Finding Needles in a Haystack: Atmospheric Characterization of Other Worlds

A PhD Thesis Proposal for the University of Toronto's Graduate Program in Astronomy & Astrophysics

Emily K. Deibert

Department of Astronomy & Astrophysics, University of Toronto
Dunlap Institute for Astronomy & Astrophysics

First Committee Meeting: May 24, 2022

Abstract

Thousands of transiting exoplanets have been discovered, but relatively little is known about their atmospheric properties and compositions. Characterizing exoplanet atmospheres is the most promising avenue through which we can learn more about the exoplanets themselves, and high-resolution spectroscopy is currently one of the best methods by which this can be accomplished. In this thesis, I will use state-of-the-art ground-based spectrographs in the near-infrared wavelength regime to detect, characterize, and understand the atmospheres of exoplanets across a wide range of parameter space. This will open the door to an era of comparative planetology that will ultimately lead to a comprehensive theory of the physics of atmospheres.

Thesis Committee

Suresh Sivanandam
Primary Advisor
Dunlap Institute for Astronomy & Astrophysics
sivanandam@dunlap.utoronto.ca
Ray Jayawardhana
Co-Advisor
Department of Astronomy, Cornell University
rayjay@cornell.edu
Diana Valencia
Committee Member
Department of Astronomy & Astrophysics
valencia@astro.utoronto.ca
Marten van Kerkwijk
Committee Member
Department of Astronomy & Astrophysics
mhvk@astro.utoronto.ca

1 Introduction

Characterizing exoplanet atmospheres is the next frontier in astronomical research because it is the most promising avenue through which we can learn more about these distant worlds. However, while thousands of transiting exoplanets have been discovered, relatively little is known about their atmospheric properties and compositions. The main limitation in characterizing an exoplanet's atmosphere lies in the extreme difference in brightness between the exoplanet and its host star, typically preventing direct atmospheric emission from being resolved. To overcome this, recent progress in the field has made use of "transmission spectroscopy" during transits, when the light from the host star passes through the exoplanet's atmosphere and allows for the detection of any atomic or molecular species present. This technique was first used by Charbonneau et al. (2002) to provide evidence for atmospheric sodium, marking the first detection of an atmosphere around a planet outside our solar system. Notable contributions since this initial discovery include detections of other chemical elements, as well as organic molecules, water vapour, and atmospheric hazes (e.g. Vidal-Madjar et al. 2003; Snellen et al. 2010; Sing et al. 2016). Despite a great deal of progress in the study of exoplanetary atmospheres, however, transmission spectroscopy has to date almost exclusively targeted high-mass hot Jupiters at low spectral resolution in the visible regime, which represents an extremely small fraction of the diverse population of exoplanets that have been discovered.

With the advent of novel methods of analysis and the continuous improvement of telescopes and observing facilities around the world, however, astronomers are poised to move into an era of true exoplanet characterization. One of the first steps towards fully understanding these alien worlds will be creating detailed, three-dimensional maps of their atmospheres, focusing not just on hot Jupiters but on exoplanets across a wide range of parameter space. The purpose of this thesis will be to use transmission spectroscopy and other novel methods to detect, characterize, and understand the atmospheres of a wide range of exoplanets, both refining the techniques that are presently available to us and pushing the limits of our observational capabilities into new, unexplored regimes. My goal is to find the atmospheric needles hidden in the proverbial exoplanetary haystack: previously-undetected atoms and molecules, atmospheric signatures in unexplored wavelength ranges, and perhaps even the first concrete detection of an atmosphere around an Earth-like exoplanet.

This proposal will proceed as follows. In section 2, I will provide a very brief introduction to the study of exoplanetary atmospheres and a summary of the current state of the field. Section 3 will describe the thesis being proposed, with motivations presented in section 3.1, details on proposed methodology presented in section 3.3, and a summary of proposed thesis projects provided in section 3.4. In section 4 I will present a timeline for completion. Conclusions will follow in section 5.

2 State of the Field

Although a full discussion on the background of this field is beyond the scope of this proposal, I will briefly summarize the current state of ground-based high-resolution spectroscopy, touching upon key discoveries.

At high spectral resolutions, molecular features in an exoplanet's atmosphere can be resolved into individual absorption lines that are unique to each molecule. For close-in planets, the large change in radial velocity of the planet during its transit means that these lines undergo large Doppler shifts, allowing them to be separated from absorption lines due to the host star or the Earth's atmosphere. For planets on wider orbits, high-contrast imaging can be used with high-resolution spectroscopy to isolate an exoplanet's spectrum using its wide spatial separation from its host star. These techniques comprise the basis of high-resolution spectroscopy. Measurements of an exoplanet's spectrum at high spectral resolution can also be used to learn more about the temperature-pressure profile of the planet's atmosphere, providing clues as to the conditions present on the planet.

