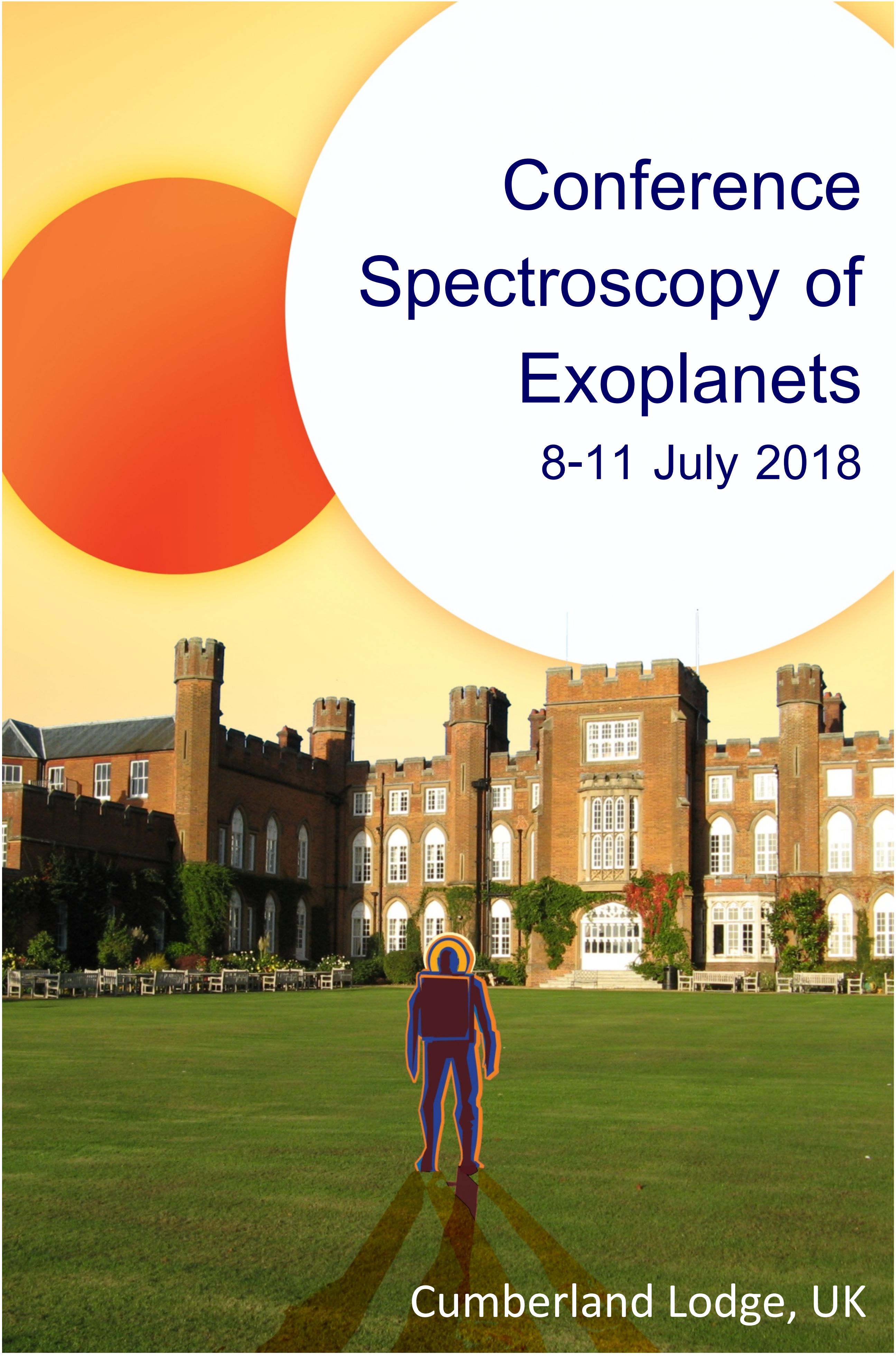

Image collage: Courtesy NASA/JPL

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Introduction

Welcome to the third conference in the ExoMol series to be held at Cumberland Lodge. These conferences are organised on the general theme of characterisation of exoplanets. This field has been given a great boost by the European Space Agency's adoption of the Ariel mission plus a variety of both spaceborne and ground based activities.

I am sure you will all agree that Cumberland Lodge provides a lovely location for these conferences. Unfortunately it is not a cheap venue but thanks to various sponsor able to reduce the full cost to all participant. I must thank Collaborative Computational Project Q (CCPQ) on "Quantum dynamics in Atomic Molecular and Optical Physics", under whose auspice a number of the codes being used by the ExoMol project were developed, UCL's Atomic, Molecular, Optical and Positron Physics and UCL's eResearch Domain. In addition funding by the European Research Council via the ExoMol project (Jonathan Tennyson), ExoLights project (Giovanna Tinetti) and ExoAI project (Ingo Waldmann) has been truly transformative in the boosting exoplanetary research at UCL.

Can I wish you all a productive and enjoyable meeting.

Jonathan Tennyson
July 2018

Programme

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14:50 - 15:10	Stephanie Merritt: *High-resolution spectroscopy for the confirmation of a temperature inversion in WASP-121b*, p. 7
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16:20 - 16:40	Simon Grimm: *HELIOS-K: The challenge of calculating opacity functions for 10^{10} molecular lines*, p. 9
16:40 - 17:00	Paul Anthony Wilson: *Signs of the beta Pictoris b Hill Sphere Transit?*, p. 10
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17:00 - 17:40	Adam Burgasser: *The Spex Prism Library Analysis Toolkit: Workshop*
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Sunday

Exoplanetary Atmospheres in 3D: multidimensional processes and opportunities

Nathan Mayne,[1] *University of Exeter*

Understanding the climates and atmospheres of exoplanets requires a multi-faceted approach. A range of theoretical models with complementary strengths and weaknesses must be used to extract the maximum knowledge from the observations, combining expertise from several areas or disciplines. In this talk I will present an overview of my own group's work building a hierarchical theoretical model framework, based on close collaboration and real-time development links with the UK Met Office and Earth climate researchers.

Using this framework, I will discuss several key results, focusing on gas giant exoplanets. Firstly, I will discuss the pure atmospheric dynamics of such planets, and and how they change as commonly made simplifications and approximations are relaxed. Secondly, I will explore the interactions of the flows with the atmospheric chemistry, and in particular show that 3D treatments are required to correctly capture the processes determining the non-equilibrium gas phase chemical abundances at pressure levels sampled by transmissions spectroscopy. Finally, I will present results from a set of 1D forward models of hot Jupiters, before moving to a 3D cloud model including time evolving, radiatively active clouds. Ultimately, the focus of these studies is the opportunity of using upcoming JWST measurements to probe the atmospheric dynamics, in 3D, especially using phase curves.

If time permits, I will briefly discuss our work on terrestrial planets, the variations of their climates, and the potential for phase curve observations of the hydrological cycle.

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High-resolution spectroscopy for the confirmation of a temperature inversion in WASP-121b

Stephanie Merritt,[1] *Queen's University Belfast*

In recent years, the atmospheres of so-called "hot Jup- iter" exoplanets have astounded us with their variety. Various detection methods have unearthed a trove of atomic and molecular species in their atmospheres, along with the discovery of cloud decks and hazes. However, one component thought to exist in the atmospheres of hot Jupiters has, until recently, eluded us: the temperature inversion. In the most irradiated of these planets, molecules such as TiO and VO are thoug- ht to exist in gaseous form, and these remarkably efficient optical absorbers cause the temperature to increase in upper layers of the atmosphere. Recent work has only just begun to uncover evidence of these inversions. Using high-resolution spectroscopic data in the optical from UVES on the VLT, and taking advantage of the planet's much greater radial velocity to disentangle planetary spectral lines from those of the parent star, my work hopes to find an unambiguous detection of TiO in the transmission spectrum of the extremely hot and inflated hot Jupiter WASP-121b, building on previous work by Evans at el (2016) and Nugroho et al (2017). This would be the first successful use of this technique using this instrument, and would pave the way for future molecular detections using powerful ground-based facilities, expanding our knowledge of these highly-unusual planets.

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Molecular Simulations for the Spectroscopic Detection of Atmospheric Volatiles

Clara Sousa-Silva,[1], J J Petkowski, S Seager, MIT

Unambiguously identifying molecules in spectra is of fundamental importance for a variety of scientific and industrial uses; a compelling modern focus is the spectroscopic detection of volatiles in exoplanet atmospheres. Analyses of observational spectra require information about the spectrum of each of its putative components. However, spectral data currently only exist for a few hundred molecules and only of fraction of those have complete spectra (e.g. H_2O, NH_3). Consequently, remote detections of molecules are vulnerable to false positives, false negatives and miss-assignments. There is a key need for spectral data for a broad range of molecules.

Using a combination of experimental measurements, organic chemistry, and quantum mechanics, ATMOS (Approximate Theoretical MOlecular Spectra) is a programme that:
a) Provides approximate spectral data (band centres and relative intensities) for thousands of molecules in seconds.
b) Assesses hundreds of molecules simultaneously, highlighting patterns and any distinguishing features. Traditional methods for obtaining spectra are extremely costly and time-consuming (i.e. months/years per molecule); ATMOS will inform prioritisation protocols for future high accuracy studies.
c) Demonstrates that, at low resolution, individual spectral features could belong to a large number of molecules. Molecular detections in spectra are often made by assigning one, or a few, spectral features to a given molecule. ATMOS can highlight ambiguities in such molecular detections and also direct observations towards spectral regions that reduce the degeneracy in molecular identification.

