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Doctoral Dissertation

**Toward Accurate Spectroscopic Characterization
of Exoplanetary Atmospheres:
A Retrieval Study of the Benchmark Brown Dwarf Binary
Luhman 16AB**

分光観測による太陽系外惑星大気の高精度な特徴づけに向けて：
ベンチマーク褐色矮星連星 Luhman 16AB のリトリバル解析

Hibiki Yama

Department of Earth and Space Science,
Graduate School of Science,
The University of Osaka

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Supervisor:
Takahiro Sumi

Abstract

More than 6000 exoplanets have been discovered to date, and in recent years, observational studies aimed at characterizing the physical and chemical properties of their atmospheres have rapidly progressed. Advances in extreme adaptive optics combined with near-infrared high-resolution spectrographs on ground-based large telescopes have enabled high-resolution spectroscopic observations of exoplanets, allowing for detailed atmospheric characterization. In particular, atmospheric retrieval analyses—an inverse problem framework that infers atmospheric physical states from observed spectra—enable not only the detection of molecular species but also the estimation of their abundances and the atmospheric temperature–pressure structure (T – P profile). Such retrieval techniques are now widely used as a standard approach for characterizing exoplanetary atmospheres.

Elemental abundances inferred from molecular compositions provide important clues for understanding the formation processes of giant gas planets. In particular, the atmospheric carbon-to-oxygen (C/O) ratio has been suggested to exhibit different behaviors depending on the dominant formation pathway, such as the core (or pebble) accretion scenario or the gravitational instability scenario, which is analogous to star formation. However, existing observational results have not yet led to a unified understanding of whether differences in gas-giant formation processes are clearly reflected in atmospheric C/O ratios.

In this context, brown dwarfs, which possess atmospheres similar to those of giant gas planets, serve as important comparative benchmarks. Brown dwarfs are thought to form through processes analogous to star formation and, owing to their higher intrinsic brightness compared to exoplanets, yield spectra with higher signal-to-noise ratios. Consequently, their atmospheric C/O ratios can provide a reference for gas planets formed via gravitational instability. Nevertheless, the number of brown dwarfs with measured C/O ratios remains limited. Furthermore, systematic uncertainties arising from differences in atmospheric models used in retrieval analyses—such as molecular line lists employed in opacity calculations and parameterizations of the T – P profile—have not yet been thoroughly investigated, despite being critical for robust comparisons of C/O ratios.

In this work, we present atmospheric retrievals of the benchmark brown dwarf binary Luhman 16AB, based on high-resolution near-infrared spectra obtained with VLT/CRIRES and the differentiable retrieval framework ExoJAX. Owing to its proximity and brightness, high-S/N data are available, and extensive external constraints exist, making the system

not only a key anchor for C/O but also a valuable testbed for evaluating model systematics and trialing new methodologies, as pursued here. We first perform retrievals with a power-law T – P profile and assess the sensitivity of inferred molecular abundances and C/O ratios to different CO line lists (ExoMol, HITEMP with air- and H₂-broadening). We then introduce a flexible Gaussian process-based T – P profile, allowing a non-parametric characterization of the thermal structure and a more conservative treatment of uncertainties. For both components, we infer C/O ratios of about 0.67, slightly above solar, with line list systematics at the 7 percent level emerging as the dominant source of uncertainty, whereas assumptions about T – P parameterization or photometric variability play a lesser role. The retrieved T – P profiles and molecular abundances are broadly consistent with atmospheric models and equilibrium chemistry. Our results establish Luhman 16AB as a key anchor for substellar C/O measurements, demonstrate the utility of flexible T – P modeling in high-resolution retrievals, and highlight the importance of systematic tests—particularly line list uncertainties—for robust comparisons between brown dwarfs and giant exoplanets.

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Chapter 1

Introduction

This chapter provides an overview of the main components of this thesis and the scientific background. Section 1.1 summarizes the physical and chemical properties of brown dwarfs and giant exoplanets—the primary targets of this thesis—and reviews the formation pathways that have been proposed. Section 1.2 describes spectroscopic observations as a key technique for characterizing these objects, together with the major approaches for analyzing the observed spectra, including the retrieval analyses performed in this work. Section 1.3 reviews the current discussion on the relationship between giant planet formation scenarios and the atmospheric carbon-to-oxygen (C/O) ratio, and highlights the potential role that brown dwarfs can play in this context. Section 1.4 further discusses open issues in current retrieval analyses that must be addressed to enable a more robust comparison of C/O ratios between brown dwarfs and gas giants.

1.1 Brown Dwarf and Giant Exoplanet

Brown dwarfs and giant exoplanets (gas giants) cannot sustain hydrogen burning and are therefore intrinsically cool and faint, making them difficult to detect. However, with advances in observational technology, the first such objects were discovered in 1995 (Nakajima et al., 1995; Mayor & Queloz, 1995). Brown dwarfs and giant planets share many physical and chemical properties. For example, their radii are nearly independent of mass and converge to roughly $1 R_J$. Their atmospheres are composed primarily of H_2 and He, containing molecules such as CO, CO_2 , CH_4 , H_2O , and NH_3 , and both classes host condensate clouds, including metal and silicate species at higher temperatures, as well as water and ammonia clouds at lower temperatures.

A frequently used practical criterion distinguishes brown dwarf and giant exoplanet by mass associated with nuclear burning: objects above $\sim 13 M_J$ ignite deuterium, whereas

hydrogen fusion requires $\gtrsim 80 M_J$ depending on metallicity and initial conditions (e.g., [Spiegel et al., 2011](#)).

1.1.1 Brown dwarfs

Brown dwarfs occupy the intermediate mass regime of $\sim 13\text{--}80 M_J$. Their central temperatures never reach the threshold for sustained hydrogen fusion, although short-lived deuterium burning occurs at young ages. Note that several theoretical studies have pointed out that deuterium burning is a short-lived process, lasting only during the first few Myr of evolution, and has a negligible impact on the subsequent thermal evolution of substellar objects ([Chabrier & Baraffe, 2000](#); [Chabrier et al., 2014](#)).

As deuterium is exhausted, brown dwarfs continue to cool over Gyr timescales, and their spectral appearance evolves accordingly. During this cooling sequence, objects with effective temperatures of approximately $T_{\text{eff}} \sim 1300\text{--}2500\text{ K}$ are classified as L dwarfs ([Kirkpatrick, 2005](#)). The onset of condensate formation marks the emergence of silicate, metal, and metal-oxide clouds in their upper atmospheres. While the earliest L dwarfs may remain largely cloud-free, mid- to late-L dwarfs are dominated by thick cloud decks that absorb and scatter efficiently at optical wavelengths. As a result, L dwarfs exhibit strongly reddened near-infrared colors and suppressed optical flux, a hallmark signature of this spectral class. As they cool further to $T_{\text{eff}} \sim 750\text{--}1500\text{ K}$, methane absorption becomes prominent in the near-infrared, marking the transition to the T spectral class ([Kirkpatrick, 2005](#), Figure 1.1). When the cooling progression reaches $T_{\text{eff}} \lesssim 500\text{ K}$, the spectral energy distributions are dominated by features of H_2O and NH_3 , and such objects are classified as Y dwarfs ([Cushing et al., 2011](#), Figure 1.1).

Brown dwarfs are thought to form through this process in a manner analogous to low-mass stars, but several mechanisms have been proposed to explain why their mass growth is halted before reaching the hydrogen-burning limit. These mechanisms include: (i) competitive accretion within the molecular cloud (e.g., [Bonnell & Bate, 2006](#)), (ii) reduced accretion rates due to tidal shear or high velocity dispersion in the surrounding environment ([Bonnell et al., 2008](#)), (iii) dynamical ejection in the early stages of mass growth (e.g., [Reipurth & Clarke, 2001](#)), (iv) gas dispersion caused by strong outflows from nascent brown dwarfs ([Machida et al., 2009](#)), and (v) photo-erosion driven by radiation from nearby OB stars (e.g., [Whitworth & Zinnecker, 2004](#)).

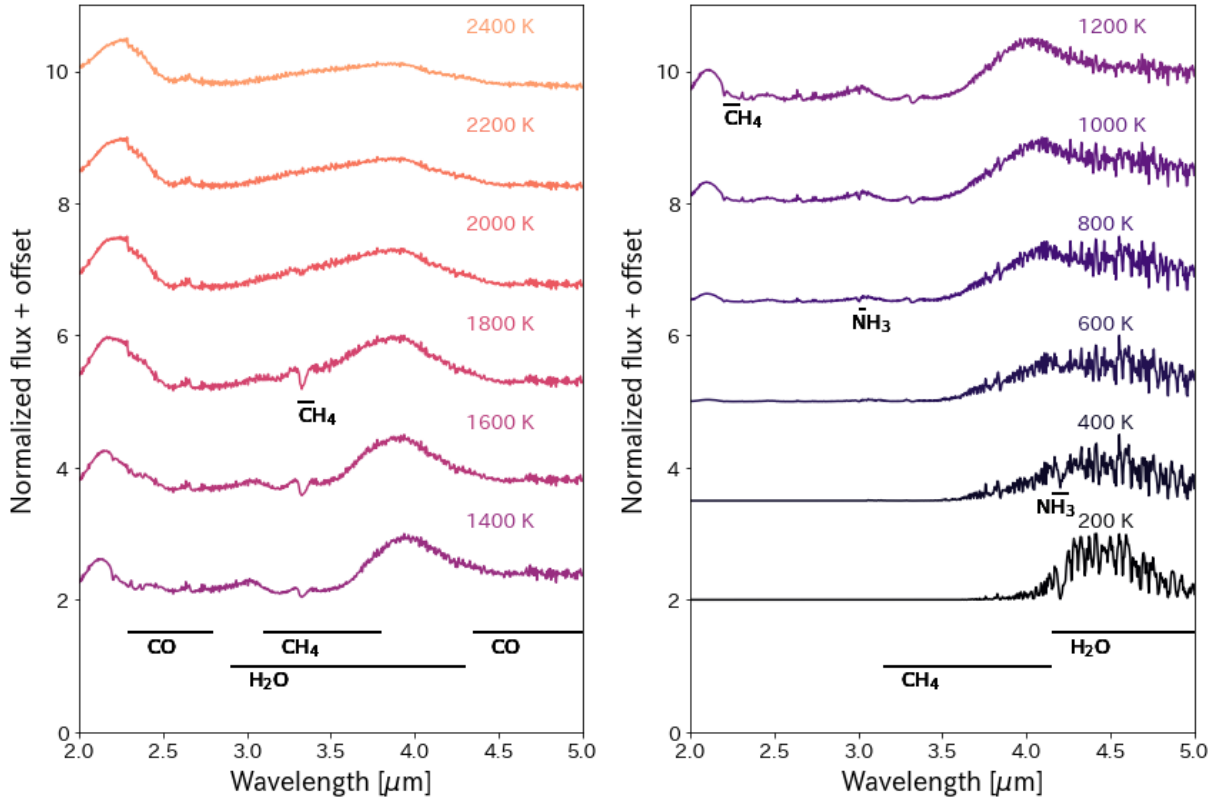


Figure 1.1: Model near-infrared spectra for different effective temperatures (Marley et al., 2021). The spectra are computed assuming cloud-free atmospheres with $\log g = 5$, $C/O = 0.5$, and $[M/H] = 0.0$.

1.1.2 Giant planets

Among the more than 6000 exoplanets have been confirmed to date, objects with masses of order a Jupiter mass and below the deuterium-burning limit ($\lesssim 13 M_J$) are referred to as giant planets. As the number of detections has increased, it has become clear that a remarkable diversity of gas giants exists—far broader than what is represented in our own Solar System. For example, hot Jupiters orbit within $\lesssim 0.1$ AU of their host stars and reach equilibrium temperatures on the order of 1000 K (e.g., Fortney et al., 2021). In contrast, systems hosting multiple cold Jupiters on wide orbits, with masses of $\sim 10 M_J$, have also been discovered, such as the HR 8799 system containing four massive planets (HR 8799 b, c, d, e; Marois et al., 2008, 2010).

This diversity of orbital configurations and mass distributions has revealed that classical Solar System-based formation theories (Hayashi et al., 1985) cannot fully account for the observed giant planet population. Consequently, multiple formation scenarios have been proposed, with two primary pathways — core accretion and gravitational collapse — being widely discussed in the literature, as outlined below. However, it remains unclear

which formation processes the gas giant planets observed to date have undergone.

Core accretion within protoplanetary disks

The standard model of giant planet formation is the core accretion scenario, in which solid particles in a protoplanetary disk coagulate and settle to form a core with a mass of a few $M_{\oplus}$ (classical core accretion: Hayashi et al. (1985); Pollack et al. (1996), pebble accretion: Ormel & Klahr (2010); Visser & Ormel (2016)). Once the core reaches a critical mass, runaway gas accretion begins, leading to the growth of the object into a giant planet.

Star-like gravitational collapse

As an alternative to the core accretion scenario, gravitational collapse has been proposed as a formation pathway for gas giant planets. The basic mechanism of this scenario is analogous to that of star formation: local density fluctuations arising within a protoplanetary disk can trigger gravitational instability, leading to the formation of gas giant planets through rapid collapse driven by self-gravity (e.g., Boss, 1997; Kratter & Lodato, 2016). In this process, regions within the disk that satisfy the Toomre instability condition begin gravitational collapse (Toomre, 1964).

1.2 Spectroscopic Techniques and Spectral Analysis

This section reviews spectroscopic observations, which are widely used to characterize brown dwarfs and exoplanets, and summarizes the main methods for analyzing the observed spectra. In spectroscopic observations, light that has passed through or originated from an exoplanetary atmosphere is dispersed in wavelength space to obtain a spectrum. Molecular absorption and emission processes in the atmosphere imprint spectral lines at specific wavelengths, whose strengths and shapes reflect presence and amount of molecules, the atmospheric temperature–pressure (T – P) structure and surface gravity. In particular, absorption lines encode information not only on molecular species and abundances and the T – P profile, but also on the projected rotational velocity through their line broadening. In addition, the presence of clouds and hazes, which scatter and absorb radiation over broad wavelength ranges, leaves characteristic signatures in the observed spectra. Spectra containing such chemical and physical information about exoplanetary atmospheres are obtained through two main observational approaches, as described below.

1.2.1 Transmission spectroscopy

For planets whose orbital planes are viewed nearly edge-on from Earth, a transit occurs when the planet passes in front of its host star, causing a temporary dimming of the observed stellar flux¹ (Figure 1.2). The effective planetary radius that blocks the stellar light depends on the atmospheric opacity of the planet. Since atmospheric opacity is wavelength-dependent (see Chapter 2 for details), the inferred planetary radius also varies with wavelength. The flux decrement during a transit is referred to as the transit depth and can be approximated by the ratio of the projected areas of the planet and the host star. Denoting the wavelength-dependent planetary radius as $R_p(\lambda)$ and the stellar radius as $R_\star$, the transit depth can be written as

$$\delta_t(\lambda) \approx \left(\frac{R_p(\lambda)}{R_\star} \right)^2. \quad (1.1)$$

By measuring $\delta_t(\lambda)$ over a range of wavelengths, one can obtain a transmission spectrum that reflects the wavelength-dependent atmospheric opacity of the planet.

The first detection of an exoplanetary atmosphere was achieved through transmission spectroscopy of the transiting planet HD 209458 b using the Hubble Space Telescope (HST)/STIS, which revealed absorption features of the Na D doublet (Charbon-

¹The method of detecting exoplanets using this phenomenon is known as the transit method.

neau et al., 2002). Subsequently, Snellen et al. (2008) demonstrated the first detection of an exoplanetary atmospheric species from the ground by identifying Na, D absorption in the atmosphere of HD 209458 b using Subaru/HDS, thereby establishing the feasibility of ground-based transmission spectroscopy. The inferred abundance was found to be consistent with results obtained from HST/STIS observations. These pioneering studies established transmission spectroscopy, using both space- and ground-based telescopes, as a powerful technique for probing exoplanetary atmospheres. Beyond the detection of individual molecular species, transmission spectroscopy has also provided evidence for the presence of clouds in gas giant atmospheres, which can act as an important source of opacity alongside molecular absorption. For instance, Wakeford & Sing (2015) analyzed transmission spectra of the hot Jupiter HD 189733 b observed with HST/STIS and Spitzer, finding strong support for the presence of clouds. Although specific chemical species responsible for the cloud opacity could not be uniquely identified, their analysis constrained the characteristic particle sizes and the vertical extent of the cloud layers. Furthermore, transmission spectroscopy can be used to discuss the escape of exoplanetary atmosphere caused by stellar irradiation (e.g., Ehrenreich et al., 2015).

Since the 2021 launch of the James Webb Space Telescope (JWST), near-infrared transmission spectroscopy has been extended to broad wavelength coverage with high photometric precision and moderate spectral resolution ($\lambda/\Delta\lambda \lesssim 2700$). These capabilities are expanding the range of detectable atmospheric species beyond the major absorbers (e.g., H_2O and CO), thereby opening a new window on atmospheric chemistry. For example, Rustamkulov et al. (2023) analyzed JWST/NIRSpec PRISM spectra ($\lambda/\Delta\lambda \sim 20 - 300$) of WASP 39 b, detecting H_2O and CO with high significance and reporting an additional absorption feature near $4\,\mu\text{m}$ consistent with SO_2 . The ability to detect trace species that can serve as diagnostics of photochemistry suggests that JWST spectra will provide stronger leverage on atmospheric processes than was previously possible. In this sense, JWST-era observations may enable more detailed constraints on atmospheric physics and chemistry, rather than merely identifying the dominant molecular absorbers. Moreover, JWST has extended transmission spectroscopy from hot Jupiters to smaller, Earth-sized planets (e.g., Lustig-Yaeger et al., 2023, *postfix*).

While transmission spectroscopy has been demonstrated to be a powerful tool for probing exoplanetary atmospheres, its sensitivity is inherently limited to the terminator region of the planet. In addition, its applicability is restricted to planets that undergo transits, such as short-period hot Jupiters. Therefore, to achieve a more comprehensive understanding of exoplanetary atmospheres, the complementary use of other observational techniques is essential.

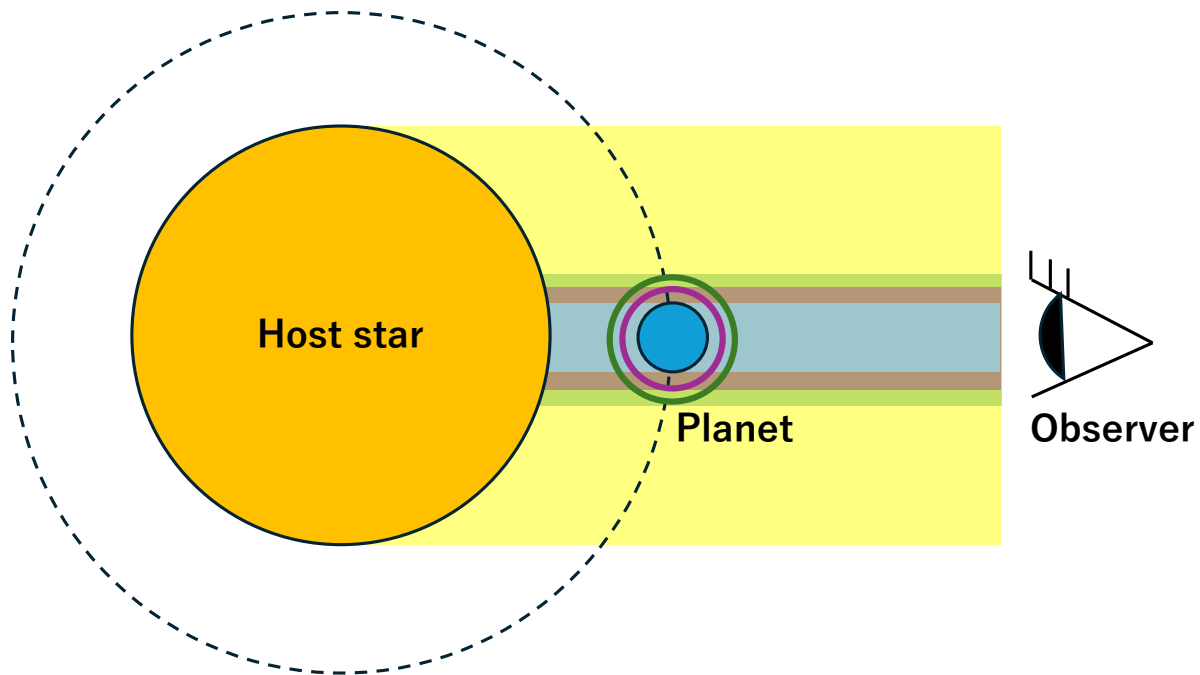


Figure 1.2: Schematic illustration of a planetary transit. In transmission spectroscopy, the wavelength-dependent transit depth is measured to infer the atmospheric opacity at each wavelength.

