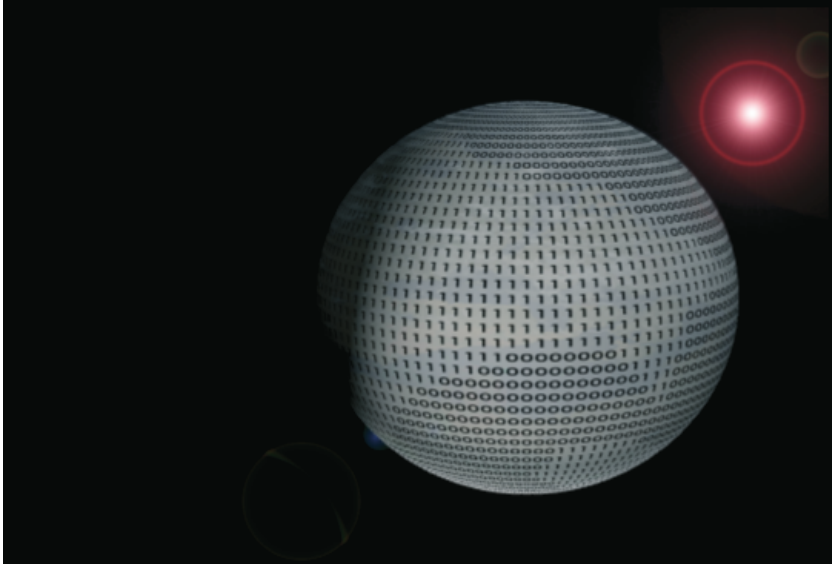
DIGITAL EXOPLANETS



Prague 2019

January 27-30

Programme

Sunday 27th January:

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15:00 - 15:20	Introduction and Welcome
15:20 - 15:40	Giuseppe Morello, "*Stellar and Exoplanetary Atmospheres Bayesian Analysis Simultaneous Spectroscopy*", p.8
15:40 - 16:00	Katy Chubb, "*ORBYTS (Original Research By Young Twinkle Students)*", p.9
16:00 - 16:20	Tea Break
16:20 - 16:40	Pierre Drossart, "*Aeronomy of exoplanets : current challenges in spectroscopy*", p.10
16:40 - 17:00	Tibor Furtenbacher, "*MARVEL*", p.11
17:00 - 17:20	Mark Phillips, "*Atmosphere and Evolutionary Models for Brown Dwarfs and Giant Exoplanets*", p.12
17:20 - 17:40	Roland Tóbiás, "*Extended MARVEL approach: a generalized model for the treatment of spectroscopic databases*", p.13
17:40 - 17:50	Jean-Loup Baudino, "*A benchmark protocol for giant exoplanet atmosphere modelling*", p.15
17:50 - 17:55	Jake Taylor, "*Using NEMESIS to Constrain Atmospheric Properties of Exoplanets*", p.16

Monday 28th January: Morning

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09:40 - 10:00	Laura McKemmish, "*Musings of a Lecturer 13 months in*", see p.19
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10:20 - 10:40	Nikku Madhusudhan, "*Exoplanetary Atmospheres - Current Trends and New Directions*", p.20
10:40 - 11:00	Jonathan Tennyson, "*The MARVEL project*", p.21
11:00 - 11:40	Coffee Break
11:40 - 12:00	Tiziano Zingales, "*ExoGAN: Retrieving Exoplanetary Atmospheres*", p.22
12:00 - 12:20	Matteo Brogi, "*Exoplanet atmospheres at high spectral resolution*", p.23
12:20 - 12:40	Jasmina Belcic, "*Complex clouds in 1D and 2D retrieval*", p.24
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Monday 28th January: Afternoon, Room 1

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16:00 - 16:40	Tutorial: Jake Taylor, "*NEMESIS*", see p.16
16:40 - 17:20	Tutorial: Tsiaras
17:20 - 19:20	Astro walk

Monday 28th January: Afternoon, Room 2

14:40 - 15:40	Tutorial: Matteo Brogi, "*Exoplanet atmospheres at high spectral resolution*", see p.23
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16:00 - 16:40	Tutorial: Tiziano
16:40 - 17:20	Tutorial: Jasmina Blecic, "*TEA and RATE, numerical and analytical thermochemical equilibrium abundances packages*", p.26
17:20 - 19:20	Astro walk

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09:00 - 09:20	Ingo Waldmann, "*3D modeling of Exoplanets*", p.27
09:20 - 09:40	Sergey Yurchenko, "*ExoCross: a general program for generating spectra from molecular line lists*", p.28
09:40 - 10:00	Paul Mollière, "*Atmospheric modeling and the impact of opacities: from structures to low and high resolution spectra*", p.
10:00 - 10:20	Vincent Boudon, "*Exo-PlanetarY high-Temperature Hydrocarbons by Emission and Absorption Spectroscopy (e-PYTHEAS project)*", p.30
10:20 - 10:40	Patricio Cubillos, "*Atmospheric retrievals from low and mid-res spectroscopy*", p.32
10:40 - 11:00	Marine Martin-Lagarde, "*ExoNoodle and MIRISim : Tools for transit spectroscopy observations simulations for JWST*", p.33
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11:40 - 12:00	Majdi Hochlaf, "*Treatment of Renner-Teller and spin-orbit effects in small molecular systems*", p.35
12:00 - 12:20	Michiel Min, "*The ARCiS framework for Exoplanet Atmospheres*", p.38
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13:00 - 14:40	Lunch

Tuesday 29th January: Afternoon, Room 1

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Tuesday 29th January: Afternoon, Room 2

14:40 - 15:40	Tutorial: Sergey Yurchenko, "*ExoCross Tutorial*", see p.28
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16:00 - 16:40	Tutorial: Subhajit Sarkar, "*ExoSim Tutorial*", see p.39

Wednesday 30th January:

