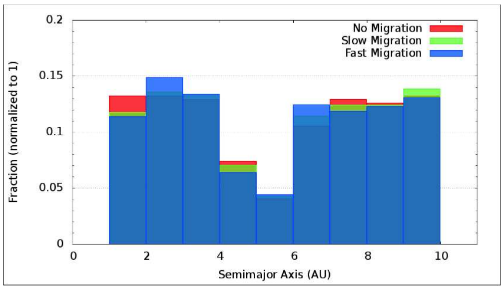

Fig. 4. Fraction of accreted solid material from a protoplanetary disk extending between 1 AU and 10 AU by a Jupiter-sized planet forming at 5.2 AU. In the cases including migration, the migration stops at 0.7 AU.

using TAU CODE (see Figure 3). Other simulations have been performed using EXOMOL spectral data of CO, CO_2 and CH_4 Moreover the calculation of cross sections of H_2O and CO have been performed in a short spectral range, using the spectral parameters provided by HITEMP, and then they were compared with the results available online from EXOMOL. Furthermore we assess the possible link between the collisional evolution of exoplanets and their atmospheric composition. This activity tackles the problem by two points of view for both of which no studies are currently available in literature.

The former is the post-formation, late accretion phase and the latter is the secular collisional evolution of hot Jupiters due to the impacts of star-grazing comets. Both aspects were addressed using the N–Body code Mercury 6.2, modified to include the possibility of planetary migration. To study the effects of late accretion a set of simulations of the collisional evolution of a Jupiter-size planet were performed, both with or without migration. The results revealed a previously unknown significant role of the inner, volatile depleted regions of proto–planetary disks (see Figure 4), which can provide ∼ 30 – 40% of the accreted material (i.e. mostly Si-based and Fe-based minerals). To study the effects of impacts by star-grazing comets, the hot Jupiter HD 189733 b was used as a template together with a family of comets modeled after the Sungrazing comets observed by SOHO in the Solar System. The results obtained highlighted the possibility of non-equilibrium effects in exoplanetary atmospheres due to a sustained delivery of exogenous materials by the impacting comets if the impact rate is high enough.

2.1. Temperate rocky planets

Super Earths are a new family of rocky exoplanets with mass ranging between 1 and 10 $M_\oplus$. While the lower bound is obvious for historical reasons the upper bound is somewhat arbitrary. It is due by the physical argument that at about $10M_\oplus$ and upper planets can retain Hydrogen and Helium in their atmospheres. Since the first Super Earth discovered GJ876d in the 200521 a set of about 60 of these special planets are confirmed up to now. Moreover the warm super Earth orbiting the M star GJ 1214b has been the first super Earth to be observed spectroscopically (Bean et al. 2010). In order to maximize the finding of habitable planets with transit search, a lot of surveys have been dedicated to search for Earth size (super Earths) planets around M stars. Due to a more favorable ratio between the radii, some small rocky companion have been discovered in the Habitable zone of these red and cold stars. In this framework it is interesting to search for biosignatures in the atmosphere of these new worlds. In particular it seems interesting to explore how the irradiation quality of a M star modifies (if it does it) the oxygen production of photosynthetic bacteria. This could be done using a environmental simulator which can control the temperature and the pressure of a mixture of gasses in order to carry out photobiology experiments by irradiating organic samples like photosynthetic bacteria. This would highlight the effects of the interaction among organics, atmospheres and radiation, allowing the identification of biomarkers and biosignatures in the atmospheric spectra. The experimental investigation (Erculiani et al. 2014) make use of environmental chamber with dedicated atmospheric cells in which the gas mixture as well as the organic materials will be confined in order to be irradiated and analyzed. Eventually the related effects will analyzed off line in a hermetic cell for measuring the absorption spectra in order to measure the optical constants and then the gas spectrum.