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HELIOS-K: The challenge of calculating opacity functions for 10^{10} molecular lines.

Simon Grimm,[1] *University of Bern*

The ExoMol database provides line lists with a very large number of transitions. For some molecules, more than 10^{10} transitions are provided. Using these line lists for exoplanetary atmospheric characterization, involves the processing of opacity functions for multiple points in temperature and pressure as well as many points in wavelength for all molecular transition lines. This set a hard computational challenge. We will present our work on the GPU opacity calculator HELIOS-K and describe how we use it to process the ExoMol line lists.

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Signs of the β Pictoris b Hill Sphere Transit?

Paul Anthony Wilson,[1] *Leiden Observatory*

The Hill sphere of the directly-imaged planet beta Pictoris b recently transited its host star resulting in the first opportunity for astronomers to study the circumplanetary environment of a young (∼23 Myr) exoplanet. The rarity of such a unique event combined with the knowledge that the next transit will not happen for another ∼23 years spurred the astronomy community to obtain a cascade of new beta Pic observations using some of the worlds largest telescopes (e.g. HST, VLT and SALT) and lead to the creation of dedicated beta Pic telescopes (e.g. bRING, PICSAT).

In this talk I will introduce the beta Pic system and give an overview of the observational efforts aimed at observing the Hill sphere transit. The talk will focus on the results of a 27 orbit HST observing campaign of beta Pic in the far-UV. I will present the variable emission and absorption signatures seen in the data and discuss their potential relationship with the Hill sphere transit.

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Improvements and developments in chemical modelling of exoplanet atmospheres

Olivia Venot,[1] *LISA*

The future JWST (2020) and ARIEL (2028) will highly improve our current knowledge on exoplanets. To interpret their observations, atmospheric models are necessary. On one hand, 1D models are able to describe the detailed atmospheric chemical composition of exoplanets, thanks to complex chemical schemes involving hundreds of compounds linked by thousands of reactions (i.e. Venot+ 2012; Moses+ 2011; Rimmer+ 2016). However, one limitation of these models concerns the description of the gas circulation, represented by the vertical Eddy diffusion. On the other hand, 3D models describe the global circulation of the gas with a very good precision, but the chemical composition can not be calculated by these models. The reason for that is the too important computational time that would required a such complete 3D model. However, developing such innovative 3D models is the key to fully understand the chemical composition of exoplanet atmospheres, which is the indispensable step to improve our knowledge of planetary formation. For this purpose, we are currently developing a reduced chemical scheme in order to couple a 3D circulation model with an accurate chemical kinetics.

Another improvement necessary for the modelling of warm exoplanet atmospheres concerns the molecular data used, in particular the VUV absorption cross sections, that describe the amount of light absorbs by species and permit to calculate their photodissociation rates. However, very few molecules have been studied at high temperature relevant for exoplanet atmospheres. To address this lack, we built an innovative project that aims at measuring the VUV absorption cross sections of the most important absorbing species of exoplanet atmospheres. We already measured the VUV absorption cross section of CO2 up to 800K (Venot+ 2013, 2018).

We will present these two improvements that are important for exoplanetary modelling.

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Monday Morning

Characterising Young Giant Exoplanet Atmospheres with Direct Imaging

Beth Biller,[1] *The University of Edinburgh*

Direct imaging uniquely yields photons from the atmospheres of wide giant exoplanets (>10 AU separation), enabling measurement of atmospheric properties and opening up a new realm of characterization possibilities. Currently, $\sim$10 young (<100 Myr), massive planets (>1 M_{Jup}) planets have been directly imaged within 100 AU of their stellar primary. These objects are detectable at near- and mid-infrared wavelengths (1-5 μm) due their own self-luminosity – at such young ages they are still hot and bright compared to similar mass objects at solar system ages. Most young giant exoplanet atmospheres are redder than brown dwarfs with similar $T_{\rm eff}$. This is likely an effect of the low surface gravity of these atmospheres, potentially allowing them to retain silicate clouds down to cooler temperatures and preferentially driving non-equilibrium chemistry in these atmospheres. Young exoplanets may also be significantly variable – multiple low-surface gravity late-L objects (PSO J318.5-22, 2M2244, W0047) that are close spectral matches to young imaged planets show high amplitude (7-10%) variability. I will discuss both current progress and the future potential for characterising giant exoplanet atmospheres via direct spectroscopy and variability monitoring. As new instruments and technologies press down to tighter separations and higher contrasts, the number of directly imaged exoplanets will likely increase dramatically, allowing us to probe both cooler atmospheres via spectroscopy as well as the statistics of planets with similar orbital separations as the gas giants in our own solar system (5-20 AU).

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Complex clouds in retrieval in the JWST era

Jasmina Blecic,[1] *New York University Abu Dhabi*

Awaiting the pending launch of the James Webb Space Telescope (JWST), which will enable probing exoplanet atmospheres from 0.6 to 28.0 μm with an unprecedented high resolution from 100 to 1550, it is of a crucial importance to develop tools that will allow us accurate characterization of exoplanetary atmospheres. These tools and observations will give us an opportunity to revolutionize what we currently know about planetary atmospheres, their composition, cloud properties, thermal structures, and their formation and evolution histories. To adequately constrain a physically plausible atmospheric structure, one must account for the uncertainties coming from our limited knowledge of the chemical, physical and dynamical processes at play. Thus, combining a retrieval framework (an observation-driven approach) and detailed theoretical models is crucial to accurately constrain atmospheric thermal structures, abundances, and cloud coverage. In particular, the formation of clouds in planetary atmospheres plays an important role in atmospheric modelling as clouds cause significant compositional and morphological changes. Being highly ubiquitous in solar system planets, clouds are also theoretically expected to be present in most temperature regimes in exoplanetary atmospheres. Regardless of their chemical composition; water, methane, sulfur in solar system planets, or iron, magnesium, silicates in hot exoplanetary atmospheres; clouds are quite difficult to model. To date two main scenarios have been proposed to understand the formation of clouds in exoplanetary atmospheres: (1) the equilibrium cloud formation scenario occurring upon vapor pressure saturation and (2) the microphysical kinetic cloud scenario that accounts for the seed particles growth and transport. We have implemented both approaches within our open-source retrieval framework, and we investigate which approach make most of the use of the current observations and which one of the future JWST observations.

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High-temperature emission spectra and updated calculated spectroscopic database of methane

Badr Amyay, Laboratoire ICB, Aline Gardez, Robert Georges, Ludovic Biennier, Institut de Physique de Rennes, Jean Vander Auwera, Service de Chimie Quantique et Photophysique, Cyril Richard, Laboratoire ICB, Vincent Boudon,[1] *Lab. ICB / UBFC / CNRS*

In the framework of the e-PYTHEAS project,[2] the C-H stretching region of methane was reinvestigated in this work using high temperature (620-1715 K) emission spectra recorded in Rennes at Doppler limited resolution. New assignments of vibration-rotation methane line positions have been achieved successfully in the Pentad system and some associated hot bands. The new assignments were injected in a global fit of methane line positions. Line intensities, based on previous existing assignments, were also refined.

This work, of interest for modelling the methane spectrum in applications to exoplanetary atmospheres has allowed to update de MeCaSDa database[3] of calculated methane lines, which is accessible through the VAMDC portal[4].

See: http://e-pytheas.cnrs.fr
Reference: B. Amyay et al.,*J. Chem. Phys.*, in press (2018).

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[2]see http://e-pytheas.cnrs.fr
[3]http://vamdc.icb.cnrs.fr/PHP/methane.php
[4]http://portal.vamdc.org

The Calculation of Atomic and Molecular Opacities for Astrophysical Applications

Richard Freedman,[1] *Seti Institute*

In order to properly model and study the emergent spectra of a variety of astronomical objects it is necessary to adequately model the opacity of their atmospheres. The objects of interest to our group span a range of temperatures from very cold solar system objects to the lower temperature limits of stellar atmospheres. There is also a large range in pressures from fractions of a millibar to hundreds of bars. An added complication is that, unlike the typical stellar atmosphere that is predominantly neutral or ionized hydrogen and helium, these objects have atmospheres that are mainly molecular hydrogen and helium. In some cases involving hypothetical rocky planets that have suffered giant impacts there may be high concentrations of water (steam) or other volatiles. This creates problems for properly defining the line broadening parameters and even the line shape itself.

I will emphasize the need for better data and discuss some of the many challenges including getting line widths for species and broadeners that are not usually studied either in the lab or through computational simulations. I will also point out what will be needed as the resolution of astronomical observations improves in the future.

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Self-consistent modelling of stellar and sub-stellar atmospheres.

Uffe G. Jørgensen,[1] *Niels Bohr Institute, Univ. of Copenhagen*

Quantitative interpretation of stellar and exoplanetary spectra requires high quality self-consistent modelling of the underlying atmospheres in order to give meaningful information about their physical and chemical structure. High resolution spectra of exoplanets, as those that are expected during the coming years, impose particular challenges and possibilities for understanding the physics in the parameter space in between well tested stellar modelling and well tested Earth climate models. We have already had very high resolution spectra of Mars for more than 50 years without being able to tell whether or not they show traces of life. Answering similar questions about exoplanets will require improved modelling, and may in particular benefit from more detailed understanding of the general cloud formation process and the basic molecular radiative processes. I will talk about some of the challenges, and about our own attempts to contribute to the progress by drawing on experience from cool stellar modelling.