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09:20 - 09:40	Paul Rimmer, "*A Lagrangian Code for Atmospheric Chemical Kinetics*", p.43
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10:00 - 10:20	Alexander Fateev, "*Far-UV spectroscopy of molecules for industrial and planetary applications*", p.45
10:20 - 10:40	Richard Hobbs, "*Constraining bulk composition using forward atmospheric models*", p.46
10:40 - 11:00	Yui Kawashima, "*Metallicity-dependence of transmission spectra of hazy exoplanet atmospheres*", p.47
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11:40 - 12:00	Svatopluk Civiš, "*Unstable species and their spectra for deeper understanding of planetary atmospheric chemistry*", p.48
12:00 - 12:20	Luis Welbanks, "*Chemical detections using optical transmission spectra of exoplanets*", p.50
12:20 - 12:40	Finishing Remarks
12:40 - 13:00	End of Meeting

Stellar and Exoplanetary Atmospheres Bayesian Analysis Simultaneous Spectroscopy

Giuseppe Morello,[†] *CEA Saclay*
Marine Martine-Lagarde, CEA Saclay
Christophe Cossou, IAS
Angelos Tsiaras, UCL
Pierre-Olivier Lagage, CEA Saclay

I introduce SEA BASS: Stellar and Exoplanetary Atmospheres Bayesian Analysis Simultaneous Spectroscopy. SEA BASS enables simultaneous derivation of four-coefficient stellar limb-darkening, transit depths and orbital parameters from multi-wavelength observations. In many cases, four limb-darkening coefficients are necessary to approximate the stellar intensity profile, but strong parameter degeneracies tend to hamper convergence of the light-curve fits with them as free parameters. Empirical estimates of the stellar limb-darkening coefficients are desirable:
1) to reduce the wavelength-dependent biases in transit depth due to the stellar-atmosphere models;
2) to validate/evaluate the current stellar-atmosphere models.
An accurate representation of the stellar limb-darkening is paramount to achieve 10^{-5}-10^{-4} precision in transit depth, required for spectroscopic studies of the exoplanet atmosphere.
I discuss the results obtained with SEA BASS both on simulated data and observation.
I also present a new open-source limb-darkening calculator and its usage in the analysis of specific transit observations. The calculator will be implemented in the ARIEL and JWST instrument simulators.

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ORBYTS (Original Research By Young Twinkle Students)

Katy Chubb,[†] *SRON*

Original Research By Young Twinkle Students (ORBYTS) is part of EduTwinkle, the education branch of the exoplanet atmosphere characterisation mission, Twinkle. ORBYTS matches a PhD student or Postdoc with a group of A-level students, aged 16-18 years, to work on a research project related to the spectroscopy of exoplanets. The MARVEL research projects that have been run as a part of ORBYTS will be discussed, along with the impact the resulting data has had on spectroscopy research within the ExoMol group.

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Aeronomy of exoplanets : current challenges in spectroscopy

Pierre Drossart,[†] *LESIA, Observatoire de Paris*

Planetary studies in the last decades have shown that the interaction between the lower atmosphere (the "meteorological" layer) and the upper layers (upper stratosphere, mesosphere up to ionosphere) exhibits a large number of complex phenomena - a particularly important phenomenon is the high temperature of the upper atmosphere of giant planets, not well modelized from one-dimensional radiative transfer balance. The evidence for wave dissipation, gravity wave in particular has been shown from several observations, with most detailed studies made in the atmosphere of Jupiter.

The aeronomy of planets is the field of complex interacting phenomena. It has a great importance for understanding the escape rate of the atmospheres, but also the composition and energy balance of the planets. The complexity comes from a combination of many different effects, in addition to the usual complexity of radiative transfer in planetary atmospheres : non-LTE effects when radiative times becomes shorter than collision time, dynamical effects, with the dissipation of waves and photochemical effects, circulation models (TGCM), involving the previous effects with connection to the meteorological deeper layers.

In exoplanets, such phenomena necessarily exist in a large variety of situations that we are just beginning to explore. The extreme situation of hot Jupiters, with a proximity to the star, potentially with active flares, will be a laboratory challenging our current understanding of the physics of planetary atmospheres. The need for molecular parameters and reaction rates in the parameter range of exoplanets is another challenge for spectroscopy.

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MARVEL

Tibor Furtenbacher,† *MTE-ELTE*
Dr. Tóbiás Roland
Prof. Attila Császár

The MARVEL (Measured Active Rotational Vibrational Energy Levels) approach enables the conversion of a set of assigned experimental rovibronic transitions to empirical rovibronic energy levels, with associated uncertainties propagated from the input transition data to the output energy levels.This conversion relies on the construction of an experimental spectroscopic network from the measured and assigned transitions, allowing an improved characterization of the high-resolution spectroscopic information. Since its inception a decade ago, the MARVEL algorithm and code was successfully employed to study the high-resolution spectra of several molecules, mostly of astronomical interest, including $^{12}C_2$, $^{48}Ti^{16}O$, $^{90}Zr^{16}O$, the H_3^+, H_2D^+, and D_2H^+ molecular ions,nine isotopologues of water, three SO_2 isotopologues, $^{12}C_2H_2$, ammonia ($^{14}NH_3$), and the parent ketene molecule. Furthermore, the MARVEL energy levels of the water isotopologues were used for determining definitive ideal-gas thermochemical functions for $H_2{}^{16}O$ and for heavy water and its three constituent isotopologues.