The instrument that will be used to carry out the experiment is LISA-SAM (see Figure 5). It is composed of a steel cylinder inside which are located six aluminum cells (volume=0.250 l) topped by a suprasil glass window transparent from UV to NIR. Inside the cells, biological samples can be placed onto a Petri dish. Cells are connected with the outer part by pipes with mechanical filters to let the gas to course and avoid biological material to go inside the cryostat chamber. Depending by the necessity, the temperature in the chamber could be raised (up to 100° C) acting on a resistance or lowered down to −25°C by means a closed circuit with liquid nitrogen (or glycol). As biological samples should be kept at a mean temperature of 20°C (the "life friendly" temperature), a Peltier cell could be used instead. The experiment will aim to measure the abundance of gaseous bioproducts (O_2) of photosynthetic bacteria placed in a simulated environment of a planet orbiting around an M star. The bacteria (*Chroococcidiopsis* and *Acharyochloris Marina*) have been selected on the basis of the know absorbance properties out of a lot of specie. In a parallel experiment, the study of spectral biomarkers or biosignatures on the gas mixtures induced mainly by UV irradiation has been performed at the DAΦNE-L laboratory at the LNF-INFN. DAΦNE-Light is a synchrotron facility operating with synchrotron and standard sources in the infrared and UV-VIS energy range is open to external users. Organic materials or bacteria can be irradiated by UV synchrotron radiation (or lamps) and real-time FTIR analysis can be carried out to follow the kinetics and the spectral evolution of the irradiated samples. Related effects on the atmospheres can be analyzed off line moving the gas mixtures inside a hermetic cell that can be arranged in the experimental setup at the INAF-IAPS lab for measuring the absorption

Fig. 5. The INAF Padova Environmental Chambre

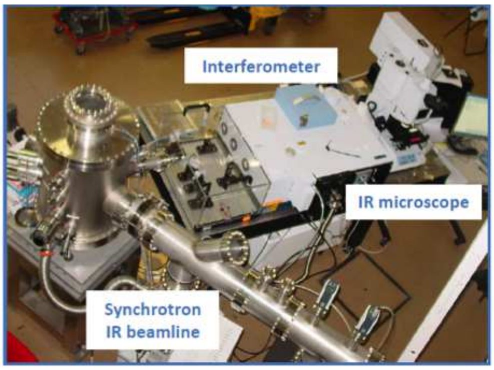

Fig. 6. The SINBAD UV-VIS source (180-650 nm)

spectra in order to find out the optical constants and then the gas spectrum. The study of the effects of radiation on biological systems (DNA, cells, tissue) is closely related to the possibility of being able to monitor in real time and in-situ modifications induced by radiation at molecular level. Infrared micro-spectroscopy is a non-destructive technique capable of measuring the molecular composition of the various biological systems with a micrometric spatial resolution. In addition, it is possible to obtain images of the molecular systems under investigation by using a multi-channel detector (Focal Plane Array).

On the SINBAD synchrotron beam line (see Figure 6) an experimental station dedicated to irradiation of different materials with UV radiation (conventional and synchrotron) is installed. The first testing experiments have shown that it is possible to follow in real time the degradation of nucleic acids, highlighted by the spectral variation of the components relating to the different chemical bonds. It is possible to perform this type of analysis also on tissues or cells, that require a microfocused beam and a magnifying optics, through the use of an infrared microscope.

2.2. Photochemestry induced modification of planetary atmosphere

Montecarlo models for multipath transmittance are needed to simulate exoplanet spectra collected by a spectroscopy based space mission like for example ARIEL. A suitable strategy to validate the models can be:

- simulating Solar System planets as investigated by ARIEL;
- considering different input to available GCM models for different class of exoplanets;
- assessing the variability of the physical quantities that ARIEL will observe, through the measured data and theoretical evaluations (e.g. GCM);
- evaluating the impact of the expected exoplanet scale of eights on the models;
- applying Bayesian formalism to evaluate retrieval capabilities.

