

Spectroscopy of Exoplanets: Over All Wavelength

High Leigh Conference Centre (Broxbourne, Hertfordshire)
26-29 June 2025

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Introduction

Welcome to the 5th conference in the ExoMol series, Spectroscopy of Exoplanets Over All Wavelengths. These conferences are organised around the general theme of exoplanet characterization.

In an era of challenging new spectroscopic observations of exoplanets, brown dwarfs, and cool stars, providing adequate atomic and molecular data for analysis and interpretation is essential. We welcome you to this meeting, where observers and data scientists can exchange ideas. We hope the discussions during this meeting will address which atomic and molecular data are needed and can be provided, given the currently available hardware and software, and how scientific research priorities should be established accordingly.

We wish you all a productive and enjoyable meeting here at the High Leigh Conference Centre, Hertfordshire, UK (near London), from June 26-29, 2025

Organisers
June 2025

Programme

Thursday – 2025 June 26th

| | | |
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| 12:00 – 13:00 | ARRIVAL | |
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| 10:00 – 10:40 | Jayne Birkby ⁹ | Exploring Complex Chemistry in Exoplanet Atmospheres at High Spectral Resolution 20 |
| 10:40 – 11:00 | COFFEE BREAK | |
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| 12:00 – 12:20 | Sushuang Ma ¹ | Exploring the Atmosphere of the Hot Jupiter WASP-39b: Using Available Opacity Data 23 |
| 12:20 – 12:40 | Charles Bowesman ¹ | Non-LTE Opacities and Radiative Transfer for Exoplanets 24 |
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| 14:40 – 15:00 | Andrei Sokolov ¹ | Temperature-Dependent Photoabsorption Spectra and Photodissociation Rates of the Carbyne Radical (CH) 26 |
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The ExoMol project: progress and updates

Jonathan Tennyson

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The ExoMol project had a major data release last year [1]. The project is continuing to (a) provide line lists for molecules of importance to exoplanetary studies with 92 currently available and studies on species such as AlF, O₂, CS₂, HCO⁺, NO⁺, OH⁺, NH⁺ and BH in progress; (b) to use the MARVEL procedure to enhance the accuracy of the line lists making them suitable for high resolution cross-correlation studies. The high resolution data can be accessed directly using the ExoMolHR front end [2]. The ExoMol database is being extended to consider ultraviolet wavelengths where (continuum) photoabsorption and photodissociation are important. A new photo dissociation database, ExoPhoto, has been launched [3] which contains temperature-dependent cross sections calculated by ExoMol and the PhoMol and UGAMOP projects, and measured by DTU and the EXACT project. Our aim to is significantly expand the ExoPhoto database. We now also provides atomic data in a new ExoMol-format database called ExoAtom [4]; these data were taken from the NIST and Kurucz compilations. We would welcome feedback on what other data are needed both in the form of specific species that should be studied and data types.

[1] J. Tennyson, S.N. Yurchenko, J. Zhang and others, The 2024 release of the ExoMol database: molecular line lists for exoplanet and other hot atmospheres, *J. Quant. Spectrosc. Rad. Transf.*, 326, 109083 (2024).

[2] Jingxin Zhang, C. Hill, J. Tennyson and S.N. Yurchenko, ExoMolHR: A Relational Database of Empirical High-Resolution Molecular Spectra, *Astrophys. J. Suppl.*, 276, 67 (2025).

[3] Qing-He Ni, C. Hill, S.N. Yurchenko, M. Pezzella, A.Z. Fateev, Zhi Qin, O. Venot and J. Tennyson, ExoPhoto: A database of temperature-dependent photodissociation cross sections, *RAS Tech. Instr.*, (*in press*).

[4] Qing-He Ni, Rujia Wang, Tianyang Xie, Jingxin Zhang, C. Hill, S.N. Yurchenko and J. Tennyson, ExoAtom: A Database of Atomic Spectra in ExoMol Format, *RAS Tech. Instr.*, (*submitted*).

High-Resolution Spectroscopy of Ultra-Hot Jupiter Atmospheres: Perspectives from the Roasting Marshmallows Program on Gemini South

Vatsal Panwar¹, Matteo Brogi², Krishna Kanumalla³, Michael R. Line³, Siddharth Gandhi¹, Peter C.B. Smith³

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Ultra-hot Jupiters (dayside temperatures > 2200 K) are a class of gas-giant exoplanets subjected to extreme stellar irradiation which causes the onset of peculiar thermochemical properties including molecular dissociation, atomic ionization, inverted thermal structures, and large day to night temperature contrast. Atmospheric characterization of gas giants lying in the transitional regime between hot and ultra-hot Jupiters can help in understanding the physical mechanisms that cause this fundamental thermochemical transition in atmospheres between the two classes of hot gas giants. In particular, ground-based high-resolution spectroscopy (HRS) is particularly suited for this as it can resolve individual spectral lines from multiple species across a wide range of pressures, and measure signatures of atmospheric dynamics. Using the near-infrared (1.4 to 2.5 microns) high-resolution spectrograph IGRINS on Gemini South, I will present the near-infrared day-side spectrum of WASP-122b ($T_{\text{day}} = 32258 \pm 54$ K), a hot gas-giant situated at this transition. I will discuss the constraints we obtain on the atmospheric chemical abundance and the thermal structure of WASP-122b using state-of-the art Bayesian retrievals. In the context of these results, I will also discuss the importance of accurate and complete line-list data for atomic and molecular species especially TiO, VO, SiO, and metal hydrides which are relevant in the temperature regime spanned by the atmospheres of ultra-hot Jupiters. In summary, I will highlight the detailed information content of ground-based HRS data, their ability to constrain complex atmospheric thermal structures and compositions, and the line-list data needed for such high-precision atmospheric characterization of ultra-hot Jupiters.

Exoplanet Atmospheric Retrieval Over All Wavelengths

Ryan MacDonald

University of St. Andrews

Atmospheric retrieval has become the most widely used technique to infer properties of exoplanet atmospheres. Retrieval codes explore millions of possible atmospheric compositions, temperature structures, and aerosol properties to uncover the range of atmospheric states consistent with an exoplanet spectrum.

With the profusion of JWST spectra and ground-based high-resolution spectrographs, alongside near-UV spectra from Hubble, retrieval codes can now extract atmospheric information from a wider and more finely-sampled wavelength range than ever before.

I will outline the fundamental principles of atmospheric retrieval, survey the retrieval landscape of 2025, and offer future prospects for the next generation of retrieval studies.

HITRAN2024 Data for Planetary Atmospheres

Robert J. Hargreaves, Iouli E. Gordon, Frances M. Gomez, Thibault Bertin & Laurence S. Rothman

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Over the past few decades, the number and variety of known exoplanets has expanded as telescopes (e.g., JWST) and detection methods (e.g., transit spectroscopy) have substantially improved. Exoplanets of the hot-Jupiter variety were the first to have their atmospheres studied, revealing distinctive spectral signatures of water and methane in high-temperature environments. As exoplanet observation and retrieval techniques have developed, molecule-rich atmospheres with temperatures approaching the terrestrial regime can now be probed. In addition, the complexity of models applied to exoplanet atmospheres require accurate spectroscopic parameters to retrieve reliable molecule abundances and infer atmospheric processes. The HITRAN database is especially well suited to provide molecular data for terrestrial-like planets, but also includes data for planetary environments such as H₂, He, or CO₂-rich atmospheres. HITRAN2024 includes 61 molecules in line-by-line parametrization, absorption cross sections for over 600 molecules, collision-induced absorption data for many collisional pairs, MT_CKD water vapor continuum, and aerosol properties. HITRAN also provides supplemental programs and files including HAPI, as well as the HITEMP database. This talk will highlight updates made for HITRAN2024 with an emphasis on the additions and improvements of relevance to (exo)planetary atmospheres.

Molecular Bands in High-Resolution Spectra of Kapteyn's Star (M1.5 VI) Across a Broad Spectral Range from 3800 to 10,400 Å

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¹ NCAC, Toruń

The primary aim of this talk is to demonstrate how recent updates in the lists of molecular lines for oxides (TiO, ScO) and hydrides (AlH, SiH, MgH, CaH, FeH) from the ExoMol database contribute to a more precise understanding of the spectra of late-type stars across the visual spectral range (3800–10,400 Å). Using MARCS atmospheric models, I synthesize the spectrum of an M1.5 red subdwarf and compare it with archival spectra of Kapteyn's Star. The choice of this star was motivated by several factors: its spectral type, where chemical abundances have been determined from atomic lines, but molecular bands are already prominent; the availability of flux-calibrated spectra (XShooter); and high-resolution spectra (HARPS, UVES) with a signal-to-noise ratio above 100. I highlight the need to introduce an enhancement of continuous opacities starting below 5600 Å, increasing towards shorter wavelengths, to match the observed flux. Modifications to the intensities of molecular bands are suggested in order to reconcile with the chemical abundances derived from atomic lines.

High-resolution overtone spectroscopy of H_3O^+

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The ro-vibrationally resolved measurement of the overtone region in the range of 6750-6950 cm^{-1} of the symmetric top molecule H_3O^+ was carried out at 120 K in a 22-pole ion trap using leak-out spectroscopy. A total of 85 lines were measured and compared with the calculations of Yurchenko et al. (2020), available in the ExoMol database, revealing their origin in the $2\nu_3$ overtone bands. The program pgopher will be used to fit the measured transitions to a Hamiltonian in order to obtain the molecular constants.

Updates and New Sections of the CoLine Database

Jeanna Buldyreva

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Elevated temperatures and high fluxes of stellar radiation characteristic for exoplanet atmospheres lead to formation of molecules and molecular ions whose spectroscopic line-shape parameters are very poorly known or simply inexistent. Whereas extensive line lists of positions and intensities of isolated spectral transitions for “ordinary” atmospheric molecules are provided in several spectroscopic databases (e.g., HITRAN [1], GEISA [2], ExoMol [3], etc.), pressure-broadening line-shape parameters, identified as the most important need [4] for experimental and theoretical studies, remain practically unknown or completely missing.

This point has been addressed recently in the framework of the European-Research-Council-funded ExoMol-HD project via a new line-broadening section created in the ExoMol database [5]. Because of “exotic” molecules needed as optically active species and a wide range of required perturbers, we provided as a first step rotationally independent estimates of pressure line-broadening parameters with their temperature dependence for infrared/microwave transitions of 52 absorbers and 12 perturbers [6] with one-value “default values” included in the ExoMol and complete datasets collected in the specifically created for this purpose ColLine (Collisional Line broadening) database.

In the present work we consider the last updates and extensions of ColLine, focusing at robust theoretical approaches to calculations of rotationally-dependent line-shape parameters over wide temperature ranges. Such data will be essential for developing appropriate database structures, including opacities, k-tables and precomputed atmospheric models.