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Future plans for HITEMP and extensions to the HITRAN broadening molecules

Robert Hargreaves,[1] S. Samuels, Y. Tan, R. V. Kochanov, L. S. Rothman, & I. E. Gordon, Harvard-Smithsonian Center for Astrophysics

The high temperatures observed for some exoplanets significantly increases the amount of lines needed to model their atmospheres. The HITEMP database[2] was developed to be used for high temperature environments, and the current version of HITEMP contains line parameters for five molecules (i.e., H_2O, CO_2, CO, NO, and OH). Some molecules omitted, due to limited or inaccurate high temperature data, have now become important for the characterization of exoplanets, cool stars and brown dwarfs (e.g., CH_4). The next major update of HITEMP will be discussed, with a brief description of the aims and difficulties that will need to be addressed.

In addition, the line broadening effect in planetary atmospheres depends on their atmospheric composition. The HITRAN database contains self- and air-broadening parameters (and exponents of temperature dependence) for all of its molecules and their isotopologues. The most recent 2016 edition of HITRAN[3] has been extended to include H_2-, He- and CO_2-broadening parameters for a significant number of molecular species relevant to planetary atmospheres. Furthermore, the effect of H_2O-broadening in the Earth's atmosphere can be observed especially in the tropics. Interestingly, it is also predicted to be important for rocky exoplanets that may have suffered giant impacts, as these are expected to have "steamy" atmospheres. An empirical law has been obtained from H_2O-broadened O_2 measurements and will be implemented into the HITRAN database for CO_2, CH_4, CO, NH_3, N_2O, OCS, CH_3CN and H_2CO.

The HITRAN Application Programming Interface, HAPI,[4] has been developed to work directly with the HITRAN and HITEMP databases, and uses the latest available partition sums.[5] HAPI can be used to calculate cross-sections at user specified temperatures (up to 9000 K for some molecules), pressures and broadening gas mixtures. Work is currently underway to increase its capability of working with large datasets.

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[2] L. S. Rothman, et al., J. Quant. Spectrosc. Radiat. Transf., 111, 2139 (2010).
[3] I. E. Gordon, et al., J. Quant. Spectrosc. Radiat. Transf., 203, 3 (2017).
[4] R. V. Kochanov, et al., J. Quant. Spectrosc. Radiat. Transf., 177, 1530 (2016).
[5] R. R. Gamache, et al., J. Quant. Spectrosc. Radiat. Transf., 203, 70 (2017).

Excursions into inversions: first results from the QUB secondary eclipse campaign

Matthew Hooton,[1] *Queen's University Belfast*

Detecting and measuring thermal emission from exoplanets immediately before and after occultation by their host stars is an important tool for studying exoplanet atmospheres. Taking this measurement over a range of wavelengths allows an emission spectrum to be built up, which alludes to atmospheric features including chemical composition, thermal structure and circulation efficiency. To date, secondary eclipse observations have largely been at wavelengths red-ward of 1 μm, in no small part due to the fact that most targets are insufficiently large or hot to have detectable secondary eclipse signals at shorter wavelengths with current instrumentation. Observations of secondary eclipses in the i- and z-bands are of particular interest as this window contains prominent TiO and VO features (compounds thought to give rise to temperature inversions in the hottest exoplanets) and is a good discriminator between models for carbon-rich and carbon-poor planets. There have also been notable discrepancies in the reported secondary eclipse depths in this window, possibly due to variability of planetary thermal emission properties as a result of storms. I will present results from the QUB secondary eclipse campaign for ultra-hot Jupiters WASP-12b and KELT-16b, including the first robust secondary eclipse detections in the i-band. I will also present our U-band secondary eclipses of the recently discovered KELT-9b - the hottest known exoplanet.

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Planetary Spectrum Generator: an accurate online radiative transfer suite for exoplanets

Geronimo Villanueva,[1] NASA Goddard Space Flight Center

We have developed an online radiative-transfer suite[2] applicable to a broad range of exoplanets (e.g., terrestrial, super-Earths, Neptune-like and gas-giants). The Planetary Spectrum Generator (PSG) can synthesize planetary spectra (atmospheres and surfaces) for a broad range of wavelengths (0.1 μm to 100 mm, UV/Vis/near-IR/IR/far-IR/THz/ sub-mm/Radio) from any observatory (e.g., JWST, HST, Keck, SOFIA, ARIEL, LUVOIR, OST, coronagraphs, transit). This is achieved by combining several state-of-the-art radiative transfer models, spectroscopic databases and planetary climatological models (e.g., Parmentier equilibrium P/T models and Kempton EOS chemistry). PSG has a 3D (three-dimensional) orbital calculator for all confirmed exoplanets, while the radiative-transfer models can ingest billions of spectral lines from hundreds of species from several spectroscopic repositories. It integrates the latest radiative-transfer and scattering methods in order to compute high resolution spectra via line-by-line calculations, and utilizes the efficient correlated-k method at moderate resolutions. PSG includes a realistic noise calculator that integrates several telescope / instrument configurations (e.g., interferometry, coronagraphs) and detector technologies (e.g., CCD, heterodyne detectors, bolometers). Such an integration of advanced spectroscopic methods into an online tool can greatly serve the planetary community, ultimately enabling to retrieve planetary parameters from remote sensing data, to efficiently plan mission strategies, to interpret current and future planetary data, to calibrate spectroscopic data and to develop new instrument/spacecraft concepts.

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[2]https://psg.gsfc.nasa.gov

Monday Afternoon

Red stars as blue planet hosts

Lalitha Sairam,[1] *Institute for Astrophysics, Göttingen*

Low mass stars make up nearly 75% of the stellar population making them the most common potential planetary hosts. They are in the focus of ongoing and planned surveys for the habitable planet. One such surveys around M dwarfs is CARMENES, which aim at detecting Earth-like planets in their habitable zone. But due to extremely low luminosities of M-dwarfs, the habitable zone moves closer to the star making the orbiting world extremely vulnerable to the effects of magnetic activity and the high-energy emission from its host. Magnetic activity manifests itself in features such as spots, flares and high-energy coronal emission. These stars are capable of producing flares of short as well as longer durations. It is essential to understand the effects of stellar activity and high-energy environment on the planetary atmosphere. Furthermore, stellar activity is also an important obstacle in planet search surveys mimicking the planetary signature. Hence, it is essential to characte rise these stars to disentangle radial velocity variation due to activity from the planetary companion. In this talk, I will give a synopsis of CARMENES survey as well as my study on the stellar activity of nearby low mass stars, which can potentially host exoplanetary systems.

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ORBYTS (Original Research by Young Twinkle Students)

Katy Chubb,[1] *UCL*

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 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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Radiative transfer in atmospheres with large aerosols

Kevin Heng,[1] *University of Bern*

Cloudy / hazy atmospheres are ubiquitous both in and beyond the Solar System, which motivates a deeper understanding of radiative transfer in the presence of aerosols. In our Solar System, geomorphic evidence points to the presence of liquid water on the surface of early Mars. A favoured explanation was the presence of carbon-dioxide ice clouds in the early Martian climate (cf. Forget & Pierrehumbert 1997), but this was later shown to be an artefact of using simplified (two-stream) radiative transfer, which overestimated the scattering greenhouse effect by about 50 K. Here, I present recent work on generalising the two-stream radiative transfer technique, such that it is capable of accurately handling the presence of medium-sized and large aerosols. This novel method retains the computational simplicity of a two-stream method, but has the accuracy of a 32-stream method, which allows for its easy inclusion in exoplanet models that aim to explore a large parameter space. It is also ripe for inclusion in three-dimensional GCMs.

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Hot Jupiters and Cool Stars Beware: A new TiO line list is here

Laura McKemmish,[1] *University of New South Wales*

A new ExoMol style line list for TiO is presented and compared against existing linelists for mid to high resolution astronomical spectroscopy. This linelist has been fitted against a large number of empirical experimental energies obtained using the MARVEL (Measured Active RoVibrational Energy Levels) program using the variational nuclear motion code Duo which enables treatment of coupled electronic states for diatomic molecules. Potential extensions of this methodology to systems like ZrO and OH are discussed.

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An Homogeneous Retrieval of Exoplanet Atmospheres

Patricio Ernesto Cubillos Vallejos,[1] *Space Research Institute, Austrian Academy of Sciences*

To date, we have observed dozens of exoplanets with multi-wavelength transmission spectra, thanks mainly to the Hubble and Spitzer Space Telescopes. However, despite these being some of the most valuable observations in existence, retrieval analyses have revealed our difficulties in establishing stringent constraints on the atmospheric properties of these planets. Given the complexity of atmospheric modeling and retrieval tools, multiple independent analyses are a valuable exercise to highlight the outcome of the assumptions taken by each approach, and ultimately, enable a better understanding of transiting exoplanet observations.

I will present an homogeneous retrieval analysis of a sample of exoplanets with HST and Spitzer observations reported in the literature. Our retrieval tool, Pyrat Bay, is an open-source package that combines advanced MCMC algorithms with an efficient radiative-transfer routine and the latest opacity databases from ExoMol or HITRAN to constrain the parameter space of exoplanet atmospheric models. I will discuss the general properties of the sample and, when applicable, compare our results to those of other retrieval tools, i.e., Line, Madhusudhan, Benneke, or Waldmann. I will also discuss the difficulties that degeneracies in the physical parameters impose in the observed spectra, the consequences that arise from modeling choices made by the researcher, and the expectations for observations from future observatories, like the James Webb Space Telescope.