1.2.2 Secondary eclipse spectroscopy and direct imaging spectroscopy

While a transit corresponds to the planet passing in front of the host star, the event in which the planet is occulted by the star is referred to as a secondary eclipse (Figure 1.3, left). During the secondary eclipse, only the stellar spectrum is observed. In contrast, spectra obtained immediately before and after the eclipse consist of the combined light from the host star and the dayside of the planet, including reflected stellar light and thermal emission from the planetary atmosphere. By taking the difference between the spectra observed outside the eclipse and those obtained during the eclipse, the planetary spectrum can be isolated. This resulting spectrum is known as the secondary eclipse spectrum and provides direct information on the thermal emission and composition of the planetary dayside.

In an effort to systematically characterize planetary atmospheres through secondary eclipse spectroscopy—thereby demonstrating the feasibility of atmospheric characterization from dayside emission—[Line et al. \(2014\)](#) analyzed spectra of nine hot Jupiters acquired with space- and ground-based facilities using a uniform retrieval framework (see Section 1.2.3). The analysis showed that, although the inferred molecular abundances generally exhibit large uncertainties, they are consistent with estimates from previous

studies based on transmission spectroscopy, despite probing different atmospheric regions (the planetary dayside for secondary eclipse spectroscopy versus the terminator region for transmission spectroscopy).

While secondary eclipse spectroscopy enables the measurement of emission spectra for transiting exoplanets, the emission spectra of planets on wide orbits, regardless of whether they transit, can instead be obtained through direct imaging spectroscopy (Figure 1.3, right). This method is particularly well suited to young and hot gas giants, which are intrinsically bright in the near-infrared. In cases where the contrast between the planet and the host star is sufficiently high, thermal emission spectra can also be obtained by combining spectroscopy with starlight suppression techniques, such as coronagraphy and adaptive optics (AO) systems.

For example, in the well-known directly imaged planetary system HR 8799, direct imaging spectroscopy has been conducted for all four of the planets discovered to date, demonstrating that direct imaging spectroscopy has also been advancing the characterization of exoplanets. [Bowler et al. \(2010\)](#) conducted near-infrared spectroscopic observations of HR 8799 b over the wavelength range of 2.12–2.23 μm using Keck II/OSIRIS, which combines a near-infrared integral-field spectrograph with adaptive optics. They investigated the presence of CH_4 absorption, which serves as a diagnostic of atmospheric temperature and a key indicator for spectral classification. Their results suggested that CH_4 is very weak or absent, and that a T2 spectral type provides the best match to the observed spectrum. Furthermore, by comparing the observed spectrum together with existing near-infrared photometric data to atmospheric models, they found that models including moderately thick clouds show relatively good agreement, while no single model is able to reproduce all observational constraints simultaneously. In addition, [Janson et al. \(2010\)](#) focused on the fact that, for young giant planets with effective temperatures of $\sim 1000\text{ K}$, the contrast between the host star and the planet becomes relatively small at wavelengths around 4 μm . Using VLT/NACO, they achieved spatially resolved spectroscopy of HR 8799 c through L' -band (3.88–4.10 μm) observations. Comparison of the resulting spectrum with thermal evolution models revealed that the continuum shape—particularly the spectral slope at wavelengths longer than 4 μm —cannot be reproduced by existing models. This discrepancy suggests that complex cloud structures, which cannot be described by simple dust assumptions, as well as departures from chemical equilibrium, may play an important role in the atmosphere of HR 8799 c. Furthermore, [Zurlo et al. \(2016\)](#) successfully obtained direct imaging spectra of HR 8799 d and e with VLT/SPHERE, showing that their spectral characteristics closely resemble those of L6–8 brown dwarfs and suggesting the possible presence of thick cloud layers in their atmo-

spheres.

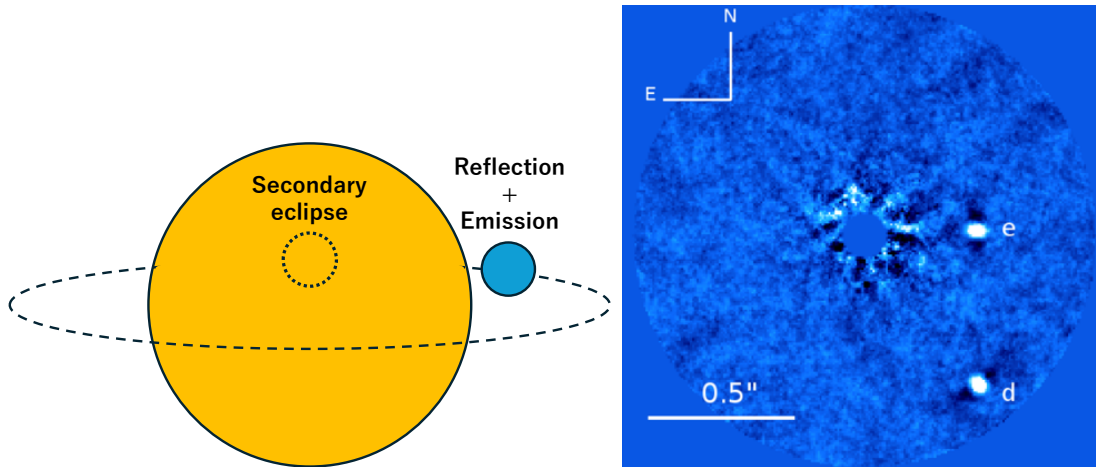


Figure 1.3: Schematic illustration of a secondary eclipse (left) and an observed direct imaging image of the HR 8799 system obtained with VLT/SPHERE using a coronagraph and an integral field spectrograph (right; Zurlo et al. 2016). In secondary eclipse spectroscopy, the planetary spectrum—consisting of thermal emission and reflected stellar light—is obtained by differencing the planetary system spectra observed outside and during the eclipse. Direct-imaging spectroscopy enables spectroscopy of a planet’s thermal emission by suppressing stellar light (e.g., with a coronagraph) and thereby reducing the star-planet contrast.

1.2.3 High-resolution spectroscopy

Transmission, secondary eclipse, and direct imaging spectroscopy enable the characterization of exoplanet atmospheres across a wide range of orbital configurations and atmospheric regions. However, in many of the previous studies discussed above, the spectral resolving power of the instruments is relatively low, or, as in the Subaru/HDS observations presented by Snellen et al. (2008), the intrinsic spectral resolution of the instrument is high but the data are binned in wavelength to improve the signal-to-noise ratio. As a result, individual molecular absorption lines are often blended into broad absorption bands, making it difficult to detect weak features and to disentangle overlapping absorption from different molecular species or clouds. Consequently, it is generally challenging to use the depths and shapes of spectral features to tightly constrain molecular abundances and the atmospheric T – P structure.

A complementary approach is high-resolution spectroscopy: with resolving powers of $\lambda/\Delta\lambda \sim 10^5$, it provides access to individual molecular absorption and emission lines and enables detailed characterization of their line shapes, including intrinsic and rotational broadening. While increasing spectral resolution inevitably reduces the S/N, recent ad-

vances combining large telescopes with near-infrared high-resolution spectrographs have substantially mitigated this limitation. As a result, high-resolution spectra of close-in exoplanets—through transmission and secondary eclipse spectroscopy—as well as of directly imaged exoplanets, are now routinely obtained from the ground. Representative examples include IRD on the Subaru Telescope (Kotani et al., 2018) and CRIRES⁺ on the Very Large Telescope (Kaeufl et al., 2004; Follert et al., 2014). These observational capabilities have opened a new regime for atmospheric characterization, in which molecular species can be detected and analyzed at the level of individual spectral lines, providing powerful constraints on atmospheric composition, dynamics, and the atmospheric T – P structure. To fully exploit the information content of high-resolution spectra, analysis techniques such as cross-correlation and atmospheric retrievals are generally employed, as discussed below.

Cross-correlation technique

As a method for analyzing high-resolution spectra of exoplanets obtained in this manner, the cross-correlation technique has been widely used to detect molecular species and characterize atmospheric properties (e.g., Snellen et al., 2010; Brogi et al., 2016; Hoeijmakers et al., 2018). In this method, observed spectra are cross-correlated with theoretical or empirical template spectra of specific molecules, coherently combining the signal from numerous weak absorption lines. Due to the orbital motion of the planet, the molecular absorption lines in the observed spectrum are Doppler-shifted. When these Doppler-shifted lines align with those in the template at a specific radial velocity, their contributions add constructively, resulting in a strong peak in the cross-correlation function. If a molecule exhibits N resolved lines within the observed wavelength range, the effective signal-to-noise ratio of the cross-correlation signal is enhanced by approximately a factor of $\sqrt{N}$. Cross-correlation is therefore particularly powerful for detecting molecular species and measuring radial velocities. This technique has enabled detections of molecules such as CO and H₂O in exoplanet atmospheres.

Snellen et al. (2010) presented the first molecular detection in an exoplanet atmosphere achieved using high-dispersion spectroscopy combined with a cross-correlation technique. By analyzing VLT/CRIRES transmission spectra of HD 209458 b, they detected carbon monoxide (CO) at a significance level of 5.6σ . Furthermore, by injecting template spectra with varying CO abundances into the observed data and comparing the resulting cross-correlation amplitudes, they demonstrated that the CO abundance (volume mixing ratio) can be constrained to $1\text{--}3 \times 10^{-3}$, although with uncertainties arising from assumptions

about the atmospheric T – P profile and from reduced sensitivity due to spectral overlap with absorption features of other molecules, most notably CH_4 .

Atmospheric retrieval

While the cross-correlation technique primarily enables the detection of molecular species, atmospheric retrieval offers a complementary and more quantitative framework for robustly constraining molecular abundances and T – P structures. By directly comparing synthetic spectra, computed via radiative transfer through a parameterized atmosphere, with observed spectra within a Bayesian framework, retrieval analyses enable the simultaneous inference of atmospheric composition, T – P structures, and dynamical parameters, together with their associated uncertainties and parameter degeneracies (see Chapter 2 for details). In this way, atmospheric retrieval provides a suitable framework for measuring the atmospheric elemental composition such as C/O ratio, owing to its ability to quantitatively constrain molecular abundances.

Recent methodological advances, such as the development of tools for high-resolution spectral retrieval (e.g., ExoJAX; Kawahara et al. 2022; Kawahara et al. 2025, petitRADTRANS; Mollière et al. 2019), allow the rich information content encoded in resolved molecular line profiles to be fully exploited. As an example of an atmospheric retrieval analysis applied to exoplanet spectra, Wang et al. (2023) combined low- and high-resolution emission spectra of HR 8799 c and performed an atmospheric retrieval analysis using petitRADTRANS. As a result, they placed physically consistent constraints on the atmospheric T – P profile and simultaneously inferred the abundances of H_2O , CO , CO_2 , and CH_4 . Furthermore, the derived carbon-to-oxygen (C/O) ratio was found to be $0.67^{+0.12}_{-0.15}$, which is consistent with that of the host star.

These advances demonstrate that atmospheric retrieval applied to high-resolution spectroscopy enables physically consistent constraints on both atmospheric structure and composition. In the following section, we review key results obtained from such retrieval studies, with particular emphasis on C/O ratios as tracers of planetary formation and atmospheric evolution.

1.3 C/O Ratio as a Formation Tracer

Differences between core accretion and gravitational collapse may be imprinted on the elemental composition of gas giant atmospheres, reflecting the distinct physical and chemical processes involved in each formation pathway. In particular, the relationship between a gas giant’s C/O ratio² and its formation process has long been discussed as an important diagnostic.

In the core accretion scenario, protoplanetary disks exhibit strong radial temperature gradients, giving rise to snow lines for volatile species. These condensation fronts cause the composition of the disk gas to vary with orbital radius. Consequently, the atmospheric composition of objects formed through core accretion reflects their formation location in the disk and does not necessarily match the elemental composition of the host star (Figure 1.4, [Öberg et al. 2011](#)). As a result, the atmospheric C/O ratio is expected to deviate from the stellar value in a manner that depends sensitively on the planet’s formation location and accretion history, making it a key diagnostic of the core accretion process. In addition to the effects of snow line formation alone, several studies have highlighted the importance of chemical evolution in the gas and solid phases driven by cosmic-ray ionization ([Eistrup et al., 2018](#)), as well as the inward transport of volatile ices embedded in pebbles from the outer to the inner regions of the disk ([Booth et al., 2017](#)).

Another key feature of the disk accretion scenario is planet migration. Planetary orbits can be altered through interactions with the surrounding disk gas, meaning that the current orbital position of a planet does not necessarily correspond to its original formation site. As a result, the observed atmospheric composition such as C/O ratio may record both the local chemical environment where the planet formed and its subsequent migration history (e.g., [Kessler & Alibert, 2023](#)).

On the other hand, in the star-like gravitational collapse scenario, little to no separation between solids and gas occurs during formation. As a result, atmospheres of objects formed in this scenario are expected to inherit the elemental composition of their natal molecular clouds essentially unchanged. Therefore, objects formed via this scenario are expected to exhibit atmospheric C/O ratios that are consistent with those of other stars formed from the same natal molecular cloud or their host stars.

²While this study focuses on the C/O ratio, elemental abundances such as [C/H] can also provide complementary diagnostics for distinguishing between planetary and brown dwarf formation pathways (e.g., [Xuan et al., 2024a](#); [Wang, 2025](#)).

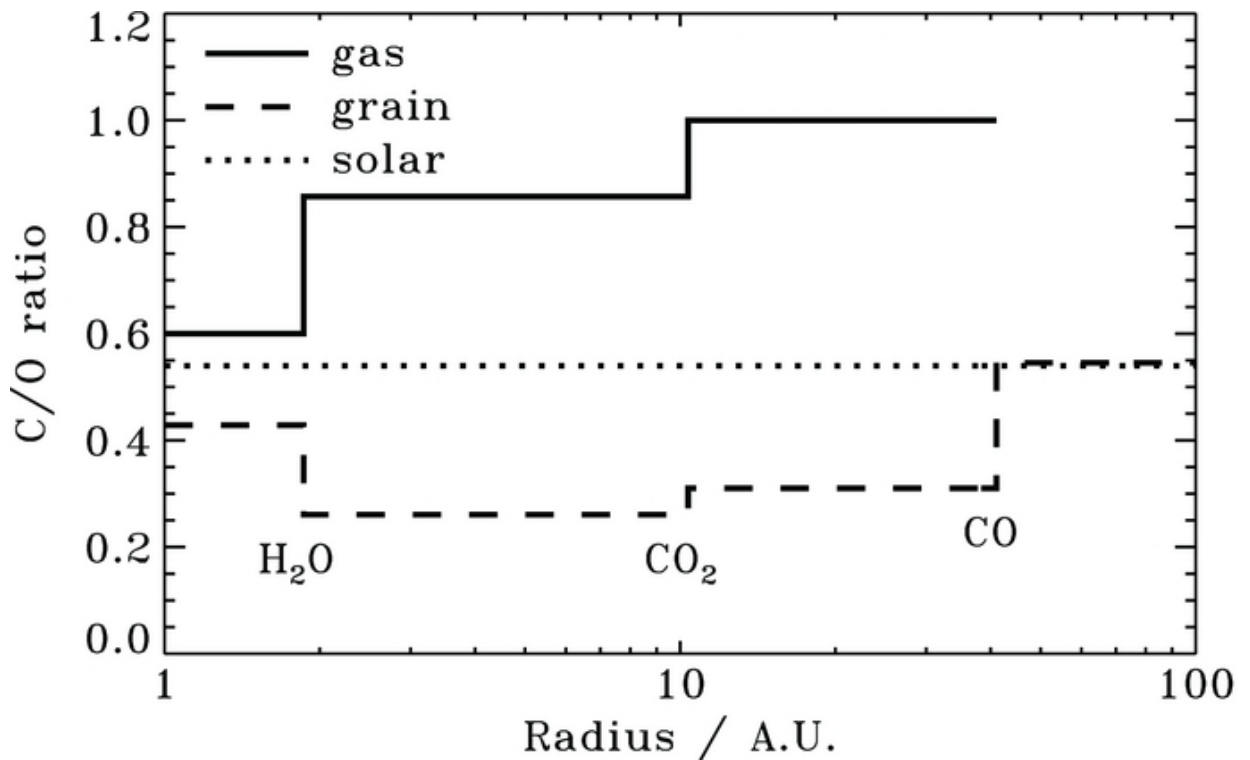


Figure 1.4: C/O ratio of the gas (solid line) and dust grains (dashed line) in a typical protoplanetary disk around a Sun-like star (reproduced from [Öberg et al. \(2011\)](#) with permission, without modification). The labeled molecular species indicate the orbital radii at which their corresponding snow lines form. This model considers only the effects associated with snowline formation.

1.3.1 Literature of C/O measurement

Close-in (transiting) giant planets, especially hot Jupiters, are well suited to atmospheric characterization via transmission and secondary-eclipse spectroscopy, and observational constraints on their atmospheric composition have steadily accumulated. Prior to JWST, such constraints were primarily built from ground- and space-based spectroscopy with facilities such as HST and Spitzer. For instance, [Changeat et al. \(2022\)](#) performed a systematic analysis of secondary eclipse spectra of 25 hot Jupiters observed with HST and Spitzer, reporting that inferred C/O ratios exhibit a large dispersion and that superstellar values are frequently obtained (green symbols in Figure 1.5). By contrast, C/O ratios inferred from recent high-precision JWST transmission spectra of transiting gas giants—although still based on a limited sample—appear to show a different tendency from the pre-JWST results, with a dispersion around substellar values (purple symbols in Figure 1.5). Meanwhile, direct imaging spectroscopy of wide-orbit gas giants has also been actively pursued with ground-based large telescopes, and such objects tend to yield C/O ratios closer to solar values than close-in planets (blue symbols in Figure 1.5; e.g., [Zhang et al. 2024a](#)). Taken at face value, the pre-JWST transiting population and the direct imaging population appear to show different behaviors in C/O ratio, potentially hinting at differences in formation pathways. However, when JWST results for transiting gas giants are taken into account, it remains unclear whether currently measured C/O ratios provide an unambiguous imprint of giant planet formation.

In addition, an important point when comparing previously measured C/O ratios is that the inferred C/O ratios for two transiting gas giants, HD 209458 b and WASP 77 Ab, have been revised downward in JWST-based analyses relative to pre-JWST estimates. Specifically, the C/O ratio of HD 209458 b has been revised from ~ 0.92 to ~ 0.11 ([Changeat et al., 2022](#); [Xue et al., 2024](#)), while that of WASP 77 Ab has been revised from ~ 0.8 to ~ 0.54 ([Changeat et al., 2022](#); [Edwards & Changeat, 2024](#)). This revision suggests that previously reported C/O ratios may have been affected by systematics arising from the atmospheric models adopted in spectral analyses.