[1] I. E. Gordon et al., JQSRT 277, 107949 (2022)

[2] T. Delahaye et al., JMS 380, 111510 (2021)

[3] J. Tennyson et al., JQSRT 255, 107228 (2020)

[4] J.J. Fortney et al., arXiv:1905.07064 (2019)

[5] J. Tennyson et al., JQSRT 326, 109083 (2024)

[6] J. Buldyreva et al., ApJS 276, 23 (2025)

Exploring the Atmospheres of Sub-Neptunes through Retrievals and Forward Modelling

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Sub-Neptunes ($1.8R_{\oplus} \leq Rp \leq 3.5R_{\oplus}$) are the most common class of exoplanets in our galaxy, yet their interior compositions remain elusive, often resulting in degenerate solutions when modelling their atmospheres. Transit observations across a broad wavelength range are essential to break these degeneracies.

For the first time, the James Webb Space Telescope (JWST) has enabled the study of exoplanet atmospheres in the near-infrared (NIR), allowing for unprecedented and detailed characterisation. Since its launch, JWST transmission spectra have been pivotal in the study of hot giant exoplanets (e.g. WASP-39b and WASP-107b).

Temperate sub-Neptunes ($T_{eq} = 200 - 400K$) are also excellent targets for JWST observations, offering valuable insights into their atmospheric composition, interior structure, and potential habitability. TOI-270 d, K2-18 b, and LHS 1140 b are examples of temperate sub-Neptunes with detected atmospheres observed by JWST.

With the influx of new and potentially transformative JWST data, there is a growing need for standardised methodologies across studies to ensure robust exoplanetary characterisation.

We present a comprehensive modelling approach to interpret JWST transmission spectra of temperate sub-Neptunes and investigate key factors influencing atmospheric retrievals. We incorporate opacity data for molecules expected in sub-Neptune atmospheres, primarily sourced from ExoMol. Our atmospheric retrieval framework includes both free and equilibrium chemistry models, enabling constraints on parameters such as metallicity and the C/O ratio. In addition, we perform self-consistent forward modelling that accounts for haze microphysics, disequilibrium chemistry, and radiative feedback, providing a physically motivated understanding of sub-Neptune atmospheres. We compare retrieval and forward model results and discuss their compatibility with current JWST observations.

Laboratory Astrophysics for Cool Stars and Exoplanets

Peter Bernath

Old Dominion University, Norfolk, VA, USA

Molecular opacities are based on line lists for small molecules and on absorption cross sections for larger molecules. In this talk research results from our laboratory will be surveyed on the preparation of line lists for diatomic molecules such as TiO, ZrO, ScO, C₂, etc. using experimental measurements with a Fourier transform spectrometer for line positions and ab initio (transition) dipole moment functions for line strengths. Our measured line lists for high temperatures for small polyatomic molecules such as methane will also be presented as well as measurements of infrared absorption cross sections for hot hydrocarbons such as ethane. Precise laboratory measurements are needed to improve the predictions of ab initio line lists and are required for high resolution cross correlation spectroscopy of exoplanets.

ExoMol Extensions: ExoAtom and ExoPhoto — Spectroscopic Databases for Atomic and Molecular Photodissociation

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Recent advances in high-resolution spectroscopy and atmospheric modeling have created a growing demand for high-accuracy molecular and atomic data. Therefore, we developed two extensions to the ExoMol framework.

The first extension is ExoPhoto database (<https://exomol.com/data/data-types/photo/>) [1]. It extends the ExoMol database to provide high-accuracy, temperature-dependent photodissociation cross-section data at short ultraviolet wavelengths. ExoPhoto combines theoretical models from three computational databases (ExoMol, UGAMOP, and PhoMol) with experimental datasets from two research groups, covering a broad range of wavelengths and temperatures. Currently, ExoPhoto includes photodissociation data for 20 molecules: AIH, HCl, HF, MgH, OH, NaO, MgO, O₂, AlCl, AlF, CS, HeH⁺, CO, CO₂, H₂O, SO₂, C₂H₂, C₂H₄, H₂CO, and NH₃. It also provides detailed branching ratios and quantum yields for selected datasets. Data are organized in JSON-based files with a consistent naming convention, and cross sections are stored in .photo files for each molecule and temperature. Future developments will include additional photodissociation data and support for non-local thermodynamic equilibrium (non-LTE) conditions.

The second extension is ExoAtom database (<https://exomol.com/data/data-types/atom/>) [2]. It extends the ExoMol database by providing atomic line lists in the ExoMol format, derived from NIST and Kurucz databases. ExoAtom uses five main file types: 'all', 'def', 'states', 'trans', and 'pf'. The 'states' file lists energy levels with quantum numbers, uncertainties, and lifetimes; the 'trans' file records transition wavenumbers and Einstein A coefficients; the 'pf' file supplies partition functions over various temperatures. Future work will expand ExoAtom to include additional ionization stages.

[1] (submitted) Ni QH, Hill C, Yurchenko SN, Pezzella M, Fateev A, Qin Z, Venot O, Tennyson J. ExoPhoto: A database of temperature dependent photodissociation cross sections. RAS Techniques & Instruments (2025)

[2] (preparation) Ni QH, Wang R, Xie T, Zhang J, Hill C, Yurchenko S.N, Tennyson J. ExoAtom: A Database of Atomic Spectra in ExoMol Format. RAS Techniques & Instruments (2025)

Exploring Complex Chemistry in Exoplanet Atmospheres at High Spectral Resolution

Jayne Birkby

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High resolution spectroscopy (HRS) is a powerful and highly versatile, ground-based technique for exoplanet atmospheric characterisation. New HRS instruments and statistical frameworks have accelerated the field dramatically in recent years, producing results on par with JWST e.g. elemental ratios for the study of planet formation, and at the same time opening new parameter space such as the 3D dynamical nature of exoplanets winds and rotation. The unique sensitivity of HRS to spectral line shape holds a wealth of information and we are only just beginning to scratch the surface of what we can learn. In this talk, I will showcase the most recent advances that will enable HRS studies of rocky exoplanets with the Extremely Large Telescopes (ELTs). I will discuss the extension to M-band wavelengths with CRIRES+ and its potential for exploring the surface composition of lava planets with existing telescopes. I will also demonstrate new results that push HRS into the warm (sub-)Neptune regime for the first time, constraining metallicity and aerosols, both in thermal emission and reflected light. I will end with a discussion on the importance of HRS in the context of robust confirmation of complex molecular species in sub-Neptune atmospheres and the necessary laboratory experiments and calculations needed to support this.

Towards a chemical survey of exoplanets

Giovanna Tinetti^{1,2,3} and ARIEL Team

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Since the discovery of the first “exoplanet” about thirty years ago, about 6000 exoplanets have been discovered in distant solar systems, with many surprising planets and planetary systems, often very different from our own. A suite of ground-based and space telescopes are currently in operation or will be launched within this decade to discover more exciting planets and unveil their nature: what are they made of? How did they form? What is the weather like there? Are they habitable?

The Ariel space telescope, to be launched in 2029 as part of the ESA Science Programme, is the first mission dedicated to the determination of the chemical composition of hundreds of exoplanets, enabling planetary science far beyond the boundaries of the Solar System.

Finding out why these new worlds are as they are and what is the Earth’s place in our galaxy and –ultimately– in the Universe, is one of the key challenges of modern astrophysics. The Ariel mission will bring a fundamental contribution to addressing this challenge, as I will illustrate in my talk.

VUV Absorption Cross-Section of HCN for Photochemistry Modelling of Hot Exoplanets

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The spectroscopic characterization of exoplanetary atmospheres is rapidly advancing thanks to observations from JWST and upcoming missions like ARIEL. Recent observations of JWST have proven that the atmospheres of warm and hot Jupiters might not be at thermochemical equilibrium. Thus, to interpret those observational infrared spectra, reliable photochemical models are needed. In hot exoplanet atmospheres, strongly irradiated by their host stars, photochemistry is driven by vacuum ultraviolet (VUV) absorption. However, available VUV absorption cross section data are mostly measured at room temperature, while exoplanet atmospheres can exceed 1500 K. The use of room-temperature absorption cross section data for high-temperature atmospheres introduces uncertainties into the predicted composition of the atmospheres. We present new experimental measurements of the VUV absorption cross-section of HCN between 300 K and 700 K over the 115-200 nm wavelength range. A clear thermal dependence is observed, with the cross-section increasing at higher temperatures. These data have been implemented in the thermo-photochemical model FRECKLL to observe their impact on the chemical composition and radiative transfer. Our results highlight the critical need for temperature-dependent spectroscopic databases to properly model and interpret UV observations of hot exoplanets. They call for continued experimental efforts to provide high-temperature data under conditions relevant to these extreme environments.

Exploring the Atmosphere of the Hot Jupiter WASP-39b Using Available Opacity Data

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Adequate atomic and molecular data are essential for the scientific interpretation of the spectroscopic data of hot Jupiters recorded from space. Recent advancements in the James Webb Space Telescope (JWST) and the upcoming Ariel mission promise unprecedented transit spectroscopic data across the optical to near and mid-infrared ranges of exoplanet atmospheres. As one of the first exoplanets meticulously observed by JWST, WASP-39b has quickly emerged as an iconic target in astrophysical research and exploration. This exoplanet has attracted considerable attention due to its unique characteristics and the extensive data available for analysis. Transit spectra captured using various instruments—including NIRISS, NIRCAM, NIRSpec G395H, NIRSpec, PRISM and MIRI—are currently accessible, paving the way for in-depth studies of its intriguing atmosphere. In this talk, we present a novel and comprehensive approach to interpreting transit spectroscopic data, with WASP-39b as our example target, using the opacity data available in the community, most of which were collected by ExoMol. Our methodology employs ab initio chemistry models alongside blind retrievals, which are used iteratively to uncover physically robust optimal solutions. By adopting this innovative approach, we successfully identify a new scenario to explain the enigmatic atmospheric composition of WASP-39b, involving the chemistry of over 20 elements and their relevant spectral signatures. Taking this study as a case, we advocate for obtaining more comprehensive opacity data, including the atomic, molecular, and aerosol species that have high abundances in our thermal chemical simulations, potentially at higher spectral resolutions for specific wavelengths to further validate and constrain the exoplanetary atmospheric compositions.

Non-LTE opacities and radiative transfer for exoplanets

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A new tool for solving radiative transfer problems and computing molecular opacities in non-LTE exoplanet atmospheres is presented. The ultra-hot Jupiter KELT-20 b is used as a case study to test the wavelengths at which non-LTE effects may be detectable. It is shown that upper atmospheric OH in vibrational non-LTE should be observable primarily via hot bands in the mid-infrared and visible. Using recent calculations for the photodissociation cross sections of OH it is shown that non-LTE effects can increase the total photodissociation rate by over three orders of magnitude, which is likely to have a significant impact on atmospheric modelling. Enhanced continuum absorption in non-LTE may significantly impact retrieved atmospheric abundances.