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The Spex Prism Library Analysis Toolkit: Tools for Characterizing Exoplanet Spectra

Adam Burgasser,[1] *UC San Diego*

The Spex Prism Library Analysis Toolkit (SPLAT) is a public curation of over 3000 near-infrared spectra of low mass stars, brown dwarfs, and planetary mass objects, primarily observed with the IRTF SpeX spectrograph. Originally conceived as a focused dataset, its scope has expanded to a "curation" model, with rich source data and data mining tools, integration of other spectral formats and user-supplied data, and an extensive analysis suite. The last includes template matching to library and user-supplied spectra, 13 sets of spectral models with associated grid-based and MCMC fitting routines, 5 sets of evolutionary models with population synthesis routines, and over 100 filter profiles and associated spectrophotometeric analysis tools. In this talk I will demonstrate a few of SPLAT's capabilities, and solicit feedback from conference participants on what tools are desired by the exoplanet community.

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Tuesday Morning

ARIEL - Science and overview of ESA's mission to study the nature of exoplanets

Göran Pilbratt,[1] *ESA/ESTEC, Noordwijk*

Since the 1990-ies thousands of exoplanets have been discovered. They orbit stars with different properties, and they display a great diversity of physical parameters and planetary system architectures.

The next logical and necessary step in exoplanet science is to independently measure chemical composition of exoplanets. This will enable them to be better modelled, which will allow addressing fundamental questions regarding their nature, in particular what they are made of, how they formed, and how they have evolved to what we observe today, and how this was affected by their parent stars.

The Atmospheric Remote-Sensing Infrared Exoplanet Large-survey (ARIEL) mission has been recently been selected by ESA as M4 in the Cosmic Vision programme for a 2028 launch. It will enable this next step in exoplanet science, by performing measurements of chemical compositions of their atmospheres. It will be devoted to observing a large population (many hundreds) of diverse known preferentially warm and hot transiting planets, opening a new discovery space in the field of extrasolar planets and enabling the understanding of the physics and chemistry of these far away worlds.

The observations will probe atmospheric chemistry and dynamics, by means of infrared spectroscopy (1.25-7.8 μm) and visible/NIR photometry in three bands (0.5-1.2 μm) with an off-axis Cassegrain telescope having a 1.1 x 0.7 m aperture. Both transit and eclipse/ occultation spectroscopy will be employed to obtain transmission and emission spectra. The photometry provides thermal and scattering properties and monitors stellar activity.

Regular timely public releases of high quality data products at various processing levels will be provided throughout the mission.

In this talk I will provide an overview of the ARIEL science objectives, and briefly outline the mission.

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Twinkle - a mission to unravel the story of planets in our galaxy

Marcell Tessenyi,[1] *UCL*

Twinkle is a small, dedicated satellite designed to measure the atmospheric composition of exoplanets. Twinkle is a cost-effective spacecraft being built on a short timescale and is planned for a launch by 2022. The satellite uses an existing platform designed by Surrey Satellite Technology Ltd, and instrumentation built by a consortium of UK institutes. Access to Twinkle is made available to universities, research institutes and national consortia worldwide. The success of this model will lead to a series of space science missions, delivered with a self-sustainable approach. We provide here an update on the funding model and the technical activities in progress for this new class of science mission.

Twinkle can observe the chemical composition and weather of at least 100 exoplanets in the Milky Way, including super-Earths (rocky planets 1-10 times the mass of Earth), Neptunes, sub-Neptunes and gas giants like Jupiter. It will also be capable of follow-up photometric observations of 1000+ exoplanets in the visible and infrared, as well as observations of Solar system objects, bright stars and disks. More information on Twinkle can be found on our website:
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Highlights from the TRES Spectrograph

Allyson Bieryla,[1] *Harvard-Smithsonian Center for Astrophysics*

The Tillinghast Reflector Echelle Spectrograph (TRES) is on the 1.5m Tillinghast Reflector at the Fred Lawrence Whipple Observatory (FLWO) located atop Mt. Hopkins in Arizona, USA. TRES is a fiber fed echelle spectrograph spanning the spectral range 3900−9100 Angstroms. It has a modest resolving power of R=44,000 but is a workhorse for exoplanet science. TRES is capable of achieving 10 m/s radial velocity precision and benefits from about two-thirds of the month on the sky with flexible observing scheduling. This enables strategic planning of observations of planet candidates at quadratures to determine velocity variation and rule out false positives more efficiently. It is difficult to determine precise radial velocities of hot stars with few spectral lines and fast rotating stars with broadened spectral features, and these planet candidates are often avoided by spectrographs, but using tools developed by Lars Buchhave and George Zhou we have begun to probe that parameter space. I will present some highlights from the TRES spectrograph.

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Supervised Machine Learning for Analysing Spectra of Exoplanetary Atmospheres

Chloe Fisher,[1] University of Bern

I am a first year PhD student in the group of Kevin Heng at the University of Bern. We have been collaborating with two computer scientists from the Biomedical Engineering department in Bern to develop a machine learning based technique for atmospheric retrieval. We have adapted the 'random forest' method of supervised machine learning, trained on a precomputed grid of atmospheric models, which retrieves full posterior distributions of the abundances of molecules and the cloud opacity. The use of a pre-computed grid allows a large part of the computational burden to be shifted offline. We demonstrate our technique on a transmission spectrum of the hot gas-giant exoplanet WASP-12b using a five-parameter model. We obtain results consistent with the standard nested-sampling retrieval method. Additionally, we can estimate the sensitivity of the measured spectrum to constraining the model parameters and we can quantify the information content of the spectrum.

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Atmospheric spectra of highly irradiated low-mass exoplanets

Masahiro Ikoma,[1] *University of Tokyo*

Diversity in measured mean density of transiting exoplanets indicates that close-in exoplanets have atmospheres of different compositions. We have recently investigated the structure and evolution of close-in Earth-like exoplanets that are subject to intense stellar radiation. Such extreme types of exoplanets include ones with rocky vapor atmospheres, hazy atmospheres, and expanding atmospheres. Here we present theoretically predicted spectra of such atmospheres and discuss their detectability.

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Atomistic simulations for Energized Processes in the Gas Phase

Markus Meuwly,[1] *University of Basel*

In this contribution I will discuss the use of classical and quantum simulations to characterize small molecular systems based on accurate potential energy surfaces. Starting from high-quality ab initio calculations the data is represented either as a parametrized force field or a reproducing kernel Hilbert space for efficient calculation of energies and forces. Using this as input to classical or quantum simulations, relevant spectroscopic or dynamical observables are determined to validate the simulations and predict properties inaccessible to direct experimentation. They include, for example, equilibrium rates of bimolecular reactions or vibrational relaxation times at very high temperatures.

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A comparison of exoplanet retrieval tools

Joanna Barstow,[1] *UCL*

In recent years, spectroscopic observations of transiting exoplanets have begun to uncover information about their atmospheres including atmospheric structure and composition, and indications of the presence of clouds. Spectral retrieval is the leading technique for interpretation of exoplanet transmission spectra. Whilst several atmospheric models and retrieval algorithms have been successfully employed, as yet the different model suites have mostly been used in isolation and so it is unknown whether results from each are comparable. As we approach the launch of the *James Webb Space Telescope* in 2020, and looking further ahead to the recently-selected *ARIEL* mission, we are entering a new data-rich era in the field of exoplanet atmospheres and so it is important that the tools that will be used to interpret these data are properly verified. We here present a comparative study of three retrieval code suites: *TauREX*; *NEMESIS*; and *CHIMERA*, and dem- onstrate that they produce comparable results for both forward and retrieval models.

We compared output transmission spectra for simple model atmospheres including only a single spectrally active gas, with isothermal temperature profiles, then moved on to comparing more realistic planet models, including simple clouds and combinations of spectrally active gases. Excellent agreement was obtained between the three forward models for the cases we tested. We then took each of the more realistic model planets and binned the spectra down to a resolution of R=100 over the wavelength range of 0.5–10 μm. These spectra were cross-retrieved between the three algorithms to assess whether spectra generated with one model can be accurately retrieved using the others. We find that in the majority of cases the cross retrievals produce the correct result, demonstrating that our retrieval codes have been successfully benchmarked against each other.

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Exoplanet Atmospheres at High Spectral Resolution

Jayne Birkby,[1] University of Amsterdam

High resolution spectroscopy is a powerful tool for exoplanet characterization. At high spectral resolution (R>20,000) the lines in a molecular band are resolved into a dense forest of numerous individual lines, with the line positions and strengths being unique to each molecular species. It is thus more difficult to mimic these signatures by random chance or instrument systematics, and makes it easier to distinguish overlapping molecular bands, when comparing to lower resolution spectroscopy. For close-in planets, we can use their significant change in Doppler shift during their orbit to disentangle their spectrum from their bright host star. Consequently, the technique works on transiting and non-transiting systems. For wide-orbit planets, we can instead use their spectrally distinct and strongly localised spatial position to dispensable them from their host stars. The extracted planet spectrum typically has very low signal-to-noise and requires template matching, e. g. cross-correlation, with models to derive the planet properties. The technique is sensitive to the shape and shift of the line, making it sensitive to measuring the planet's true mass, atmospheric composition and structure, day-to-night winds, rotation, heat circulation, clouds, and potentially even its atmospheric surface features. I will overview the advances of this technique since its first successful detections in 2010 as well as its limitations. I will highlight its future directions with the upcoming ELTs, and its complementary to other characterisation techniques and missions such as JWST and ARIEL.

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Wednesday

ExoAI: Deep learning in exoplanet spectroscopy

Ingo Waldmann,[1] *UCL*

The field of exoplanetary spectroscopy is as fast moving as it is new. Analysing currently available observations of exoplanetary atmospheres often invoke large and correlated parameter spaces that can be difficult to map or constrain. This is true for both: the data analysis of observations as well as the theoretical modelling of their atmospheres. Modelling both sets of correlations in data and modelling is key to understanding the nature of exoplanet atmospheres.