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Atmosphere and Evolutionary Models for Brown Dwarfs and Giant Exoplanets

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Isabelle Baraffe, University of Exeter
Pascal Tremblin, CEA Saclay
Gilles Chabrier, University of Exeter

The study of brown dwarfs and giant exoplanets is rapidly evolving as ever-improving instrumentation becomes sensitive to cooler objects. Accurate and reliable atmosphere and evolutionary models are important for placing mass and age constraints on newly discovered objects, and understanding the rich chemistry and physics taking place in their atmospheres. We are expanding on the widely used COND evolutionary models by developing a grid of model atmospheres (Teff=200-2000K, log(g)=2.5-5.5) with our state-of-the-art 1D radiative-convective equilibrium code ATMO. ATMO includes the latest opacities for important molecular absorbers such as H_2O, CH_4 and NH_3, and takes into account the condensation of H_2O and NH_3 which are important for the coolest atmospheres (Teff=200-350K). These model improvements allow us to follow the evolution of Jupiter mass objects down to the coolest temperatures (Teff=200K). I will present comparisons of these new models to previous model grids and to observations in colour-magnitude diagrams. I will also highlight the uncertainty surrounding the highly pressure broadened potassium resonance doublet, and its impact on predicted near-infrared spectra. Our future work will involve expanding on this initial grid, to investigate the effects of metallicity, C/O ratio and non-equilibrium chemistry in cool brown dwarfs and giant exoplanets.

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Extended MARVEL approach: a generalized model for the treatment of spectroscopic databases

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Jonathan Tennyson, University College London
Attila G. Császár, MTA-ELTE Complex Chemical Systems Research Group

Several improvements are introduced into the conventional MARVEL (Measured Active Rotational-Vibrational Energy Levels) protocol [1,2] to facilitate the accurate inversion of a huge set of measured transitions with significantly different accuracies to empirical energy levels. The most important algorithmic developments, leading to an extended MARVEL (extMARVEL) scheme [3], can be summarized as follows:
(a) when the transitions of the data sources are processed, they are divided into (data-source) segments by the user in the input file;
(b) line-by-line input uncertainties are replaced with estimated segment uncertainties (ESU);
(c) experimental rovibrational lines are blocked by the ESUs of their segments;
(d) refined segment uncertainties (RSU) are determined using the ESU values and spectroscopic cycles;
(e) transitions are blocked by the orders of magnitude of their RSUs;
(f) based on sequential addition of blocks of increasing RSUs, a constrained weighted least-squares procedure is utilized to provide even more accurate (constrained) energy levels;
(g) automated recalibration is performed for those data-source segments where recalibration is allowed by the user;
(h) combination difference relations are employed to reduce residual uncertainties in the resulting dataset of constrained empirical energy levels; and
(i) improved classification of the lines and energy levels is devised, based on their accuracy and dependability.

To show the effectiveness of the novel algorithm, extMARVEL has been applied for the analysis of the complete set of highly accurate H216O transitions. As a result, more than 200 highly accurate energy levels of H216O are obtained in the energy range of 0-6000 cm^{-1}. The database of constrained energy levels, derived from highly accurate, measured rovibrational lines with the extMARVEL protocol, is considerably larger and more accurate than the best previous datasets [4] in the literature.

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[1] T. Furtenbacher, A. G. Császár, and J. Tennyson, J. Mol. Spectry., 2007, 245, 115-125.
[2] T. Furtenbacher and A. G. Császár, J. Quant. Spectr. Rad. Transfer, 2012, 113, 929-935.
[3] R. Tóbiás, T. Furtenbacher, J. Tennyson, and A. G. Császár, Phys. Chem. Chem. Phys., 2019 (in press, DOI: 10.1039/C8CP05169K)
[4] R. Lanquetin, L. H. Coudert, and C. Camy-Peyret, J. Mol. Spectrosc., 2001, 206, 54–67.

A benchmark protocol for giant exoplanet atmosphere modelling

Jean-Loup Baudino,† *University of Oxford*
Paul Mollière (Observatory of Leiden), Olivia Venot (Université Paris-Est Créteil), Pascal Tremblin (CEA-Saclay), Bruno Bézard (Observatoire de Paris), and Pierre-Olivier Lagage (CEA-Saclay)

In Baudino et al. 2017 we presented a benchmark protocol to the community and how we successfully obtained similar results for 3 forward models after converging on a minimal model agreement. To go further, we need more models to be tested in same conditions, with the idea to find new non-negligible physical phenomenon or molecules to add to this minimal model.

This hands-on session introduces an easy way to have access to the data of Baudino et al. 2017, including the protocol, commented dataset (spectra and profiles) and plot routines. Everything is available in a Jupyter notebook: https://gitlab.physics.ox.ac.uk/baudino/tutorial-exoplanet-benchmark/

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Using NEMESIS to Constrain Atmospheric Properties of Exoplanets

Jake Taylor,[†] *University of Oxford*
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The **N**on-linear optimal **E**stimator for **M**ultivariat**E** spectral analy**SIS** code (NEMESIS) is a radiative transfer and retrieval framework which was developed to study bodies in the Solar System and has since been adapted to study bodies outside the Solar System, e.g. exoplanets. We will show how the code can be used to generate emission spectra based on the exoplanet WASP-43b. By adding noise to the generated model, we will use this as a mock data set to recover the information in the atmosphere using Bayesian techniques.

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3D modeling of Exoplanets.

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James Manners, Ian Boutle (UK Met Office)
D. Sing (Univ. Johns Hopkins), C. Helling (Univ. St Andrews), G. Lee (Univ Oxford/Bern)

I will present results from the University of Exeter hierarchical modeling framework, focusing on three recent effects requiring 3D modeling to capture. I will introduce the framework, then detail the application applications exploring the dynamics of Super Earths/Warm Neptunes, 3D mixing in hot Jupiters, and cloud structures in hot Jupiters. Firstly, we will demonstrate how the resolved flow, using a 3D model, differs when commonly made approximations to the underlying dynamical equations are made. Secondly, we will detail wind-driven mixing of CH_4/CO, impacting on the synthetic observations, and operating over 3 dimensions. Finally, I will show results from 3D models including two separate cloud schemes, both incorporating radiative feedback. Finally, if time permits, I will outline results from terrestrial planets on the water cycle, and impacts of dust on the atmosphere.