Characterizing Hot Rocky Exoplanets: Insights from Lava Oceans and Atmospheric Interactions

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In the current Era of Exoplanet Characterization, hot rocky exoplanets are the new frontier, particularly those orbiting close to their stars, which are more accessible to detailed observations. These unique planets suffer from intense stellar irradiation, causing lava oceans to be present on their day-side surfaces. The direct interaction between these molten surfaces and their overlying atmospheres offers unique insights into the planets' internal compositions, making them exceptional planets different than the rocky planets in our Solar System. In this presentation I will discuss methodologies for modelling outgassed magma oceans and their interactions with atmospheric volatiles, highlighting the processes shaping these exoplanetary environments. Additionally, I will present state-of-the-art models that integrate outgassing, radiative transfer, and atmospheric chemistry, providing fits to recent JWST observations of exoplanets like 55 Cnc e and K2-141b. The talk will also address the critical need for enhanced atomic and molecular data to resolve the existing ambiguities in these complex models, towards more precise characterizations of exoplanetary atmospheres.

Temperature-dependent photoabsorption spectra and photodissociation rates of the carbyne radical (CH)

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Understanding photodissociation rates is essential for chemical modeling in various astrophysical environments, particularly in UV-rich regions like the interstellar medium and exoplanetary atmospheres [1]. Traditional models often assume 0 K conditions, which may be insufficient for high-temperature systems and non-LTE conditions. This has motivated the development of new temperature-dependent approaches to calculation of dissociation rates and photoabsorption spectra [2]. In this work, we are using new quantum chemistry data for CH [3] supplemented by a number of experimental photodissociation data for this radical, together with Duo [4] and ExoCross [5] to obtain improved, temperature-dependent photodissociation rates and photoabsorption spectra. Our results are compared with the Leiden database CH data [6] and can be used in astrophysical studies to accurately describe hot or excited carbon-rich environments.

[1] Heays et al., 2017, 10.1051/0004-6361/201628742

[2] Pezzella et al., 2021, 10.1039/D1CP02162A

[3] Hou and Liu, 2024, 10.1039/D4CP03298E

[4] Yurchenko et al., 2016, 10.1016/j.cpc.2015.12.021

[5] Yurchenko et al., 2018, 10.1051/0004-6361/201732531

[6] Van Dishoeck, 1987, 10.1063/1.452610

UV Dual Comb Spectroscopy – Ultra-High Resolution Molecular Spectra in Milliseconds

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Dual comb spectroscopy (DCS) is a novel method that enables the measurement of atomic and molecular spectra at ultra-high spectral (MHz - GHz) and temporal resolution (fs pulses) with measurement times of 500 ms to a few seconds. The principle of DCS is based on the difference in repetition rate between two laser frequency combs generating a beat note that down-converts the optical signals into the radio regime, enabling detection with standard photodiodes. Spectral information is then reconstructed via fast Fourier transformation (FFT). This method offers high stability due to its lack of moving parts, rapid acquisition times, broad spectral coverage, and precise wavelength accuracy. Recent advancements have expanded this method into the UV regime using nonlinear frequency-upconversion, allowing access to not only rotational and vibrational, but also electronic transitions.

The UV regime is critical for the investigation of exoplanet atmospheres, because it drives atmospheric chemistry through photodissociation and provides a unique view into the upper layers of the atmosphere, enabling the detection of trace gases that are difficult to detect in the IR. Investigating this by atmospheric modelling requires precise knowledge of both reaction rates and spectral signatures to be able to predict the abundances and spectral detectability of atmospheric constituents. Many key species for atmospheric chemistry, including potential biosignatures, are expected to be present in such atmospheres only in trace amounts or have weak spectral features in the IR. One such example, NO_2 , is difficult to observe in the MIR due to being overshadowed by H_2O . Here, the UV/VIS regime offers a promising alternative due to higher absorption cross-sections and less interference. With upcoming missions like the habitable worlds observatory (HWO), such molecules may be detected.

Analysing observed spectra, accurately simulating expected absorption and modelling their atmospheric chemistry require expansive molecular databases at a wide range of temperatures. Current databases in the UV regime are often incomplete or lack high resolution data, particularly at higher temperatures. Simulated spectra derived from theoretical line list calculations come with significant uncertainties, especially in the absence of high-quality reference data. This method was used to investigate formaldehyde (HCHO) in the NUV region around 350 nm with a resolution of 1 GHz. We were able to detect over 100 previously unresolved lines, with the measurements being in excellent agreement with ab-initio calculations. Subsequently, benzene (C_6H_6) and SO_2 were studied at 262 nm. Like with formaldehyde, we were able to resolve previously unseen weak lines of benzene. All of these measurements are comparable to or even improve existing state-of-the-art literature with the spectral resolution being Doppler-limited. Good SNR can be achieved with measurement times from a few seconds to as low as 500 ms. By providing high-precision laboratory measurements, DCS helps refine line positions, intensities, and broadening parameters, improving databases such as HITRAN, ExoMol, and UV spectral atlases. Our high resolution data provides experimental validation to existing line lists and can also provide a basis for new models.

Missing Opacity in the Atmospheres of Uranus and Neptune?

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JWST NIRSpec observations have measured the continuous near-infrared spectrum of solar system's giant planets in greater detail than ever measured before. From these new data, new challenges for spectral modelling have emerged.

In the case of Uranus and Neptune, much of the faint near-infrared reflectance spectrum has been revealed for the first. While much of the spectrum can be modelled accurately, we are finding inconsistencies between observed and modelled spectra that suggest a significant source of opacity is missing from our models in windows of otherwise weak methane and hydrogen collision induced ($\text{H}_2 - \text{H}_2$, $\text{H}_2 - \text{He}$) absorption (e.g. 2.7-3.1 μm ; 3200–3700 cm^{-1}). The strength of the additional absorption needed to match the data suggests that the missing opacity is gaseous rather than due to aerosols. Given the smooth spectral shape, we speculate that the missing opacity may be collision induced absorption from $\text{H}_2 - \text{CH}_4$ collisions, which have yet to be characterised by lab or theoretical work in the near-infrared. In this presentation, we will present the case and argue the need for further laboratory and/or theoretical work on $\text{H}_2 - \text{CH}_4$ collision induced absorption, with potential relevance to all cold, hydrogen and methane rich worlds.

Hydrogen Deficient Carbon-Rich Supergiant Stars: Tracing their Atmosphere Rich in Oxygen-18 Isotope to their White-Dwarf Merger Origin

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Hydrogen-deficient Carbon (HdC) stars are supergiants characterised by highly unusual chemical compositions, believed to result from mergers between carbon-oxygen (CO) and helium (He) white dwarfs. Following an overview of our current understanding of these enigmatic and rare stars - whose first known example, R CrB, was discovered over 200 years ago - I will present our latest findings. In a recent study, Mehla et al. (2025) analysed high-resolution K-band spectra ($R \sim 75,000$) of six R Coronae Borealis (RCB) stars and six dustless Hydrogen-deficient Carbon (dLHdC) stars. These two subgroups of HdC stars are thought to represent the high- and low-mass ends, respectively, of the CO-He white dwarf merger population. A semi-automated fitting routine was developed to measure oxygen $^{16}\text{O}/^{18}\text{O}$ isotope ratios using the latest ExoMol line lists. It revealed that all dLHdC stars have ratios consistently lower than 1, while RCB stars exhibit ratios above 4. Notably, a trend of decreasing $^{16}\text{O}/^{18}\text{O}$ ratios with increasing effective temperature was observed, aligning with theoretical predictions of white dwarf merger models, although current models overpredict the low $^{16}\text{O}/^{18}\text{O}$ ratios in dLHdC stars by two orders of magnitude. Additionally, abundances analysis uncovered a correlation between ^{14}N and ^{18}O abundances, suggesting α -capture processes converting a fixed fraction of ^{14}N to ^{18}O from partial He-burning occurring during the merger phase. We are currently extending this work with the analysis of over 30 high-resolution optical spectra of HdC stars obtained using the AAT/VELOCE spectrograph - representing the largest such sample studied to date.

Temperature-Dependent Photodissociation Cross Sections and Rates for H₂S and NH

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The photodissociation of molecules impacts the composition and dynamics of many astronomical systems. The vacuum ultraviolet irradiation of exoplanets by their host star leads to complex photochemistry in their upper atmosphere. In the study of observable exoplanets and other hot astronomical bodies, it is thus critical to understand the effect of temperature on such processes. For instance, H₂S is an important equilibrium sulfur species in exoplanetary atmospheres that is expected to yield a variety of subsequent photochemical products. This is of particular importance with recent James Webb Space Telescope (JWST) detections of SO₂. Accordingly, this work presents preliminary temperature-dependent photodissociation cross sections for both H₂S and NH. All nuclear motion calculations were performed with exact kinetic energy operators using ab initio potential energy, coupling and transition dipole moment surfaces/curves. These data are compared to experimental measurements at room temperature and photodissociation rates are calculated for several important radiation fields.

Blue Skies Space – a new model for the future of space-based research data

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Blue Skies Space has developed an innovative funding and delivery model for science satellites. This new model leverages recent advancements in space technology and the rapidly evolving global scientific landscape, enabling us to drastically reduce satellite development time and costs. Our vision is to accelerate and expand the availability of new datasets to researchers worldwide, complementing the facilities delivered by space agencies.

Our first satellite, Mauve, is designed to monitor the flaring activity of stars, including those that are hosts to potentially habitable exoplanets. Mauve's data will help scientists understand the impact of powerful stellar flares on their atmospheres. The satellite, launching in October 2025, is equipped with a 13 cm telescope and a UV spectrophotometric instrument with a wavelength coverage from 200 to 700 nm.

Twinkle, our flagship mission, features an infrared spectrometer to study extrasolar objects and solar system bodies with a 45 cm telescope in the visible and infrared wavelengths (0.5- 4.5 μm). Twinkle will deliver spectroscopy of thousands of targets, enabling scientists to produce transformative research on exoplanet atmospheres, solar system objects, stars and stellar discs.

In our presentation, we will deliver updates on our satellites and discuss how this new approach is set to increase global access to valuable scientific data. To learn more, please visit bssl.space.