In recent years, bayesian atmospheric retrieval algorithms have become the norm in exoplanet characterization. Traditional atmospheric retrievals are limited by the sampling time required to fully map the likelihood space of the solution. Such large sampling processes do consequently require the atmospheric forward model to be fast, and hence simplistic. Whilst simple forward models are sufficient for the resolution and signal-to-noise of currently available Hubble data, this will not be the case in the era of JWST or Ariel. Though, more complex forward models require more computation time, making them the paramount bottleneck of next generation atmospheric retrievals.

In this talk I will discuss how these improvements in deep learning can be applied to solve correlations in the models as well as speeding up the statistical sampling.

By designing deep neural networks, we can significantly speed up data analysis and interpretation and allow our current models to 'learn from experience'. Such AI driven systems will help to resolve model correlations, and allow us to incorporate complex forward models in the atmospheric retrieval of extrasolar planets.

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The peculiar atmospheric chemistry of KELT-9b

Daniel Kitzmann,[1] *University of Bern*

The atmospheric temperatures of the ultra hot-Jupiter KELT-9b straddle the transition between gas giants and stars, and therefore between two traditionally distinct regimes of atmospheric chemistry. It also makes the atmosphere of KELT-9b, which is expected to be cloudfree, a tightly constrained chemical system that lends itself to a clean set of theoretical predictions and an ideal target for spectral characterisation.

In this talk, we will present the peculiar chemical composition of this ultra hot atmosphere and its implications for observations. For example, we predict the abundance of water to vary by several orders of magnitude across the atmospheric limb depending on temperature, which makes water a sensitive thermometer. Carbon monoxide is predicted to be the dominant molecule under a wide range of scenarios, rendering it a robust diagnostic of the metallicity and allowing to directly obtain the C/H or O/H element abundance from spectroscopic measurements.

Additionally, we will show that atoms and ions of metals are abundantly present in Kelt-9b's atmosphere and could potentially be directly observed. For example, neutral atomic iron is predicted to be seen through a forest of optical and near-infrared lines, which makes KELT-9b an ideal target for high-resolution, ground-based spectroscopy with HARPS-N or CARMENES. We will present theoretical predictions for detecting iron at high spectral resolution and summarise the future observational prospects of characterising the atmosphere of KELT-9b with the Hubble Space Telescope, James Webb Space Telescope, and CHEOPS.

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Atmosphere models for cool brown dwarfs and giant exoplanets

Mark Phillips,[1] *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 (T_{eff}=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 (T_{eff}=200-350K). These model improvements allow us to follow the evolution of Jupiter mass objects down to the coolest temperatures (T_{eff}=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, the treatment of condensates through rainout, and the calculation of low temperature chemical equilibrium abundances. 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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Atmospheric retrievals across the LT transition using 1 - 15um spectroscopy

Ben Burningham,[1] *University of Hertfordshire*

I will present a brief summary of progress in using Brewster to estimate atmospheric properties of brown dwarfs across the L5 - T4.5 spectral range using spectra spanning 1 - 15 microns. I will highlight key results revealing cloud properties, thermal profiles and chemical abundances in the context of predictions from self-consistent radiative-convective equiliubrium models.

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Spectral decomposition: a method to classify exoplanets spectra

Karan Molaverdikhani,[1] *University of Colorado*
Paul Molliere, Max Planck Institute for Astronomy
Thomas Henning, University of Colorado

We introduce a simple but powerful technique to estimate the contribution of each atmospheric constituent in its spectrum, averaged over all pressures. Estimating these contribution coefficients provides us with a tool to quantitatively study relative importance of individual species in both emission and transmission spectra.

We employ this spectral contrast between molecular features, namely water and methane, to explore the parameter spaces where either methane or water is the dominant spectral feature. We propose a classification scheme, with four classes, for irradiated planets based on the dominancy of water and methane features in their atmospheric spectra and the association of their boundary with planetary effective temperature, surface gravity, metallicity and their host star's spectral type.

We find C/O<1 is not a global indicator for a water-dominated atmosphere and neither C/O>∼1 is a ubiquitous indication of methane-dominancy. Consequently, the best temperature range to look for CH4 features is somewhat not very cold as one might expect, ranging from 800k to 1500k and requiring carbon to oxygen ratio to be about 0.7 or higher. This temperature range is also in favor of less cloudy atmosphere in contrast to colder planets, however the presence of clouds is not unlikely and consequently the TP structure as well as species abundances might alter, and similarly non-equilibrium chemistry could also change the spectral appearance of these planets. We present the effect of non-equilibrium chemistry on these regions and show how non-equilibrium chemistry modifies the classification and the regions where it can be neglected.

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The legacy of HST/WFC3: a prototype for future population studies of exoplanets

Angelos Tsiaras,[1] *UCL*

Today, more that 3500 exoplanets have been detected and, despite the significant progress in the field of atmospheric characterisation in the last decade, we still have a limited understanding for a small number of planets. Similarly to the field of exoplanetary detection, atmospheric population studies are the way forward in constraining, which is the current condition of planets, how did they form, and how have they evolved. One of the most successful instruments for observing exoplanetary atmospheres is the Wide Field Camera 3 (WFC3) on-board the Hubble Space Telescope. In particular, the use of the spatial scanning technique has given the opportunity for even more efficient observations of the brightest targets, achieving the necessary precision of 10 to 100 ppm to the flux of the star.

In this presentation, I will discuss the main characteristics of the WFC3/IR instrument, the process followed to develop an automatic analysis pipeline, and the lessons learnt from this process, focusing on the parallel development of both data analysis and simulation software. I will also present the result of this study: an extended catalogue of consistently analysed spectra from HST/WFC3 for cases ranging from super-Earth to Jupiter sizes, from warm to hot temperatures, from clear to cloudy atmospheres. The collective behaviour of these planets with respect to their atmospheric conditions, as well as exceptional cases, such as the super-Earths in the Trappist-1 and 55-Cancri systems will be discussed in more detail. Following a scalable approach is vital for observation planning and data processing in the future, as more dedicated instruments will provide a large number of observations.

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The ExoMol project: progress and perspectives

Sergei N. Yurchenko,[1] *Jonathan Tennyson, Katy L. Chubb, Phillip A. Coles, Daniel Darby-Lewis, Maire N. Gorman, Barry Mant, Laura K. McKemmish, Alec Owens, Oleg N. Polyansky and the ExoMol Team, UCL*

The ExoMol project aims to provide molecular line lists for exoplanets and other atmosphere with a particular emphasis on those atmospheres which are significantly hotter than the Earth's. The ExoMol database underwent a major reformat and upgrade in 2016; it now provides information on a variety of topics including, of course, line lists, cross sections (generated from the same line lists), lifetimes and Landé *g*-factors. So far ExoMol has generated line lists for more than 30 key molecular species and more than 20 line lists have been collected from other sources. In 2017, ExoMol was updated with the line lists for NO,[2] SiH,[3] PO, PS,[4] SH and NS,[5] ^{17}H2O and ^{18}H2O.[6] The update from 2018 will include AlH,[7] BeH,[8] SiH_4,[9] H_2O,[10] C_2,[11] C_2H_2, C_2H_4,[12] CH_3Cl,[13] CH_3F,[14] NH_3 and MgO. Our new flexible code ExoCross can rapidly generate cross sections even from huge line lists. ExoCross also allows facile conversion between ExoMol and HITRAN formats. Methods for efficient production, storage and usage of line lists as well as further data needs will be discussed.

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Posters

Vertical Mixing in Hot Jupiter Atmospheres: 2D post-processing coupling general circulation and disequilibrium chemistry

Robin Baeyens,[1] *KU Leuven*

In the study of exoplanets and their atmospheres, numerical models are indispensible tools. Simulations with various degrees of sophication are used to aid in the interpretation of observational results, and to provide a thorough understanding of the often complex interplay between the physical and chemical processes at play in exoplanet atmospheres.

In order to constrain the abundances of chemical species in the atmospheres of hot Jupiters, a three-dimensional general circulation model[2] and a pseudo-two-dimensional chemistry code[3] were applied in series. By adopting this approach, the degree of vertical mixing in the atmosphere was quantified locally and used as a well-constrained input parameter for the chemistry code. The latter was then employed to solve for the molecular abundances in the atmosphere, taking into consideration both photochemistry and the dynamical disequilibrium effects caused by wind advection.

From the general circulation a localized region of strong vertical mixing was identified at the night side of the planet. Eddy diffusion coefficients in this region can be up to an order of magnitude larger than the atmospheric average. Furthermore, it was found that the mixing in this region has a significant effect on the abundances of molecules such as CH4, CO2 and NH3, when compared to equilibrium chemistry or previously adopted values for the eddy diffusion coefficient.

In the future we plan on further investigating the physical nature of this localized mixing region, as well as continuing to characterize the physical and chemical nature of exoplanet atmospheres using this setup.

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[3] Agundez et al., 2014

Are we ready to characterise exoplanet atmospheres with the James Webb Space Telescope observations?

Jean-Loup Baudino,[1] *University of Oxford*

The James Webb Space Telescope (JWST) will open a new area in the domain of exoplanet atmosphere characterisation and will require accurate models to interpret the observations. In this context, we propose a protocol to compare various atmospheric codes, to identify and discuss the significant differences in the results and to help the codes evolve to become as consistent as possible. We applied this protocol on 3 forward models and one retrieval. We updated them to account for the major differences and we are now able to identify the remaining differences observable with the JWST.