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3D planets, 1D models, what can possibly go wrong ?

Vivien Parmentier,[†] *University of Oxford*

Most accessible exo-atmospheres are surrounding tidally locked planets in close-in orbits. Large scale cloud, temperature and chemical inhomogeneities are expected. Unfortunately most observations are sensible to some sort of spatially averaged atmospheric state. I will discuss when these large gradients are expected and in which cases the 1D approach no longer provides an acceptable interpretation of the data and needs to be improved.

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Musings of a Lecturer 13 months in

Laura McKemmish,[†] *University of New South Wales*

Alongside all the new responsibilities and new opportunities, my first year as a Lecturer at the University of New South Wales has been a time of deep self-reflection as I seek to understand my research strengths and key interests, articulate what will make my research team unique, motivated and strong, and to decide on my group's core and supplementary research objectives: in short, as I define what The McKemmish Group at UNSW Chemistry is. In this lecture, I will explain to you some of the answers I have come up with as I take you through my research history up to this point and preview some of my group's upcoming research.

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Exoplanetary Atmospheres - Current Trends and New Directions

Nikku Madhusudhan,† *University of Cambridge*

Exoplanetary discoveries in the past two decades have unveiled an astonishing diversity in the physical characteristics of exoplanetary systems, including their orbital properties, masses, radii, equilibrium temperatures, and stellar hosts. Exoplanets known today range from gas-giants to nearly Earth-size planets, and some even in the habitable zones of their host stars. Recent advances in spectroscopic observations and theoretical methods are now leading to unprecedented constraints on the physicochemical properties of exoplanetary atmospheres. I will discuss some of the latest developments and future prospects of this new era of exoplanetary characterization.

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The MARVEL project

Jonathan Tennyson,[†] *University College London*

The measured active vibration rotation energy level (MARVEL) procedure is now a well established method for inverting measured and assigned high resolution molecular spectra. The MARVEL procedure is used to determine and validate the most accurate empirical energy levels and hence transition frequencies. The MARVEL procedure has been applied to an increasing list of small molecules, most of them important for exoplanets.

MARVEL is by design active; that is the procedure can be updated and re-run if and when new measurements become available. As the project becomes more mature it would seem that appropriate to put the project into some sort of steady state were there is a single point from which the energy levels and input data can be accessed, and datasets updated in a fairly seemless fashion once new sources become available. Ideas in this direction will be presented at the meeting.

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ExoGAN: Retrieving Exoplanetary Atmospheres

Tiziano Zingales,[†] *Laboratoire d'Astrophysique de Bordeaux*
Ingo P. Waldmann, University College London

Atmospheric retrievals on exoplanets usually involve computationally intensive Bayesian sampling methods. Large parameter spaces and increasingly complex atmospheric models create a computational bottleneck forcing a trade-off between statistical sampling accuracy and model complexity. It is especially true for upcoming JWST and ARIEL observations. We introduce ExoGAN, the Exoplanet Generative Adversarial Network, a new deep-learning algorithm able to recognize molecular features, atmospheric trace-gas abundances, and planetary parameters using unsupervised learning. Once trained, ExoGAN is widely applicable to a large number of instruments and planetary types. The ExoGAN retrievals constitute a significant speed improvement over traditional retrievals and can be used either as a final atmospheric analysis or provide prior constraints to subsequent retrieval.

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Exoplanet atmospheres at high spectral resolution

Matteo Brogi,[†] *University of Warwick*
Michael R. Line, Arizona State University, USA

In recent years a new observational technique to study the atmospheres of exoplanets has emerged. This is based on the use of very high resolution spectroscopy (R > 25,000) to resolve molecular bands into the individual lines and subsequently co-add their signal by cross correlating with template spectra. At high resolving power it is also possible to detect the changing Doppler shifts of exoplanet spectra while planets moving along their orbits, which helps us filtering out the main contaminants (the Earth's and stellar spectra). This method enables unique science cases such as the study of non-transiting planets, previously impossible, and the measurement of rotation and winds. A Bayesian framework has also been formalised to combine high- and low-resolution spectroscopy to benefit from their complementary information. However, modelling template spectra for cross correlation heavily relies on accurate molecular line lists at high temperature (T > 1000K). Even for key molecules such as H_2O, there are inconsistencies between current databases in both frequency and intensity of lines. I will show how these might affect the detectability of molecular species and consequently the interpretation of exoplanet spectra. With high-resolution spectroscopy becoming a leading observational technique, more effort is required to (cross-)validate molecular databases for their subsequent use on spectral modelling.

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Complex clouds in 1D and 2D retrieval

Jasmina Blecic,[†] *New York University Abu Dhabi*

Understanding the nature of clouds and hazes in exoplanetary atmospheres is crucial for interpreting transit observations, particularly those made with JWST, as aerosols are extremely common in planetary atmospheres and dramatically change the appearance of spectral features and underlying thermal structure. The inclusion of clouds is one of the largest outstanding issues in exoplanetary atmospheres characterization. To date, there have been two approaches to understanding cloud formation: (i) the phase-non-equilibrium concept of kinetic dust formation (Wiotke & Helling 2003; Wiotke & Helling 2004) and (ii) the phase-equilibrium concept of thermal stability (e.g., Ackerman & Marley 2001). Together with my collaborators, I implemented a complex microphysical kinetic cloud model (Heling and Woitke 2006) in retrieval (Blecic 2019a in prep; Blecic 2019b in prep). In addition, I developed a fully automatized code that can perform forward model exploration and I applied this approach to several hot-Jupiter planets. We have also developed a thermal-stability cloud model, inspired by Ackerman and Marley 2001 and Benneke 2015, and implemented it in 1D and 2D retrieval and applied it to two promising JWST targets (Kilpatrick, et al., ApJ, 156, 103, 2018.; Venot et al 2019, in prep). Both complex cloud models are implemented in an open-source PyratBay retrieval framework (Cubillos, Blecic, Harrington 2019, in prep), and are able to provide the cloud location, extent, distribution, and particle sizes in 1D, and in 2D, in addition to these, the variation in thermal structures, molecular abundances, and cloud coverage with phase.