Probing the Most Revealing Layers of the Giant Planets

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The upper atmospheres of Jupiter and Saturn, located several hundred kilometers above the planet's visible cloud decks, are extraordinarily thin, with number densities below 10^{12} cm^{-3} . Being "basically space", however, is not a weakness, but a strength; it makes the region highly sensitive to physical and chemical processes on the planet and to interactions between the planet and its space environment. In this talk, I will focus on two major processes that shape these upper atmospheres: the polar aurorae, which dominate the planet's global upper-atmospheric energy balance, and Saturn's eroding rings, which deposit material into the atmosphere and dominate chemistry. The latter has interesting implications for the evolution and ultimate fate of Saturn's rings. By the end of this talk, I hope to convince you that, if it can be detected, this most revealing layer is worth investigating outside of the solar system.

The Importance of UV-Optical Spectra of Giant Exoplanets

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UV observations probe unique characteristics of exoplanet atmospheres. The mid- to near-UV (MUV 200-300 nm and NUV 300-400 nm) can provide constraints on the presence of strong UV absorbers/scatterers [e.g., Gao et al. 2017; Sing et al. 2019], atmospheric escape [e.g., Bourrier et al. 2018; dos Santos et al. 2023], and enhanced scattering due to aerosol (cloud and/or haze) opacities [e.g., Parmentier et al. 2016; Ohno & Kawashima 2020]. With the advent of JWST, these UV measurements are even more vital providing quantifiable information content to atmospheric interpretation inaccessible at longer wavelengths [e.g., Fairman, Wakeford, & MacDonald 2024]. Aerosols are a core driver for changes seen in UV spectra of transiting exoplanets, yet we still have limited understanding of their particle size and composition, distribution, and dynamics. On an individual basis, this is hard to discern with low-resolution spectra, but as a collective we can look for trends across the population and determine the main drivers of UV opacity. I will highlight how Hubble is leading the way in UV-optical studies through multiple large programs to assess atmospheric escape and low-resolution spectroscopy programs. I will also look to the future and discuss the current instruments and the need for new UV-optical spectroscopy missions and instrumentation beyond 2035.

The Opportunities and Challenges of Using Near-Infrared High-Resolution Spectroscopy to Detect Atmospheric Technosignature Gases in Exoplanets

Mitchell John Yzer¹, Jayne Birkby¹ Raymond Pierrehumbert²

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The search for atmospheric technosignature gases using high-resolution spectroscopy in the near-infrared is a valuable extension of the search for general biosignatures and low-abundance gases in exoplanet atmospheres. High-resolution cross-correlation spectroscopy (HRCCS) is the best technique currently available for this, since it can disentangle faint potential technosignatures from features of more significant atmospheric constituents, such as H_2O , and use the light-collecting power of the Extremely Large Telescopes. My research explores the viability of searching for technosignature gases with next-generation, high-resolution spectrographs, such as ANDES/HARMONI/METIS on the ELT, setting realistic expectations on the likelihood of being able to detect these gases on nearby exoplanets, as a function of their concentration. One of the current limitation in this search is the availability of accurate line lists for important technosignature gases. In this talk, I will present a simulated search for sulphur hexafluoride (SF_6) on rocky exoplanets, which has potential to exist as an industrial pollutant, and as an intentionally released artificial greenhouse gas on planets with insufficient natural CO_2 production. SF_6 is non-toxic, relatively chemically inert, and has an atmospheric lifetime of ~ 1000 years, making it a prime technosignature target. However, there are no sufficiently accurate line lists for SF_6 in the wavelength ranges and spectral resolutions of existing and upcoming high-res spectroscopes, only absorption cross-section data. During this talk, I will demonstrate the challenges in HRCCS that need to be addressed for this technosignature search, including the required spectral resolution and light-collecting power, and the availability of detailed and accurate line lists, when considering observations from ground and space with e.g. JWST, the ELTs, and the Habitable Worlds Observatory.

Next Generation Methods for Simulating Exoplanet Atmospheres

Ahmed Al-Refaie

University College London

The era of Hubble brought about many advancements and discoveries in the field of exoplanet atmospheric characterisation. However, the spectral resolution and density of data from JWST and the upcoming ESA Ariel Space Mission requires us to re-evaluate the fundamental assumptions we make in how we infer and interpret observations. This talk examines the limitations of current methods and how new-generation tools and TauREx are addressing these challenges. In particular we will see how the TauREx framework handles problems such as cloud-modelling through YunMa, stellar contamination with ASteRA and disequilibrium with FRECKLL. We will also look at the application of machine learning in addressing both modelling and retrieval challenges.

Spectroscopy of Free-Floating Planetary-Mass Objects and their Disks with JWST

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Free-floating planetary-mass objects (FFPMOs) in star-forming regions represent the low end of the stellar initial mass function and overlap in mass with the high end of the exoplanet population. As such, they share characteristics with both brown dwarfs and giant planets. We will present new findings on eight FFPMOs from near- and mid-infrared spectroscopy using the NIRSpec and MIRI instruments on the James Webb Space Telescope. We derive fundamental properties of these targets, and find spectral types of M9.5 to L4, with effective temperatures of 1900-1600 K. The photospheric spectra of our targets clearly show a diversity at similar temperatures, especially in the 3-5 micron range, not accounted for by current atmosphere models. We find silicate absorption features in the photospheres of two of our targets, the first such detections in very young FFPMOs, indicating silicate clouds in their cool atmospheres. The remaining six objects show mid-infrared excess emission above the photosphere, as well as silicate emission features, demonstrating the presence of dusty disks. The shape and strength of the silicate features constitute strong evidence of grain growth and crystallization, similar to what is seen in young brown dwarfs and stars. We also detect emission lines from hydrocarbon molecules in the disks of several targets most notably Cha 1107-7626, which shows unambiguously methane and ethylene lines as well as hydrogen recombination lines, the latter implying ongoing accretion. Its disk spectrum looks remarkably similar to that of a very low mass star with a carbon-rich disk, and a model assuming gas temperatures of a few hundred Kelvin in the inner disk can account for its hydrocarbon lines. These are the lowest mass objects found so far with silicate and hydrocarbon emission features arising in their disks, and are worthy of follow-up spectroscopy at high resolution.

Irradiated Brown Dwarfs and their Desert

author Sarah Casewell

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Brown dwarfs are often described as failed stars, however the flip side of this description is that they can also be described as over-ambitious planets. With masses between 13-70 Jupiter masses they have cool atmospheres dominated by cloud features, molecules and show features due to weather. These atmospheres have a lot of similarities with atmospheres we see in planets in our solar system, and also directly imaged exoplanets. The question then is: How like hot Jupiters are irradiated brown dwarfs? I will discuss the phenomenon known as the brown dwarf desert and what we know about the atmospheres of irradiated brown dwarfs and their similarities with irradiated exoplanets including recent results from HST and JWST.

Investigating the Influence of Asymmetric Error Bars in Retrievals of Exoplanet Transmission Spectra

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In a Bayesian retrieval framework, the goodness-of-fit of a model to the observed data is quantified by computing the value of a likelihood function. This informs the pipeline of the suitability of the tested parameters and iteratively updates the system's knowledge in response. However, current pipelines assume a Gaussian form of the likelihood which imposes limitations on our analysis.

Many datasets have now been published which exhibit different upper and lower error bars. These emerge from the asymmetric form of the posterior distributions when fitting the transit depths across wavelength channels in lightcurve data. The Gaussian likelihood can only accept one value for the width of the distribution and, as such, we are forced to average between the two quoted errors. The extent to which this approximation could influence the resultant predictions has been given little attention up to this point. Perhaps it was safe in an age of lower quality data but we have now become sensitive to its influence with improved observing capabilities with the James Webb Space Telescope (JWST).

Given that many JWST datasets are now available to the community, we test this assumption and seek to reaffirm our confidence in our predictions. We incorporate an asymmetric likelihood function in a retrieval and test its ability to accurately retrieve the parameters of a simulation scattered by an asymmetric distribution. Results are compared to the currently accepted, Gaussian case in several scattering regimes and, in doing so, we are able to probe the retrieval's sensitivity to this effect at different scales.

On data scattered by realistic error bars (in terms of their scale and the level of asymmetry), we find the Gaussian assumption to be sufficient. However, when we test the retrieval's sensitivity to these effects with extreme cases of asymmetry, we find that we can improve on the Gaussian approximation as long as the exact shape of the error distribution is well known.

New Mean-Opacity Tables for Probing Stable Stratification in Giant Planets

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Interior models of giant planets traditionally assume convection as the dominant heat transport mechanism in the molecular hydrogen envelope. However, several observations of Jupiter are challenging to explain under this assumption, including the measured abundances of CO and water in the atmosphere, as well as the depth of the zonal winds. A stable layer located around the kilobar level has been proposed to reconcile these observations, an idea that has gained more support with recent Juno measurements of alkali metals, which suggest a depletion in the deep atmosphere. While the presence of a stable layer around the kilobar level appears promising, the degree of alkali depletion required to sustain it remains unclear. In this presentation, I will introduce new mean opacity tables to determine the specific atmospheric compositions that can give rise to stable stratification in the outer envelopes of Jupiter, Saturn, and giant planets in general. These tables extend to higher pressures than those commonly used, making them particularly relevant for modeling planetary interiors and deep atmospheres. I will highlight the key opacity sources that control the presence of stable stratification in the outer envelopes of gas giants and point to species with missing or incomplete opacity data that may also play a significant role.

Predicting the Rotational Dependence of Line Broadening using Machine Learning

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Correct pressure broadening is essential for modelling radiative transfer in atmospheres, however data are lacking for the many exotic molecules expected in exoplanetary atmospheres. Here we explore modern machine learning methods to mass produce pressure broadening parameters for the molecules in the ExoMol database. To this end, state-of-the-art machine learning models have been used to fit to existing, empirical air-broadening data from the HITRAN database. A computationally cheap method for large-scale production of pressure broadening parameters is developed, which is shown to be reasonably (69%) accurate for unseen active molecules. This method has been used to augment the previously insufficient ExoMol line broadening data, providing air-broadening data for all ExoMol molecules, so that the ExoMol database has a full and more accurate treatment of line broadening. Suggestions are made for improved air broadening parameters for species present in atmospheric databases. Further work is in progress to incorporate data for line broadening by other perturbative species. This should lead to a final pipeline which can provide reasonable estimates of pressure broadening for any active-perturbing molecule pair.

Some like it hot, some like it cold, some like it mild but old: Chemical kinetics of (exo)planetary atmospheres

Éric Hébrard

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Chemical kinetics is used in many fields of science. In combustion to describe the degradation of fuels. In air quality to describe the transformation of primary pollutants into secondary pollutants. When chemical kinetics data are obtained, they are usually obtained with these specific applications in mind. However, new applications could be found, and here I will present some examples in the field of astrophysics, specifically in the study of (exo)planetary atmospheres. I will share results obtained from our 3D coupled hydrodynamics-radiation-chemistry model, the Met Office Unified Model, adapted to simulate these environments within our Exoplanet Theory Group (ETG, exoclimatology.com), a multi-disciplinary research group focused on the study of (exo)planetary climates. Hopefully sparking interest in an interdisciplinary collaboration between astrophysicists and chemical kineticists, I will show (1) how combustion chemical kinetics data are used to study the atmospheric composition of hot Jupiters and warm Neptunes, and (2) how Earth's air quality (photo)chemical kinetics data are used to model the atmospheres of terrestrial exoplanets.