Atmospheric composition of exoplanets is linked to the formation and evolution of the systems that host them. However, as in all inverse problems, such a link is not easy to unfold. Giant planets offer a unique opportunity to investigate the relationship between formation, evolution and atmospheric composition, as is shown by the case of our Solar System. We plan to investigate how tools and models developed for the Solar System case can be applied to the study of extrasolar planets. Assessing what are the sources and the composition of the materials accreted by the forming giant planets will be crucial to constrain their effects on atmospheric compositions. Presently, we are conducting a case study using the data available on Jupiter as a planetary analogue, to preliminary test the sensitivity of the methods we intend to use for the exoplanets. So a 1D spherical radiative transfer model applicable to describe transmission spectra of close-in extrasolar planets was implemented. The model requires temperature and pressure profiles of the atmosphere, together with the volume mixing ratios of the atmospheric constituents. All these quantities are free to vary within the atmosphere as functions of the altitude. The microphysics of the atmosphere is treated in detail. In particular, molecular absorption coefficients are computed as functions of pressure and temperature. The model allow the use of different line profiles, including standard ones like the Voigt function and other kind of description, like the Van Vleck – Weisskopf profile valid under the assumption that collisions are infrequent but sufficient strong to change the orientation of the molecular dipole moment in a fully random way. The code, validated against pre-existing models, will be used in the development of auxiliary routines handling micro- and macrophysics. At the end of the validation phase, the radiative transfer module itself shall be upgraded to a 3D geometry, incorporating multiple scattering. We shall consider vectorial radiative transfer through a suitable MonteCarlo technique. Furthermore, in order to start with photochemical experiment, we study the feasibility of a cell in which a mixture of gases ("the atmosphere") will be confined and irradiated with different radiation sources. Materials, pumping system, sizes and design of the cell have been investigated for the construction. The gas mixing line of the LIFE laboratory has been assembled and there is an ongoing activity for its testing and calibration (see Figure 7). The mixing line will be used to prepare the mixture of gasses. Furthermore the modeling of effects of high energy radiation on planet atmospheres is on going. Young stars are powerful X-ray emitters (see Figure 8).

X-rays have a larger penetration depth than UV photons, and they induce in the gas a chemistry with peculiar features, mainly driven by a cascade of secondary electrons, following the slowing-down of the primary in the atmosphere. a) A photo-chemical model of X-ray dominated regions has been constructed, and there is an ongoing activity to validate the code against the important problem of the detection of IR signatures from nascent molecular hydrogen. b) Subsequently, the code will be applied to the atmosphere of exoplanets, known to be illuminated by intense X-ray fields.

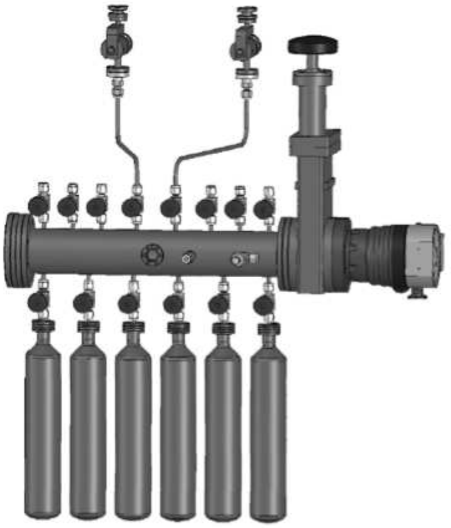

Fig. 7. Gas Line sketch

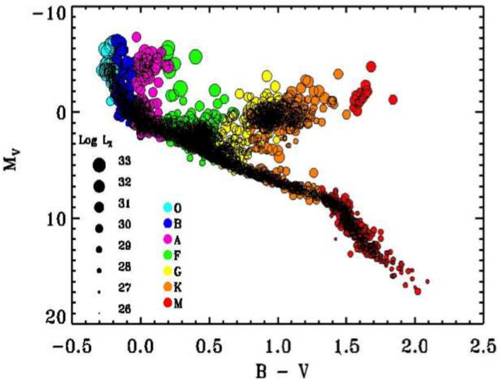

Fig. 8. X-Ray emission along the HR diagram

3. Conclusions

The main characteristics of the project "Atmosphere in a Test Tube" have been outlined. Furthermore we shown the synergy and the possible application in order to interpret future data that will gather by space mission.

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