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Hands-on MARVEL demonstration

Laura McKemmish,[†] *University of New South Wales*
Katy Chubb, SRON Netherlands Institute for Space Research
Attila Császár, Eotvos University
Tibor Furtenbacher, Eotvos University
Jonathan Tennyson, University College London

In this tutorial session, you will get hands-on experience using the MARVEL (Measured Active Ro-Vibrational Energy Levels) online program to determine empirical energy levels from experimental assigned transitions. This program has proven exceptionally useful in consolidating all existing experimental data into a single authoritative data set useful for modern data science applications particularly construction of high quality list lists (energy levels and transition intensities of molecules). The methodology readily enables identification of mis-assignments and typos through enforcing self-consistency of the spectroscopic networks created. As a web-based tool, MARVEL Online opens up the power of the MARVEL algorithms to non-experts in a user-friendly manner without the need for installation or compilation, and is thus suitable for both student projects and cutting-edge research.

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TEA and RATE, numerical and analytical thermochemical equilibrium abundances packages

Jasmina Blecic,[†] *New York University Abu Dhabi*

Thermochemical equilibrium calculations are the starting point for initializing models of any planetary atmosphere. Thermochemical equilibrium largely governs the composition of the deep planetary atmospheres of giant planets, however, in cooler atmospheres equilibrium calculations are the necessary baseline for further disequilibrium assessment. It provides a first-order approximation for species abundances as a function of pressure, temperature, and metallicity. I will present and do tutorials on two open-source codes, TEA (Blecic et al. 2016. Blecic and Cubillos 2019, in prep) and RATE (Cubillos, Blecic, Dobbs-Dixon 2019, in press). TEA, Thermochemical Equilibrium Abundances, is a numerical code that uses the Gibbs-Free Minimization method together with the Lagrangian optimization scheme to find the equilibrium abundances given the temperature, pressure and elemental abundances at each atmospheric layer. The code executes in couple of seconds, and can explore the temperature ranges from 200 to 6000K and metallicities several magnitudes higher and lower than solar. RATE, Reliable Analytical Thermochemical Equilibrium, is an analytical code that calculates the equilibrium abundances using an improved, more reliable, and more widely applicable analytical scheme than originally developed by Heng & Tsai (2016). The code can explore the temperature range from 200 to ∼2000 K, pressures from 10^{-8} to 10^{3} bar, and CNO elemental abundances from 10^{-3} to $\sim 10^{2}$ × solar for hydrogen-dominated atmospheres. RATE executes in microseconds and presents a perfect tool for Bayesian phase space exploration, when millions of models need to be evaluated fast, in a self-consistent way.

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3D modeling of Exoplanets

Ingo Waldmann,[†] *UCL*
Quentin Changeat, Kai Yip, & Angelos Tsiaras, UCL

The TauREx retrieval code (Waldmann et al. 2015a,b) is an open-source, fully bayesian retrieval algorithm written in python. In this conference, I will introduce some of the key features of TauREx and how to run and setup retrievals and forward models for transmission and eclipse measurements. I will then proceed to discuss some of the new features of TauREx, in particular the light curve retrieval mode (L-retrieval). Unlike standard retrievals that take 1D spectra as input, the L-retrieval goes one step closer to the date and takes transit/eclipse light curves as direct input. This allows us to take into account the correlation of spectral features with correlations in orbital or stellar limb-darkening paramters and map a consistent, common likelihood.

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ExoCross: a general program for generating spectra from molecular line lists

Sergey Yurchenko,† *University College London*
Sergey Yurchenko, Ahmed Al-Refaie, Katy Chubb, Laura McKemmish and Jonathan Tennyson, UCL

We present ExoCross, an open-access Fortran code for generating spectra (emission, absorption) and thermodynamic properties (partition function, specific heat etc.) from molecular line lists. Input is taken in several formats, including ExoMol and HITRAN. ExoCross is efficiently parallelized showing also a high degree of vectorization. It can work with several line profiles such as Doppler, Lorentzian and Voigt and support several broadening schemes. Voigt profiles are handled by several methods allowing fast and accurate simulations. Two of these methods are new. ExoCross is also capable of working with the recently proposed method of *super-lines*: a super-fast method of handling billions of transitions on-the-fly. ExoCross supports calculations of lifetimes, cooling functions, specific heats and other properties. It can be used to convert between different formats, such as HITRAN, ExoMol and Phoenix. It is capable of simulating non-LTE spectra using a simple two-temperature approach. Different electronic, vibronic or vibrational bands can be simulated separately using an efficient filtering scheme based on the quantum numbers.

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Atmospheric modeling and the impact of opacities: from structures to low and high resolution spectra

Paul Mollière,[†] *Leiden Observatory*

Understanding the structures of exoplanet atmospheres and their spectra is not possible without properly modeling the underlying radiative transfer. For this, a complete and accurate opacity database is crucial. One important opacity contributor are line absorbers, and I will, among other things, show how even single lines can strongly affect the atmospheric structure, under the 'right' conditions. Moreover, JWST will give the opportunity to study spectra of exoplanets in the mid-IR. With this it may be possible to unambiguously identify cloud species for the first time. I will show how parameters such as the cloud particle size, but also the internal structure and shape of the condensates will affect the spectra.

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

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and the e-PYTHEAS Team

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, such as retrieved by ESA's M4 space mission ARIEL.

Our consortium of 5 French laboratories and associated partners proposes to improve the existing high-temperature spectroscopy data for several molecular species detected in exoplanets. 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.