How to Characterise Uncertainties in Molecular Opacities: An ExoMol Study

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Accurate molecular opacities are paramount for reliable exoplanet atmospheric characterisation and the interpretation of observed spectra. The ExoMol opacities (ExoMolOP) are based on line lists for over 100 molecules and 300 isotopologues, amounting to nearly a trillion individual transitions. The quality of the lines provided can vary significantly, ranging from high spectroscopic resolution to being only applicable for low-resolution applications. This information is recorded in individual line uncertainties, provided alongside the description of molecular or atomic states. However, this information is not propagated to the opacity tables. As a result, high-quality spectroscopic regions can be mixed with low-quality data. In this talk, I will discuss ideas on how uncertainties of the molecular opacities can be defined and present our methodology for a robust propagation of the line uncertainties to the molecular cross sections. The associated data format for storing this information in the database, as well as prospects for integrating these uncertainties into atmospheric retrievals, will also be discussed.

Multi-modal Atmospheric Characterization of β Pictoris b : Adding High-Resolution Continuum Spectra from GRAVITY

Matthieu Ravet

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The characterization of giant exoplanets such as β Pic b is now routinely performed with multiple spectrographs and imagers exploring different spectral bandwidths and resolutions, allowing for atmospheric retrieval of spectra with or without the conservation of the planet spectral continuum. The accounting of data multi-modality in the analysis can provide a more comprehensive determination of the planets physical and chemical properties and inform on their formation history. As both data and models are becoming increasingly complex, new analysis techniques are being developed to better characterize these objects. We present the first VLTI observations at R 4000 of β Pic b, the first obtained on an exoplanet with GRAVITY at such resolution. We upgrade the forward modelling code ForMoSA to account for the data multi-modality, including low- medium- and high-resolution spectroscopy both based on direct model-data comparison and the analysis of cross-correlation signals. We use ForMoSA to refine the constraints on the atmospheric properties of the exoplanet and evaluate the sensitivity on the retrieved values to the input dataset. We obtain four high signal-to-noise (S/N 20) spectra of β Pic b at K-band with GRAVITY conserving both the pseudo-continuum and the pattern of molecular absorptions. We use ForMoSA with four grids of self-consistent forward models (Exo-REM, ATMO, BT-Settl, and Sonora) exploring different T_{eff} , $\log g$, metallicity, C/O, and $^{12}\text{CO}/^{13}\text{CO}$ ratio. We then combine the GRAVITY spectra with published 1-5 μ photometry (NaCo, VisAO, NICI, SPHERE), low- to medium- resolution (R 700 broad band, 0.9-7 μ) spectra, and echelle spectra covering narrower bandwidths (R 100000, 2.1-5.2 μ).

RACER (RAPid Calculation of Exoplanetary Radiative Opacities): a new PYTHON Package to Efficiently Calculate Opacities

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With the expected revolution in high-resolution characterization of exoplanets with the ELT, accurate modeling of spectral features requires precise cross-sections of atoms and molecules. In this talk, I will present a new, easy-to-use Python package I am developing for calculating high-resolution opacities. A key feature is its numerical efficiency as the line lists are growing. For instance, the ExoMol methane line list currently contains about 50 billion lines, which significantly increases the computational time for opacity calculations. The rapid calculation of the individual line profiles is therefore crucial. To tackle this, our package combines a sampling method for molecular lines (M. Min, 2017) with the Humlíček approximation of the Voigt profile to speed up the line profile calculations. This combination enables processing up to 2×10^6 lines per second per CPU core (depending on the pressure and resolution), making it possible to handle even the largest line lists efficiently. The package also allows the user to include sub-Lorentzian line wing treatments and multiple line broadening approaches, offering flexibility for various use cases. As input, the package supports the major spectroscopic databases ExoMol, HITRAN, HITEMP, VALD, and Kurucz. The resulting opacity data can be used directly with petitRADTRANS, a widely used atmospheric modeling and retrieval code, but can also be formatted in any other way that is specified by the user. At this workshop, I will ask for community input regarding additional features that may enhance usability in the community.

Three Years of Transiting Exoplanet Spectroscopy with JWST

Jo Barstow

Open University

Over the last three years, JWST has revolutionised our ability to characterise exoplanets via transit, eclipse and phase curve spectroscopy. Results have highlighted the diversity of gas giant atmospheres and delivered several surprises along the way. Within this talk, I will present some highlights of transiting gas giant spectroscopy during the first three JWST cycles, and how these results have informed our understanding of atmospheric chemistry and dynamics. I will also discuss some of the challenges involved in interpreting these datasets, arising from instrument choice, observation geometry, and sometimes quirks of the target itself. Underpinning all of these results is the requirement for accurate absorption data for the chemical species under consideration, a list that is rapidly expanding as we begin to characterise cooler and smaller planets.

Constraining Atmospheric Evaporation Rate From Gas Giants by Simultaneous Modelling of Lyman- α , H α and Helium Transit Spectra

Gopal Hazra, Subhadip Pal and Arnob Ghosh

IIT Kanpur

Evaporation of atmospheres from giant planets is well observed in various spectral lines, for example in Ly-alpha, H-alpha and helium lines. This atmospheric evaporation is driven by X-ray and Ultraviolet (XUV) radiation from the host star but total evaporation rate does not solely depend on XUV radiation. The complex photochemistry of the atmosphere also play a significant role on the evaporation rate. We model the atmospheric evaporation by considering a hydrogen-helium atmosphere using a self-consistent radiation-driven atmospheric escape model. We include the self-consistent hydrogen-helium photochemistry in the atmosphere. After successfully modelling the evaporating atmosphere, we compute synthetic Ly-alpha, H-alpha and helium spectra. We compare our synthetic transit spectra with the observed Ly-alpha, H-alpha and helium spectra simultaneously for gas giants (e.g., HD189733b) to constrain some uncertain parameters and put a stringent constraint on the evaporation rate. As the initial fractional composition of hydrogen and helium in the atmosphere and the incident stellar XUV radiation remain sources of uncertainty, we first estimate those values by comparing our synthetic transit spectra with observed ones and then compute the evaporation rate. Our findings will be discussed in detail.

The Earth 2.0 (ET) Space Mission

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The Earth 2.0 (ET) space mission will deploy a space observatory consisting of six wide-angle transit telescopes and one microlensing telescope in a halo orbit near the Sun-Earth Lagrange L2 point. By combining the transit and microlensing methods, the mission aims to search for habitable Earth-like exoplanets orbiting solar-type stars, measure their occurrence rate, and conduct a comprehensive population census of both terrestrial and free-floating planets. This will help reveal the origins of these planets and provide new candidates and perspectives for the search for extraterrestrial life. The ET mission's observations, statistical studies, and theoretical analyses will address key scientific questions, including: (1) How common are habitable Earth-like planets orbiting solar-type stars? (2) What are the properties of terrestrial-like exoplanets? (3) How common are free-floating Earth-mass planets, and what are their origins? In addition, the ET mission will provide vast amounts of high-precision, high-frequency, and long-baseline photometric data, advancing research in fields such as asteroseismology, galactic archaeology, time-domain astronomy, binary stars, and binary black holes.

Addressing Laboratory Challenges in the VUV for Exoplanet Atmospheres: Photodissociation and Photoionization

Helgi Hróðmarsson

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VUV photons are important drivers of chemical processes in exoplanet atmospheres. In order to accurately simulate the photo-driven chemistry within, it is important to accurately characterize and constrain photodissociation and photoionization cross sections of molecules. Obtaining cross sections experimentally is significantly challenging, but more challenges arise in terms of translating laboratory data into quantities used in photochemical models as there are multitudes of photoprocesses unaccounted for, either due to the lack of laboratory/theoretical data or due to accidental ignorance of what photo-processes are potentially important, such as photodissociation branching ratios, electronically excited photoproducts, fluorescence, and more. The objective of this talk will be to give an overview of the current state of knowledge of quantified photo-driven processes that are being exploited, and the potential blind spots that could be sources of important photochemistry unaccounted for in modern exoplanetary atmospheric models.

Towards a Spectroscopic potential energy surface for Methanol CH₃OH

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Electronic potential energy surfaces form the basis of spectroscopic calculations. Achieving spectroscopic accuracy in *ab initio* calculations remains a difficult task. Here we apply the approach previously used to obtain the highly accurate surface computed for methyl chloride (Owens et al. 2015). The main contribution is computed using the explicitly correlated CCSD(T)-f12b method extrapolating to the complete basis set limit using the aug-cc-pVTZ-f12b/aug-cc-pVQZ-f12b basis sets. We then consider core-valence effects, higher-order correlation, the diagonal Born-Oppenheimer correction and scalar relativistic corrections. The potential energy function is represented by a fully symmeterised series expansion fit using weighted least squares on the *ab initio* data consisting of 49537 grid points.

Owens, Alec, Sergei N. Yurchenko, Andrey Yachmenev, Jonathan Tennyson, and Walter Thiel. "Accurate Ab Initio Vibrational Energies of Methyl Chloride." *The Journal of Chemical Physics* 142, no. 24 (June 28, 2015): 244306. <https://doi.org/10.1063/1.4922890>

A Study of Very High-Resolution Visible Spectra of Titan: Line Characterisation in Visible CH₄ Bands and the Search for C₃

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The atmosphere of Titan is a unique natural laboratory for the study of atmospheric evolution and photochemistry akin to that of the primitive Earth, with a wide array of complex molecules discovered through infrared and sub-mm spectroscopy. Here, we present the results of the exploration of original, ground-based, very high-resolution visible spectra of Titan, obtained with VLT-UVES. We have developed a new, Doppler-based line detection method which allowed to retrieve an empirical, high resolution ($R = 100.000$) list of methane absorption lines between 525 nm and 618 nm, for which no similar line lists are yet available, identifying and characterising more than 90 new high energy CH₄ lines.

Furthermore, we searched for the predicted, but previously undetected carbon trimer molecule, C₃, on the atmosphere of Titan, at its 405.1 nm band, by comparing VLT-UVES Titan spectra with a line-by-line model spectrum of Titan's atmosphere with C₃. Our results are consistent with the presence of C₃ at the upper atmosphere of Titan, with a column density of 10^{13} cm⁻². This study of Titan's atmosphere with very high-resolution visible spectroscopy presents a unique opportunity to observe a planetary target with a CH₄-rich atmosphere, from which CH₄ optical properties can be studied. It also showcases the use of a close planetary target to test new methods for chemical retrieval of minor atmospheric compounds, in preparation for upcoming studies of temperate small exoplanets.