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A Benchmark to Consistently Model Haze Precursors in Exoplanet Atmospheres

Sarah Blumenthal,[1] *University of Exeter*

We present the benchmark of the the long-chain carbon chemical network from Venot et al. (2015) into the 1D atmospheric code, ATMO.[2] ATMO is capable of modelling pressure-temper- ature profiles consistently with equilibrium and non-equilibrium chemical compositions, hydrostatic equilibrium, and radiative convective equilibrium. Drummond et al. (2016) implemented the C0-C2 chemical network from Venot et al. (2012) to consistently model the pressure-temperature profiles of HD 209458b and HD 189733b. We repeat this work adding the C0-C6 chemical network from Venot et al. (2015)

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[2]Tremblin et al. 2015

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

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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.

See: http://e-pytheas.cnrs.fr

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Frequency Comb Spectroscopy at Extreme Temperature and Pressure in Support of Exoplanet Research

Ryan K. Cole,[1] *Nathan Malarich, Paul J. Schroeder, Torrey R. S. Hayden, Anthony D. Draper, and Gregory B. Rieker, University of Colorado Boulder*

We present a suite of laboratory facilities for high-resolution absorption spectroscopy covering a wide range of temperature and pressure. These facilities include multiple atmospheric-pressure burners covering 1400-2200K, a low-pressure three-zone tube furnace covering 0-1atm and 300- 1300K with tunable uniformity, and a high-pressure, high-temperature optical cell capable of up to 100atm and up to 1000K. The facilities are instrumented with a dual frequency comb absorption spectrometer to record spectra in the 1-2 μm range with a resolution of $\sim$0.0014 nm and 10-5 nm wavelength accuracy. A new mid-infrared dual frequency comb spectrometer will enable operation beyond 3 μm. The combination of the broadband, high-resolution spectrometers with high pressure, high temperature measurement capabilities provides a unique opportunity for developing and validating absorption models for exoplanetary atmospheres in a controlled laboratory setting.

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Synthetic spectra of BeH, BeD and BeT using vibronically resolved R-Martrix data for modelling of emission from the JET plasma

Daniel Darby-Lewis,[1]; J. Tennyson, UCL; K. D. Lawson, CCFE, Abingdon; S. N. Yurchenko, UCL; M. F. Stamp, A. Shaw, CCFE, Abingdon; JET Contributors[2]

In order to predict the erosion of the Be first wall in fusion devices such as ITER, an understanding of the release and transport of Be is an essential requirement. BeD release was shown to contribute more than 50% to the total erosion in certain cases of JET D plasma.[3] A study of the molecular spectra, such as those for BeH, BeD and BeT can provide valuable input to codes used for modelling these processes.[4] To this end, transition energies and A-values have been derived from fitted potential energy curves (PECs)[5,6,7] and *ab initio* dipole curves.[8]

Ab initio R-matrix data provides electron electronic-excitation cross sections,[9,10] which along with electron temperature dependent energy distributions can be used to calculate state to state transition rates. Geometry resolved R-matrix calculations will be rotationally-vibrationally averaged to determine vibronic transition rates. These calculations can lead to a non-Boltzmann fitting for the population of states and more accurate estimations for electron temperatures.

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Extrapolating and Interpolating Hydrocarbon Cross Sections

Brendan Devlin-Hill, Barry Mant,[1] *and Sergey Yurchenko, UCL*

The calculation of line lists for large molecules is very intensive in terms of CPU time and memory. Our recent ethylene line[2] list required 100s of hours of CPU time and terabytes of data. However, for many larger hydrocarbons it appears infrared absorption cross sections show simple temperature dependence.[3] We present work on modeling the temperature dependence of ethylene, propene and propane absorption cross sections using model Exomol line list[2] and experimental data.[4,5] A simple polynomial fit to infrared cross sections is shown to give reliable interpolation between measured temperatures and modest extrapolation to higher temperatures. This simple model can reproduce band shapes relatively well as well as retain integrated absorption cross sections. This method, as well as more sophisticated models,[6] should allow the temperature dependence of many hydrocarbons to be accounted for in a cheap and simple manner.

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An Updated Mission Reference Sample for ARIEL

Billy Edwards,[1] *UCL*

ARIEL (Atmospheric Remote-sensing Infrared Exoplanet Large-survey) has been selected as the next ESA medium-class science mission and is due for launch in 2028. During its 4-year mission, ARIEL aims to observe 1000 exoplanets ranging from Jupiter and Neptune-size down to super-Earth size in the visible and the infrared with its meter-class telescope.

The analysis of ARIEL spectra and photometric data will deliver a homogenous catalogue of planetary spectra which will allow the extraction of the chemical fingerprints of gases and condensates in the planet's atmosphere, including the elemental composition for the most favourable targets. It will also enable the study of thermal and scattering properties of the atmosphere as the planet orbit around the star.

An updated study of the suitability of currently-known exoplanets for study with ARIEL has been undertaken. A recent prediction of the TESS yield has resulted in simulated targets around a catalogue of stars and these have also been included to create a list of potential targets. This list of planets has been utilised to form an example Mission Reference Sample to determine whether ARIEL's mission goals could be met from this planetary population.

We find that ARIEL should be able to observe ∼1000 planets at various resolutions over the primary mission life. This sample of the exoplanet population has a diverse range of sizes, temperatures and stellar hosts. The target list will continue to evolve as new planets are discovered.

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Exoplanetary Science with Twinkle

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Twinkle is a 45cm space telescope conceived to characterise extrasolar planets and Solar System objects over a broad wavelength range (0.4 μm). From a sun-synchronous polar orbit vantage point, Twinkle's highly-stable instrument will allow the photometric and spectroscopic observation of a wide range of planetary classes around different types of stars, with a focus on bright sources close to the ecliptic. The planets will be observed through transit and eclipse photometry and spectroscopy, as well as phase curves, eclipse mapping and multiple narrow-band time-series.

The ability of Twinkle's infrared spectrometer to characterise the currently known exoplanets has been assessed. The spectral resolution achievable by combining multiple observations has been studied for various planetary and stellar types. Spectral retrievals have been simulated for some well-known planets (HD 209458 b, GJ 3470 b and 55 Cnc e).

From the exoplanets known today it has been found that Twinkle could probe a large number of planets at low spectral resolution, useful to refine planetary, stellar and orbital parameters, search for TTV and monitor stellar activity through time. For planets orbiting very bright stars, Twinkle observations at higher spectral resolution will enable to probe atmospheric chemical and thermal properties, with the potential to revisit them many times over the mission lifetime to detect variations such as non-uniform cloud cover.

Further surveys will reveal thousands of new exoplanets, of which many will be located within Twinkle's field of regard. TESS in particular is predicted to discover many targets around bright stars which will increase the number of exoplanets Twinkle could observe and simulated TESS detections have been analysed to confirm this.

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Generation of line lists for the manganese bearing diatomics of MnH, MnF and MnCl

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At present, to the best of our knowledge, there are no line lists in the literature for MnH, MnF and MnCl: hence this work opens up the possibility of detection of these molecules in space. It has been speculated that MnH could exist in the ISM and, coupled with the favourable abundance of manganese this acts as motivation for this work.

This line list created for MnH as part of the ExoMol group consists of 10 low-lying electronic states. Using the available experimental data for the $A^7\Pi$ - $X^7\Sigma^+$ system, the Potential Energy Curves (PECs) of the X and A states were refined to an accuracy of around 0.5 cm^{-1}. The experimentally derived term values presented by Balfour (1990, 1992) for the $a^5\Sigma^+$, $b^5\Pi$, $c^5\Sigma^+$, $d^5\Pi$ and $e^5\Sigma^+$ states were processed and used in the final line list. Our line list has a coverage in J up to 50 which we show to be more than adequate for temperatures up to 3000 K and a wavelength range extending from around 0.3 to 10 microns.

For MnCl and MnF, unrefined line lists covering the first 8 electronic states have been created. Future work will be to refine the *ab initio* curves to the available experimental measurements for the $X^7\Sigma^+$, $A^7\Pi$, $a^5\Sigma^+$, $b^5\Pi$, $c^5\Sigma^+$, $d^5\Pi$ and $e^5\Sigma^+$ for MnF and the $X^7\Sigma^+$ state for MnCl hence producing refined line lists.

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Refined line lists for the ions of ArH^+, KrH^+ and XeH^+

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Here we present refined ground state ($X^1\Sigma^+$) line lists for the ions of ArH^+, KrH^+ and XeH^+. The various isotopologues considered are $^{36}ArH^+$, $^{38}ArH^+$, $^{40}ArH^+$, $^{84}KrH^+$, $^{129}XeH^+$, $^{131}XeH^+$ and $^{132}XeH^+$. To date, $^{36}ArH^+$ has been found in the Crab Nebula and both $^{36}ArH^+$ and $^{38}ArH^+$ have been detected in the direction of the lensed blazar PKS 1830 - 211. As far as we are aware neither KrH^+ or XeH^+ have been detected in space. *Ab initio* Potential Energy and Dipole Moment curves where calculated using MRCI/aug-cc-pVQZ level of theory and the former refined by fitting experimental data to an Extended Morse Oscillator to accuracies of $\sim$0.60 cm^{-1} (ArH^+) and $\sim$0.0009 cm^{-1} (KrH^+, XeH^+). All line lists contain 400 states and 4000 - 7000 transitions covering appropriate vibrational and rotational states up to dissociation. Further work will now include adapting the Dipole moment curves to take into account the difference in position between centre of mass and centre of charge for these ions.

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High resolution day-side spectroscopy of the hot gas giant HD 102195b

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Recent observations of the transiting hot Jupiter HD189733b with the GIANO infrared (0.9-2.45) μm spectrograph at the Telescopio Nazionale Galileo have successfully proven that a 4-m class telescope with a performing high-resolution spectrograph can successfully study the atmospheres of exoplanets at high spectral resolution (R$\sim$50,000).