1.3.2 Brown dwarfs as benchmarks for atmospheric C/O ratios

To advance these discussions, brown dwarfs serve as important comparison targets, providing benchmark reference points for gas giants. Brown dwarfs are generally thought to form in a star-like manner and are therefore expected to inherit the elemental composition of their natal clouds. At the same time, their atmospheres are broadly similar to those of gas giant planets, making them particularly useful reference objects. Moreover,

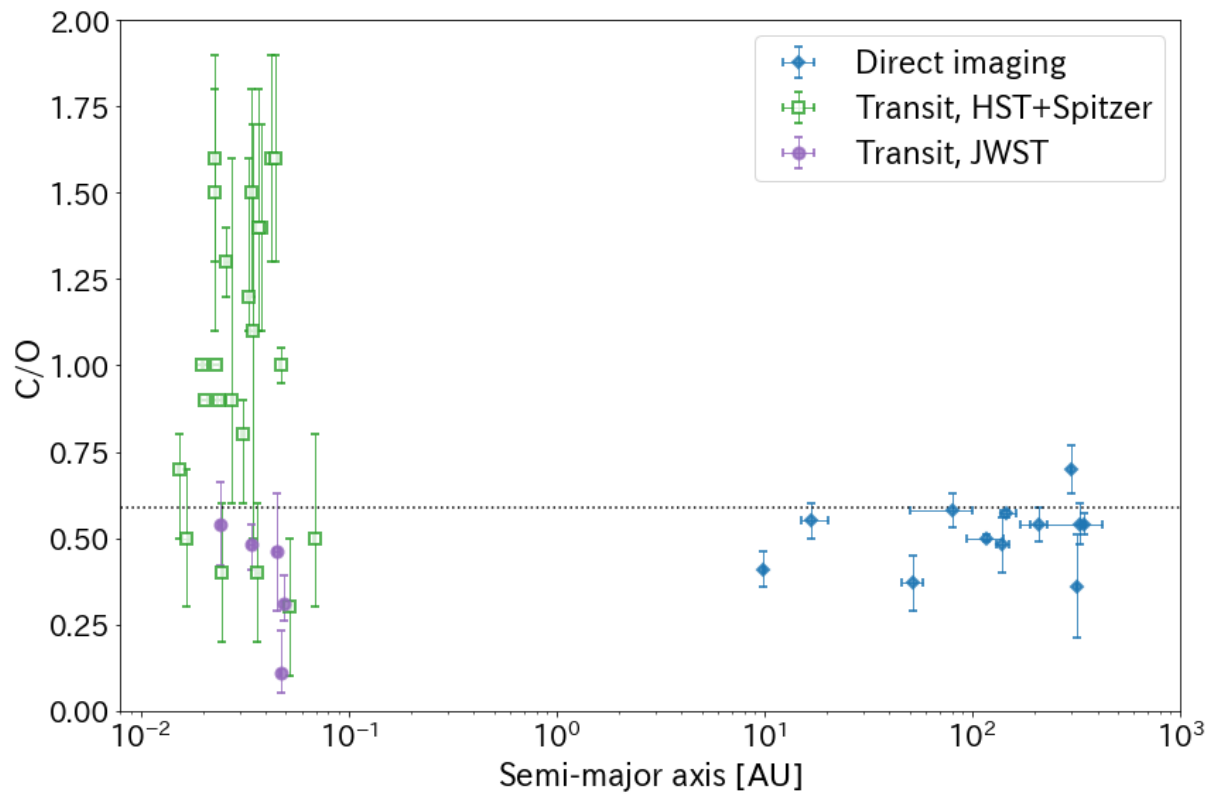


Figure 1.5: Comparison of C/O ratios versus semi-major axis for directly-imaged gas giants (blue symbols) and transit gas giant planets (green symbols; observed with HST+Spitzer, purple symbols; observed with JWST). Literature values and properties are summarized in Table A.1. The horizontal dot line shows Solar C/O ratio (0.59; [Asplund et al., 2021](#)).

brown dwarfs can typically be observed at higher signal-to-noise ratios than planetary-mass objects, enabling stringent tests of systematic uncertainties in atmospheric retrieval analyses. In this way, brown dwarfs can provide a baseline for atmospheric C/O ratios and help interpret gas giant formation scenarios inferred from C/O measurements.

In practice, when comparing the C/O ratios measured for directly imaged gas giants with those derived for brown dwarfs from high-resolution direct imaging spectroscopy, brown dwarfs tend to show values closer to the solar C/O ratio (Figure 1.6; e.g., [Hsu et al. 2024](#); [González Picos et al. 2024](#)). However, to discuss more statistically what C/O ratios brown dwarfs should exhibit as a baseline outcome of star-like formation via gravitational collapse, it is necessary to increase the sample size of brown dwarfs with C/O measurements. Moreover, in order to perform accurate comparisons using measured C/O ratios, it is crucial to properly quantify systematic uncertainties in C/O inferences that arise from atmospheric-model assumptions, as discussed in Section 1.3.1.

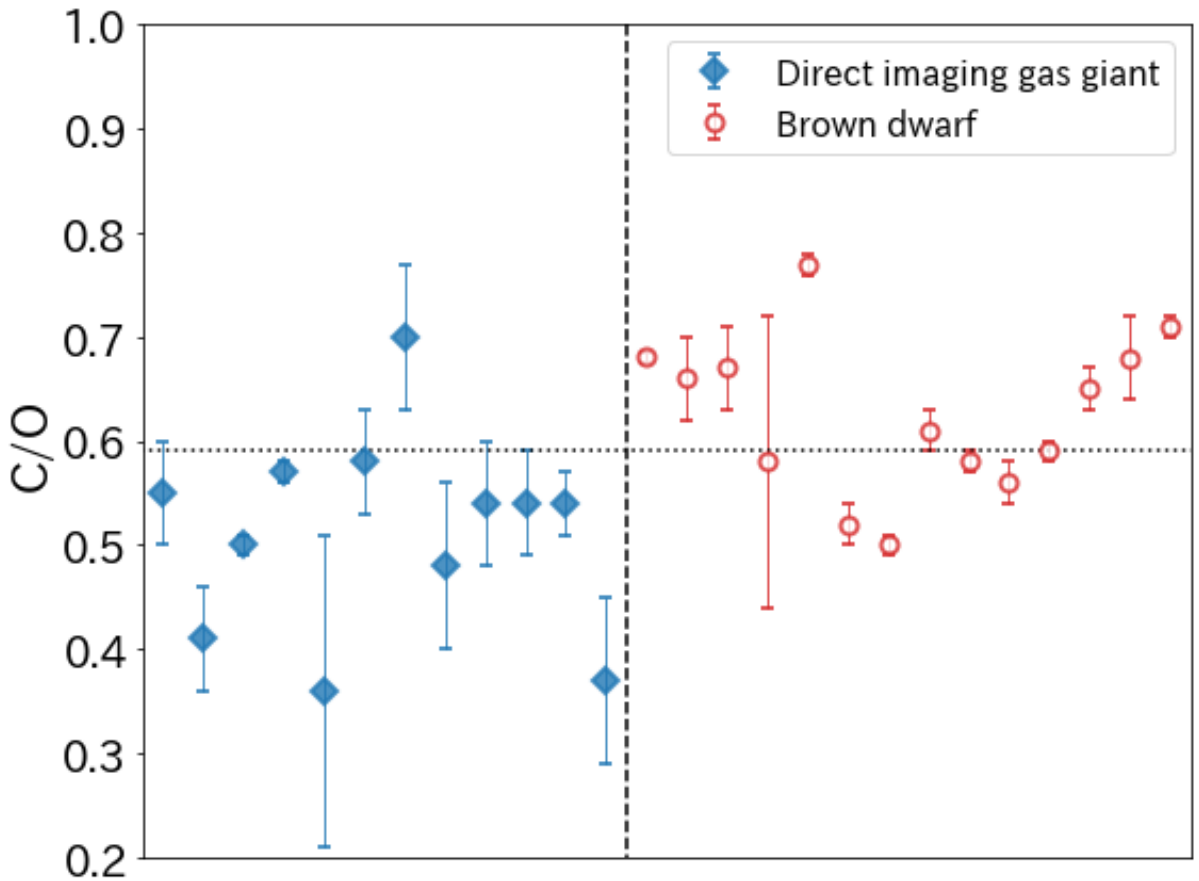


Figure 1.6: Comparison of C/O ratios of directly-imaged gas giants (blue symbols) and brown dwarfs (red symbols). Literature values and properties are summarized in Table A.1. The horizontal dot line shows Solar C/O ratio (0.59; [Asplund et al., 2021](#)).

1.4 Open Issues in Atmospheric Retrieval

Despite the rapid progress of atmospheric retrieval, systematic uncertainties associated with atmospheric modeling remain, particularly for high-resolution retrievals. At present, a community-wide standard has not been established for key ingredients such as molecular opacities, T – P profile parameterizations, and cloud modeling, and the choice of these assumptions can lead to different inferred atmospheric parameters, including molecular abundances and the C/O ratio.

First, molecular opacities rely on precomputed line lists that tabulate line strengths and coefficients controlling line shapes (e.g., pressure broadening; see Section 2.3.1 for details). Multiple line lists often exist for the same molecule, and no single line list has been adopted as a unique standard. Differences among line lists can lead to different line shape parameters and therefore different absorption line profiles even under identical conditions. As a result, inferred atmospheric parameters from line shapes of observed spectra, such as molecular abundances and the C/O ratio, can depend on the adopted line list. As an example, [de Regt et al. \(2024\)](#) performed retrievals of the high-resolution spectrum of the brown dwarf DENIS J0255 using two different H₂O line lists and reported differences not only in the inferred metallicity and the ¹²CO/¹³CO isotopologue ratio but also in the C/O ratio, at the $\sim 4\%$ level between the two line list choices.

Second, retrieval models typically treat the T – P profile in a parameterized form, yet different parameterizations have been adopted in the literature (see Section 2.5 for details). The choice of parameterization can change the inferred T – P structure, thereby modifying the relative line strengths and line shapes and ultimately affecting retrieved molecular abundances and the C/O ratio. Indeed, [González Picos et al. \(2024\)](#) reported that retrievals of the high-resolution spectrum of the brown dwarf/super-Jupiter GQ Lup b with two different T – P parameterizations yield different estimates of the surface gravity. They also demonstrated that the inferred C/O ratio differs substantially depending on how the T – P structure is treated: adopting a fixed T – P profile calculated self-consistently under radiative–convective equilibrium yields $\text{C/O} = 0.70 \pm 0.01$, whereas using a parameterized T – P prescription yields $\text{C/O} = 0.50 \pm 0.01$.

Finally, clouds are expected to be present in the atmospheres of brown dwarfs and gas giants, yet cloud modeling is likewise not unique; a variety of prescriptions are used for the wavelength dependence and vertical distribution of cloud opacity (e.g., [Ackerman & Marley 2001](#); [Inglis et al. 2024](#); [Kasagi et al. 2025](#); see Section 2.3.3 for details). Because cloud opacity can be degenerate with molecular opacity, differences in cloud modeling may also impact the inferred molecular abundances and the C/O ratio. For example, [Inglis et al.](#)

(2024) performed retrievals of the spectrum of the directly imaged gas giant ROXs 42B b using cloud models with different wavelength dependences and vertical distributions, and found that the inferred C/O ratio shifts at the $\sim 6\%$ level between cloud prescriptions in their analysis, highlighting that cloud modeling can introduce non-negligible systematics in C/O inferences.

Therefore, robust comparisons of C/O ratios from high-resolution retrievals—and their use as formation diagnostics—require a careful quantification of model-dependent systematics and a conservative uncertainty budget that propagates these effects into the inferred atmospheric parameters. In the next section, we outline the scope of this thesis and the approach taken to address these challenges.

1.5 Scope of This Thesis

In this thesis, we investigate the atmospheric properties of the benchmark brown dwarf binary Luhman 16AB—taking advantage of its proximity, brightness, and extensive external constraints—using high-resolution spectroscopy and atmospheric retrieval techniques, with a particular focus on the C/O ratio and related elemental abundances as tracers of formation environments. In parallel, we assess systematic uncertainties in inferred atmospheric parameters—especially the C/O ratio—arising from the choice of CO molecular line lists and from the treatment of the atmospheric T – P structure. In particular, we develop and apply a flexible T – P profile representation and quantitatively evaluate its impact using high-quality observational data. Such assessments are essential both for comparative planetology and for improving the robustness of atmospheric retrieval methodologies.

The remainder of this thesis is organized as follows. In Chapter 2, we describe the radiative transfer framework for brown dwarf and giant planet atmospheres and derive the thermal emission spectral models employed in the retrieval analyses. In Chapter 3, we perform atmospheric retrievals for Luhman 16AB and measure its C/O ratio. We also examine the dependence of the inferred atmospheric properties on the choice of CO molecular line lists within a power-law T – P parameterization. We then introduce a more flexible Gaussian-process-based representation of the T – P profile, demonstrate its utility, and discuss how assumptions about the thermal structure propagate into retrieved parameters and their interpretation. Finally, Chapter 4 summarizes the main findings of this thesis, discusses their implications for the formation of brown dwarfs and giant planets, and outlines directions for future observational and theoretical work.

Chapter 2

Radiative Transfer for Brown Dwarfs and Gas Giants

In this chapter, we summarize the radiative transfer calculations for brown dwarfs and gas giants (substellar objects) and the formulation of atmospheric opacities used in this study, to the extent necessary for the retrieval framework discussed later.

2.1 Optical Depth

Light propagating through the atmosphere of a substellar object is attenuated by absorption and scattering due to atmospheric constituents. In other words, the atmosphere becomes opaque owing to the presence of material along the line of sight. A convenient quantity to characterize this opacity is the optical depth τ , defined as

$$\tau \equiv \int n \sigma dx, \quad (2.1)$$

where n [$/\text{cm}^3$] is the number density of atmospheric material and σ [cm^2] is the cross section, which represents the probability that an incident photon is absorbed or scattered by the material. When a photon travels a distance dx through an atmospheric layer, the infinitesimal probability for interaction with the material is

$$dp = n \sigma dx = d\tau. \quad (2.2)$$

The probability that a photon passes through this thin layer without interaction is therefore $(1 - dp)$, and by multiplying this over the entire atmosphere one obtains

$$p_{\text{sur}} = \prod_{i=1}^N (1 - \Delta p_i) \quad (2.3)$$

$$= \lim_{N \rightarrow \infty} \left(1 - \frac{\tau}{N}\right)^N \quad (2.4)$$

$$= e^{-\tau}. \quad (2.5)$$

Thus, the characteristic depth to which photons can propagate on average is determined by the location where

$$\tau \sim 1 \quad (2.6)$$

is satisfied. In other words, the radiation observed at a given wavelength predominantly originates from the atmospheric layer where the optical depth at that wavelength is $\tau \sim 1$.

2.2 Radiative Transfer

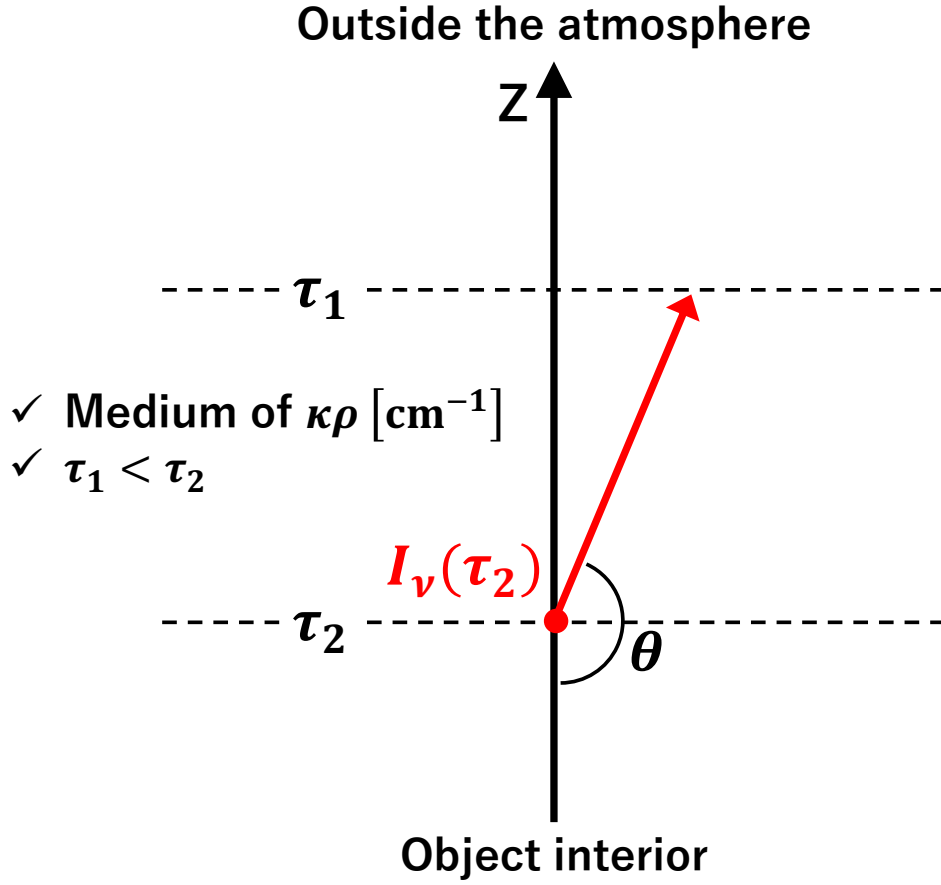


Figure 2.1: Schematic of the coordinate system used for radiative transfer. The z -axis is defined to point from the interior of the object toward the outer atmosphere. The optical depth τ is defined in the opposite direction, increasing inward from the outside of the atmosphere, such that $\tau_2 > \tau_1$.

We next describe the propagation of radiation in the atmosphere, i.e., radiative transfer. In what follows, the subscript ν is assumed to denote the wavenumber in units of cm^{-1} . A schematic of the coordinate system is shown in Figure 2.1.

Let $d\varepsilon_\nu$ [erg] be the energy carried by radiation within a wavenumber interval $d\nu$ that passes through an area element dA [cm^2] during a time interval dt [s] into a solid angle $d\Omega$ [str]. The specific intensity I_ν [$\text{erg}/\text{cm}^2/\text{s}/\text{str}/\text{cm}^{-1}$] is then defined by

$$d\varepsilon_\nu = I_\nu dA dt d\Omega d\nu. \quad (2.7)$$

We set the z -axis to point upward from the interior toward the top of the atmosphere and consider radiation propagating from the deeper layers to the upper atmosphere. When

radiation enters a thin cylinder whose top and bottom faces are perpendicular to the z -axis, it experiences absorption and scattering by the medium inside the cylinder in proportion to I_ν . The proportionality coefficient is the opacity κ_ν [cm^2/g], which quantifies the extinction of the specific intensity due to absorption and scattering per unit mass of the medium. Using a path length ds [cm] and the density ρ [g/cm^3] of the cylinder, the amount of I_ν absorbed or scattered per unit time within the cylinder can be written as

$$-(\kappa_\nu \rho I_\nu ds) dA dt d\Omega d\nu = dI_\nu dA dt d\Omega d\nu, \quad (2.8)$$

which leads to

$$dI_\nu = -\kappa_\nu \rho I_\nu ds. \quad (2.9)$$

On the other hand, radiation emitted from within the cylinder is described by the emission coefficient η_ν [$\text{erg}/\text{g}/\text{s}/\text{str}/\text{cm}^{-1}$] as

$$dI_\nu = \eta_\nu \rho ds. \quad (2.10)$$

The net change in I_ν within the cylinder is therefore

$$dI_\nu = -\kappa_\nu \rho I_\nu ds + \eta_\nu \rho ds. \quad (2.11)$$

Introducing the source function $\mathcal{S}_\nu$ as

$$\mathcal{S}_\nu \equiv \frac{\eta_\nu}{\kappa_\nu}, \quad (2.12)$$

the radiative transfer equation can be written as

$$\frac{dI_\nu}{\kappa_\nu \rho ds} = -I_\nu + \mathcal{S}_\nu. \quad (2.13)$$

The optical depth τ can also be defined in terms of the opacity κ_ν and the column mass $\tilde{m}$ [g/cm^2], defined as the mass per unit area obtained by integrating the density of the medium along the vertical direction. Under hydrostatic equilibrium, the column mass is related to the pressure as $P = \tilde{m}g$, where g is the gravitational acceleration. The optical depth is then given by

$$\tau \equiv \int \kappa_\nu d\tilde{m}. \quad (2.14)$$

When the optical depth is measured from the outside of the atmosphere toward the

interior, one obtains

$$d\tau = \kappa_\nu d\tilde{m} \tag{2.15}$$

$$= -\kappa_\nu \rho dz. \tag{2.16}$$

Defining θ as the angle between the specific intensity and the z -axis, and $\mu \equiv \cos \theta$, the geometrical relation $dz = \mu ds$ yields

$$d\tau = -\mu \kappa_\nu \rho ds. \tag{2.17}$$

Substituting this into Eq. 2.13, the radiative transfer equation in terms of τ becomes

$$\mu \frac{dI_\nu}{d\tau} = I_\nu - \mathcal{S}_\nu. \tag{2.18}$$

2.3 Atmospheric Opacities

The atmospheric opacity κ_ν contains contributions from both absorption and scattering, and can be written as the sum of an absorption component κ_a and a scattering component κ_s :

$$\kappa_\nu = \kappa_a + \kappa_s. \quad (2.19)$$

Absorption corresponds to processes in which photons are converted into internal energy of atmospheric molecules and atoms (e.g., ionization plus kinetic energy of the released electrons, or excitation of bound states), whereas scattering corresponds to processes in which atoms, molecules, or electrons respond to the incident electromagnetic field and re-emit radiation, causing photons to emerge in directions different from the incident one.