NRMolCol: Inelastic Scattering Data for (exo)Planetary Atmospheres

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The study of molecular scattering is an essential step for understanding a large number of phenomena, from the dynamics and evolution of planetary and exoplanetary atmospheres, the population evolution in plasmas, to the understanding of spectral broadening observed during retrievals [1]. The importance of this field is evident from the vast number of computational methodologies developed over the years (from full quantum methodologies, to quasi classical trajectories, passing by semiclassical approaches) [2]. and the existence of well-recognised databases in the community (KIDA, BaseCol, etc) [3].

This contribution will present the progress made in the improvement of the semiclassical approach (full quantum vibrations, classic rotation and translation) introduced by Billing [4], extending the range of applications of the code (introduction of different functionalities that allows the treatment of rotational-dependent cross sections, etc), and improving the code performances (different parallelisations schemes, GPU porting etc).

Our code is tested against full quantum simulations, using CS+He as a test case [5]. CS has been observed in a variety of objects such as carbon-rich stars, star forming regions, dense interstellar clouds, and recently proposed as sulphur bearing species in WASP-39 b [6]. We found that the difference in rates between the two models is within the accuracy of the two approaches. We explored the convergences of our results when changing the number of vibrational states and the number of classic trajectories. We will extend the range of available data to cover the vibrational ladder up to dissociation.

[1] G. Graziano, Nat. Rev. Chem 2 (2018), 0127.C.-H. Shon and T. Makabe, IEEE Trans. Plasma Sci. 32 (2004) 390-398. P. W. Anderson, Phys. Rev. 76 (1949), 647.

[2] W.H. Miller, J. Chem. Phys. 53, 3578 (1970). Jeremy M. Hutson, C. Ruth Le Sueur, Comput. Phys. Commun. 241 (2019), 9-18. Yang, Dongzheng, et al. J. Chem. Phys. 158. 5 (2023).

[3] D. Talbi and V. Wakelam J. Phys. Conf. Ser., 1 (2001), 300. M.L. Dubernet et al A&A, 683 (2024) A40.

[4] G. D. Billing Comp. Phys. Rep. 1 (1984) 237-296.

[5] F. Lique, A. Spielfiedel and J. Cernicharo A&A, 451 3 (2006) 1125-1132.

[6] M. Agundez, J. Cernicharo, ApJ, 650 (2006), 374. G. Bilalbegovic, G. Baranovic MNRAS, 446 (2015), 3118 c) SM. Tsai, E. K. H. Lee, D. Powell et al. Nature 617 (2023), 483-487.

Upper-Atmosphere Exoplanet Constraints from Ultraviolet Transmission Observations

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The discovery of thousands of exoplanets has unveiled a staggering diversity in their physical properties and environments. It is thought that the observed distribution of planetary masses and radii is the direct outcome of planet formation processes and subsequent evolutionary interactions with their host stars. These processes can be further understood by studying the structure, composition, and loss of exoplanetary atmospheres. Of particular importance is the study of the uppermost layers of an atmosphere (below 1 micro-bar), where atmospheric escape is expected to take place. Detecting and characterizing escaping species in these regions enables us to constrain key properties such as thermal structure, mass loss rates, compositional changes, and star-planet interactions. In this presentation, I will provide an overview of current efforts to probe the upper atmospheres of exoplanets through ultraviolet and optical observations. I will discuss the implications of these observations for our understanding of atmospheric mass-loss regimes, as well as the observational, laboratory-data, and modeling challenges associated with these studies.

FT-UV emission spectroscopy of the $B^2\Sigma^+ - X^2\Sigma^+$ system of $^{12}C^{16}O^+$ and $^{12}C^{17}O^+$

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Abstract The CO^+ molecule is a cation of the second most abundant molecule in space, carbon monoxide. The main isotopologue i.e. $^{12}C^{16}O^+$ was successfully detected towards the interstellar medium (ISM) by the lowest rotational transitions and also in the comets by the $A^2\Pi_i - X^2\Sigma^+$ system bands (see [1] and references therein). There is no evidence about the presence of the $^{12}C^{17}O^+$ cation in space. However, CO molecules bearing the isotope seventeen of oxygen have already been detected in ISM, despite a very low natural abundance of the ^{17}O (about 0.04%).

The CO^+ isotopologues have been studied recently in the Materials Spectroscopy Laboratory at the University of Rzeszów through the $B^2\Sigma^+ - X^2\Sigma^+$ system using FT-UV emission spectroscopy technique: $^{12}C^{16}O^+$ [1] and $^{12}C^{17}O^+$ [this work]. In total, about 1000 ro-vibronic transitions, belonging to the $0 - 0, 0 - 1, 0 - 2$ and $0 - 3$ bands, have been measured with an absolute accuracy of $0.005 - 0.010 \text{ cm}^{-1}$. The experimental data were analyzed using the PGOPHER program [2], which resulted in a set of high accuracy molecular constants and ro-vibronic level positions for the $X^2\Sigma^+, v = 0 - 3$ and $B^2\Sigma^+, v = 0$ levels for both isotopologues.

References 1. W. Szajna, R. Kępa, R.W. Field, R. Hakalla, FT emission spectroscopy of the $0 - v''$ progression bands of the $B^2\Sigma^+ - X^2\Sigma^+$ system of $^{12}C^{16}O^+$, J. Quant. Spectrosc. Radiat. Transf. 324, 109059 (2024). [10.1016/j.jqsrt.2024.109059](https://doi.org/10.1016/j.jqsrt.2024.109059)

2. C.M. Western, PGOPHER: A program for simulating rotational, vibrational and electronic spectra. J. Quant. Spectrosc. Radiat. Transf. 186:221-42 (2018). [10.1016/j.jqsrt.2016.04.010](https://doi.org/10.1016/j.jqsrt.2016.04.010).

Ab initio Spectroscopic Investigation of Hydrogen Fluoride

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Hydrogen fluoride (HF) is a chemically simple but astrophysically significant molecule, with strong rovibrational features that make it a useful probe in exoplanetary atmospheres. It has been detected in various astronomical environments, including sunspots, the atmosphere of Venus, red giant stars, and the interstellar medium. In this study, we perform a detailed ab initio investigation of the rovibronic spectroscopy of the HF molecule. High-level quantum methods are used to model the electronic structure of the HF molecule, including potential energy curves, transition dipole moments, and allowed couplings for relevant excited states. These data are then combined with accurate nuclear motion calculations to characterize the rovibronic structure and spectral features of HF. The resulting theoretical spectra provide reliable molecular data that is applicable to astrophysical modeling, particularly in the context of exoplanetary atmospheres and interstellar chemistry. This work contributes to a deeper understanding of molecular signatures in the ultraviolet (UV) region and supports the interpretation of spectroscopic data from current and future space-based observatories.

Machine Learning for Isotopologue Extraction

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Accurate isotopologue line lists are essential for modelling and interpreting high-resolution astronomical spectra, particularly for molecules like carbon monoxide (CO) that play a key role in the atmospheres of exoplanets, brown dwarfs, and cool stars. Existing approaches to isotopologue extrapolation used by ExoMol typically apply corrections based on variational calculations for the main isotopologue, assuming mass-dependent shifts and shared residuals across isotopologues [1]. While this method is effective and has proved useful [2], it can struggle with higher accuracy requirements at elevated vibrational or rotational states, and/or for minor isotopologues. In this work-in-progress, the application of machine learning (ML) techniques is explored to improve isotopologue extrapolation for CO. Predicting isotopologue rovibrational energy levels and transition frequencies using ML on a combination of variational calculations, hybrid line list data, and available experimental results. By learning paYerns in the residuals between computed and corrected energy levels, these models are expected to generalize to isotopologues with sparse experimental data, such as $^{12}\text{C}^{17}\text{O}$, $^{13}\text{C}^{17}\text{O}$ or $^{13}\text{C}^{18}\text{O}$. Several machine learning architectures are currently being evaluated including kernel-based methods and neural networks, with plans to benchmark against traditional extrapolation techniques in terms of accuracy and robustness across a range of energy levels.

[1] O.L. Polyansky, A.A. Kyuberis, L. Lodi, J. Tennyson, Sergei N. Yurchenko, R.I. Ovsyannikov, and N.F. Zobov, *Mon. Not. R. astr. Soc.*, 466, 1363-1371.(2017).

[2] Ya.V. Pavlenko, S.N. Yurchenko, L.K. McKemmish and J. Tennyson, *Astron. Astrophys.*, 42, A77 (2020).

High-resolution Rovibrational and Rovibronic Spectra of $^{12}\text{C}^{16}\text{O}$

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Carbon monoxide (CO) plays a crucial role in understanding the atmospheric composition and chemical processes of exoplanets, as it is a key indicator of planetary atmospheric chemistry, thermal structure, and potential habitability. The availability of reliable CO spectroscopic data enhances the robustness of retrievals in exoplanet characterization and directly supports the scientific goals of present and future missions such as Ariel, JWST, and Twinkle. Available tools, such as MARVEL (Measured Active Rotational-Vibrational Energy Levels), and ab-initio calculations are necessary to achieve such goal. In MARVEL, the input consists of experimentally observed transition frequencies, each with an associated uncertainty and quantum state label. These transitions are validated and processed to create a spectroscopic network (SN) where nodes represent energy levels and edges represent transitions. By solving the network using weighted least-squares fitting, MARVEL yields a set of term energies that best reproduce the measured data within their uncertainties. In this work, accurate, MARVEL experimental rovibrational and rovibronic energy levels, with associated labels and uncertainties, are reported for the ground and lowest low-lying singlet and triplet electronic states of the diatomic $^{12}\text{C}^{16}\text{O}$ molecule. The energy levels are obtained through careful analysis of high-resolution experimental spectra of CO from more than seventy-five literature sources. The obtained data is used to fit energy levels that were obtained in previous work through ab-initio methods. Comparisons of our results with published work show remarkable agreement.

Collisional-broadening line-shape parameters of rovibronic transitions in the $^{12}\text{C}^{16}\text{O}$ $\text{a}^3\Pi - \text{X}^1\Sigma^+(1, 0)$ band

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Line-shape parameters of rovibronic transitions have become a subject of increasing study since they are needed for modeling of visible and ultraviolet radiation transport in exoplanetary atmospheres. Getting their experimental values represents however a formidable task, so that a very limited number of measurements is available in the literature for NO, CO and OH self-perturbed and perturbed by N₂, CO₂, H₂O and Ar.