Although high-resolution spectroscopic techniques (described in section 3.3) have been used in numerous studies, to date they have only been successful in definitively detecting 7 multi-line atmospheric species in 10 separate planets. These are summarized in Table 1. It should be noted that this does not include detections made at low-resolutions or with space-based instruments.

Of these planets, the smallest is roughly half the mass of Jupiter. Detections of single-line (i.e. atomic) species have also been reported, but are likewise limited to large, close-in exoplanets. The field is clearly still in its infancy and ripe with further advancements to be made.

3 Thesis Proposal

3.1 Motivations

As is clear from Table 1, only a very narrow subset of exoplanets have had their atmospheres probed at high spectral resolutions, and even fewer in the near-infrared (NIR) regime. Ground-based NIR spectroscopy is particularly challenging due to intervening absorption from the Earth's atmosphere; at wavelengths of $\sim 1.3 - 1.5$ μm, the contamination is severe. However, there is a wealth of molecular absorption lines present in the NIR regime that are also expected to be present in exoplanetary atmospheres: CO, CO_2, TiO, and H_2O, to name a few. Being able to resolve features in this regime is therefore of significant interest, and for that reason will be the focus of my thesis.

3.2 Summary of Proposal

This thesis will be built on three main goals: the development and usage of novel ground-based observational facilities at the forefront of astronomical instrumentation, the implementation of innovative data analysis techniques, and the creation of a detailed inventory of exoplanet atmospheres. I will make use of observations from well established high-resolution ground-based instruments (e.g. GRACES from Gemini-N and HDS from Subaru; see Deibert et al. 2019 and section 3.4.1), as well as instruments that have only recently become available for use (e.g. SPIRou from CFHT and the soon-to-be-completed MAPS instrument at the MMT observatory; see section 3.4.3). This will position me as an experienced observational astronomer, with work across a wide range of instruments, exoplanets, and wavelength regimes.

3.3 Methodology

As my thesis will focus on high-resolution ground-based atmospheric characterization of exoplanets, the majority of the work I undertake will be based around the Doppler cross-correlation technique pioneered by Snellen et al. (2010), which is currently the best method known to search for atmospheric absorption in exoplanetary atmospheres. Briefly, this method takes advantage of the large change in radial velocity of a close-in exoplanet throughout its transit to disentangle the exoplanet's signal from that of the star and the Earth's atmosphere. A model of the exoplanet's atmosphere can be cross-correlated with observations of the exoplanet during its transit and then phase-folded to the planet's radial velocity in order to detect any absorption due to the planet's atmosphere. This method has proven successful in a number of cases, some of which are summarized in section 2 and Table 1.

3.4 Proposed Projects

3.4.1 Previous Work

The groundwork for this thesis has already been laid in a research project completed during the first year of my PhD (Deibert et al. 2019), in which I presented transmission spectroscopy of some of the smallest hot Jupiters to have had their atmospheres probed at high spectral resolution from ground-based facilities (namely, the GRACES

Table 1: A summary of the current detections made with high-resolution ground-based spectroscopy. Table adapted from Birkby (2018).

Planet	Mass (M_J)	Species Detected	Instrument	Citation
HD 209458 b	0.69	CO, H_2O, HCN	CRIRES	Snellen et al. (2010); Hawker et al. (2018)
HD 189733 b	1.142	CO, H_2O	CRIRES, GIANO	Brogi et al. (2016, 2018)
KELT-9 b	2.88	Ti+, Fe, Fe+	HARPS-N	Hoeijmakers et al. (2018)
KELT-2A b	1.486	H_2O	NIRSPEC	Piskorz et al. (2018)
WASP-33 b	2.1	TiO	HDS	Nugroho et al. (2017)
τ Boo b	5.84	CO, H_2O	CRIRES, NIRSPEC	Brogi et al. (2012); Lockwood et al. (2014)
51 Peg b	0.47	CO, H_2O	CRIRES	Brogi et al. (2013); Birkby et al. (2017)
HD 179949 b	0.92	CO, H_2O	CRIRES	Brogi et al. (2014)
HD 88133 b	0.3	H_2O	NIRSPEC	Piskorz et al. (2016)
ups And b	> 0.62	H_2O	NIRSPEC	Piskorz et al. (2017)

instrument at Gemini-N and the HDS instrument at Subaru). I made use of a sophisticated Doppler cross-correlation technique which involves correlating highly-detailed model spectra with our observations, taking advantage of the large shifts in radial velocity of the exoplanets in question. While this method had been used in previous studies to make atmospheric detections around several hot Jupiters, the atmospheres of cooler, lower-mass planets remain elusive. My work in Deibert et al. (2019) focused on "warm Saturns", a smaller class of the massive hot Jupiter population, and served as a stepping-stone between the atmospheres of these giant hot Jupiters and detailed analyses of super-Earth atmospheres. This project was an ideal introduction to the field, and will guide the research that will be undertaken for my thesis.