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Atmospheric retrievals from low and mid-res spectroscopy

Patricio Cubillos,[†] *Space Research Institute (IWF), Austria*

To date, space and ground-based telescopes have allowed us to probe the transmission and emission spectra of dozens of exoplanets, covering from infrared to ultraviolet wavelengths, with low- and mid-resolution spectra. The theoretical modeling of these observations enable us to constrain the atmospheric properties of these planets, their temperature, composition, and dynamics. A robust interpretation of the data requires the development of sophisticated tools, involving the combined and advanced knowledge of physical processes, bayesian statistics, and software development.

In this talk I will discuss the opportunities that low- and mid-resolutions spectroscopy offer to characterize the atmospheres of extrasolar planets, the challenges faced to implement such complex analyses, and the expectations that future observatories and open-science data will offer, to ultimately enable a better understanding of planetary physics.

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ExoNoodle and MIRISim : Tools for transit spectroscopy observations simulations for JWST

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The launch and commissioning of the James Webb Space Telescope (JWST) in 2021 will open new perspectives in astrophysics and especially in exoplanet observations. Among all the instruments embedded in the telescope, MIRI (Mid-InfraRed Instrument) and its Low Resolution spectrometer will carry out transit spectroscopy observations for exoplanets atmosphere characterization. In order to prepare the analysis and interpretation of these observations, several pieces of software have been developed to create synthetic data of such observations. First, a simulator of the instrument (MIRISim) itself have been created to reproduce as accurately as possible the instrument noises and systematics, for all the different modes and usage of MIRI. It has been developed by the MIRI consortium and is available [1]. We have developed ExoNoodle, a Python tool (ExoNoodle) to generate time-series spectra expected from star-planet systems, varying over time as the planet orbits around the star, to provide MIRISim with input files. Given that MIRISim cannot handle sources variable in time, we have to launch a new MIRISim simulation at each time step. Next we will introduce all kind of systematics in the simulation. The simulated data will be used to test and improve the data reduction, retrieval techniques and analysis codes the community is building.

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Reference:

[1] MIRISim Documentation : http://miri.ster.kuleuven.be/pub/Public/MIRISim_Public/MIRISim.pdf

Treatment of Renner-Teller and spin-orbit effects in small molecular systems

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Renner-Teller effect is present in tri-, tetra- and polyatomic molecules electronic ground and/or excited states correlating to doubly degenerate electronic state at linearity. Many of them are of atmospheric or planetary or astrophysical interest, or relevant for combustion or environment. Accurate predictions of their spectra are crucial for their identification in these media and for fully understanding of their reactivity there.

For molecular systems presenting Renner-Teller effect, couplings between the electronic, vibrational and rotational angular momenta are in action [1]. For molecular systems having non-zero spin-orbit interaction (states of spin-multiplicity other than singlet), further complications exist since these angular momenta may also couple with spin-orbit. All these couplings complicate even more the patterns of the resulting spin-rovibronic levels [1]. These spectra cannot be predicted by simple considerations. Instead, we observe Born-Oppenheimer approximation breaking, where strong perturbations in the patterns of the rovibronic levels occur especially close to barriers to linearity. They were evidenced experimentally by means of high resolution spectroscopic techniques.

From a theoretical point of view, difficulties reside in the simultaneous description of the couplings between the electronic, spin-orbit, vibrational and rotational angular momenta present in degenerate electronic states of linear molecules close and far from linearity. To solve the nuclear problem, we adopt the variational approaches developed by Carter and co-workers for triatomics [2-3]. For tetraatomics, an extension by Jutier and co-workers is also available [5,6]. These treatments are performed in internal coordinates (valence distances and in-plane angles and torsion coordinates) or in Jacobi coordinates. The corresponding hamiltonians exhibit complex forms. These hamiltonians are expressed on specific basis sets for the stretchings (e.g. Hermit polynomes), the

bending (e.g. Legendre polynomes) and torsions (Fourier transform expansions). The energies and the rovibronic wave functions are optimized variationally. The sizes of the corresponding matrices grow rapidly and become too large, so that they are hard to handle. This limits the extension of such approaches to larger polyatomic systems. Alternatively, Peric and co-workers developed a simpler approach in reduced dimensionality where only bendings modes (subject to strong modified patterns) are treated. This approach was used to treat tri-, tetra and even penta-atomic Renner-Teller systems (mostly of linear/linear cases) [7]. For illustration several examples will be presented. Several examples will be presented. [8-17]

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The ARCiS framework for Exoplanet Atmospheres

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Exoplanet atmospheres are very complex environments. Dynamics, (non equilibrium) chemistry and cloud formation all act together. Modelling of exoplanet atmospheres thus requires making careful decisions on the assumptions made. Analysing observations through retrieval requires even more care as here the computations have to be fast enough to allow tens to hundreds of thousands of models to be computed. Here we will present a new modelling framework, the artful modelling framework ARCiS, where we carefully consider which parts of physics and chemistry are included and which are parameterised. This framework will bridge the gap between current parameterised retrieval models and the highly complex and computationally demanding GCM type models. In this presentation I will also focus on the recently developed cloud formation model as a good example of the modelling philosophy.

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Simulated transit observations with ExoSim

Subhajit Sarkar,[†] *Cardiff University*

There are many time-dependent processes that can interfere with a transit spectroscopic observation. These include the effects of instrumental systematics, stellar surface inhomogeneities and time-correlated astrophysical or instrumental random noise. These can affect the accuracy and/or precision of the final reconstructed planet spectrum and thus the scientific conclusions of an observation. We developed ExoSim as a time domain simulator of transit spectroscopy representing both the astrophysical scene and the instrument, generating data akin to a real observation. Into ExoSim can be put complex time dependent effects, and their consequences projected to the level of the final planet spectrum, obtaining better assessments for the final error bar sizes and any residual biases, which then can feed into spectral retrieval algorithms. ExoSim can be used to assess performance of an instrument operating with complex time-dependent effects, or provide fake data for testing data reduction pipelines. ExoSim has been used to assess the impact of stellar pulsations and granulations on transit spectroscopic observations, the impact of star spots and faculae, and the effects of correlated noise sources such as pointing jitter. It has been extensively applied to Phase A and Phase B of the ARIEL mission, but its core structure is generic and applicable to other instruments.