In the present work we analyse transitions in the $\text{a}^3\Pi - \text{X}^1\Sigma^+(1, 0)$ band of $^{12}\text{C}^{16}\text{O}$ recorded in SOLEIL Synchrotron at 300 K [1]. The broadening and shift coefficients obtained for different values of the rotational quantum number J are compared to CO-CO measurements of Q-branch transitions in the B - X(0,0) band by DiRosa et al. [2] who reported no observed dependence on rotational quantum state.

Our measurements represent an alternative way to obtaining rovibronic line-shape parameters at room and elevated temperatures (above 1000K) needed for exoplanets. They enable also probing of various buffer gases. The J -dependence of broadening and shift coefficients opens a prospective of more advanced theoretical calculations going beyond the traditional "phase-shift" theory previously applied to NO and OH [3].

[1] S. Mahmoud et al. (in preparation).

[2] M.D. Di Rosa, R.L. Farrow, JQSRT 68, 363-375 (2001).

[3] J. Buldyreva, R.P. Brady, S.N. Yurchenko, J. Tennyson, JQSRT 313, 108843 (2024).

Rovibrational Overtone and Combination Bands of the HCNH⁺ Ion

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The HCNH⁺ ion, a linear closed-shell species of considerable relevance in interstellar chemistry, has been the subject of extensive laboratory investigations. While recent studies have concentrated on the hyperfine-resolved pure rotational spectra, the present work focuses on the vibrational spectra in the 6200–6900 cm⁻¹ region, specifically covering overtones and combination bands associated with the principal N-H (ν_1) and C-H (ν_2) stretching modes. Rovibrationally resolved spectra have been obtained for the first overtones $2\nu_1$ and $2\nu_2$, the combination band $\nu_1 + \nu_2$, and another combination band $\nu_2 + \nu_3 + 2\nu_5^0$, where ν_3 corresponds to the C-N stretch and ν_5 to the HNC bending mode. Notably, this last combination band possesses a calculated intensity of merely 0.06 km mol⁻¹, approximately 10⁴ times weaker than the ν_1 fundamental band (482 km mol⁻¹). Such high sensitivity was achieved using a “kick-out” enhanced multi-step laser-induced reaction (LIR) scheme. The endothermic reaction with C₂H₄ was employed; however, the resulting products underwent further reaction with C₂H₄, forming up to C₅H₇⁺ ions, which were subsequently monitored as the spectroscopic signal. The experimental findings are supported by theoretical calculations at the CCSD(T)-F12b/cc-pCVQZ-F12 level.

Low-Lying Electronic States for CO

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My research focuses on studying the spectroscopy of carbon monoxide (CO) molecules in exoplanets. The motivation for investigating the molecular spectroscopy lies in its crucial role in deciphering the compositions of exoplanet atmospheres. In my study, my focus is specifically on the lower-energy states of CO, with the aim of compiling a comprehensive list detailing the transitions between various electronic states for CO. This compilation will serve to enhance the existing ExoMol database. The generated list will be valuable for spectral characterization, simulation, and will act as input for atmospheric models applied to exoplanets. In essence, my research has implications for remote sensing of planetary atmospheres and contributes to climate monitoring efforts. The methodology for constructing the CO line list heavily relies on the DUO program and a well-established spectroscopic model, which I will personally develop using relevant programs and laboratory data acquired beforehand.

Atmospheric Characterisation with the Twinkle Space Telescope Following Advancements from JWST Observations

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London, United Kingdom.

The Twinkle Space Telescope is a general observatory designed for on-demand spectroscopic observations of a wide range of extrasolar and solar system objects, equipped with a 0.45 m diameter telescope and a spectrometer covering wavelengths from 0.5 to 4.5 μm simultaneously. Twinkle is one of the first in a series of innovative science satellites managed and operated by Blue Skies Space Ltd. Leveraging recent advances from JWST observations, we present updated simulations evaluating Twinkle's observational capabilities in the context of exoplanet atmospheres. Through retrieval analyses of HD 209458 b, WASP-107 b, GJ 3470 b, and 55 Cnc e, we demonstrate how increasing observational investment enhances the retrieval of atmospheric parameters and molecular abundances. Our sensitivity study highlights Twinkle's capability to detect less abundant/detectable molecules depending on the observing strategies adopted. This work provides practical guidance for developing targeted observational strategies, maximising Twinkle's scientific outcomes, and effectively preparing the community for its upcoming observation planning phase.

SOLIS: An accurate IR/Vis line list for sulfur monoxide ($^{32}\text{S}^{16}\text{O}$) & UV photoabsorption and photodissociation cross section predictions

R.P. Brady, S.N. Yurchenko & J. Tennyson

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We present a rovibronic IR/Vis line list for the transient diatomic sulfur monoxide ($^{32}\text{S}^{16}\text{O}$) computed through our variational code Duo using a semi-empirical spectroscopic model consisting of potential energy curves, spin-orbit curves, electronic angular momentum curves, (transition) dipole moment curves as well as other couplings. The underlying *ab initio* spectroscopic model of SO was taken from Brady et al. (2022) which was refined by fitting to a comprehensive experimentally derived set of energies of SO. To this end, an experimental set of 50106 transitions, 49613 of those being non-redundant, have been compiled through the analysis of 29 experimental sources. A self-consistent set of 8850 rovibronic energy levels for the $X^3\Sigma^-$, $a^1\Delta$, $b^1\Sigma^+$, $A^3\Pi$, $B^3\Sigma^-$, and $C^3\Pi$ electronic states has been generated with the MARVEL algorithm covering rotational and vibrational quantum numbers $J \leq 69$ and $v \leq 30$, respectively, and energies up to 52350.40 cm^{-1} ($\geq 191 \text{ nm}$). A large gap in our network between $12300\text{-}20500 \text{ cm}^{-1}$ exists due to lack of vibrational data for $X^3\Sigma^-$, $a^1\Delta$, and $b^1\Sigma^+$ with no coverage of the $c^1\Sigma^-$, $A'^3\Delta$, and $A''^3\Sigma^+$ states. Our refined spectroscopic model reproduces the $X^3\Sigma^-$, $a^1\Delta$, $b^1\Sigma^+$, and $A^3\Pi$ MARVEL energies with a weighted root-mean-square error of $3.13 \times 10^{-3} \text{ cm}^{-1}$, $1.08 \times 10^{-3} \text{ cm}^{-1}$, 0.27 cm^{-1} , and 0.24 cm^{-1} .

We are currently refining the UV region of the spectroscopic model, which was not done originally because of the many perturbations in the $B^3\Sigma^-$, and $C^3\Pi$ electronic state energies due to their overlapping potentials and large coupling. However, we present novel predicted UV absorption cross sections for the SO radical, highlighting specific wavelengths for its potential detection. Furthermore, we provide initial photodissociation cross sections, crucial for understanding SO's behaviour in astrophysical environments, particularly the atmospheres of hot Jupiter exoplanets.

High-resolution FT spectroscopy of the $^{12}\text{C}^{16}\text{O } a^3\Pi - X^1\Sigma^+$ system

S. Ryzner^{1,2}, A. Stasik^{1,2}, M. I. Malicka³, W. Szajna¹, R. W. Field⁴, W. Ubachs⁵, K. F. Lai⁵, A. Pashov⁶, P. Jasik^{7,8}, J. E. Sienkiewicz^{7,9}, N. de Oliveira¹⁰, R. Hakalla¹

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Carbon monoxide (CO) is one of the key molecules in the study of planetary and exoplanetary atmospheres, as well as processes occurring in outer space. Precisely determining the energy of its energy levels and describing the processes governing them is fundamental for modelling astrophysical phenomena and the dynamics of astronomical environment and objects.

Research performed at the Materials Spectroscopy Laboratory at the University of Rzeszow focuses on precise measurements of the frequency of diatomic molecules of great astronomical and astrophysical importance. The result of our studies was to obtain 806 spectral lines of the ($v' - 0$) progression of the forbidden by selection rules, Cameron system ($a^3\Pi - X^1\Sigma^+$). The band range concerns the lowest, regular region, free from the rotational unimolecular perturbations, thus $v' = 0-3$. The spectra were obtained using vacuum ultraviolet absorption spectroscopy (VUV) with a Fourier-transform spectrometer installed on the DESIRS beamline at the SOLEIL synchrotron in St. Aubin (France).

The MARVEL (Measured Active Rotational-Vibrational Energy Levels) algorithm was applied to merging of a wide range of experimental terms of $^{12}\text{C}^{16}\text{O}$ molecule to build the ExoMol database for the carbon monoxide molecule. The use of MARVEL enabled the integration of results from 17 previous studies, leading to the verification of 5,213 rovibronic transitions and the determination of 2,586 energy levels, covering the six lowest electronic states of the CO molecule. This algorithm serves as an advanced tool for unifying spectroscopic data and providing a coherent interpretation. Thanks to it, previously unknown high-rotation lines can be generated for the systems studied in this work.

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Empowering Space Science Research in Jordan through Spectroscopic Data Generation and Global Collaboration

Ala'a Azzam

Department of Physics, University of Jordan; Research Department, AstrJo Institute, Amman, Jordan

Significant progress in space sciences and molecular spectroscopy is currently underway in Jordan, driven by the Astronomy, Astrophysics, and Space Technology Research Group (AASTG) at the University of Jordan and the AstroJo Institute. Over the past 2.5 years, a coordinated national effort involving 30 Jordanian researchers has focused on producing high-precision empirical rovibrational energy levels for a range of astrophysically and atmospherically relevant molecules and their isotopologues using the MARVEL (Measured Active Rotational-Vibrational Energy Levels) protocol.

This initiative marks a major capacity-building milestone for the region, representing one of the largest space science training programs in the Arab world. The project has been carried out in close collaboration with Prof. Jonathan Tennyson (University College London) and Prof. Attila G. Csaszar (Eotvos Lorand University), both of whom have played key advisory roles in the scientific direction and quality assurance of the MARVEL analyses.

The resulting datasets are of direct relevance to high-resolution spectroscopic applications such as exoplanet atmosphere modelling, astrophysical observations, and remote sensing. They contribute to global efforts in refining molecular databases like ExoMol, HITRAN, and CDMS. Beyond scientific outcomes, this work has established a highly trained local research workforce capable of contributing rapidly and effectively to international projects.

We now seek to expand this momentum through new international collaborations, offering a large, trained team ready to accelerate molecular spectroscopy research and data production on short timescales. This Jordanian initiative demonstrates how regional investment in space science infrastructure and training can have global impact.