3.4.2 Current Work

I am currently working on characterizing the atmosphere of 55 Cnc e, a low-density $\sim 8.5 M_\oplus$ super-Earth orbiting a Sun-like star. Of the known super-Earths, 55 Cnc e is perhaps the best target for ground-based atmospheric characterization. Its host is both nearby and among the brightest planet-hosting stars, and its orbit is incredibly short—only $\sim$ 18 hours—making it one of the hottest super-Earths discovered to date. For this reason it has been studied in considerable detail; a full summary of previous work is beyond the scope of this proposal, but to date only one atmospheric detection has been reported (Tsiaras et al. (2016) made a detection of HCN using the WFC3 instrument aboard the *Hubble Space Telescope*, but caution that additional spectroscopic observations are needed to confirm their results).

My current project makes use of high-resolution NIR spectra from the CARMENES instrument at the Calar Alto Observatory. Similar to Esteves et al. (2017), this analysis will take advantage of the large wavelength coverage and high spectral resolution of the data to search for the signature of thousands of absorption lines produced by molecules in the exoplanet's atmosphere. However, while Esteves et al. (2017) focused solely on water features visible in the optical wavelength range, this analysis will focus on molecules visible in the relatively-unexplored NIR regime: CO, CO_2, and HCN, in addition to H_2O. This work will therefore serve as a test for the HCN detection reported by Tsiaras et al. (2016), and may provide evidence of additional molecular species present in 55 Cnc e's atmosphere that have to date remained undetected.

In the context of my dissertation, this work serves as an ideal follow-up to the work I completed in Deibert et al. (2019). It builds upon the techniques I developed in that work, and gives me the chance to explore both a new type of exoplanet and a new wavelength regime. This will further prepare me for future observational work.

3.4.3 Future Work

Following the work described in section 3.4.2, there are a number of research projects I plan to pursue. As a direct follow-up to my analysis of 55 Cnc e's atmosphere using CARMENES data, I plan to continue my analysis with NIR observations I have recently obtained from the high-resolution SPIRou instrument at the Canada-France-Hawai'i Telescope (CFHT). I was the principal investigator for these observations, and determined the observing parameters necessary for atmospheric characterization. This project will allow for a further exploration of 55 Cnc e's atmosphere; perhaps providing the data necessary to make detections, if the CARMENES data prove to be insufficient. Furthermore, as my proposal was accepted for SPIRou's very first observing semester, this work will be among the first science results from the instrument and will therefore be of great interest to astronomers in the field. Working with a new instrument like SPIRou will also help to position me as an experienced observational researcher, and will provide me with the challenging but important experience of working with an uncharacterized instrument.

After this, I will focus the remainder of my thesis on work undertaken with the MMT Adaptive Optics Exo-

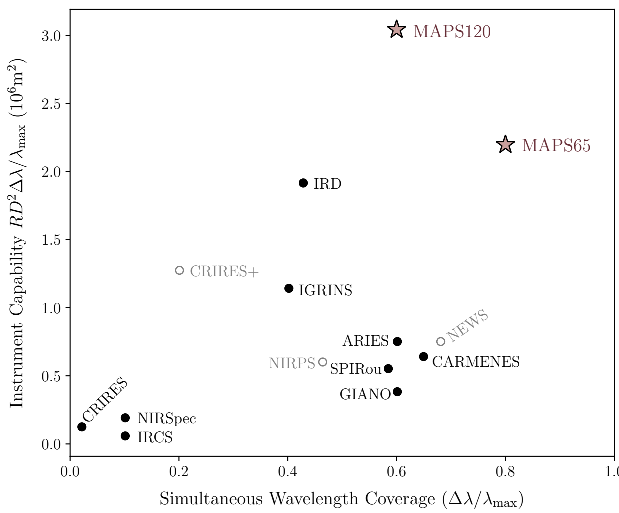

Figure 1: A comparison of existing (filled circles) and planned (unfilled circles) near-infrared spectrographs. The instrument capability metric shown on the y-axis combines the spectral resolution (R), collecting area (D^2), and simultaneous wavelength coverage ($\Delta\lambda/\lambda_{\max}$) in order to quantify the efficacy of each instrument at performing high-resolution spectroscopy (Crossfield 2016). The MAPS instrument provides a dramatic increase in instrument capability compared to all other existing and planned spectrographs in this wavelength regime. Figure adapted from the MAPS NSF Project Description.