Assuming isotropic scattering, let J_ν denote the total (angle-integrated) intensity of the scattered radiation. The mean intensity is then defined as

$$\frac{J_\nu}{4\pi} \equiv \frac{1}{4\pi} \int_0^{2\pi} \int_{-1}^1 I_\nu d\mu d\phi. \quad (2.20)$$

If molecules and atoms that have absorbed photons re-emit according to the Planck function B_ν , the emission coefficient η_ν can be written as

$$\eta_\nu = \kappa_a B_\nu + \kappa_s \frac{J_\nu}{4\pi}. \quad (2.21)$$

Introducing the single-scattering albedo ω_0 as

$$\omega_0 \equiv \frac{\kappa_s}{\kappa_a + \kappa_s}, \quad (2.22)$$

the source function obtained from Eqs. 2.12, 2.19, and 2.21 becomes

$$\mathcal{S}_\nu = (1 - \omega_0) B_\nu + \omega_0 \frac{J_\nu}{4\pi}. \quad (2.23)$$

For the thermal emission of substellar objects, absorption generally dominates over scattering in the opacity (i.e., $\kappa_s \ll \kappa_a$), and the source function reduces to $\mathcal{S}_\nu \simeq B_\nu$. In what follows, we therefore focus on the physical processes responsible for the attenuation of radiation in the atmosphere (primarily absorption) and consider the corresponding variation of optical depth $\Delta\tau$ in the vertical direction.

2.3.1 Atomic & molecular absorption

Absorption of radiation propagating through an atmosphere occurs when atoms and molecules interact with photons and undergo quantum-mechanical transitions. The relevant types of transitions include electronic transitions as well as vibrational and rotational transitions of molecules. In what follows, we focus on electric dipole transitions¹.

Electronic transition

We first consider absorption due to electronic transitions using the Bohr model of the hydrogen atom. With Planck constant denoted by h , the energy of a photon with frequency $\tilde{\nu}$ is $h\tilde{\nu}$. Absorption associated with an electronic transition occurs when a photon of appropriate energy excites an electron in a hydrogen atom from a lower energy level E_j to a higher energy level E_k ,

$$E_k = E_j + h\nu. \quad (2.24)$$

In the Bohr model, the orbital angular momentum L of the electron is quantized:

$$L = m_e r v = n\hbar, \quad (n = 1, 2, 3, \dots), \quad (2.25)$$

where m_e is the electron mass, r the orbital radius, and v the orbital velocity. Combining this condition with the kinetic and potential energies of the system, the total energy of the electron in the n th orbit is

$$E_n = -R_H h c \frac{1}{n^2}, \quad (2.26)$$

where R_H is the Rydberg constant for hydrogen and c is the speed of light. From Eqs. 2.24 and 2.26 together with $\tilde{\nu} = c\nu$, the wavenumber of a photon absorbed when the hydrogen atom transitions from E_j to E_k is

$$\nu = R_H \left(\frac{1}{j^2} - \frac{1}{k^2} \right). \quad (2.27)$$

In substellar atmospheres, such electronic transitions are not the dominant contributors to opacity. Electronic transitions typically require high-energy photons in the ultraviolet or visible range, whereas the radiation field corresponding to the effective temperatures of substellar objects (a few hundred to ~ 2000 K) contains very few photons at such high energies. Under these conditions, molecules remain in their electronic ground states, and the molecular absorption spectrum is mainly composed of transitions between

¹In reality, transitions associated with electric quadrupole moments also exist, but they are generally much weaker than dipole transitions and are often neglected in spectral analyses.

rotational and vibrational levels built upon the ground electronic state.

To separate the internal degrees of freedom of a molecule into electronic, vibrational, and rotational parts, one exploits the fact that the timescales of electronic and nuclear motion differ significantly, treating the nuclei as nearly stationary parameters when solving for the electronic states. This is the Born–Oppenheimer approximation. Under this approximation, the nuclei move on a single potential energy surface determined by the electronic state. At typical substellar atmospheric temperatures, most molecules reside on the potential energy surface of the electronic ground state, so the majority of observed molecular absorption lines can be described as transitions between rotational and vibrational levels on this ground electronic surface, while transitions between excited electronic states are usually negligible. In what follows, we therefore assume the electronic ground state and focus on rotational and vibrational transitions that govern molecular absorption in substellar atmospheres.

Rotational and vibrational transition

We next consider absorption associated with rotational and vibrational transitions. For simplicity, we first assume that the separation between the two atoms in a diatomic molecule is fixed and treat the molecule as a rigid rotor to describe rotational transitions. Let the atomic masses be m_1 and m_2 , and define the reduced mass $m_{\text{red}} = (m_1 m_2) / (m_1 + m_2)$. If r_e is the equilibrium bond length, the moment of inertia I about an axis passing through the center of mass and perpendicular to the molecular axis is

$$I = m_{\text{red}} r_e^2. \quad (2.28)$$

The Schrödinger equation and Hamiltonian for the rigid rotor can then be written using the angular momentum operator $\hat{\mathbf{L}}$ as

$$\hat{H}_{\text{rot}} \psi = E_J \psi, \quad (2.29)$$

$$\hat{H}_{\text{rot}} = \frac{\hat{\mathbf{L}}^2}{2I}. \quad (2.30)$$

Because angular momentum is quantized, the rotational energy levels E_J are discrete and can be expressed in terms of the rotational quantum number J :

$$E_J = \frac{\hbar^2}{2I} J(J+1), \quad (J = 0, 1, 2, \dots). \quad (2.31)$$

Introducing

$$B \equiv \frac{\hbar^2}{2I} = \frac{h^2}{8\pi^2 m_{\text{red}} r_e^2}, \quad (2.32)$$

we can rewrite this as $E_J = B J(J+1)$. For electric dipole transitions, the selection rule is $\Delta J = \pm 1$, and in absorption the dominant process is $J \rightarrow J+1$. The corresponding energy difference is

$$\Delta E_J = E_{J+1} - E_J = 2B(J+1), \quad (2.33)$$

which equals the energy $h\nu_{J \rightarrow J+1}$ of the absorbed photon, so

$$\nu_{J \rightarrow J+1} = \frac{\Delta E_J}{hc} = \frac{2B}{hc}(J+1) = 2\tilde{B}(J+1), \quad (2.34)$$

where $\tilde{B} = B/(hc) = h/(8\pi^2 m_{\text{red}} r_e^2 c)$ is the rotational constant in wavenumber units. Thus, for a rigid rotor, the pure rotational spectrum appears as a series of lines in wavenumber space separated by $2\tilde{B}$. More explicitly, the wavenumber of an absorbed photon can be approximated as

$$\nu_{J \rightarrow J+1} \doteq 33.5 (J+1) \left(\frac{m_{\text{red}}}{m_p} \right)^{-1} \left(\frac{r_e}{1 \text{ [\AA]}} \right)^{-2} [\text{cm}^{-1}], \quad (2.35)$$

indicating that rotational transitions typically occur at wavenumbers of order $\nu_J \sim 10 \text{ cm}^{-1}$.

We now consider vibrational transitions. The stretching motion of the bond in a diatomic molecule can be approximated as a harmonic vibration about the equilibrium bond length r_e . Writing the displacement from equilibrium as q , we have

$$r = r_e + q. \quad (2.36)$$

Using the reduced mass m_{red} and the force constant k of the bond, the Hamiltonian for the one-dimensional harmonic oscillator corresponding to the stretching vibration is

$$\hat{H}_{\text{vib}} = -\frac{\hbar^2}{2m_{\text{red}}} \frac{\partial^2}{\partial q^2} + \frac{1}{2} k q^2. \quad (2.37)$$

The energy levels of the harmonic oscillator are quantized and can be written in terms of the vibrational quantum number v as

$$E_v = \hbar \sqrt{\frac{k}{m_{\text{red}}}} \left(v + \frac{1}{2} \right), \quad (v = 0, 1, 2, \dots). \quad (2.38)$$

Expressed in wavenumber units, these levels become

$$\nu_v = \frac{1}{2\pi c} \sqrt{\frac{k}{m_{\text{red}}}} \left(v + \frac{1}{2} \right). \quad (2.39)$$

For electric dipole transitions in the harmonic oscillator, the selection rule is

$$\Delta v = \pm 1, \quad (2.40)$$

and the dominant absorption process is the transition from the ground vibrational state v to $v + 1$. The wavenumber of the absorbed photon is then

$$\nu_{v \rightarrow v+1} = \frac{1}{2\pi c} \sqrt{\frac{k}{m_{\text{red}}}} \doteq 4.1 \times 10^3 \left(\frac{k}{1000 [\text{N/m}]} \right)^{\frac{1}{2}} \left(\frac{m_{\text{red}}}{m_{\text{p}}} \right)^{-\frac{1}{2}} [\text{cm}^{-1}]. \quad (2.41)$$

Typical force constants for diatomic molecules lie in the range 10^2 – 10^3 N/m, so we have used $k = 1000$ N/m in the above expression. In the harmonic oscillator approximation, all fundamental vibrational transitions $v \rightarrow v + 1$ therefore appear at the same wavenumber, typically of order 10^3 – 10^4 cm^{-1} .

In reality, molecular potentials deviate from the harmonic oscillator form, especially on the bond-stretching side where the potential is asymmetric and ultimately leads to dissociation. A more realistic model is the Morse potential,

$$V(q) = D_e (1 - e^{-aq})^2, \quad (2.42)$$

where D_e is the dissociation energy (the depth of the potential well) and a is the Morse parameter that controls the width of the potential. With the Morse potential, the wavenumber of the $v \rightarrow v + 1$ transition is

$$\nu_{v \rightarrow v+1} = \frac{1}{2\pi c} \sqrt{\frac{k}{m_{\text{red}}}} (1 - 2x_e (v + 1)), \quad (2.43)$$

where x_e is a dimensionless anharmonicity constant. Unlike the harmonic case, the level spacing decreases with increasing v , and as a result the wavenumber of the fundamental transition $v \rightarrow v + 1$ is shifted slightly to lower values than the harmonic-oscillator prediction. Anharmonicity also allows transitions with $\Delta v = \pm 2, \pm 3, \dots$, although their transition probabilities decrease rapidly with increasing $|\Delta v|$.

For simplicity, if we neglect the coupling between vibrational and rotational motions, the wavenumber of an absorption line corresponding to a rotational transition $J \rightarrow J \pm 1$

combined with a vibrational transition $v \rightarrow v + 1$ can be approximated at zeroth order as

$$\hat{\nu} \simeq \nu_{J \rightarrow J+1} + \nu_{v \rightarrow v+1}, \quad (2.44)$$

i.e., as the sum of the vibrational and rotational contributions. In practice, a vibrational transition first produces a band center in the near- to mid-infrared, and around this center numerous rotational lines appear at nearly equal spacings, forming the P-branch ($\Delta J = -1$) on one side and the R-branch ($\Delta J = +1$) on the other (Figure 2.2).

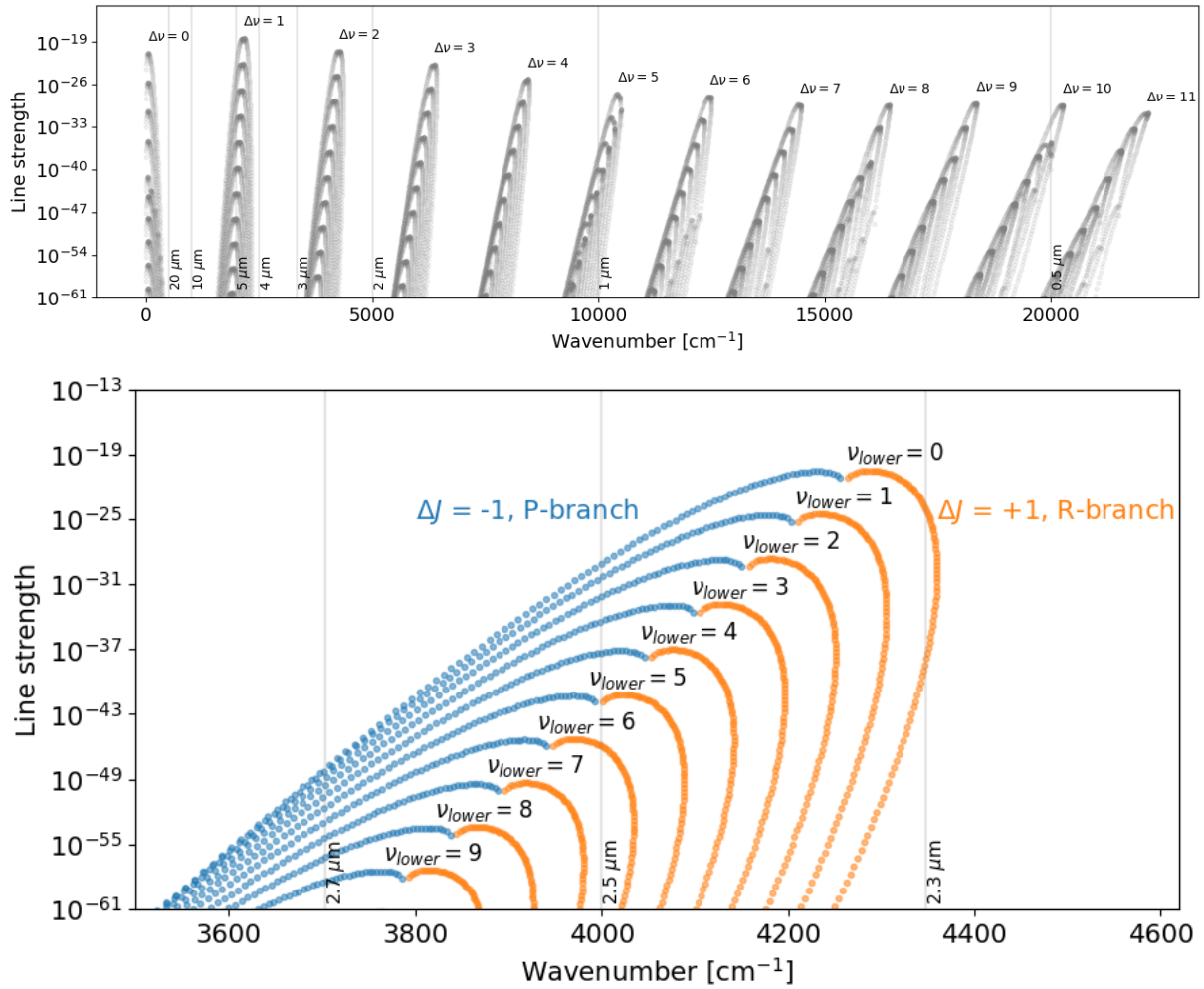


Figure 2.2: Wavenumbers and line strengths of rotational and vibrational transitions of CO based on the ExoMol line list (Li et al., 2015). (Top panel) Distribution of wavenumbers and line strengths for different vibrational transitions. (Bottom panel) Wavenumbers and line strengths of rotational transitions within the $\Delta v = 2$ vibrational band, with v_{lower} indicating the lower vibrational state.

Line profile

Absorption lines formed in a spectrum do not appear as delta functions at the wavenumber $\hat{\nu}$, but instead have finite widths in wavenumber space. This line broadening is determined by the combined effects of natural broadening (arising from the quantum-mechanical uncertainty principle), Doppler broadening due to the thermal motion of molecules, and pressure broadening caused by collisions with surrounding particles. The functional form describing the broadened line shape is the Voigt profile, $V(\nu; \hat{\nu})$. It is normalized as

$$\int V(\nu; \hat{\nu}) d\nu = 1. \quad (2.45)$$

Consider a given molecular transition l between levels j and k at temperature T . The cross section $\sigma_l(\nu)$ of this line can be factorized into the Voigt profile $V(\nu; \hat{\nu})$ and the line strength $S_{j,k}(T)$:

$$\sigma_l(\nu) = S_{j,k}(T) V(\nu; \hat{\nu}). \quad (2.46)$$

Here the line strength $S_{j,k}$ is defined as

$$S_{j,k}(T) \equiv \int \sigma_l(\nu) d\nu \quad (2.47)$$

and can be derived from quantum and statistical mechanics. We now derive $S_{j,k}$ for a two-level system with energies $E_j < E_k$.

Let n_j and n_k denote the number densities of molecules in the lower and upper levels, respectively. The probability per unit time that a molecule in the upper level k undergoes a spontaneous transition to the lower level j , independent of the external radiation field, is called the Einstein A-coefficient A_{kj} [s^{-1}]. The probability per unit time that a molecule in the lower level j is excited to the upper level k by absorbing a photon from the surrounding radiation field is described by the Einstein B-coefficient B_{jk} , while the probability of stimulated emission from k to j induced by the incident radiation is described by B_{kj} . Each Einstein B-coefficient multiplies the energy density of the radiation field to give a transition rate per unit time. The Einstein A- and B-coefficients are not independent but are related through statistical weights. In terms of these coefficients, and defining n as the total number density of particles, the line strength is given by

$$S_{j,k}(T) = \frac{h\hat{\nu}(n_j B_{jk} - n_k B_{kj})}{n}. \quad (2.48)$$

The populations of the two levels and the transition rates are related by the principle

of detailed balance:

$$\mathcal{E} (n_j B_{jk} - n_k B_{kj}) = n_k A_{kj}, \quad (2.49)$$

where $\mathcal{E}$ is the energy density of the radiation field per unit wavenumber². Under local thermodynamic equilibrium (LTE), the ratio of the level populations follows the Boltzmann distribution,

$$\frac{n_k}{n_j} = \frac{g_k}{g_j} \exp \left(-\frac{hc\hat{\nu}}{k_B T} \right), \quad (2.50)$$

where g_j and g_k are the statistical weights of levels j and k , respectively. The radiation field in thermal equilibrium follows the Planck distribution:

$$\mathcal{E} = \frac{4\pi B_{\hat{\nu}}}{c} = 8\pi hc\hat{\nu}^3 \left(e^{hc\hat{\nu}/k_B T} - 1 \right)^{-1}. \quad (2.51)$$

From Eqs. 2.49, 2.50, and 2.51, we obtain

$$g_j B_{jk} = g_k B_{kj}, \quad (2.52)$$

$$A_{kj} = 8\pi hc\hat{\nu}^3 B_{kj}. \quad (2.53)$$

The relation between the total number density n and the population n_j of level j can be expressed using the partition function $Q(T) = \sum_i g_i \exp(-E_i/k_B T)$ as

$$\frac{n_j}{n} = \frac{g_j}{Q(T)} \exp \left(-\frac{E_j}{k_B T} \right). \quad (2.54)$$

Combining Eqs. 2.48, 2.52, and 2.54, we arrive at

$$S_{j,k}(T) = \frac{g_k}{Q(T)} \frac{A_{kj}}{8\pi c\hat{\nu}^2} \exp \left(-\frac{E_j}{k_B T} \right) \left(1 - \exp \left[-\frac{hc\hat{\nu}}{k_B T} \right] \right). \quad (2.55)$$

Molecular line databases commonly used in modeling substellar atmospheres, such as ExoMol and HITEMP/HITRAN, provide values of $\hat{\nu}$, A_{kj} , g_k , and related quantities so that line strengths can be computed in the form of Eq. 2.55 (or in equivalent forms using reference values; see below for details).