Comprehensive MARVEL Analysis of Empirical Rovibrational Energy Levels for Twelve Carbon Dioxide Isotopologues

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We present a systematic analysis of empirical rovibrational energy levels for twelve isotopologues of carbon dioxide (CO₂), employing the MARVEL (Measured Active Rotational-Vibrational Energy Levels) protocol. This work integrates over 125,000 experimentally measured transitions compiled from more than 350 literature sources, covering wavenumber ranges from 2 to 14,076 cm⁻¹. The MARVEL approach enables construction of spectroscopic networks and rigorous validation of experimental data, resulting in the extraction of over 58,800 empirical energy levels with quantified uncertainties. Detailed rovibrational datasets are provided for rare and asymmetric isotopologues including 828 (¹⁸O¹²C¹⁸O), 728 (¹⁷O¹²C¹⁸O), 838 (¹⁸O¹³C¹⁸O), and the third to fifth most abundant species: 628 (¹⁶O¹²C¹⁸O), 638 (¹⁶O¹³C¹⁸O), 627 (¹⁶O¹²C¹⁷O), among others. The number of validated transitions and derived energy levels per isotopologue ranges from hundreds to tens of thousands, spanning polyads up to $P = 17$. Notably, the 626M24 dataset for the parent (¹²C¹⁶CO₂), isotopologue comprises 44,828 line measurements and yields 8,268 empirical energy levels. All MARVEL-generated energy levels were critically compared with established line lists from CDS-296, Ames-2021, and HITRAN2020. The comparisons confirm excellent agreement, while also highlighting areas for potential refinement in the databases. Our results are of direct relevance to high-resolution atmospheric and astrophysical spectroscopy, including the detection and characterization of CO₂ isotopologues in exoplanetary atmospheres.

Empirical Rovibrational Energy Levels of Hydrogen Cyanide Isotopologues via MARVEL for High-Resolution Exoplanetary Spectroscopy

Saja Obaidat^{1,2}, Waed O.H. Al-Nashash¹, Sana A.E. Abzakh¹, Lina M.T. Alshobki^{1,2}, Dunia Alatoom^{1,2}, Mohammad Taha I. Ibrahim¹, Ala'a A.A. Azzam^{1,2}, Jonathan Tennyson³, Tibor Furtenbacher⁴, Attila G. Cs'aszaar⁴

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We report high-accuracy empirical rovibrational energy levels for eight isotopologues of hydrogen cyanide (HCN), derived using the MARVEL (Measured Active Rotational-Vibrational Energy Levels) protocol. These include the most astrophysically relevant isotopologues: H¹²C¹⁴N (124), H¹³C¹⁴N (134), H¹²C¹⁵N (125), D¹²C¹⁴N (224), D¹²C¹³N (234), D¹²C¹⁵N (225), and D¹³C¹⁵N (235). The MARVEL procedure validates and refines rovibrational transitions collected from a wide range of literature sources spanning seven decades (1952-2019), resulting in an extensive and error-corrected spectroscopic dataset.

For 124 and 134, the two most abundant isotopologues, 29,796 (20,515 unique) and 17,062 (11,719 unique) transitions were analyzed, covering the spectral ranges 500-18,400 cm⁻¹ and 522-12,604 cm⁻¹, respectively. The third most abundant, 125, was examined using 13,762 (11,754 unique) transitions over 60-9,700 cm⁻¹, with polyads up to $P = 37$.

Rare isotopologues D¹²C¹⁴N, D¹³C¹⁴N, D¹²C¹⁵N, and D¹³C¹⁵N yielded 2,493 / 1,321 / 64 / 1,190 empirical energy levels, respectively, based on 8,931 / 3,526 / 407 / 3,427 measured transitions. After critical evaluation, subsets of questionable transitions were removed (e.g., 1,322 transitions from 224), ensuring dataset integrity. The energy levels span wavenumber ranges from below 1 cm⁻¹ to over 5,000 cm⁻¹, across up to 77 vibrational bands depending on the isotopologue.

Cross-comparison with ExoMol, Ames-2021, HITRAN, and CDMS databases demonstrates strong agreement, while also identifying areas for refinement, especially for the deuterated isotopologues. The validated datasets produced here enhance the precision of molecular line lists essential for the detection and modeling of exoplanetary atmospheres rich in HCN and its isotopic variants.

The First International Earth 2.0 (ET) Science Conference: Charting the Mission Roadmap

Haitao Li^{1,2}, Jian Ge³ the ET team

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We are pleased to announce that the first annual science meeting of the Earth 2.0 (ET) space mission will be held in Shanghai this August. The meeting will focus on relevant scientific research and promote the development of the mission. Major topics to be covered include (but are not limited to): Transit Exoplanets, Microlensing Exoplanets, Follow-up Observations, Asteroseismology, Stellar Activity and Archaeology of the Galaxy, Time Domain Astronomy, Binary Stars and Black Hole Binary Stars, Solar System Science and Solar System Science. The main agenda and content include: (1) The first in-person meeting and collaboration of the full ET science team, including invited plenary talks, contributed talks, panel discussions, parallel sessions, and poster sessions; (2) Official establishment of multiple Science Working Groups (SWGs). Each SWG will introduce and discuss its key scientific questions, how ET data can be used to address these questions, and how to organize team efforts in preparation for the 2028 satellite launch – including target selection, observation and data analysis, ET observation simulations, pipeline development, and follow-up observation plans; (3) Official announcement of the ET data rights and publication policy, as well as the procedures and guidelines for becoming a formal member of the ET science team; (4) Discussion of future ET science conferences and sub-meetings.

A Population of 20 Exoplanet Atmospheres Observed with the Hubble Space Telescope Reveals Evidence for Widespread Stellar Activity

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We present a population study of 20 transiting exoplanets, currently the largest sample of exoplanet atmospheres observed to date in the spectral range near-UV to near-IR. Archive data obtained with the Hubble STIS and WFC3 instruments are uniformly analysed using the Iraclis pipeline and a suite of spectral retrieval plugins integrated in TauREx 3.1, including the stellar activity plugin ASteRA and the cloud microphysics plugin YunMa. Most exoplanets included in the sample were observed multiple times with the STIS G430L and/or G750L gratings, allowing for the study of temporal variability caused by changes in the exoplanet atmosphere, due to e.g. cloud/haze variability and/or stellar magnetic activity. Our analysis reveals significant differences among the observations obtained with STIS at various epochs for about half of the planets included in the sample. These data show amplitudes and patterns that are suggestive of time-varying stellar surface heterogeneities that cause contamination in the exoplanetary spectra.

We assessed the presence of an active star for all planets in our sample using a variety of statistical metrics. Our findings demonstrate the significant role that stellar contamination may have in all exoplanet spectra observations. Therefore, comprehending, modelling, and correcting for the impact of stellar activity is important for a complete characterisation of exoplanet atmospheres. This issue becomes particularly relevant with the ongoing JWST observations of small planets, statistically more likely to orbit active stars. Additionally, addressing stellar activity becomes even more pertinent in anticipation of the extensive chemical surveys to be conducted by next-generation space telescopes in the coming decade. For these reasons, targeted campaigns aimed at investigating the activity of exoplanets' stellar hosts through time would significantly contribute to the success of the exoplanet field.

Ab initio Potential Energy and Dipole Moment Surfaces of the HOPO Molecule

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Recent atmospheric photochemical studies show that phosphorus-hydrogen-oxygen (PHO) photochemical network can play a key role in gas giant hydrogen-dominated atmosphere. Among the main phosphorus contained absorbers, HOPO, PO and P₂ are the dominant P carriers for HD 189733b-like hot Jupiters at pressures important for transit and emission spectra, rather than PH₃. Even for GJ1214b-like warm Neptune atmospheres at 10 and 100 times Solar metallicity, small oxygenated phosphorus molecules such as HOPO and PO dominate for both thermochemical and photochemical simulations. Here we present an initial quantum-chemistry study of the potential energy surface of HOPO. A new potential energy and dipole moment surfaces of HOPO have been constructed at the CCSD(T)-F12b/cc-pVTZ-F12 level of theory for the cis- and trans-HOPO conformers, at an energy range up to 20,000 cm⁻¹. Electronic structure calculations are performed with MOLPRO. These surfaces were parameterised using 6D analytic expansions covering both cis- and trans-isomers in single non-rigid representations. A new exact kinetic energy operator of this system was derived and implemented in the variational program TROVE. Preliminary results of energy calculations will be presented.

ExoMol line lists for 12 isotopologues of CO₂

ExoMol Hackathon team: Sergei N. Yurchenko, Marco Barnfield, Charles Bowesman, Ryan Brady, Kyriaki Kefala, Qinghe Ni, Oleksyi Smola, Armando Perri, Chenyi Tao, Andrei Sokolov, Jonathan Tennyson

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London, United Kingdom.*

Extensive rovibrational line lists for 12 isotopologues of carbon dioxide, ¹²C¹⁶O₂, ¹³C¹⁶O₂, ¹²C¹⁷O₂, ¹³C¹⁷O₂, ¹²C¹⁸O₂, ¹³C¹⁸O₂, ¹⁶O¹²C¹⁷O, ¹⁶O¹²C¹⁸O, ¹⁶O¹³C¹⁷O, ¹⁶O¹³C¹⁸O, ¹⁷O¹²C¹⁸O, ¹⁷O¹³C¹⁸O have been constructed for hot exoplanetary applications. We used accurate empirical potential energy surfaces Ames-2 and Ames-X01d by Huang et al., accurate *ab initio* dipole moment surface Ames-2021–40K by Huang et al. and the variational rovibrational program TROVE to solve the Schrödinger equation and generate associated Einstein A coefficients. We then applied empirical energies from the most recent MARVEL, HITRAN and CDSO studies of CO₂ to replace the calculated energies where available. We used a combination of Machine learning algorithms handled by a separate estimator built as a VotingClassifier to assign the AFGL quantum numbers where they are not available. The line lists and all associated data will be provided at www.exomol.com.

Useful Information

Venue Address

High Leigh Conference Centre

Lord Street, Hoddesdon

Hertfordshire

EN11 8SG

01992 463016

highleigh@cct.org.uk

Travel Information

To Drive: High Leigh is seven miles from the M25. From Junction 25, take the northbound A10 dual carriageway towards Hertford. Leave the A10 at the junction for Hoddesdon and follow the road towards the town. At the roundabout take the third exit signed 'Town Centre' (alongside Morrisons). Turn right at the church into Pauls Lane and bear left into Taverners Way. Take the first right into Lord Street and continue up the hill for just under a mile. High Leigh is on the left.

By Rail: The local train station is Broxbourne station (1.7 miles). There is a regular service from London Liverpool Street, which also connects with the Underground Victoria Line at Seven Sisters or Tottenham Hale. <https://www.thetrainline.com/>

By Taxi: There are plenty of taxis at reasonable rates (typically £6) from Broxbourne station. A local taxi company is Broxbourne Taxis who can be contacted via telephone on: 01992 464 007.

By Air: The local airport, Stansted Airport, is 40 minutes away by road or a 35 minute train journey from Broxbourne.

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