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petitRADTRANS: a Python radiative transfer package for clear and cloudy atmospheres

Paul Mollière,[†] *Leiden Observatory*

petitRADTRANS is a Python package that can calculate emission and transmission spectra at low resolution, using the correlated-k approximation, or at high resolution, using line-by-line radiative transfer. petitRADTRANS will soon be officially published, but is already available upon request, or at this workshop. Parameters describing the planetary atmosphere can be changed on the fly, and a few lines are sufficient to obtain spectra, within a few seconds. This code is fast enough to allow for retrievals, when run in parallel. The code also allows to include clouds of various species (MgSiO3, Na2S, Fe, H2O, ...), where the cloud mass fraction, mean cloud particle size and particle shape can be varied. In this hands-on session we will go through a few examples for calculating clear and cloudy spectra, and also how to get diagnostics such as emission and transmission contribution functions.

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The Pyrat Bay package for atmospheric modeling and retrieval

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The Pyrat Bay package is a user-friendly (written in Python) but efficient tool (and in C) to produce forward-model spectra of exoplanets and retrieve their atmospheric properties. The modular design of the package allows the user to run high level tasks (such as a MCMC atmospheric retrieval) or specific low-level tasks that are part of atmospheric forward modeling.

In this workshop I will walk through the main capabilities of the Pyrat Bay package: to generate temperature-profile, abundance, and transmission/emission forward models, and to run atmospheric retrievals of transit/eclipse observations.

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Considerations for High-Precision Atmospheric Retrievals of Brown Dwarfs

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Nikku Madhusudhan, Institute of Astronomy, Cambridge

Isolated brown dwarfs provide remarkable laboratories for understanding atmospheric physics in the low-irradiation regime, and can be observed more precisely than exoplanets thanks to their higher temperatures and remoteness from stars. As such, they provide a glimpse into the future of high signal-to-noise observations of exoplanets, which will place atmospheric models under increasing scrutiny. I investigate the importance of considering model uncertainties when interpreting high-quality spectra with atmospheric retrievals, and show that it can be important to allow for model uncertainty explicitly in the retrieval in order to correctly infer atmospheric properties. I will also present a new parametrisation for the P-T profile which avoids over-fitting of the spectrum, and show that it works successfully with test retrievals on simulated data. By analysing the origins of the spectrum as a function of depth within the atmosphere, it is evident that pressures as high as a few tens of bar can be probed with near-infrared spectra of T-dwarfs. The new P-T model therefore allows for a suitable amount of flexibility at high pressures. Finally, I will demonstrate the new retrieval framework on a high-precision spectrum of a brown dwarf.

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A Lagrangian Code for Atmospheric Chemical Kinetics

Paul Brandon Rimmer,[†] *University of Cambridge*

I will briefly discuss the ARGO photochemical model, a Lagrangian chemical kinetics model that uses the STAND2019 Chemical Network. This code incorporates over 5000 reactions, including ion-neutral chemistry, complete for simple gas-phase H/C/N/O chemistry, and includes a smaller network of reactions for other species such as He, Ar, Fe, Si, Mg and Ti. The network is valid for temperatures between 200 K and 30000 K. It has been benchmarked for the present-day Earth, Mars, Jupiter, Hot Jupiters, and Ultra-Hot Jupiters. Most of this talk will be on what parameters this model requires, and the uncertainties in those parameters. The photochemistry relies on UV absorption spectra and quantum yields, which need to be measured in the lab or calculated, and are temperature-dependent. The other rates are parameterized by bimolecular and termolecular rate constants, and the values of these also need to be measured in a lab or calculated. The disagreement between measurement and calculation, and between different measurements, and between different calculations, can span more than an order of magnitude, especially for termolecular reactions. This is especially problematic for parameters where a factor of two change in the parameter can result in more than an order of magnitude change in the result. I will conclude with suggested ways to determine which are the critical parameters, and to use a combination of observation, theory and experiment to constrain these parameters.

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Atmospheric modeling and the impact of opacities: from structures to low and high resolution spectra

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N. Bowles, A. Braude, R. Garland, J. Taylor, J.L. Baudino (University of Oxford); P. Coles, S. Yurchenko, J. Tennyson (University College London)

An analysis of currently available ammonia (NH3) visible-to-near-infrared gas absorption data was recently undertaken (Irwin et al., Icarus 302, 426–436, 2018) to help interpret Very Large Telescope (VLT) MUSE observations of Jupiter from 0.48–0.93 μm, made in support of the NASA/Juno mission. Since this analysis a newly revised set of ammonia line data, covering the previously poorly constrained range 0.5–0.833 μm, has been released by the ExoMol project, "C2018" (Coles et al., 2018), which demonstrates significant advantages over previously available data sets, and provides for the first time complete line data for the previously poorly constrained 5520- and 6475-Åbands of NH3. In our most recent paper (Irwin et al., Icarus 321, 572-582, 2019) we compare spectra calculated using the ExoMol-C2018 data set with spectra calculated from previous sources to demonstrate its advantages. We conclude that at the present time the ExoMol-C2018 dataset provides the most reliable ammonia absorption source for analysing low- to medium-resolution spectra of Jupiter in the visible/near-IR spectral range, but note that the data are less able to model high-resolution spectra owing to small, but significant inaccuracies in the line wavenumber estimates. This work is of significance not only for solar system planetary physics, but for future proposed observations of Jupiter-like planets orbiting other stars, such as with NASA's planned Wide-Field Infrared Survey Telescope (WFIRST). In this presentation we will review in particular our method of dealing with the very large number of very weak lines in databases such as ExoMOL through the use of a 'pseudo-continuum' treatment, which we find very much improves the speed with which we can calculate k-distribution look-up tables, with negligible loss of accuracy.

