Isotopes and the characterization of extrasolar planets

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Summary

How did we come into existence? Are we alone? The origin of life and our place in the universe have been enduring quests of human beings. It was only three decades ago when astronomers began studying exoplanets, planets outside our solar system. In 1995, the first exoplanet around a main sequence star, 51 Pegasi b, was discovered, leading to the development of exoplanetary science. Since then, the field has proceeded rapidly with more than 5000 diverse exoplanets discovered to date. These discoveries include a population of close-in planets to their host stars, known as hot Jupiters, a class of young massive giant planets, called super Jupiters, and planets with intermediate sizes between the Earth and the Neptune, named super-Earths and mini-Neptunes. The presence of these strange worlds that have no counterparts in the solar system poses challenges to our perception of planet formation and evolution but also opens exciting new windows of understanding.

With the number of detected exoplanets growing rapidly, we are entering an era of characterizing their properties in detail. Observations of exoplanet atmospheres open an essential avenue for a further level of characterization beyond the dimension of planet masses and sizes. The study of exoplanet atmospheres aims at unveiling their chemical compositions, which play a vital role in retracing the formation history of planets, assessing the habitability and searching for extraterrestrial life. This can be achieved by spectroscopic observations, that is, dispersing lights into different wavelengths (or colors). As different species absorb lights at different wavelengths and result in unique signatures in the spectra, hence the chemical constituents can be identified through spectroscopy.

The spectral characterization of exoplanet atmospheres benefits from high resolving power, which resolves the atomic or molecular features into individual spectral lines that facilitate the disentanglement of different species and even isotopologues. In addition, the position and shape of spectral lines bears a wealth of information on dynamical processes in atmospheres. As such, the spectral analyses allow us to chart thermal structures, winds, clouds/hazes, and atmospheric escapes of exoplanets. The application of high resolution spectroscopy in studying atmospheres of gas giant exoplanets is explored in chapter 2-5 of this dissertation.

In the quest for giant planet formation, while three major scenarios have been proposed, including core accretion, gravitational instability, and cloud fragmentation, fundamental questions remain unanswered. Linking atmospheric composition to planet formation has been one of the most challenging frontiers of planetary science. The atmospheric elemental abundance ratios, such as the carbon-to-oxygen (C/O) and nitrogen-to-carbon (N/C) ratios, are believed to provide important clues. As temperature decreases in protoplanetary disks with the distance from the central star, molecules freeze out onto dust grains and are removed from the gas phase to the solid phase, changing the elemental abundance ratios in the gas and solid reservoirs. Planets formed at different locations with respect to molecular icelines and/or incorporated different amounts of solids are expected to show distinct chemical abundance ratios in their atmospheres, providing implications

for formation pathways, birth locations, and the relative contributions of gas versus solid accretion. Similarly, isotope abundance ratios, such as D/H and $^{12}C/^{13}C$, are suggested to be powerful tracers for the formation and evolution history of planets. With state-of-the-art facilities and techniques, it becomes feasible to combine multiple observational probes to disentangle the subtleties of planet formation processes. This is investigated in chapter 2 and 3 in particular.

Chapter 2: First detection of minor isotopologue ^{13}CO in an exoplanet
Isotopologues in planetary atmospheres are believed to be able to reveal how planets were formed. This idea is inspired by measurements of isotopic ratios (such as deuterium-to-hydrogen ratios) in our own solar system, which vary significantly across different planets. These variations are likely linked to the isotope ratios in protoplanetary disks, which are affected by temperature and irradiation-dependent processes known as fractionation. By detecting and analyzing isotopes in exoplanet atmospheres, we can constrain where the planet formed, how much gas and solids contributed to its formation, and how much atmospheric loss it has experienced (as heavy isotopes are less prone to escape from atmospheres). This chapter presents the first detection of the minor isotopologue of carbon monoxide ^{13}CO in the atmosphere of a super Jupiter named YSES-1 b using the near-infrared integral-field spectrograph SINFONI at the VLT, marking the first time that isotopic measurements have been extended to exoplanets. Through modeling of planetary atmospheres and Bayesian retrieval analyses, we determined the carbon isotope ratio in the planetary atmosphere to be $^{12}CO/^{13}CO$~31, which means a factor of two enhancement of ^{13}C compared to the local interstellar medium ($^{12}C/^{13}C$~68). This finding suggests that the planet was plausibly formed outside the CO iceline and mainly acquired carbon from accretion of ^{13}C-enriched ices. It opens up an exciting new avenue of connecting atmospheric characteristics to planet formation.

Chapter 3: First detection of minor isotopologue ^{13}CO in a brown dwarf
After detecting ^{13}CO in the exoplanet YSES 1b, we extended our method to an exoplanet analog called 2M0355, which is a young, isolated brown dwarf with comparable mass and effective temperature to the super Jupiter companion. Interestingly, this study revealed no ^{13}CO enrichment in the brown dwarf based on archival observations taken with the high-resolution spectrograph NIRSPEC at the Keck observatory. The carbon isotope ratio in the brown dwarf ($^{12}CO/^{13}CO$~100) is in stark contrast to that in the exoplanet, hinting at different formation processes. To further investigate this benchmark object, we conducted follow-up observations of this brown dwarf using the upgraded state-of-the-art spectrograph CRIRES at the VLT, and were able to confirm the constraint on the carbon isotope ratio. Additionally, we suggest that the oxygen isotope ratio ($^{16}O/^{18}O$) can now be studied in bright super Jupiters and brown dwarfs using high-resolution spectroscopy. The comparison of atmospheric compositions in giant exoplanets and brown dwarfs plays an important role in unraveling their distinction in terms of formation pathways.