Here we report on day-time spectroscopy observations with GIANO of the non-transiting hot giant planet HD102195b, aimed at detecting water vapour in its atmosphere. We employ a technique to disentangle the Doppler-shifted planet spectrum (whose individual lines are resolved at high spectral resolution) from the stationary telluric/stellar components. We then extract the planetary signal by cross-correlating the residual spectra with template models of the planet atmosphere computed through line-by-line radiative transfer calculations, and containing molecular absorption lines from water and methane. Based on this analysis, we present a preliminary detection of water in the atmosphere of HD102195b, and a first estimate of the planet's true mass and inclination angle of the orbital plane.

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Precision Spectroscopy and Comprehensive Analysis of Perturbations in the $\mathbf{A}^1\Pi(v=0)$ State of $^{13}\mathbf{C}^{18}\mathbf{O}$

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We have reanalysed the $\mathrm{A}^1\Pi(v=0)$ level of $^{13}\mathrm{C}^{18}\mathrm{O}$ by investigating the high-resolution spectra obtained via multi-photon laser excitation as well as with synchro- tron-based Fourier-transform absorption spectroscopy of the $\mathrm{A}^1\Pi - \mathrm{X}^1\Sigma^+(0,0)$, $\mathrm{e}^3\Sigma^- - \mathrm{X}^1\Sigma^+(1,0)$, $\mathrm{d}^3\Delta - \mathrm{X}^1\Sigma^+(4,0)$, $\mathrm{a'}^3\Sigma^+ - \mathrm{X}^1\Sigma^+(9,0)$, and $\mathrm{a}^3\Pi - \mathrm{X}^1\Sigma^+(11,0)$ bands. In addition, Fourier-transform emission spectroscopy in the visible range is performed on the $\mathrm{B}^1\Sigma^+ - \mathrm{A}^1\Pi(0,0)$ band. Spectra of the $\mathrm{B}^1\Sigma^+ - \mathrm{X}^1\Sigma^+$ band are measured in order to tie information from the latter emission data to the level structure of $\mathrm{A}^1\Pi(v=0)$. The high pressures in the absorption cell at the synchrotron and the high temperatures in the emission discharge permitted monitoring of high rotational quantum levels in $\mathrm{A}^1\Pi(v=0)$ up to $J=43$. All information, in total over 900 spectral lines, was included in an effective-Hamiltonian analysis of the $\mathrm{A}^1\Pi(v=0,J)$ levels that are directly perturbed by the $\mathrm{e}^3\Sigma^-(v=1)$, $\mathrm{d}^3\Delta(v=4)$, $\mathrm{a'}^3\Sigma^+(v=9)$, $\mathrm{D}\,^1\Delta(v=0)$, $\mathrm{I}\,^1\Sigma^-(v=0,1)$ close-lying levels and the $\mathrm{e}^3\Sigma^-(v=0,2)$, $\mathrm{d}^3\Delta(v=3,5)$, $\mathrm{a'}^3\Sigma^+(v=8,10)$ remote levels, as well being indirectly influenced by the $\mathrm{a}^3\Pi(v=10,11)$ state. The influence of six further perturber states and their interactions was investigated and are not significant for reproducing the present experimental data. This analysis leads to a much improved description in terms of molecular constants and interaction parameters, compared to previous studies of the same energy region for other CO isotopologues. This work is the next stage of the global project [2,3,1,4,5,6] of precise and comprehensive deperturbation analysis of the $\mathrm{A}^1\Pi$ state in carbon monoxide using complementary spectroscopic techniques.

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Fourier-transform Spectroscopy and Deperturbation Analysis of the $A^1\Pi(v=0)$ Level in the $^{12}C^{17}O$ Isotopologue

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The present study focuses on a first analysis of spectroscopic data for the $A^1\Pi(v=0)$ level in the $^{12}C^{17}O$ isotopologue. Fourier-transform spectroscopy (1.71 m Bruker IFS 125HR) was used to obtain the Ångström $(B^1\Sigma^+ - A^1\Pi)(0,0)$ band spectrum under 0.018 cm^{-1} resolution. The discharge was conducted in the air-cooled, carbon hollow-cathode lamp. The temperature of dc-plasma at the center of the cathode was about 1000 K. The estimated absolute calibration uncertainty (1σ) was 0.005 cm^{-1}. The fitting uncertainty of the line frequency measurements was estimated to be 0.005 cm^{-1}. The spectrum was combined with high-resolution photoabsorption measurements of the $^{12}C^{17}O$ $B^1\Sigma^+ - X^1\Sigma^+(0,0)$ and $C^1\Sigma^+ - X^1\Sigma^+)(0,0)$ bands[2] recorded with an accuracy of 0.01 cm^{-1} using the vacuum ultraviolet Fourier-transform spectrometer, installed on the DESIRS beamline at the SOLEIL synchrotron. An effective Hamiltonian used in deperturbation analysis was performed up to $J=39$, quantitatively addressing complex, multistate interactions with the $e^3\Sigma^-(v=1)$, $d^3\Delta(v=4)$, $a'^3\Sigma^+(v=9)$, $D\,^1\Delta(v=0)$, and $I\,^1\Sigma^-(v=0,1)$ rovibrational levels. The comprehensive data set, 281 spectral lines belonging to 3 bands, was included in the fit. The $A^1\Pi$ and perturber states were described in terms of a set of deperturbed molecular constants, spin-orbit and L-uncoupling interaction parameters, individual and equilibrium constants, term values, as well as isotopologue-independent spin-orbit and rotation-electronic perturbation parameters. This work is a member of a sequence of studies analysing the $A^1\Pi(v=0)$ level in the CO isotopologues [3,4,5,6,7]

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FT spectroscopy of the comet-tail ($A^2\Pi_i \to X^2\Sigma^+$) system bands in $^{12}C^{17}O^+$

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In the emission spectrum of $^{12}C^{17}O^+$ molecule new observations and analyses were performed. Two bands ($1-0$ and $1-1$) of the comet – tail ($A^2\Pi_i \to X^2\Sigma^+$) system in the 18900 to 22100 cm^{-1} region were recorded with the Fourier transform spectrometer (BRUKER IFS 125-HR). The absolute accuracy of wavenumbers was about 0.005 cm^{-1}. The measurement cycle included 128 scans within 1.5 h. As a source of the studied spectrum an air-cooled, carbon hollow-cathode (HC) lamp operated at 780 V, 54 mA dc was used. The lamp was filled with a static mixture of $^{17}O_2$ (70 %) and $^{16}O_2$ (30 %) at a pressure of ∼1 Torr. During the discharge process, the O_2 molecules react with the ^{12}C atoms ejected from the carbon filler placed inside the cathode, thus forming $^{12}C^{17}O$ and $^{12}C^{17}O^+$ molecules in the gas phase, in amounts sufficient to finally achieve a signal-to-noise ratio (SNR) of 100:1 for the $^{12}C^{17}O^+$ ion. Spectra were analyzed using a commercial software OPUS™.[2], which finds peaks and calculates various spectral parameters (wavenumbers, FWHM, etc). As a result of a detailed spectral analysis the individual molecular constants of both $A^2\Pi_i$ and $X^2\Sigma^+$ states were obtained. For the upper $A^2\Pi_i$ state all these constants were delivered for the first time. The parameters for the lower $X^2\Sigma^+$ state were also calculated and can be compared with these determined previously.[3][4][5]

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Experimental and Theoretical Investigations on the Visible Spectrum of AlD^+

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The emission spectrum of the AlD^+ ion has been studied by Fourier transform spectroscopy technique, as a further step of our investigation of the AlD neutral molecule.[2] The $0-0$ and $1-1$ bands of the $AXpI$ system have been recorded in the $27,000 - 29,000$ cm^{-1} region with an instrumental resolution of 0.03 cm^{-1}. In total, almost 500 rotational frequencies were measured with an absolute accuracy of about 0.005 cm^{-1}. It improved the experimental accuracy of the determined frequencies by the factor 10 compared to the previous work.[3] The rotational analysis has shown irregularities in the $\Lambda-$ doubling splitting of the ApI $v = 0, 1$. Consequently, the ApI state has been represented by the rotational term values, while the regular XpI state by the molecular constants. The causes of the irregularities were identified in the interaction between the ApI state the lying higher the BpI state.

Ab initio calculations on the ion were performed using a parallel version of the MOLPRO[4] (version 2010.1) suite of quantum chemistry codes. The static electron correlation was calculated using SA−CASSCF method.[5] The active space consisted of all the occupied valence orbitals of the aluminum atom plus the $1s$ orbital from the deuterium atom. The $1s$ orbital of the Al^+ atom is kept frozen while the $2s2p$ orbitals are closed (kept doubly occupied in all configurations). In addition, SA−CASSCF can be used to calculate the excited electronic states corresponding to the $\mathrm{Al^+(^3P) + D(^2S)}$ asymptote so a total of five states are included ($2\times$ $^2\Sigma^+$, $^2\Pi$, $^4\Sigma^+$, $^4\Pi$). The accuracy of the potentials can be improved by including dynamic electron correlation, that was handled here by using MRCI method.[6]

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Detection of Iron and Titanium in the atmosphere of Kelt-9 b

Jens Hoeijmakers,[1] *CSH Bern / Geneva Observatory*

Kelt-9 b was discovered in 2017 to orbit a bright, hot early-type (A0) star in a 3.4 day orbit, and is the hottest hot-Jupiter known to date, with an expected equilibrium temperature of over 4000 K. This extreme temperature implies an atmospheric chemistry that is distinct from cooler, more commonly detected hot Jupiters with temperatures around 3000 K or less. We have predicted that at the limb, the atmosphere is in chemical equilibrium over a large range in pressure; meaning that the chemistry is fully constrained by the temperature and the metallicity.[2] Another consequence is the expected absence of clouds, making the transmission spectrum less prone to degeneracies that plague retrieval analyses for planets with lower temperatures, that are often cloudy.