planet Characterization System (MAPS) instrument at the University of Arizona's MMT Observatory. The MAPS project, which is currently underway and slated to be operational by the end of 2019, is a technical upgrade to the existing Arizona Infrared Echelle Imager and Spectrometer (ARIES) and MMT Adaptive Secondary Mirror (ASM)-based Adaptive Optics (AO) system. The new MAPS instrument will be composed of two high-resolution modes: MAPS65, which will have instantaneous spectral coverage from 1-5 μm with a resolution of $R = 65,000$; and MAPS120, which will deliver a resolution of $R = 120,000$ over a 1.5 μm subset of the full 1-5 μm band. The primary science goal of this upgrade will be characterizing the atmospheric composition of exoplanets, and by doing so it will serve as the definitive high-resolution spectroscopic follow-up counterpart to *Kepler*, *TESS*, and eventually JWST. Fig. 1 situates MAPS in the context of other NIR spectrographs.

I will have access to the MAPS instrument as soon as it is operational, meaning that I will be able to carry out work on innovative new projects that will revolutionize the field of atmospheric characterization. Potential projects may include follow-up of currently-known exoplanets of interest or soon-to-be-discovered *TESS* exoplanets.

Additionally, I am a co-investigator of the One Hit Wonders survey based out of the Dunlap Institute. This survey will focus on following-up the thousands of single-transit events that will be detected by *TESS*, yielding a population of long-period exoplanets that will fill a region of parameter space that has to date been unexplored with high-resolution spectroscopy. Through this survey I will thus have unparalleled access to newly-discovered exoplanets that I can follow-up on with MAPS, setting me apart from other researchers in the field.

Finally, I recently served as a co-investigator on a letter of intent for a GRACES/Gemini-N and HDS/Subaru Large and Long Program (LLP). This program, if accepted, will focus on exploring the diversity of exoplanet atmospheres at high-spectral resolution in the visible regime. Targets that I help discover with the One Hit Wonders survey and later follow-up on with MAPS in the NIR regime will be ideal for this program: they can be further studied in visible wavelengths, strengthening any detections I make or providing the additional data needed to make detections in the first place. Together, these programs will comprise an unprecedented survey of exoplanet atmospheres, and will propel the field forward into a new era of atmospheric characterization.

3.5 Contingency Plan

As is the case with any observational-based thesis—especially one for which the instruments to be used are not currently operational—there is a risk of either not obtaining data due to unforeseen circumstances or not being able to access desired instruments before the nominal thesis end date. In the event that the work described in the latter portions of section 3.4.3 cannot be completed for any reason, there are a number of other avenues I can explore. With either a Gemini Fast Turnaround proposal or regular observing semester proposals for currently-operational instruments, I can carry out additional projects similar to the work I did in Deibert et al. (2019). If for some reason I am also unable to obtain data through these means, there are ample unexplored archival observations available for various instruments that I can use to carry out additional projects.

4 Proposed Timeline

With the publication of one thesis chapter already complete (Deibert et al. 2019) and an additional two chapters underway (see the CARMENES project described in section 3.4.2 and the SPIRou project described in section 3.4.3), my dissertation is well on its way to being completed by August 2022 (my nominal program completion date). Work with MAPS and the One Hit Wonders survey will comprise the final chapters of my dissertation.

A timeline for this thesis is presented in Fig. 2, with major projects indicated by coloured bars and various project milestones indicated by stars. Today's date is also marked.