We now discuss the Voigt profile, the other ingredient required to describe the cross section, in terms of the broadening mechanisms that contribute to it. We first consider Doppler broadening, which arises from the thermal motion of molecules. If a molecule has a velocity v_x along the line of sight to the observer, the Doppler effect shifts the line center from $\hat{\lambda}$ to $\lambda = \hat{\lambda}(1 + v_x/c)$. In wavenumber space, the shift is $\Delta\nu = -\hat{\nu}(v_x/c)$.

²Energy densities per unit wavelength or per unit frequency are also used in some contexts; care must be taken when converting between them.

At temperature T , the distribution of the line-of-sight velocity v_x of molecules of mass m follows the one-dimensional Maxwell distribution:

$$p(v_x) = \sqrt{\frac{m}{2\pi k_B T}} \exp\left(-\frac{mv_x^2}{2k_B T}\right) \quad (2.56)$$

$$= \sqrt{\frac{m}{2\pi k_B T}} \exp\left(-\frac{mc^2 \Delta\nu^2}{2k_B T \hat{\nu}^2}\right) \quad (2.57)$$

$$= \frac{\hat{\nu}}{\sqrt{2\pi c \beta}} \exp\left(-\frac{\Delta\nu^2}{2\beta^2}\right), \quad (2.58)$$

where

$$\beta = \sqrt{\frac{k_B T}{m}} \frac{\hat{\nu}}{c}. \quad (2.59)$$

Since Doppler broadening follows this distribution, the line profile is Gaussian. The half-width at half-maximum (HWHM) γ_D is related to β by

$$\gamma_D = \sqrt{2 \log 2} \beta. \quad (2.60)$$

If we denote the Doppler line profile by Φ_D , then the relation $p(v_x) dv_x = \Phi_D d\nu$ implies

$$\Phi_D d\nu = p(v_x) dv_x = p(v_x) \left| \frac{dv_x}{d\nu} \right| d\nu = p(v_x) \frac{c}{\hat{\nu}} d\nu. \quad (2.61)$$

Rewriting Φ_D in terms of γ_D yields

$$\Phi_D = \sqrt{\frac{\log 2}{\pi}} \frac{1}{\gamma_D} \exp\left\{-\log 2 \left(\frac{\nu - \hat{\nu}}{\gamma_D}\right)^2\right\}. \quad (2.62)$$

In contrast, natural broadening and pressure broadening both give rise to a Lorentz profile,

$$\Phi_L(\nu; \hat{\nu}) = \frac{\gamma_L/\pi}{(\nu - \hat{\nu})^2 + \gamma_L^2}, \quad (2.63)$$

where γ_L is the HWHM of the Lorentz profile.

In substellar atmospheres, pressure broadening due to collisions between molecules³ is particularly important and largely determines the shape of the line wings. Pressure broadening arises because collisions between molecules perturb the energy level spacing associated with absorption. At a given pressure P , the Lorentz width γ_L^p due to pressure broadening is usually parameterized in terms of the reference broadening coefficient γ_{ref} for collisions with the background atmosphere, the self-broadening coefficient γ_{self} for

³Here we follow the van der Waals approximation, which is commonly used in substellar atmospheric analyses.

collisions between identical molecules, and the temperature exponent n :

$$\gamma_L^p = \left(\frac{T}{T_{\text{ref}}} \right)^{-n} \left\{ \gamma_{\text{ref}} \left(\frac{P - P_{\text{self}}}{P_{\text{ref}}} \right) + \gamma_{\text{self}} \left(\frac{P_{\text{self}}}{P_{\text{ref}}} \right) \right\}, \quad (2.64)$$

where T_{ref} and P_{ref} are the reference temperature and pressure adopted by the line list (typically $T_{\text{ref}} = 296$ K and $P_{\text{ref}} = 1$ atm). Collisions also cause shifts in the line center. The shifted line center can be expressed using the pressure shift coefficient δ_{ref} as

$$\hat{\nu}^* = \hat{\nu} + \delta_{\text{ref}} \left(\frac{P}{P_{\text{ref}}} \right). \quad (2.65)$$

However, the effect of pressure shifts is usually small. Moreover, some line lists commonly used in substellar atmospheric studies, such as ExoMol, do not provide δ_{ref} , and it is therefore often neglected in practice. In the retrieval framework adopted in this work, we also ignore pressure shifts, and henceforth we simply write the line center wavenumber as $\hat{\nu}$.

Natural broadening is the line broadening associated with the uncertainty principle, and its contribution becomes important at low pressures compared to pressure broadening. The Lorentz width due to natural broadening, γ_L^n , can be written in terms of Einstein A-coefficients as

$$\gamma_L^n = \frac{\sum_j A_{kj}}{4\pi c}. \quad (2.66)$$

The combined effect of pressure broadening and natural broadening corresponds to the convolution of their respective Lorentz profiles. For two functions $f(x)$ and $g(x)$, the convolution is defined as

$$f(x) * g(x) \equiv \int_{-\infty}^{\infty} f(x') g(x - x') dx'. \quad (2.67)$$

Thus, the convolution of the pressure-broadened and naturally broadened Lorentz profiles is

$$\Phi_L^p(\nu; \hat{\nu}) * \Phi_L^n(\nu; \hat{\nu}) = \int_{-\infty}^{\infty} \Phi_L^p(\nu'; \hat{\nu}) \Phi_L^n(\nu - \nu'; \hat{\nu}) d\nu' \quad (2.68)$$

$$= \frac{(\gamma_L^p + \gamma_L^n) / \pi}{(\nu - \hat{\nu})^2 + (\gamma_L^p + \gamma_L^n)^2}. \quad (2.69)$$

Therefore, when both pressure and natural broadening are considered, the effective Lorentz width γ_L can be written as

$$\gamma_L = \gamma_L^p + \gamma_L^n. \quad (2.70)$$

The Voigt profile, which describes the overall line shape, is the convolution of the Doppler and Lorentz profiles (including both pressure and natural broadening):

$$V(\nu; \hat{\nu}) = \Phi_D(\nu; \hat{\nu}) * \Phi_L(\nu; \hat{\nu}). \quad (2.71)$$

Because each broadened line contributes over a finite range of wavenumbers, the total cross section at a given wavenumber ν is obtained by summing over all transitions:

$$\sigma = \sum_l \sigma_l \quad (2.72)$$

$$= \sum_l S_l(T) V(\nu; \hat{\nu}), \quad (2.73)$$

where the index l labels transitions $j \rightarrow k$. Using this total cross section σ , the change in optical depth due to molecular absorption, $\Delta\tau_{\text{mol}}$, in a layer of thickness Δz is

$$\Delta\tau_{\text{mol}} = -n\sigma \Delta z, \quad (2.74)$$

where n is the number density of the absorbing molecules⁴. If we further assume that the atmosphere is in hydrostatic equilibrium, the relation between a small change in altitude Δz and a small change in pressure ΔP is

$$\Delta z = -\frac{1}{\rho g} \Delta P, \quad (2.75)$$

where ρ is the atmospheric density and g is the gravitational acceleration. Substituting this into Eq. 2.74, the change in optical depth due to molecular absorption can be expressed in terms of the volume mixing ratio $\text{VMR}(P)$ of the molecule, the mean molecular weight μ of the gas phase, and the atomic mass unit m_u as

$$\Delta\tau_{\text{mol}} = \frac{\text{VMR}(P)}{\mu m_u g} \sigma \Delta P. \quad (2.76)$$

Thus, under hydrostatic equilibrium, $\Delta\tau_{\text{mol}}$ can be described as a function of pressure rather than altitude. In practice, atmospheric structure is typically defined as a function of pressure, and Eq. 2.76 is therefore the standard form used in discussions of substellar atmospheres.

⁴The change in optical depth due to atomic absorption, $\Delta\tau_{\text{atm}}$, has the same functional form.

2.3.2 Collision-induced absorption

Symmetric molecules such as H_2 , O_2 , and N_2 have no permanent electric dipole moment and therefore do not exhibit absorption through electric dipole transitions⁵. However, when these molecules collide with other molecules or atoms, the interaction transiently distorts the electron clouds and induces a dipole moment (an induced dipole). Absorption associated with transitions of this induced dipole is called collision-induced absorption (CIA). Because the duration of the collision-induced excitation is extremely short, the energy width of the transition is broadened by the uncertainty principle ($\Delta E \Delta t \geq \hbar/2$). As a result, CIA manifests not as discrete spectral lines but as broad, quasi-continuous absorption features.

Since CIA arises from collisions between molecules, its absorption strength is proportional to the product of the number densities of the colliding species ($n_A \times n_B$). Denoting the CIA absorption coefficient by $\alpha_{A,B}^{\text{CIA}}$, the change in optical depth due to CIA, $\Delta\tau_{\text{CIA}}$, over a layer of thickness Δz is

$$\Delta\tau_{\text{CIA}} = -n_A n_B \alpha_{A,B}^{\text{CIA}} \Delta z. \quad (2.77)$$

Values of $\alpha_{A,B}^{\text{CIA}}$ are provided, for example, by molecular opacity databases such as HITRAN. Under hydrostatic equilibrium, we can use the ideal gas law to rewrite this expression in terms of a small pressure increment ΔP as

$$\Delta\tau_{\text{CIA}} = n_A n_B \alpha_{A,B}^{\text{CIA}} \frac{k_B T}{\mu m_u g} \frac{\Delta P}{P}, \quad (2.78)$$

where T is the temperature, μ the mean molecular weight of the gas, m_u the atomic mass unit, and g the gravitational acceleration.

In high-pressure, H_2 - and He-rich atmospheres of substellar objects, CIA by H_2 – H_2 and H_2 –He pairs contributes significantly to the spectral shape and effectively sets the continuum level.

2.3.3 Cloud opacity

In addition to line absorption by molecules and atoms, substellar atmospheres can host condensate cloud particles that act as absorbers and scatterers of photons.

According to thermal evolution models of substellar objects, these bodies cool by radiating away the internal heat acquired during their formation (e.g., through gravitational

⁵Several detections of absorption due to quadrupole transitions of H_2 in substellar atmospheres have been reported (Ishikawa et al., 2025).

contraction and deuterium burning). As the atmospheric temperature cools to values characteristic of mid-L dwarfs, metals such as Fe, oxides such as Al_2O_3 , and silicates such as Mg_2SiO_4 and MgSiO_3 are expected to condense and form clouds. At still lower temperatures, corresponding to late-T and Y dwarfs, the formation of NH_3 and H_2O clouds is predicted (Lunine et al., 1986; Chabrier et al., 2000; Saumon & Marley, 2008).

Observationally, it is well established that the near-infrared colors of L dwarfs redden as they cool, which has been attributed to the presence of thick silicate clouds in the upper atmosphere (Cushing et al., 2006, 2008; Faherty et al., 2016). In addition, absorption bands associated with the solid-state vibrational modes of silicate grains appear around $10\,\mu\text{m}$, and these features have been detected in several L dwarfs (Cushing et al., 2006; Suárez & Metchev, 2022; Hoch et al., 2025).

If we approximate cloud particles as spheres with radius r , their cross section can be written as

$$\sigma = Q_{\text{ext}} \pi r^2, \quad (2.79)$$

where Q_{ext} is the extinction efficiency. Under hydrostatic equilibrium, the increment in optical depth due to clouds, $\Delta\tau_c$, in a layer with cloud particle number density n_c is

$$\Delta\tau_c = -n_c Q_{\text{ext}} \pi r^2 \Delta z \quad (2.80)$$

$$= n_c Q_{\text{ext}} \pi r^2 \frac{k_B T}{\mu m_u g} \frac{\Delta P}{P}, \quad (2.81)$$

where T is the temperature, μ the mean molecular weight of the gas, m_u the atomic mass unit, and g the gravitational acceleration.

The extinction efficiency Q_{ext} depends on the size parameter

$$x = \frac{2\pi r}{\lambda}, \quad (2.82)$$

and for spherical particles, Mie theory gives

$$Q_{\text{ext}} = \frac{2}{x^2} \sum_{n=1}^{\infty} (2n+1) \text{Re}(a_n + b_n), \quad (2.83)$$

where a_n and b_n are the Mie coefficients defined in terms of Riccati–Bessel functions (Bohren & Huffman, 1983).

The extinction efficiency can be decomposed into contributions from absorption and scattering,

$$Q_{\text{ext}} = Q_a + Q_s, \quad (2.84)$$

where Q_a and Q_s are the absorption and scattering efficiencies, respectively. In the Rayleigh limit, where the particle size is much smaller than the wavelength ($x \ll 1$),

$$Q_a \propto x, \quad Q_s \propto x^4, \quad (2.85)$$

so absorption dominates. In contrast, when the particle size is much larger than the wavelength ($x \gg 1$), corresponding to the geometric optics limit of Mie theory,

$$Q_{\text{ext}} \approx 2 \quad (2.86)$$

is obtained.

A detailed computation of the exact extinction efficiency for a given cloud species generally requires solving the full Mie problem and is therefore computationally expensive. In practice, empirical functional forms for Q_{ext} are often adopted. For example, [Lee et al. \(2013\)](#) proposed an empirical form that depends only on the size parameter x ,

$$Q_{\text{ext}} = \frac{5}{Q_0 x^{-4} + x^{0.2}}, \quad (2.87)$$

where Q_0 is a constant that depends on the cloud composition, with typical values $Q_0 \sim 100$ for volatile species such as H_2O and $Q_0 \sim 10$ for silicates.

A widely used cloud model for substellar atmospheres is that of [Ackerman & Marley \(2001\)](#), which incorporates the vertical structure of clouds by balancing the upward transport of condensates by turbulent mixing against their downward transport by sedimentation. In this model, the increment in cloud optical depth $\Delta\tau_c$ in a given atmospheric layer is written as

$$\Delta\tau_c = -\frac{3}{2} \frac{\epsilon \rho_a q_c}{\rho_p r_{\text{eff}}} \Delta z, \quad (2.88)$$

$$r_{\text{eff}} = r_w f_{\text{sed}}^{1/\alpha} \exp \left[-\frac{\alpha + 1}{2} (\log \sigma_g)^2 \right], \quad (2.89)$$

where ϵ is the ratio of the condensate molecular weight to the mean molecular weight of the atmosphere, ρ_a and ρ_p are the mass densities of the gas and the cloud particles, respectively, q_c is the mole mixing ratio of condensates relative to the gas, r_w and α are parameters related to the particle sedimentation velocity, and f_{sed} is the sedimentation efficiency. A larger f_{sed} corresponds to more efficient sedimentation (larger particles residing deeper in the atmosphere), whereas a smaller f_{sed} implies stronger lofting of particles to higher altitudes by turbulent mixing. The parameter σ_g is the width of the log-normal

particle size distribution; Ackerman & Marley (2001) adopted $\sigma_g = 2$. They further assumed $Q_{\text{ext}} = 2$ in deriving Eq. 2.88. Under hydrostatic equilibrium, Eq. 2.88 can be rewritten in terms of a small pressure increment ΔP as

$$\Delta\tau_c = \frac{3}{2} \frac{\epsilon q_c}{\rho_p r_{\text{eff}} g} \Delta P. \quad (2.90)$$

2.4 Intensity-based Solutions of Radiative Transfer

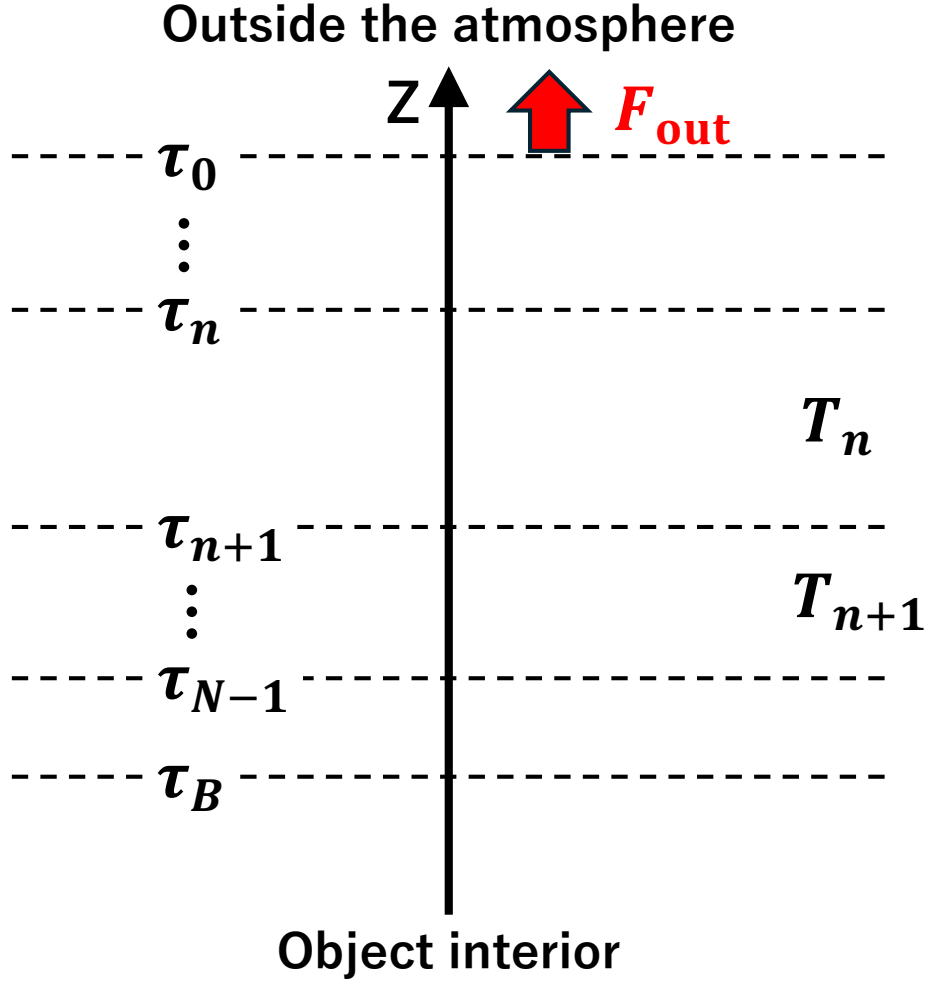


Figure 2.3: Schematic illustration of an atmosphere discretized into N layers, as adopted in intensity-based solutions of the radiative transfer equation.

In this section, we summarize how to solve the radiative transfer equation in an intensity-based formulation for a purely absorbing atmosphere, under the assumptions of a plane-parallel geometry and local thermodynamic equilibrium (LTE). We neglect scattering and assume a purely absorbing atmosphere; this approximation constitutes the default setup for the radiative transfer calculations in this work. In particular, following Section 4.2.1 of [Kawahara et al. \(2025\)](#), we derive the flux density emerging at the top of a generic substellar atmosphere. The optical depth τ and the opacity κ_ν appearing below follow the definitions introduced in the previous section.

For a purely absorbing atmosphere, omitting the explicit subscript ν for the wavenum-

ber, the radiative transfer equation can be written as

$$\mu \frac{dI}{d\tau} = I - \mathcal{S} \quad (2.91)$$

$$= I - B(\tau), \quad (2.92)$$

where, under LTE and in the absence of scattering, the source function reduces to $\mathcal{S} = B(\tau)$. To obtain a formal solution, we multiply both sides by $e^{-\tau/\mu}$ and integrate from the top of the atmosphere ($\tau = 0$) to the bottom layer ($\tau = \tau_B$), yielding

$$I_0(\mu) = I(\tau_B, \mu) e^{-\tau_B/\mu} + \frac{1}{\mu} \int_0^{\tau_B} B(\tau) e^{-\tau/\mu} d\tau, \quad (2.93)$$

where $I_0(\mu)$ is the specific intensity emerging at the top of the atmosphere.