Assuming a non-inverted atmosphere, we predicted to be able to detect absorption by neutral Iron (Fe) in the transmission spectrum of the planet, using a high-resolution cross-correlation-based analysis.

We subsequently were able to perform this analysis on a single transit observation by the HARPS-N instrument, and detected the absorption signal of Fe, and unexpectedly, much stronger absorption by Fe^{+} and Ti^{+} - implying high temperatures - above the equilibrium temperature of the planet. This work is currently under review at Nature; and in this talk I will present the analysis and our interpretation of these exciting detections.

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[2] Kitzmann et al. 2018, under review

The Impact of Opacities on Radiative Transfer Calculations

Matej Malik,[1] *University of Bern*

I will present self-consistent radiative transfer calculations of atmospheres of hot and very hot Jupiters. Specifically, I will discuss the impact of using various line lists and differences in line treatment (e.g. wing cut-off) on atmospheric temperatures and emission spectra and the consequences of neglecting vs. including important opacity sources like metals, ions, and atomic lines.

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Optical Transmission Spectra with IMACS on Magellan Baade

Erin May,[1] *University of Michigan*

Transmission Spectroscopy is an exciting observational technique which allows us to gain insight into the atmospheres of gaseous exoplanets while they transit their host stars. Using IMACS on the Magellan Baade telescope, we have started a survey (MOPSS: the Michigan Optical Planetary Spectrum Survey) to study the atmospheres of exoplanets at optical wavelengths, with hopes of measuring Rayleigh scattering slopes and compositions, as well as constrain the existence of alkali absorption features. Here I present results for several of our current data sets, as well as future plans and progress towards our southern hemisphere survey goals.

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A Multi-Parameter Approach to Habitability (M-PAtH)

Sarah McIntyre,[1] *Australian National University*

Recent research has shown that a planet's ability to maintain liquid water and potentially host life depends on the type of star, the planet's density, atmospheric composition and planet-star interactions. Additionally, there are a variety of previously undefined factors such as magnetic field, albedo, impact events, and plate tectonics that could also affect habitability. Analysing the interrelatedness of these factors on detected exoplanets would help to generate a revised model of planetary habitability and suggest a suitable strategy for future astrobiological and biosignature observations of life in the universe. In conjunction with the rapidly increasing information from exoplanet databases expected within the next 2 years, this research will help provide a flexible framework for prioritisation to determine optimal targets for near-future ground- and space-based spectroscopic observations of planetary atmospheres and the potential detection of life in space.

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ExoMol line lists – XXIX. The rotation-vibration spectrum of methyl chloride up to 1200 K

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The recent interstellar detection of methyl chloride[2] has undermined the possibility of CH_3Cl as a realistic biosignature gas in the search for life outside of our Solar system. [3] The fact that CH_3Cl can be formed abiotically, and possibly delivered by cometary impact to young planets, means it is now far more relevant in the context of newly formed rocky exoplanets. Here, we present comprehensive rotation-vibration line lists for the two main isotopologues of methyl chloride, $^{12}CH_3{}^{35}Cl$ and $^{12}CH_3{}^{37}Cl$. [4] The line lists, OYT-35 and OYT-37, are suitable for temperatures up to $T = 1200$ K and consider transitions with rotational excitation up to $J = 85$ in the wavenumber range $0-6400\,cm^{-1}$ (wavelengths $\lambda > 1.56\ \mu m$). Over 166 billion transitions between 10.2 million energy levels have been calculated variationally for each line list. The OYT line lists show excellent agreement with newly measured high-temperature infrared absorption cross-sections, reproducing both strong and weak intensity features across the spectrum. The line lists are available from the ExoMol database.

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The spectrum of sodium hydride and its detection in the atmospheres of cool red dwarfs

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In the paper "ExoMol molecular line lists – X. The spectrum of sodium hydride"[2] published in 2015, we provided rotational, rotational-vibrational, and rotational-vibrational-electronic line lists for sodium hydride in its ground and excited electronic states, and for the two isotopes NaH and NaD. This was achieved by using potential energy curves from literature sources[3] obtained using spectroscopic data, and with *ab initio* dipole moment curves. The PECs and DMCs were used as inputs for the diatomic code LEVEL,[4] which then produced the energy levels of the molecules and the intensities of the transitions.

In 2018, a group from the Australian National University in Canberra combined this line list with astronomical observations to claim that NaH is present in the atmospheres of two well-known red dwarfs: Proxima Centauri and Wolf 359.

In this poster I will discuss the methods used to produce the NaH line lists, and the brief history of the detection of NaH in astrophysical objects.

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ExoMol line lists XXV: a hot line list for silicon sulphide, SiS

Apoorva Upadhyay,[1] *UCL*

The ExoMol project aims to provide line lists of spectroscopic transitions for key molecular species that are likely to be important in the atmosphere of extrasolar planets and cool stars. This is essential for the continued exploration of newly discovered astrophysical objects such as exoplanets, for which there is an increasing desire to characterize their atmospheric compositions. In this poster I will discuss the methodology of the ExoMol project, using silicon sulphide (SiS) as an example.

SiS has long been observed in the circumstellar medium of the carbon-rich star IRC+10216 CW Leo. In our work, comprehensive and accurate rotation–vibrational line lists and partition functions are computed for 12 isotopologues of silicon sulphide in its ground electronic state. The calculations employ an existing spectroscopically accurate potential energy curve (PEC) derived from experimental measurements and a newly computed ab initio dipole moment curve (DMC). The SiS line list for the parent isotopologue includes 10 104 states and 91 715 transitions. These line lists are available from the ExoMol website.

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Conference Delegates

Surname	First name	Institution
Baeyens	Robin	KU Leuven
Barstow	Joanna	UCL
Baudino	Jean-Loup	University of Oxford
Bieryla	Allyson	Harvard-Smithsonian Center for Astrophysics
Biller	Beth	University of Edinburgh
Birkby	Jayne	University of Amsterdam
Blecic	Jasmina	New York University Abu Dhabi
Blumenthal	Sarah	University of Exeter
Boudon	Vincent	Lab. ICB / UBFC / CNRS
Burningham	Ben	University of Hertfordshire
Burgasser	Adam	UC San Diego
Chubb	Katy	UCL/SRON
Clark	Victoria	UCL
Cubillos	Patricio	Austrian Academy of Sciences
Darby-Lewis	Daniel	UCL
Dhesi	Mekhi	UCL
Edwards	Billy	UCL
Fisher	Chloe	University of Bern
Freedman	Richard	Seti Institute
Gorman	Maire	University of Aberystwyth
Grimm	Simon	University of Bern
Guilluy	Gloria	Unito
Hakalla	Rafal	University of Rzeszów
Hargreaves	Robert	Harvard-Smithsonian Center for Astrophysics
Heng	Kevin	University of Bern
Hoeijmakers	Jens	CSH Bern/ Geneva Observatory
Hooton	Matthew	Queen's University Belfast
Howe	Alex	University of Michigan
Ikoma	Masahiro	University of Tokyo
Jørgensen	Uffe G.	University of Copenhagen
Kitzmann	Daniel	University of Bern
Korcakova	Daniela	Astronomical Institute, Charles University
Lavie	Baptiste	Observatory of Geneva
Leconte	Jérémy	Université de Bordeaux

Surname	First name	Institution
Lynas-Gray	Anthony Eugene	UCL / University of Oxford
Malik	Matej	University of Bern
May	Erin	University of Michigan
Mayne	Nathan	University of Exeter
McIntyre	Sarah	Australian National University
McKemmish	Laura	University of New South Wales, Australia
Mendoza	Claudio	Western Michigan University
Merritt	Stephanie	Queen's University Belfast
Meuwly	Marcus	University of Basel
Molaverdikhani	Karan	Max Planck Institute for Astronomy
Owens	Alec	Universität Hamburg
Pilbratt	Göran	ESA
Phillips	Mark	University of Exeter
Pluriel	William	LAB UMR 5804 CNRS
Rivlin	Tom	UCL
Sairam	Lalitha	George-August University
Shea	Christopher	Intrepid Pursuits
Sousa-Silva	Clara	MIT
Talens	Geert Jan	Leiden Observatory
Tennyson	Jonathan	UCL
Tessenyi	Marcell	UCL
Tinetti	Giovanna	UCL
Tsiaras	Angelos	UCL
Upadhyay	Apoorva	UCL
Venot	Olivia	LISA
Villanueva	Geronimo	NASA Goddard Space Flight Center
Waldmann	Ingo	UCL
Wilson	Paul Anthony	Leiden Observatory
Yurchenko	Sergey	UCL

Useful Information

Venue Address

Cumberland Lodge
The Great Park
Windsor
Berkshire
SL4 2HP, UK

01784 432 316

http://www.cumberlandlodge.ac.uk

Travel Information

Rail: Egham station is 3.5 miles (10 minutes by taxi) from Cumberland Lodge.
http://www.nationalrail.co.uk

Taxi: Three taxi firms suggested by Cumberland Lodge are Windsor Cars (01753 677 677), Egham Taxis (01784 433 933) and Egham Cars (01784 434 484).

Organisers' Contact Details

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Jonathan Tennyson:

Grateful thanks are extended to the organising committee:

Victoria Clark
Tom Rivlin
Jonathan Tennyson
Giovanna Tinetti
Ingo Waldmann
Sergey Yurchenko