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Far-UV spectroscopy of molecules for industrial and planetary applications

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Recent developments in VUV sensitive array detectors give possibilities for implementing a new measurement technique in far-UV spectral range (110-200 nm) suitable for various industrial applications on Earth. The technique is based on use broad-band optical absorption spectroscopy with hot gases and does not require expensive low-pressure (pumps) and light-source (synchrotron) solutions. Spectroscopy in far-UV is typically Rydberg state spectroscopy that characterizes with much larger absorption cross sections compare to those in UV/IR spectral range making molecule detection less demanding for instrumental resolution and therefore much easy to detect. In the presentation an overview of the new measurement technique and measurement methods is given. Several examples of laboratory measurements in far-UV spectral range on group's unique high-temperature flow gas cells (up to 1500C) are given. Spectroscopy of molecules (as e.g. CO_2, CH_3Cl, NH_3 and H_2CO) relevant for both industrial and planetary applications is discussed. Practical applications of the new technique are demonstrated in two industrial environments: on-line measurements on the producer gas (gasification) and on stack gas (natural gas combustion).

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Constraining bulk composition using forward atmospheric models

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The composition of exoplanets gives key insights into their formation and evolution, and the most powerful observation for gaining this constraint is through atmospheric spectroscopy. Whether obtained in transmission or emission, however, spectroscopic observations probe limited pressure windows of planetary atmospheres and are directly sensitive to only a limited, spectroscopically active, species set. It is therefore critical to have forward models that can relate retrieved atmospheric compositions to an atmosphere's bulk physical and chemical state. To this end we have created a new Eulerian 1-D chemical kinetics code for modelling exoplanet atmospheres, Levi.

Using Levi, and the Stand2019 chemical network, we investigate how variations in bulk C/O and N/O affects observable exoplanet atmospheric chemistry. For typical Hot Jupiters we demonstrate the strong sensitivity of molecular detections to the atmospheric C/O: with current observations neither NH_3 nor HCN could be detected without super-solar carbon. N/O is less discriminatory, although highly super-solar N/O can decrease the bC/O required for HCN and NH_3 detection down to solar-like values. We also evaluate recent reported detections of CO, H_2O and HCN. We show that our models are consistent with these species having been detected in retrieval, albeit with a narrow compositional window: approximately a C/O > 0.9 (1.6 times solar) was required to meet the minimum reported value for HCN, while an approximate C/O < 1 (1.8 times solar) was required to fit the expected H_2O abundance.

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Metallicity-dependence of transmission spectra of hazy exoplanet atmospheres

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Recently, properties of exoplanet atmospheres have been constrained via multi-wavelength transit observation, which measures an apparent decrease in stellar brightness during planetary transit in front of its host star (called transit depth). Sets of transit depths so far measured at different wavelengths (called transmission spectra) for some exoplanets are featureless or flat, inferring the existence of haze particles in the atmospheres. Previous studies that addressed theoretical modeling of transmission spectra of hydrogen-dominated atmospheres with haze used some assumed distribution and size of haze particles. In Kawashima & Ikoma (2018), we developed new photochemical and microphysical models of the creation, growth, and settling of haze particles for deriving their size and number-density distributions in hydrogen-dominated atmospheres of close-in warm (< 1000 K) exoplanets. In this presentation, we show the metallicity-dependence of the production rate of haze and the resultant transmission spectra, and also discuss implications for observations.

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Unstable species and their spectra for deeper understanding of planetary atmospheric chemistry

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Spectra of ions, radicals and atoms have played important role in development of knowledge about stars and other objects in the Universe and the lack of reliable data has become a crucial problem for further progress [1]. Although, for decades, the most of spectral lines used by astrophysicist were in optical or ultraviolet range, the correct interpretation of new high-resolution astrophysical spectra, require an increasing number of high qualitymolecular and atomic data, such as level energies, oscillator strengths and photoionisation cross-sections, including those related to the infrared spectral region [2, 3]. Infrared astronomy is very promising in studies of dust-obscured objects and interstellar clouds, cool objects such as brown dwarfs, and objects at cosmological distances from Earth [4]. Since the long-range interaction between atoms as well as their interaction with other particles and external electric field is determined by dynamic polarizability, calculations of its values for excited atomic states are required for gas-laser physics, plasma physics and upper-atmosphere physics fields involving collisions of excited atomic particles. Polarizability values for atoms in their excited states are also important for the interpretation of electron scattering experiments (where the formation of temporary negative ions and channel-opening effects are observed [5]; for compensating the varying Doppler shift under laser cooling of metastable atoms [6], for optimizing the loading dynamics of optical traps [7] and Rydberg quantum gate (as one of the possible schemes for quantum computations) [8].

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Chemical detections using optical transmission spectra of exoplanets

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Transit spectroscopy provides a unique opportunity to study atmospheres of exoplanets. A main goal of spectroscopic characterisation of exoplanets is to discover chemical species in their atmospheres and estimate their abundances. The combination of detailed retrieval techniques and data in the optical can allow robust chemical characterisation along with constraints on clouds/hazes in the atmospheres. I will present two of the latest results in chemical detections using optical spectra: the detection of Li in WASP-127b and AlO in WASP-33b. I will highlight how the inclusion of new data, both observations as well as atomic data, in the optical wavelengths is fundamental for these new discoveries. This showcases the potential of current (e.g. GTC, VLT) and upcoming ground-based facilities (e.g. ELT) as well as the importance of developing tools to interpret this data accurately.

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