To solve the radiative transfer equation numerically, we discretize the atmosphere into N layers and approximate each layer as isothermal (Figure 2.3). Denoting the temperature of the n -th layer by T_n , we approximate

$$B(\tau) \approx B(T_n) \quad (2.94)$$

within that layer. Equation 2.93 can then be rewritten as

$$I_0(\mu) = B(T_B) e^{-\tau_B/\mu} + \frac{1}{\mu} \int_0^{\tau_B} B(\tau) e^{-\tau/\mu} d\tau \quad (2.95)$$

$$\approx B(T_B) e^{-\tau_B/\mu} + \frac{1}{\mu} \sum_{n=0}^{N-1} \int_{\tau_n}^{\tau_{n+1}} B(T_n) e^{-\tau/\mu} d\tau \quad (2.96)$$

$$= B(T_B) e^{-\tau_B/\mu} + \sum_{n=0}^{N-1} B(T_n) (e^{-\tau_n/\mu} - e^{-\tau_{n+1}/\mu}), \quad (2.97)$$

where we used the boundary condition $I(\tau_B, \mu) = B(T_B)$.

The upward flux density at optical depth τ is defined as

$$F_{\uparrow} \equiv \int_0^{2\pi} d\phi \int_0^1 \mu I(\tau, \mu) d\mu. \quad (2.98)$$

Thus, the flux density at the top of the atmosphere is

$$S_{\text{raw}} = \int_0^{2\pi} d\phi \int_0^1 \mu I_0(\mu) d\mu \quad (2.99)$$

$$= 2\pi \int_0^1 \mu I_0(\mu) d\mu. \quad (2.100)$$

The angular integration can be evaluated numerically using Gauss–Legendre quadrature. In an N -stream scheme, the number of upward streams is $N' = N/2$, and we approximate

$$S_{\text{raw}} = 2\pi \int_0^1 \mu I_0(\mu) d\mu \quad (2.101)$$

$$\approx 2\pi \sum_{i=1}^{N'} \mu_i \mathbf{w}_i I_0(\mu_i) \quad (2.102)$$

$$= 2\pi \sum_{i=1}^{N'} \mu_i \mathbf{w}_i \left\{ B(T_B) e^{-\tau_B/\mu_i} + \sum_{n=0}^{N-1} B(T_n) (e^{-\tau_n/\mu_i} - e^{-\tau_{n+1}/\mu_i}) \right\}, \quad (2.103)$$

where μ_i and $\mathbf{w}_i$ are the Gauss–Legendre nodes and weights, respectively. If x_i and w_i denote the standard nodes and weights on the interval $[-1, 1]$, then they are related to the half-range quadrature by $\mu_i = (1 + x_i)/2$ and $\mathbf{w}_i = w_i/2$.

In this way, we obtain the intensity-based formulation of the radiative transfer solution for a purely absorbing atmosphere. The emergent emission from a substellar atmosphere is thus determined by the temperature T_n and optical depth distribution in each atmospheric layer. In practical spectral calculations, this expression is evaluated at each wavenumber, combining the optical depth profile $\tau_\nu(P)$ constructed from molecular lines, collision-induced absorption, and cloud opacity (introduced in the previous subsections) with an assumed temperature–pressure structure to generate synthetic spectra of substellar atmospheres.

2.5 Temperature–Pressure Profile

In the previous section, we showed that the solution of the radiative transfer equation is determined by the optical depth and temperature structure of the atmosphere. Consequently, the emergent flux is governed by the atmospheric temperature–pressure (T – P) profile, $T(P)$, together with the vertical distributions of the mixing ratios of molecules, cloud particles, and other opacity sources. Therefore, to infer the physical state of a substellar atmosphere from observations, it is essential to first discuss the general properties of atmospheric T – P profiles and how they are modeled.

One way to describe substellar atmospheric T – P profiles is to employ semi-analytic models under the assumption of radiative equilibrium. For example, [Guillot \(2010\)](#) introduced wavelength-weighted mean opacities in the visible and infrared, κ_v and κ_{ir} (a two-band gray approximation), and derived a radiative-equilibrium temperature structure that incorporates both internal heat flux and external irradiation, using only a small number of parameters. The model of [Guillot \(2010\)](#), in which the temperature structure is specified by the internal flux F_{int} and the effective irradiation temperature T_{irr} , can be written as

$$T^4(\bar{\tau}) = \frac{3}{4}T_{\text{int}}^4 \left(\bar{\tau} + \frac{2}{3} \right) + \frac{3}{4}T_{\text{irr}}^4 \xi(\bar{\tau}), \quad (2.104)$$

where $\bar{\tau} \equiv \kappa_{\text{ir}}\tilde{m}$, $T_{\text{int}}^4 = F_{\text{int}}/\sigma$, and $\xi(\bar{\tau})$ is a function that encodes the geometric effects of stellar irradiation and the impact of scattering. Although this expression is written as a function of the optical depth $\bar{\tau}$, the gray approximation with constant κ_{ir} implies $\bar{\tau} = (\kappa_{\text{ir}}/g)P$, so that the temperature can be expressed as a function of pressure. Such analytic T – P models have the advantage of providing idealized radiative-equilibrium structures at low computational cost, and are often used as parametrizations of the T – P profile (e.g., [Nugroho et al., 2020](#)).

In real substellar atmospheres, however, wavelength-dependent opacities, vertical variations in chemical composition, the contributions of cloud formation and condensation, and convective heat transport are all important. It is generally difficult to capture all of these processes in closed analytic form. Instead, they are treated in detail in one-dimensional numerical radiative–convective equilibrium models. In the Sonora model grid ([Marley et al., 2021](#); [Karalidi et al., 2021](#); [Morley et al., 2024](#); [Mukherjee et al., 2024](#)), ATMO ([Phillips et al., 2020](#)), PHOENIX ([Husser et al., 2013](#)), and similar frameworks, multi-wavelength radiative transfer, convection, chemical equilibrium/non-equilibrium, and cloud formation are computed in a self-consistent manner, at the expense of much higher computational cost and complexity compared to analytic models.

These detailed 1D radiative–convective equilibrium models are indispensable for providing a comprehensive description of the thermal structure and composition of substellar atmospheres. However, they are not always well suited for direct use in atmospheric retrieval analyses. In addition to their computational cost, such models rely on a number of physical assumptions, including the treatment of chemical equilibrium or disequilibrium, cloud formation and properties, vertical mixing, and radiative–convective coupling. Adopting a specific radiative–convective model in a retrieval framework therefore implicitly imposes strong prior constraints on the atmospheric thermal structure, which may bias the inferred atmospheric parameters, such as molecular abundances and elemental ratios. For this reason, retrieval studies commonly employ parametric T – P profiles that are designed to be flexible and computationally efficient, allowing the thermal structure to be constrained primarily by the observational data rather than by model-dependent assumptions.

The power-law T – P profile adopted in this work is an empirical parametrization that aims to reproduce the typical temperature structures suggested by these semi-analytic solutions and 1D radiative–convective models, while maintaining a balance between flexibility and computational efficiency suitable for retrieval (Section 3.3).

Chapter 3

ExoJAX Retrievals of VLT/CRIRES Spectra of Luhman 16AB: C/O Ratios and Systematic Uncertainties

*This chapter is based on the peer-reviewed publication:
Yama, H., Masuda, K., Kawashima, Y., Kawahara, H. (2026),
The Astrophysical Journal, Volume 997, Number 1, pp.118.*

3.1 Introduction

In this study, we perform atmospheric retrieval analyses of high-resolution infrared spectra of the nearby benchmark brown dwarf binary Luhman 16AB obtained with VLT/CRIRES. In particular, we systematically quantify the systematic uncertainties in the retrieval outcomes arising from the choice of carbon monoxide (CO) line lists, which dominate the absorption in the CRIRES wavelength range, and from different parameterizations of the temperature–pressure (T – P) profile, and on that basis derive a conservative estimate of the atmospheric C/O ratio of Luhman 16AB.

3.1.1 Luhman 16AB

Luhman 16AB is a binary brown dwarf system consisting of an L7.5 primary (A) and a T0.5 secondary (B), discovered in 2013 from WISE observations (Luhman, 2013; Burgasser et al., 2013). Sahlmann & Lazorenko (2015) measured a parallax of $\varpi = 500.5 \pm 0.11$ mas, corresponding to a distance of 1.9980 ± 0.0004 pc from Earth, making it the nearest known pair of brown dwarfs. Because it is the closest and one of the brightest substellar

systems discovered to date—MKO K -band magnitudes of 9.44 ± 0.07 for component A and 9.73 ± 0.09 for component B (Burgasser et al., 2013)—high-S/N observations across many instruments are available, providing a rich set of empirical constraints. Consequently, Luhman 16AB is not only valuable as a benchmark system for C/O ratios, but also serves as an ideal testbed for evaluating systematic errors and validating new analysis methodologies. Astrometric measurements have determined dynamical masses of $M_A = 33.2 \pm 0.3 M_J$ and $M_B = 28.6 \pm 0.3 M_J$ (Lazorenko & Sahlmann, 2018). More recently, clustering analyses based on 6D kinematics using Gaia DR3 have shown that Luhman 16AB is likely a member of the Oceanus moving group, implying an estimated age of 510 ± 95 Myr (Gagné et al., 2023). Combining these external constraints with brown-dwarf evolutionary models (Baraffe et al., 2003) enables us to place informative priors on the surface gravity. Such external priors help break the common degeneracy between metallicity and $\log g$ in high-resolution spectroscopic retrievals, thereby yielding more robust estimates of elemental abundances (Line et al., 2015; Snellen, 2025). Moreover, the binary nature of the system itself provides an internal consistency check for retrieval results across both components.

3.1.2 Chapter Outline

This chapter is organized as follows. Section 3.2 outlines the retrieval framework. In Section 3.3, we assess the line-list dependence in retrievals based on a power-law T – P profile. Section 3.4 then introduces a more flexible Gaussian-process (GP) T – P profile, demonstrates its utility, and discusses how assumptions about the T – P structure propagate into other parameters and their interpretation. Finally, Section 3.5 summarizes the results, highlights the significance of this work, and discusses directions for future studies.

3.2 Retrieval Framework

3.2.1 Data

In this work, we analyze the K -band (2.288–2.345 μm) high-resolution spectra of Luhman 16AB obtained with the CRyogenic high-resolution InfraRed Echelle Spectrograph (CRIRES; Kaeuff et al., 2004) mounted on the Very Large Telescope (VLT), i.e., the same data used for Doppler imaging by Crossfield et al. (2014). The observations were carried out for 5 hr on UT 2013-05-05. The stacked spectrum achieves a resolving power of $R \sim 10^5$ with $S/N \sim 180$. Because CRIRES records spectra on four detectors aligned in the dispersion direction, the analyzed data are further divided into four wavelength segments within the observed bandpass; in what follows we refer to these as chip 1–4 from shorter to longer wavelengths. Each segment is normalized independently (Figure 3.1).

3.2.2 Spectrum Model

We modeled the high-resolution spectra of Luhman 16AB with the ExoJAX spectral framework (Kawahara et al., 2022; Kawahara et al., 2025). ExoJAX solves the radiative transfer by computing, for each pressure interval ΔP between adjacent levels, the optical-depth increment as the sum of the molecular contribution in a given layer $\sum_i \Delta\tau_{\text{mol},i}$, collision-induced absorption (CIA) $\Delta\tau_{\text{CIA}}$, and cloud opacity $\Delta\tau_{\text{c}}$:

$$\Delta\tau(\nu) = \sum_i \Delta\tau_{\text{mol},i}(\nu) + \Delta\tau_{\text{CIA}}(\nu) + \Delta\tau_{\text{c}}, \quad (3.1)$$

where ν is the wavenumber. We discretize the atmosphere into 101 pressure levels, logarithmically spaced from 10^{-4} – 10^2 bar. Here, the molecular contribution in a given layer $\Delta\tau_{\text{mol},i}$ is

$$\Delta\tau_{\text{mol},i}(\nu) = \frac{\text{VMR}_i}{\mu m_u g} \sigma_i(\nu) \Delta P, \quad (3.2)$$

where VMR_i denotes the volume mixing ratio of absorbing species i , m_u is the atomic mass unit, and g is the surface gravity. The mean molecular weight μ is calculated self-consistently from the adopted VMRs of all atmospheric components, accounting for both the absorbing species and the bulk gases. The molecular cross section σ_i is computed from line strengths $S(T)$ and Voigt profiles $V(\nu, \beta, \gamma_L)$ as

$$\sigma_i(\nu) = \sum_l S_l(T) V(\nu - \hat{\nu}, \beta_l(T), \gamma_{L,l}(T, P)). \quad (3.3)$$

Here, l indexes the absorption lines ($l = 1, \dots, N_l$) and $\hat{\nu}$ is the line center. ExoJAX evaluates the Voigt profiles only for the lines located within the specified wavelength range, and for each line the Voigt function is computed over that interval. The Gaussian (thermal) width is

$$\beta = \sqrt{\frac{k_B T}{M_i m_u}} \frac{\hat{\nu}}{c}, \quad (3.4)$$

where M_i is molecular mass of species i and c is the speed of light. The pressure broadening parameter γ_L and the line strengths $S_l(T)$ are computed from the line lists HITRAN/HITEMP (Gordon et al., 2022; Rothman et al., 2010) and ExoMol (Tennyson et al., 2016; Tennyson et al., 2024) in combination with the assumed temperature–pressure structure $T(P)$ (see Sections 3.3, 3.4.1). We explicitly include the trace absorbers $i = \text{CO}, \text{H}_2\text{O}, \text{CH}_4, \text{HF}$, with free, vertically uniform VMRs; inclusion of HF is motivated by its reported K -band detection in Luhman 16AB from high-resolution IGRINS/Gemini South spectroscopy (Ishikawa et al., 2025). The remainder of the atmosphere is assigned to the bulk gas, H_2 and He. After specifying the four trace-species VMRs, the residual fraction $1 - \sum_i \text{VMR}_i$ is distributed between H_2 and He according to the solar mass ratio 0.74:0.25 (Asplund et al., 2021). Because the retrieval is performed in VMR, we convert this mass ratio into a volume ratio by weighting with the molecular masses, i.e., in proportion to $(0.74/M_{\text{H}_2}) : (0.25/M_{\text{He}})$, which ensures that the total across every included species—CO, H_2O , CH_4 , HF, H_2 , and He—sums to unity. The collision-induced absorption (CIA) contribution $\Delta\tau_{\text{CIA}}$ is

$$\Delta\tau_{\text{CIA}}(\nu) = (n_{\text{H}_2}^2 \alpha_{\text{H}_2-\text{H}_2}(T, \nu) + n_{\text{H}_2} n_{\text{He}} \alpha_{\text{H}_2-\text{He}}(T, \nu)) \frac{k_B T}{\mu m_u g} \frac{\Delta P}{P}, \quad (3.5)$$

where n_{H_2} and n_{He} are number densities, μ is the mean molecular weight, and $\alpha_{\text{CIA}}(T, \nu)$ are CIA coefficients taken from the HITRAN database. The cloud optical depth per layer, $\Delta\tau_c$, is modeled as a Gaussian in $\log_{10} P$ with width w_c and central pressure P_c :

$$\Delta\tau_c = \frac{C}{\sqrt{2\pi w_c^2}} \exp \left[-\frac{(\log_{10} P - \log_{10} P_c)^2}{2w_c^2} \right], \quad (3.6)$$

where C is the (dimensionless) column optical depth of the cloud. This functional form is motivated by the vertical cloud opacity profiles in the Sonora diamondback models (Morley et al., 2024). Given the narrow wavelength range analyzed here, we neglect any wavelength dependence of the cloud optical depth. Because w_c and P_c are strongly degenerate, we fix $w_c = 0.3$. To emulate an effectively optically thick gray deck, we fix the column optical depth to a large arbitrary constant, $C = 500$.

Using the resulting $\Delta\tau(\nu)$, we solve the radiative transfer with an eight-stream approximation to obtain the local one-dimensional emergent spectrum $S_{\text{raw}}(\nu)$. We then convolve with a rotational broadening kernel computed from the limb-darkening law and the projected rotational velocity $V \sin i$ to obtain the disk-integrated spectrum $F_{\text{raw}}(\nu)$. For limb darkening, we adopt the quadratic law with the (q_1, q_2) parametrization as proposed by [Kipping \(2013\)](#).

To model the Earth-observed, per-chip normalized spectra, we first apply the Doppler shift due to the brown dwarf radial velocity RV . For an intrinsic wavenumber ν_0 , the observed wavenumber is

$$\nu_{\text{obs}} = \nu_0 \frac{c}{c + RV}. \quad (3.7)$$

Because the observed spectra are normalized per detector, the model is likewise normalized in each wavelength segment. Denoting the model for the four detector segments by $\mathbf{F}_i$ ($i = 1, 2, 3, 4$) and their mean values by $\bar{\mathbf{F}}_i$, the normalized spectra are

$$\mathbf{f}_i = \frac{\mathbf{F}_i}{A_i \bar{\mathbf{F}}_i}, \quad (3.8)$$

with A_i a per-segment normalization factor. The final model used in the analysis is the concatenation

$$\mathbf{f} = [\mathbf{f}_1, \mathbf{f}_2, \mathbf{f}_3, \mathbf{f}_4]. \quad (3.9)$$

3.2.3 Inference

ExoJAX is implemented with JAX ([Bradbury et al., 2018](#)), a high-performance Python library that supports GPU acceleration and automatic differentiation. Consequently, our spectral model can be evaluated on GPUs and differentiated with respect to arbitrary parameters, enabling gradient-based inference.

Leveraging these features, we infer posterior distributions of the model parameters with Hamiltonian Monte Carlo (HMC; [Neal, 2011](#)) and the No-U-Turn Sampler (NUTS; [Hoffman & Gelman, 2014](#)) implemented in NumPyro. With prior $p(\boldsymbol{\theta})$, the posterior is given by Bayes' theorem:

$$p(\boldsymbol{\theta} \mid \mathbf{d}) \propto \mathcal{L}(\boldsymbol{\theta}) p(\boldsymbol{\theta}). \quad (3.10)$$

To account for correlated noise, we use a Gaussian-process (GP) likelihood ([Kawahara et al., 2022](#)),

$$\mathcal{L}(\boldsymbol{\theta}) = \frac{1}{\sqrt{(2\pi)^n |\boldsymbol{\Sigma}|}} \exp \left[-\frac{1}{2} (\mathbf{d} - \mathbf{f}(\boldsymbol{\theta}))^T \boldsymbol{\Sigma}^{-1} (\mathbf{d} - \mathbf{f}(\boldsymbol{\theta})) \right], \quad (3.11)$$

where $\mathbf{d}$ is the n -point observed spectrum and $\mathbf{f}(\boldsymbol{\theta})$ is the model. The covariance matrix is

$$\Sigma_{ij} = K_{ij} + \sigma_{e,i}^2 \delta_{ij}, \quad (3.12)$$

with $\sigma_{e,i}$ the i -th data uncertainty and δ_{ij} the Kronecker delta. We adopt an RBF kernel,

$$K_{ij} = a_{\text{GP}} \exp \left[-\frac{(\lambda_i - \lambda_j)^2}{2\tau_{\text{GP}}^2} \right], \quad (3.13)$$

where λ_i, λ_j are wavelength of i -th and j -th data, a_{GP} is the GP amplitude, and τ_{GP} (in Å) is the correlation length.

The set of inferred parameters and their priors is listed in Table 3.1. For $\log g$, we imposed Normal priors informed by external constraints. Using the system age of 510 ± 95 Myr from Gagné et al. (2023) together with the dynamical masses $M_A = 33.5 \pm 0.3 M_J$ and $M_B = 28.6 \pm 0.3 M_J$ from Lazorenko & Sahlmann (2018), we interpolated the brown dwarf evolutionary model of Baraffe et al. (2003) to obtain surface gravities. Since the surface gravity is given by $g = GM/R^2$ with brown dwarf mass M , radius R , and the gravitational constant G , we propagated the quoted mass uncertainties ($\sim 1\%$) and assumed a 10% fractional uncertainty on the radius to set the prior widths, yielding Normal priors $\log g_A = 4.93 \pm 0.09$ and $\log g_B = 4.86 \pm 0.09$, each truncated at 3σ . Sampling used HMC-NUTS with a dense mass matrix. For numerical stability and mixing, parameters were affinely re-scaled so that the prior support maps to $\mathcal{O}(1)$ in the sampler's internal coordinates. Sampling/adaptation were performed in the transformed space and results are reported after back-transformation.