Chapter 4: Search for He I airglow emission from hot Jupiter
Gaseous planets that orbit very closely to their host stars can undergo significant atmospheric erosion due to the intense high-energy radiation from their stars. This process

is especially relevant for planets that are smaller than Neptune, driving the evolution of their atmospheres. One powerful way to study atmospheric escape in these planets is to look for the absorption of helium atoms in their atmospheres, which has been successfully detected in a dozen of exoplanet atmospheres during transiting. However, the helium absorption is inconclusive in determining the atmospheric mass loss on its own because it is difficult to separate the effects of atmospheric escape from the exospheric temperature using helium absorption alone. To overcome this challenge, we aimed at searching for helium airglow emission to be combined with the absorption to better constrain the upper atmospheres. We carried out this search in the non-transiting hot Jupiter τ Bootis b using the near-infrared spectrograph CARMENES at the Calar Alto Observatory. Although it resulted in a non-detection, our study provides important information about the detection limits of helium airglow emission in exoplanets, and we believe that next-generation telescopes will be able to measure this emission. Detecting helium airglow emission will be crucial in studying the atmospheric structure, mass loss rates, and bulk-atmospheric evolution of gaseous planets that are located very close to their host stars.

Chapter 5: Disentangle hydrostatic and exospheric regimes of ultra-hot Jupiters
The strong high-energy stellar irradiation on close-in hot Jupiters results in two distinct regimes in their atmospheres, the hydrostatic lower atmosphere and the hydrodynamic exosphere. Understanding the dynamics of these regions requires the measurement of different atoms or molecules. In this chapter, we characterized the atmosphere of the ultra-hot Jupiter MASCARA-4b, which has an equilibrium temperature above 2000 K, using transmission spectroscopic observations taken with the optical high-resolution spectrograph ESPRESSO at the VLT. Our measurements detected a variety of absorbing species, including H I, Na I, Fe I, and Fe II in the planetary atmosphere. To put the results into context, we compared our findings to those of seven other ultra-hot Jupiters and investigated the trend of these atomic absorption strengths. We found that neutral metal species trace the hydrostatic regime, while hydrogen and ionized metals probe the hydrodynamic exosphere and atmospheric escape. This comparison allowed us to take the first step towards analyzing high-resolution spectroscopic results at a population level, making it possible to distinguish between different dynamic regimes of highly-irradiated atmospheres.

Chapter 6: Diverse outcomes of binary-disk interactions
To gain insights into planet formation, it is necessary to understand circumstellar disks, the birthplace of planets. As approximately half of solar-type stars are born in multiple stellar systems, the presence of stellar companions can modify the morphology and evolution of disks, potentially influencing the outcomes of planet formation. In this chapter, we used polarimetric differential imaging with SPHERE/IRDIS at the VLT to resolve circumstellar disks in three multiple systems: CHX 22, S CrA, and HP Cha, as part of the Disk Evolution Study Through Imaging of Nearby Young Stars (DESTINYS) large program. The observed disk morphology, in combination with astrometric and orbit analyses for the stellar companions, allows for a better understanding of the interplay between disks and companions. The comparison of the three systems spans a wide range of binary separations (50 – 500 au) and illustrates the decreasing influence of companions on disk structures with increasing separation. This finding is consistent with the statistical analysis of exoplanet populations

in binaries, which suggests that planet formation is likely hindered around close binary systems, while it is not suppressed in wide binaries.

Outlook: unravel the origin of planets

Moving forward, a key step to better understand the origin of exoplanets is to extend the characterization of exoplanet atmospheres to a larger sample. With the ability to reliably retrieve formation tracers, such as elemental and isotopic compositions, from near-infrared high-resolution spectra, we will be able to address the questions through population-level analyses of young giant planets and brown dwarfs and compare different classes of sub-stellar objects. This will enable us to explore the trends in atmospheric constituents with stellar and planetary properties, such as mass and orbital separation, and assess the plausibility of various formation scenarios. The census of chemical composition will contribute to bridging the gap between atmospheric observations and planet formation and evolution, and addressing the fundamental question of what sets the boundary between planets and brown dwarfs.

Looking towards the future, the upcoming thirty-meter class telescopes, such as the Extremely Large Telescope (ELT) with first light expected in five years, and the next-generation flagship space telescope, will routinely deliver characterizations of smaller exoplanets with the potential of investigating atmospheric biosignatures and habitability. The ELT will be particularly promising for probing rare isotopes, such as deuterium, in exoplanets, which is one of the most informative tracers of planet formation and atmospheric evolution. Hopefully, we will begin answering the ultimate questions of how unique our solar system is and how we got here.