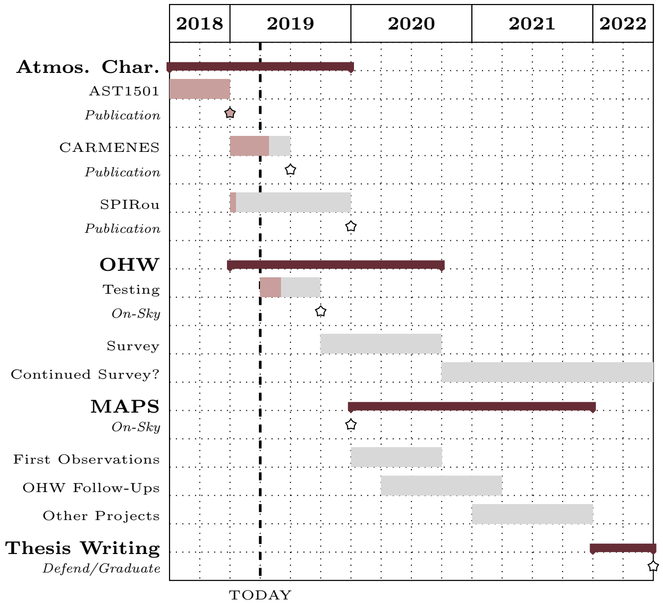

Figure 2: A visualization of the the timeline for this thesis, with specific goals based on the work described in section 3. The shaded regions correspond to the amount of each goal that has been completed to date, and the stars correspond to various progress milestones. Note that some of these projects will have started before or will continue past these dates, and I have indicated only the times during which I will be involved in each project.

In general, the projects listed for the earlier years of the thesis (i.e. up until the end of 2019) are likely to be completed as projected by Fig. 2. The later projects are less certain; however, a rough timeline would involve getting started working on the One Hit Wonders survey by September 2019, with targets being detected throughout the next year. Targets could then be followed-up on as soon as MAPS is operational, with a projected on-sky date of early 2020. The latter years of the thesis would involve determining best follow-up targets, arranging for observations with MAPS (and potentially high-resolution visible wavelength counterparts), and carrying out further high-resolution spectroscopic work. My thesis will be written throughout 2022, with an expected defense date of August 2022.

5 Conclusion

The goal of the thesis presented in this proposal will be to characterize a diversity of exoplanet atmospheres at high-spectral resolution in the near-infrared regime. This will be accomplished using both existing instruments (e.g. CARMENES and SPIRou) and the soon-to-be-operational MAPS instrument at the MMT observatory. The result will be a large-scale survey of exoplanet atmospheres across an unprecedented area of parameter space, ranging in size from massive hot Jupiters to small, potentially habitable Earth-like exoplanets. In the field of exoplanet science, a catalogue of exoplanet atmospheres such as this is crucial: it will provide astronomers with the context that is lacking by studying just the planets in our Solar System or the largest planets throughout the galaxy, and will open the door to an era of comparative planetology that will ultimately lead to a comprehensive theory of the physics of atmospheres.

References

Birkby, J. 2018, Multi-Dimensional Characterization of Distant Worlds Workshop Slides

Birkby, J. L., de Kok, R. J., Brogi, M., Schwarz, H., & Snellen, I. A. G. 2017, AJ, 153, 138

Brogi, M., de Kok, R. J., Albrecht, S., et al. 2016, ApJ, 817, 106

Brogi, M., de Kok, R. J., Birkby, J. L., Schwarz, H., & Snellen, I. A. G. 2014, A&A, 565, A124

Brogi, M., Giacobbe, P., Guilluy, G., et al. 2018, A&A, 615, A16

Brogi, M., Snellen, I. A. G., de Kok, R. J., et al. 2012, Nature, 486, 502

—. 2013, ApJ, 767, 27

Charbonneau, D., Brown, T. M., Noyes, R. W., & Gilliland, R. L. 2002, ApJ, 568, 377

Crossfield, I. J. M. 2016, arXiv e-prints, arXiv:1604.06458

Deibert, E. K., de Mooij, E. J. W., Jayawardhana, R., et al. 2019, AJ, 157, 58

Esteves, L. J., de Mooij, E. J. W., Jayawardhana, R., Watson, C., & de Kok, R. 2017, AJ, 153, 268

Hawker, G. A., Madhusudhan, N., Cabot, S. H. C., & Gandhi, S. 2018, ApJ, 863, L11

Hoeijmakers, H. J., Ehrenreich, D., Heng, K., et al. 2018, Nature, 560, 453

Lockwood, A. C., Johnson, J. A., Bender, C. F., et al. 2014, ApJ, 783, L29

Nugroho, S. K., Kawahara, H., Masuda, K., et al. 2017, AJ, 154, 221

Piskorz, D., Benneke, B., Crockett, N. R., et al. 2016, ApJ, 832, 131

—. 2017, AJ, 154, 78

Piskorz, D., Buzard, C., Line, M. R., et al. 2018, AJ, 156, 133

Sing, D. K., Fortney, J. J., Nikolov, N., et al. 2016, Nature, 529, 59

Snellen, I. A. G., de Kok, R. J., de Mooij, E. J. W., & Albrecht, S. 2010, Nature, 465, 1049

Tsiaras, A., Rocchetto, M., Waldmann, I. P., et al. 2016, ApJ, 820, 99

Vidal-Madjar, A., Lecavelier des Etangs, A., Désert, J.-M., et al. 2003, Nature, 422, 143