Table 3.1: Parameters and priors for the spectral model

Parameter	Unit	Prior	Description
General parameters			
$\log g$	–	$\mathcal{N}_{[4.66, 5.20]}(4.93, 0.09)$ (A), $\mathcal{N}_{[4.59, 5.13]}(4.86, 0.09)$ (B)	Surface gravity
RV	km s^{-1}	$\mathcal{U}(20, 30)$	Radial velocity
$\log_{10} \text{VMR}_{\text{CO}}$	–	$\mathcal{U}(-6.0, -1.0)$	VMR of $^{12}\text{C}^{16}\text{O}$
$\log_{10} \text{VMR}_{\text{H}_2\text{O}}$	–	$\mathcal{U}(-6.0, -1.0)$	VMR of H_2^{16}O
$\log_{10} \text{VMR}_{\text{CH}_4}$	–	$\mathcal{U}(-6.0, -1.0)$	VMR of CH_4
$\log_{10} \text{VMR}_{\text{HF}}$	–	$\mathcal{U}(-10.0, -5.0)$	VMR of HF
$\log_{10} P_c$	–	$\mathcal{U}(-2.0, 2.0)$	Cloud center pressure
$V \sin i$	km s^{-1}	$\mathcal{U}(10, 20)$ (A), $\mathcal{U}(20, 30)$ (B)	Projected rotational velocity
q_1	–	$\mathcal{U}(0.0, 1.0)$	Limb darkening parameter
q_2	–	$\mathcal{U}(0.0, 1.0)$	Limb darkening parameter
$\log_{10} \tau_{\text{GP}}$	–	$\mathcal{U}(-1.5, 0.5)$	GP amplitude
$\log_{10} a_{\text{GP}}$	–	$\mathcal{U}(-4.5, 2.0)$	GP length scale
A_1	–	$\mathcal{U}(1.0, 1.2)$	Normalization factor (chip 1)
A_2	–	$\mathcal{U}(1.0, 1.2)$	Normalization factor (chip 2)
A_3	–	$\mathcal{U}(1.0, 1.2)$	Normalization factor (chip 3)
A_4	–	$\mathcal{U}(1.0, 1.2)$	Normalization factor (chip 4)
Power-law T–P profile			
T_0	K	$\mathcal{U}(1000, 1700)$	Temperature at 1 bar
α	–	$\mathcal{U}(0.05, 0.20)$	Power-law index
GP T–P profile			
$T_{0,m}$	K	$\mathcal{U}(1000, 1700)$	Temperature at 1 bar (mean model)
α_m	–	$\mathcal{U}(0.05, 0.20)$	Power-law index (mean model)
$\log_{10} a_u$	–	$\mathcal{U}(-1.0, 0.5)$	GP amplitude for T – P
$\log_{10} \tau_u$	–	$\mathcal{U}(-0.5, 1.4)$	GP length scale for T – P

3.3 Retrievals Using a Power-Law T – P Profile

In this section, we adopt a simple power-law T – P profile given by

$$T(P) = T_0 \left(\frac{P}{1 \text{ bar}} \right)^\alpha. \quad (3.14)$$

In high-resolution retrievals of brown dwarf and exoplanet atmospheres, line shapes depend on the pressure broadening parameters provided by the molecular line lists, which can in turn impart systematic effects on the inferred molecular abundances and atmospheric structure. To assess the robustness of the results, it is therefore essential to analyze a given target with multiple line lists. Motivated by this, we focus on the CO line list and compare three models based on ExoMol and HITEMP.

3.3.1 Line Lists

High-resolution retrievals for brown dwarfs commonly use line lists from ExoMol and HITEMP. ExoMol provides theoretically computed line data tailored to brown dwarf and exoplanet atmospheres, assuming an H_2 –He background. HITEMP, by contrast, is based largely on high-temperature laboratory measurements and typically adopts an Earth background (air) for pressure broadening. More recently, an H_2 –He broadened variant of HITEMP has become available, obtained by converting the air-broadening parameters; the conversion employs semi-empirical models anchored to validated laboratory measurements and theoretical predictions (Tan et al., 2022).

ExoMol

According to Tennyson et al. (2016), ExoMol supplies transition wavenumbers $\hat{\nu}$, Einstein coefficients A , state energies E , and statistical weights g , from which the line strength $S(T)$ can be computed as

$$S(T) = \frac{g_{\text{up}}}{Q(T)} \frac{A}{8\pi c \hat{\nu}^2} e^{-hcE_{\text{low}}/k_B T} (1 - e^{-hc\hat{\nu}/k_B T}), \quad (3.15)$$

where E_{low} is the lower-state energy¹ and g_{up} is the upper-state statistical weight. For pressure broadening in an H_2 background, ExoMol provides the reference broadening coefficient $\gamma_{\text{ref}}(J_{\text{low}})$ and temperature exponent $n(J_{\text{low}})$ as functions of the lower-state

¹The units are $[\text{cm}^{-1}]$, normalized by hc .

rotational quantum number. The pressure-broadened Lorentz width is then

$$\gamma_L^p = \gamma_{\text{ref}} \left(\frac{T}{T_{\text{ref}}} \right)^{-n} \left(\frac{P}{P_{\text{ref}}} \right), \quad (3.16)$$

with $T_{\text{ref}} = 296 \text{ K}$ and $P_{\text{ref}} = 1 \text{ bar}$.

HITEMP

According to Rothman et al. (2010), HITEMP provides $\hat{\nu}$, $S(T_{\text{ref}})$ at $T_{\text{ref}} = 296 \text{ K}$, and E_{low} , from which

$$S(T) = S(T_{\text{ref}}) \frac{Q(T_{\text{ref}})}{Q(T)} \frac{e^{-hcE_{\text{low}}/k_{\text{B}}T}}{e^{-hcE_{\text{low}}/k_{\text{B}}T_{\text{ref}}}} \frac{1 - e^{-hc\hat{\nu}/k_{\text{B}}T}}{1 - e^{-hc\hat{\nu}/k_{\text{B}}T_{\text{ref}}}} \quad (3.17)$$

is obtained. HITEMP further provides air-broadened reference widths $\gamma_{\text{ref,air}}$ and temperature exponents n_{air} for each line, yielding

$$\gamma_L^p = \gamma_{\text{ref,air}} \left(\frac{T}{T_{\text{ref}}} \right)^{-n_{\text{air}}} \left(\frac{P}{P_{\text{ref}}} \right) \quad (3.18)$$

with $P_{\text{ref}} = 1 \text{ atm}$. For some molecules, H_2 -broadened parameters $\gamma_{\text{ref,H}_2}$ and n_{H_2} are available, allowing H_2 -background pressure broadening to be computed via Eq. (3.18) (Tan et al., 2022). In what follows, we refer to air-broadened HITEMP as $\text{HITEMP}_{\text{Air}}$ and H_2 -broadened HITEMP as $\text{HITEMP}_{\text{H}_2}$. Nominally, air broadening parameters are not appropriate for brown dwarf atmospheres. However, the laboratory experiment by Hosokawa et al. (2025) suggests that these parameters are not necessarily incorrect, so we include them in the comparison.

Adopted Line Lists in This Study

Given that brown dwarf atmospheres are dominated by H_2 , we adopt the ExoMol POKAZATEL for H_2O (Polyansky et al., 2018), ExoMol MM for CH_4 (Yurchenko et al., 2024), and the ExoMol Coxon–Hajig line list for HF (Coxon & Hajigeorgiou, 2015). To assess the impact of the CO line list—which exhibits prominent absorption in the K band—on the retrieval results, we consider the following three CO line list configurations:

ExoMol CO: ExoMol CO line list Li2015 (Li et al., 2015), assuming an H_2 background.

HITEMP_{Air} CO: HITEMP CO line list (Li et al., 2015) with air-broadening parameters.

HITEMP_{H₂} CO: An H₂-broadened version of HITEMP CO based on the semi-empirical models constructed on available and validated experimental measurements and theoretical predictions (Tan et al., 2022).

For all three CO line lists, the same Voigt profile treatment is applied, so that the differences in the retrieval results originate only from the broadening parameters. The selection of molecular species was referenced from the *K*-band high-resolution spectral analysis of Luhman 16AB with IGRINS/Gemini South reported by Ishikawa et al. (2025). We also searched for the isotopologue ¹³CO, but it was not detected in the present analysis. This is consistent with Ishikawa et al. (2025), who did not detect ¹³CO in the same wavelength region. Therefore, we did not include ¹³CO opacity in the spectral model.

3.3.2 Results

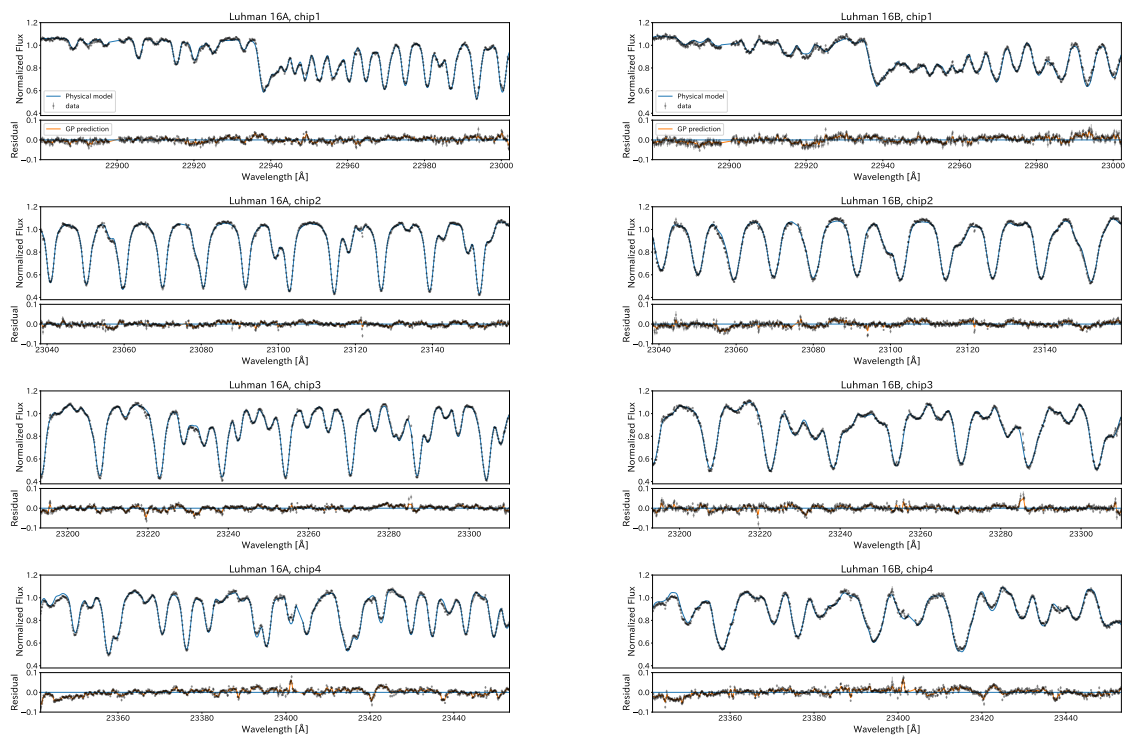


Figure 3.1: Retrieval results for the VLT/CRIRES high-resolution spectra of Luhman 16A (left) and Luhman 16B (right), modeled with the HITEMP_{H₂} CO line list and a power-law T - P profile. The wavelength coverage is split into four detector segments (chips 1–4). For each chip, the top panel shows the normalized flux data (black points) and the best-fit physical model (blue line). The bottom panel shows the residuals (data minus the best-fit model); orange lines indicate the correlated noise predicted by the GP. Each chip is normalized independently.

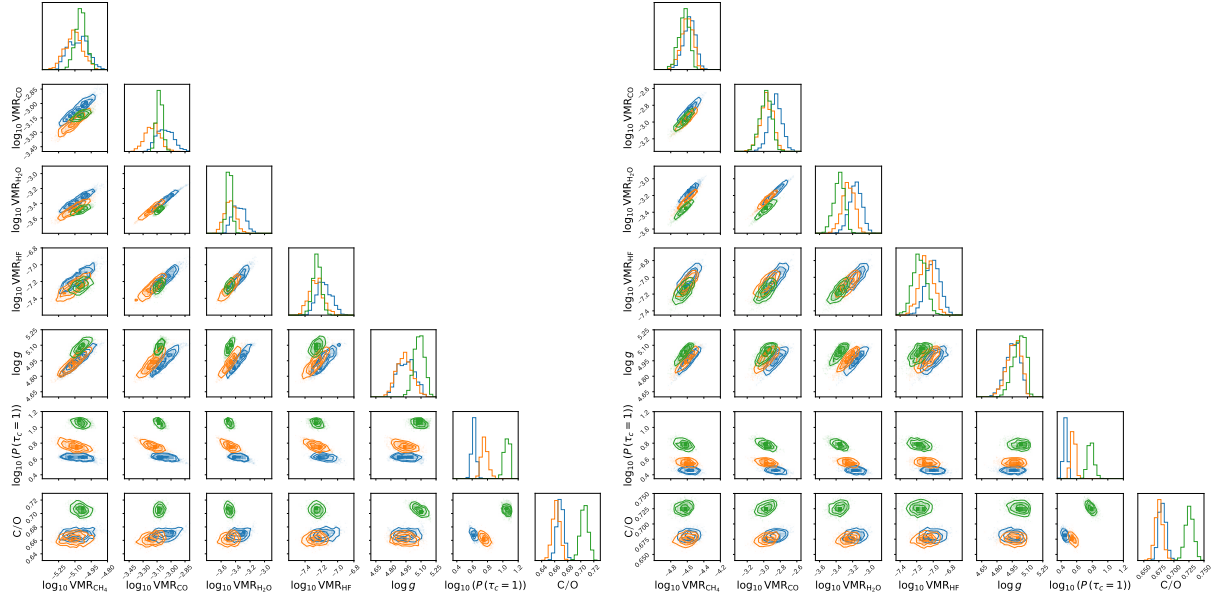


Figure 3.2: Corner plots for the posterior samples obtained by fitting the spectra with models that use CO line lists from ExoMol CO (orange), HITEMP_{Air} CO (green), and HITEMP_{H2} CO (blue). (Left) Luhman 16A. (Right) Luhman 16B.

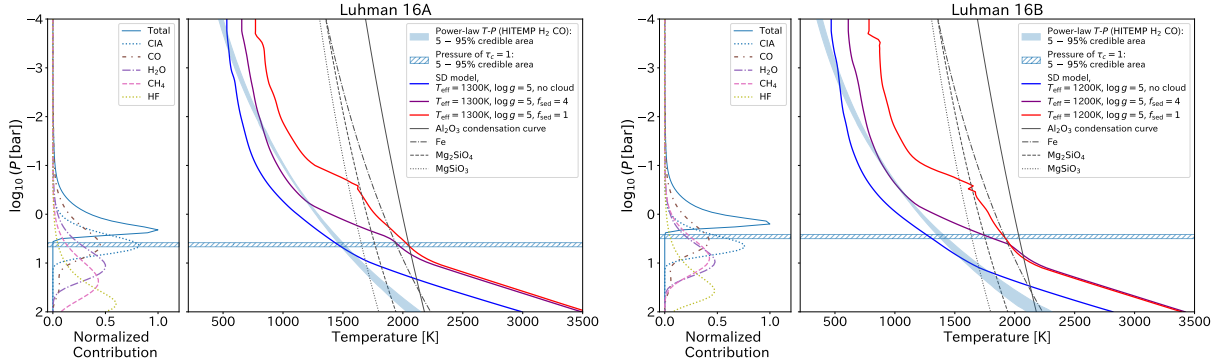


Figure 3.3: Retrieved T - P profiles and normalized contribution functions for Luhman 16A (left) and Luhman 16B (right) under the HITEMP_{H2} CO configuration. For each object, the left panel shows the contribution function, and the right panel shows the posterior T - P profile. The horizontal shaded band marks the inferred cloud deck pressure, $\log_{10} P(\tau_c = 1)$. Note that τ_c denotes the cumulative optical depth due only to cloud opacity. Blue, purple, and red lines are Sonora Diamondback (SD) T - P models (Morley et al., 2024). Black curves in the right panels indicate condensation curves for the principal brown dwarf cloud species identified by Morley et al. (2024) (condensation curve formulas from Visscher et al. 2010; Wakeford et al. 2017).

Using spectral models based on each CO line list, we performed NUTS sampling and obtained posterior distributions for all parameters. Posterior summaries are listed in Tables 3.2 and 3.3.

Figure 3.1 compares, for both components of Luhman 16, the data and the best-fitting

spectral models computed with a power-law T – P profile, a gray-cloud prescription, and HITEMP_{H₂} CO. Overall, the models reproduce the high-resolution spectra well: the residual panels show no conspicuous absorption features that are clearly misfit. The largest residual structures may reflect limitations of the spectral model (e.g., line list incompleteness or pressure broadening uncertainties), although residual telluric contamination or detector-related systematics cannot be ruled out. Although not shown, the other two CO line lists yield comparably good fits.

To examine posterior structure, Figure 3.2 overlays selected parameters from the three line list runs in a corner plot. From Eq. (3.2), the molecular optical depth increment scales as $\Delta\tau_{\text{mol},i} \propto \text{VMR}_i/(\mu g)$ (at fixed T and line shape), where the mean molecular weight μ is computed self-consistently from the adopted VMRs of all species at each sampling step. Since the variation in μ is negligibly small, its effect on the opacity is minor, and the spectra primarily constrain the ratio VMR_i/g . Increases in g can therefore be offset by proportional increases in VMR_i , producing the observed positive covariance between $\log g$ and the molecular VMRs. In our spectra the key features of each species are largely separated in wavelength, so the relative line depths directly constrain abundance ratios; accordingly, the retrieved VMRs exhibit positive covariance. These correlations between $\log g$ and the VMRs appear as diagonally elongated contours in the off-diagonal panels of Figure 3.2. However, this correlation does not translate into a simple one-to-one trend in the one-dimensional summaries (Tables 3.2 and 3.3), because the correlation structures in the joint posteriors can also shift due to line-list-dependent systematics and the inferred cloud-deck pressure.

The retrieved T – P profiles under the power-law + gray-cloud + HITEMP_{H₂} CO configuration are shown for each object in Figure 3.3. Across all line lists, the inferred temperature ranges in the regions of largest contribution are consistent with the Sonora diamondback models (Morley et al., 2024) at the literature effective temperatures. Here, τ_c denotes the cumulative optical depth due only to the gray-cloud opacity integrated downward from the top of the atmosphere, and the pressure level at $\tau_c = 1$ corresponds to the cloud deck in our model. The inferred cloud-deck pressures fall within the altitude ranges predicted by the condensation curves in the Sonora Diamondback models, indicating broad physical consistency with the cloud-base pressures of plausible condensates, although we do not attempt to identify a specific cloud species.

We use the VMR in the retrieval, so that the number density of each species is directly

represented as $n_i = \text{VMR}_i$. From these, the elemental number densities are derived as

$$n_{\text{C}} = n_{\text{CO}} + n_{\text{CH}_4}, \quad (3.19)$$

$$n_{\text{O}} = n_{\text{CO}} + n_{\text{H}_2\text{O}}, \quad (3.20)$$

$$n_{\text{F}} = n_{\text{HF}}, \quad (3.21)$$

$$n_{\text{H}} = 2n_{\text{H}_2} + 4n_{\text{CH}_4} + 2n_{\text{H}_2\text{O}} + n_{\text{HF}}, \quad (3.22)$$

and the carbon-to-oxygen ratio

$$\text{C/O} = \frac{n_{\text{C}}}{n_{\text{O}}}. \quad (3.23)$$

We also compute $[\text{C/H}]$, $[\text{O/H}]$, $[\text{F/H}]$, and $[(\text{C} + \text{O})/\text{H}]$ as

$$[\text{X/H}] = \log_{10} \left(\frac{n_{\text{X}}}{n_{\text{H}}} \right) - \log_{10} (\text{X/H})_{\odot}, \quad \text{X} \in \{\text{C}, \text{O}, \text{F}\}, \quad (3.24)$$

$$[(\text{C} + \text{O})/\text{H}] = \log_{10} \left(\frac{n_{\text{C}} + n_{\text{O}}}{n_{\text{H}}} \right) - \log_{10} \left(\frac{\text{C} + \text{O}}{\text{H}} \right)_{\odot}, \quad (3.25)$$

where the solar ratios $(\text{X/H})_{\odot}$ follow [Asplund et al. \(2021\)](#). For both Luhman 16A and 16B, the VMR-inferred C/O is ~ 0.67 —slightly above solar (Figure 3.2). We nevertheless find that the inferred C/O shifts by $\sim 7\%$ depending on the adopted line list. Differences in the line shapes alter the inferred cloud-deck pressure and, in turn, the relative VMRs.

To interpret the retrieved abundances, we computed thermochemical-equilibrium VMRs with FastChem including equilibrium condensation ([Stock et al., 2018](#); [Kitzmann et al., 2024](#)). In these calculations, we adjusted the solar C, O, and F abundances of [Asplund et al. \(2021\)](#) by our retrieved $[\text{X/H}]$ values (all other elements fixed to solar). [Asplund et al. \(2021\)](#) tabulate $A(\text{X}) \equiv \log_{10}(n_{\text{X}}/n_{\text{H}}) + 12$ with $A(\text{H}) = 12$; accordingly we adopt

$$A(\text{X}) = A_{\odot}(\text{X}) + [\text{X/H}], \quad \text{X} \in \{\text{C}, \text{O}, \text{F}\}, \quad (3.26)$$

evaluated separately for Luhman 16A and 16B using their respective $[\text{X/H}]$. Numerically, $A_{\odot}(\text{C}) = 8.46$, $A_{\odot}(\text{O}) = 8.69$, and $A_{\odot}(\text{F}) = 4.40$ ([Asplund et al., 2021](#)). The equilibrium VMRs computed with these inputs and the retrieved T – P profiles (Figure 3.4) agree well for CO, H₂O, and HF, indicating compatibility with chemical equilibrium under the inferred thermal structures. By contrast, the retrieved CH₄ VMRs for both objects are about an order of magnitude lower than the FastChem predictions; we revisit this discrepancy in Section 3.4.3.

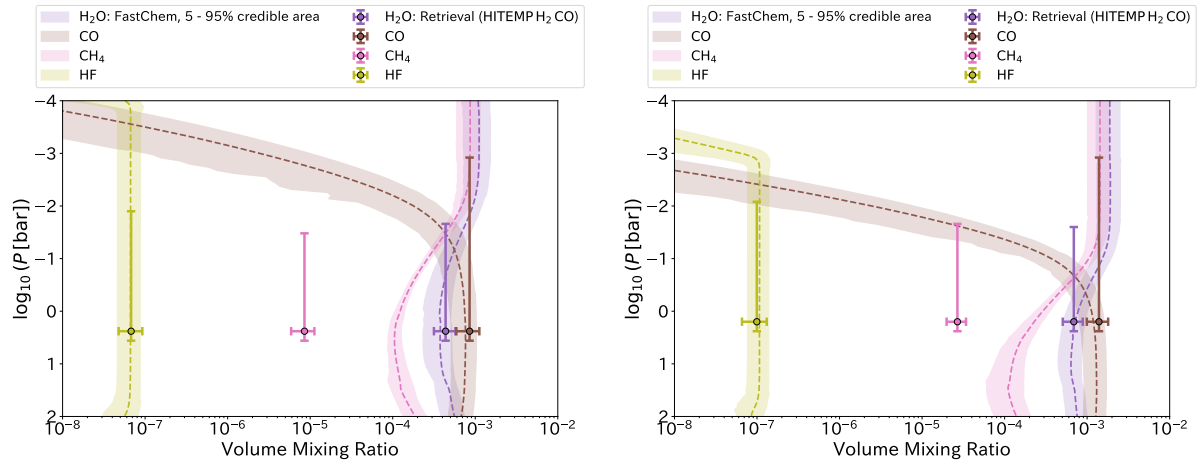


Figure 3.4: Retrieved VMRs of H₂O (purple), CO (brown), CH₄ (pink), and HF (yellow) for Luhman 16A (left) and Luhman 16B (right). Points are plotted at the pressure of the contribution function peak; the vertical extent indicates the pressure range that contributes appreciably for each molecule, with the upper bound truncated at the cloud-deck pressure. For comparison, thermochemical-equilibrium VMRs computed with FastChem, including equilibrium condensation, are shown as 5–95% credible bands.

Table 3.2: Parameter estimates for Luhman 16A under each modeling configuration.

Parameter	Unit	PL T - P ExoMol CO	PL T - P HITEMP _{Air} CO	PL T - P HITEMP _{H₂} CO	GP T - P HITEMP _{H₂} CO
$\log g$	cgs	$4.93^{+0.07}_{-0.09}$	$5.08^{+0.04}_{-0.06}$	$4.95^{+0.08}_{-0.09}$	$5.06^{+0.08}_{-0.07}$
RV	km s ⁻¹	$28.13^{+0.03}_{-0.04}$	$28.19^{+0.05}_{-0.05}$	$28.17^{+0.03}_{-0.04}$	$28.16^{+0.03}_{-0.04}$
$\log_{10} \text{VMR}_{\text{CO}}$	—	$-3.20^{+0.06}_{-0.10}$	$-3.12^{+0.03}_{-0.04}$	$-3.07^{+0.09}_{-0.09}$	$-3.04^{+0.07}_{-0.08}$
$\log_{10} \text{VMR}_{\text{H}_2\text{O}}$	—	$-3.47^{+0.08}_{-0.07}$	$-3.49^{+0.03}_{-0.03}$	$-3.36^{+0.09}_{-0.08}$	$-3.31^{+0.08}_{-0.07}$
$\log_{10} \text{VMR}_{\text{CH}_4}$	—	$-5.17^{+0.10}_{-0.07}$	$-5.10^{+0.05}_{-0.05}$	$-5.11^{+0.08}_{-0.09}$	$-5.04^{+0.08}_{-0.05}$
$\log_{10} \text{VMR}_{\text{HF}}$	—	$-7.27^{+0.08}_{-0.09}$	$-7.25^{+0.05}_{-0.05}$	$-7.17^{+0.07}_{-0.11}$	$-7.15^{+0.1}_{-0.07}$
[C/H]	—	$0.11^{+0.09}_{-0.07}$	$0.19^{+0.03}_{-0.03}$	$0.26^{+0.07}_{-0.09}$	$0.28^{+0.07}_{-0.06}$
[O/H]	—	$0.06^{+0.08}_{-0.08}$	$0.11^{+0.04}_{-0.03}$	$0.21^{+0.06}_{-0.09}$	$0.23^{+0.07}_{-0.05}$
[F/H]	—	$-3.96^{+0.09}_{-0.08}$	$-3.95^{+0.05}_{-0.05}$	$-3.85^{+0.09}_{-0.09}$	$-3.84^{+0.07}_{-0.07}$
[(C + O)/H]	—	$0.08^{+0.08}_{-0.08}$	$0.14^{+0.04}_{-0.03}$	$0.23^{+0.06}_{-0.10}$	$0.25^{+0.07}_{-0.05}$
C/O	—	$0.662^{+0.005}_{-0.006}$	$0.704^{+0.007}_{-0.006}$	$0.668^{+0.005}_{-0.006}$	$0.660^{+0.005}_{-0.007}$
$\log_{10} P_c$	bar	$1.66^{+0.03}_{-0.06}$	$1.95^{+0.05}_{-0.02}$	$1.52^{+0.02}_{-0.03}$	$1.90^{+0.09}_{-0.05}$
$\log_{10} P (\tau_c = 1)$	bar	$0.76^{+0.05}_{-0.03}$	$1.05^{+0.05}_{-0.02}$	$0.62^{+0.02}_{-0.03}$	$1.00^{+0.10}_{-0.04}$
$V \sin i$	km s ⁻¹	$16.21^{+0.37}_{-0.51}$	$15.89^{+0.22}_{-0.29}$	$17.09^{+0.27}_{-0.22}$	$15.62^{+0.19}_{-0.23}$
q_1	—	$0.82^{+0.17}_{-0.12}$	$0.73^{+0.26}_{-0.11}$	$0.90^{+0.10}_{-0.05}$	$0.77^{+0.23}_{-0.13}$
q_2	—	$0.43^{+0.17}_{-0.15}$	$0.53^{+0.14}_{-0.14}$	$0.29^{+0.09}_{-0.10}$	$0.63^{+0.15}_{-0.12}$
$\log_{10} a_{\text{GP}}$	—	$-3.96^{+0.02}_{-0.02}$	$-3.87^{+0.02}_{-0.02}$	$-3.95^{+0.01}_{-0.02}$	$-4.03^{+0.02}_{-0.02}$
$\log_{10} \tau_{\text{GP}}$	Å	$-1.27^{+0.01}_{-0.01}$	$-1.22^{+0.02}_{-0.01}$	$-1.27^{+0.01}_{-0.01}$	$-1.30^{+0.01}_{-0.02}$
A_1	—	$1.140^{+0.001}_{-0.001}$	$1.140^{+0.001}_{-0.001}$	$1.141^{+0.001}_{-0.001}$	$1.140^{+0.001}_{-0.001}$
A_2	—	$1.134^{+0.001}_{-0.001}$	$1.134^{+0.001}_{-0.001}$	$1.134^{+0.001}_{-0.001}$	$1.133^{+0.001}_{-0.001}$
A_3	—	$1.138^{+0.001}_{-0.001}$	$1.138^{+0.001}_{-0.001}$	$1.139^{+0.001}_{-0.001}$	$1.139^{+0.001}_{-0.001}$
A_4	—	$1.109^{+0.001}_{-0.001}$	$1.108^{+0.001}_{-0.001}$	$1.109^{+0.001}_{-0.001}$	$1.108^{+0.001}_{-0.001}$
<i>(Power-law T-P)</i>					
T_0	K	1293^{+6}_{-6}	1258^{+5}_{-5}	1283^{+6}_{-6}	—
α	—	$0.109^{+0.003}_{-0.003}$	$0.108^{+0.002}_{-0.003}$	$0.107^{+0.003}_{-0.003}$	—
<i>(GP T-P)</i>					
$T_{0,m}$	K	—	—	—	1285^{+158}_{-143}
α_m	—	—	—	—	$0.110^{+0.027}_{-0.041}$
$\log_{10} a_u$	—	—	—	—	$-0.34^{+0.10}_{-0.18}$
$\log_{10} \tau_u$	—	—	—	—	$-0.40^{+0.06}_{-0.10}$
<i>(Negative log-likelihood)</i>					
Normalized high-resolution spectra	—	-13177	-13090	-13167	-13257
JWST medium-resolution flux density	—	13	-29	-24	-1
Total	—	-13164	-13119	-13190	-13258

Table 3.3: Parameter estimates for Luhman 16B under each modeling configuration.

Parameter	Unit	PL T - P ExoMol CO	PL T - P HITEMP _{Air} CO	PL T - P HITEMP _{H₂} CO	GP T - P HITEMP _{H₂} CO
$\log g$	cgs	$4.97^{+0.08}_{-0.06}$	$5.03^{+0.08}_{-0.05}$	$4.96^{+0.07}_{-0.07}$	$5.03^{+0.07}_{-0.05}$
RV	km s ⁻¹	$25.66^{+0.07}_{-0.06}$	$25.59^{+0.07}_{-0.07}$	$25.54^{+0.06}_{-0.08}$	$25.52^{+0.06}_{-0.06}$
$\log_{10} \text{VMR}_{\text{CO}}$	—	$-2.96^{+0.09}_{-0.07}$	$-2.97^{+0.09}_{-0.05}$	$-2.86^{+0.07}_{-0.09}$	$-2.95^{+0.06}_{-0.08}$
$\log_{10} \text{VMR}_{\text{H}_2\text{O}}$	—	$-3.25^{+0.09}_{-0.05}$	$-3.36^{+0.08}_{-0.05}$	$-3.16^{+0.08}_{-0.07}$	$-3.21^{+0.06}_{-0.07}$
$\log_{10} \text{VMR}_{\text{CH}_4}$	—	$-4.65^{+0.08}_{-0.07}$	$-4.69^{+0.06}_{-0.06}$	$-4.61^{+0.10}_{-0.06}$	$-4.61^{+0.07}_{-0.05}$
$\log_{10} \text{VMR}_{\text{HF}}$	—	$-7.08^{+0.10}_{-0.07}$	$-7.17^{+0.08}_{-0.07}$	$-7.00^{+0.10}_{-0.07}$	$-7.10^{+0.09}_{-0.07}$
[C/H]	—	$0.36^{+0.09}_{-0.07}$	$0.35^{+0.06}_{-0.06}$	$0.47^{+0.09}_{-0.08}$	$0.36^{+0.05}_{-0.07}$
[O/H]	—	$0.30^{+0.09}_{-0.06}$	$0.25^{+0.07}_{-0.05}$	$0.41^{+0.10}_{-0.07}$	$0.31^{+0.06}_{-0.06}$
[F/H]	—	$-3.76^{+0.08}_{-0.09}$	$-3.85^{+0.07}_{-0.08}$	$-3.69^{+0.07}_{-0.10}$	$-3.82^{+0.10}_{-0.07}$
[(C + O)/H]	—	$0.33^{+0.09}_{-0.06}$	$0.29^{+0.06}_{-0.07}$	$0.43^{+0.06}_{-0.07}$	$0.33^{+0.06}_{-0.07}$
C/O	—	$0.674^{+0.005}_{-0.008}$	$0.725^{+0.007}_{-0.006}$	$0.679^{+0.006}_{-0.006}$	$0.660^{+0.007}_{-0.007}$
$\log_{10} P_c$	bar	$1.45^{+0.03}_{-0.03}$	$1.68^{+0.03}_{-0.04}$	$1.35^{+0.03}_{-0.02}$	$1.93^{+0.07}_{-0.03}$
$\log_{10} P (\tau_c = 1)$	bar	$0.55^{+0.02}_{-0.03}$	$0.78^{+0.03}_{-0.04}$	$0.45^{+0.03}_{-0.02}$	$1.04^{+0.07}_{-0.03}$
$V \sin i$	km s ⁻¹	$27.65^{+0.28}_{-0.53}$	$27.30^{+0.43}_{-0.37}$	$27.79^{+0.46}_{-0.48}$	$26.93^{+0.56}_{-0.47}$
q_1	—	$0.81^{+0.19}_{-0.08}$	$0.81^{+0.18}_{-0.09}$	$0.80^{+0.19}_{-0.09}$	$0.79^{+0.21}_{-0.11}$
q_2	—	$0.36^{+0.12}_{-0.11}$	$0.40^{+0.12}_{-0.12}$	$0.34^{+0.11}_{-0.12}$	$0.48^{+0.14}_{-0.14}$
$\log_{10} a_{\text{GP}}$	—	$-3.83^{+0.02}_{-0.02}$	$-3.75^{+0.02}_{-0.02}$	$-3.83^{+0.02}_{-0.02}$	$-3.88^{+0.02}_{-0.02}$
$\log_{10} \tau_{\text{GP}}$	Å	$-1.32^{+0.01}_{-0.02}$	$-1.28^{+0.02}_{-0.02}$	$-1.32^{+0.01}_{-0.02}$	$-1.35^{+0.01}_{-0.01}$
A_1	—	$1.141^{+0.001}_{-0.001}$	$1.141^{+0.001}_{-0.001}$	$1.142^{+0.001}_{-0.001}$	$1.140^{+0.001}_{-0.001}$
A_2	—	$1.141^{+0.001}_{-0.001}$	$1.141^{+0.001}_{-0.001}$	$1.141^{+0.001}_{-0.001}$	$1.140^{+0.001}_{-0.001}$
A_3	—	$1.141^{+0.001}_{-0.001}$	$1.140^{+0.001}_{-0.001}$	$1.142^{+0.001}_{-0.001}$	$1.142^{+0.001}_{-0.001}$
A_4	—	$1.108^{+0.001}_{-0.001}$	$1.107^{+0.001}_{-0.001}$	$1.108^{+0.001}_{-0.001}$	$1.108^{+0.001}_{-0.001}$
<i>(Power-law T-P)</i>					
T_0	K	1219^{+7}_{-9}	1177^{+6}_{-6}	1215^{+8}_{-9}	—
α	—	$0.129^{+0.003}_{-0.006}$	$0.123^{+0.005}_{-0.004}$	$0.128^{+0.004}_{-0.005}$	—
<i>(GP T-P)</i>					
$T_{0,m}$	K	—	—	—	1165^{+82}_{-143}
α_m	—	—	—	—	$0.104^{+0.023}_{-0.044}$
$\log_{10} a_u$	—	—	—	—	$-0.36^{+0.11}_{-0.19}$
$\log_{10} \tau_u$	—	—	—	—	$-0.37^{+0.08}_{-0.13}$
<i>(Negative log-likelihood)</i>					
Normalized high-resolution spectra	—	—12239	—12165	—12251	—12295
JWST medium-resolution flux density	—	—28	—14	—13	—28
Total	—	—12268	—12179	—12265	—12323

Comparison with Medium-Resolution Flux Density

Although the retrievals above were performed on normalized spectra, the forward models also provide absolute flux densities. Since observational measurements of the absolute flux are available, checking their consistency with the model is also important for validating the retrieval. We therefore compared the JWST medium-resolution flux density with the model flux densities computed using each CO line list at the chip1 central wavelength $\lambda_1 = 2.30 \mu\text{m}$ (Figure 3.5). To enable a direct comparison, we converted the mean emergent flux density per wavenumber from ExoJAX, $\bar{F}_{\text{model}} [\text{erg}/\text{cm}^2/\text{s}/\text{cm}^{-1}]$, to the observed flux density in JWST units $F_{\text{JWST}} [\text{W}/\text{m}^2/\mu\text{m}]$ via

$$F_{\text{JWST}}(\lambda_1) = \left(\frac{R_{\text{BD}}}{D} \right)^2 \bar{F}_{\text{model}} \frac{10}{\lambda_1^2}, \quad (3.27)$$

where λ_1 is in μm and the prefactor $10/\lambda_1^2$ results from $1 \text{ erg} = 10^{-7} \text{ J}$, $1 \text{ cm}^{-2} = 10^4 \text{ m}^{-2}$, and $d\nu/d\lambda_\mu = 10^4/\lambda_\mu^2$ for wavenumber $\tilde{\nu}$ in cm^{-1} and wavelength in μm . The brown dwarf radius $R_{\text{BD}} = \sqrt{GM/g}$ is sampled from the retrieved surface gravity g and mass prior, and the distance D is computed from the parallax $\varpi = 500.5 \pm 0.11 \text{ mas}$ measured by [Sahlmann & Lazorenko \(2015\)](#). We also include a 3% photometric uncertainty to account for systematic errors in JWST spectroscopy ([Biller et al., 2024](#)). We find that the observations and predictions show reasonable agreement for both Luhman 16A and 16B across all line lists. Thus, our models are consistent not only in spectral morphology but also in the absolute flux density. While the strong prior on $\log g$ and the well-constrained mass and distance contribute to the agreement in the absolute flux density, the retrieved temperature structure and cloud properties also play a significant role. Therefore, the flux density agreement is not trivial; rather, it provides a valuable cross-check between the observed spectra and the model predictions. Because the prior on $\log g$ was informed by evolutionary models, this comparison also provides an external consistency check with those evolutionary constraints.

To assess the agreement across line lists, we compared the total negative log-likelihoods from the combined CRIRES spectra and JWST flux density; the values are shown in the bottom of Table 3.2 and 3.3. Among the three CO line lists, HITEMP_{Air} consistently yielded the poorest fit for both Luhman 16A and B. The remaining two, ExoMol CO and HITEMP_{H₂} CO, performed similarly, with HITEMP_{H₂} CO providing the best agreement for Luhman 16A and nearly matching ExoMol CO for Luhman 16B. We therefore focus on the HITEMP_{H₂} CO results hereafter, noting that our conclusions are insensitive to the choice of line list.

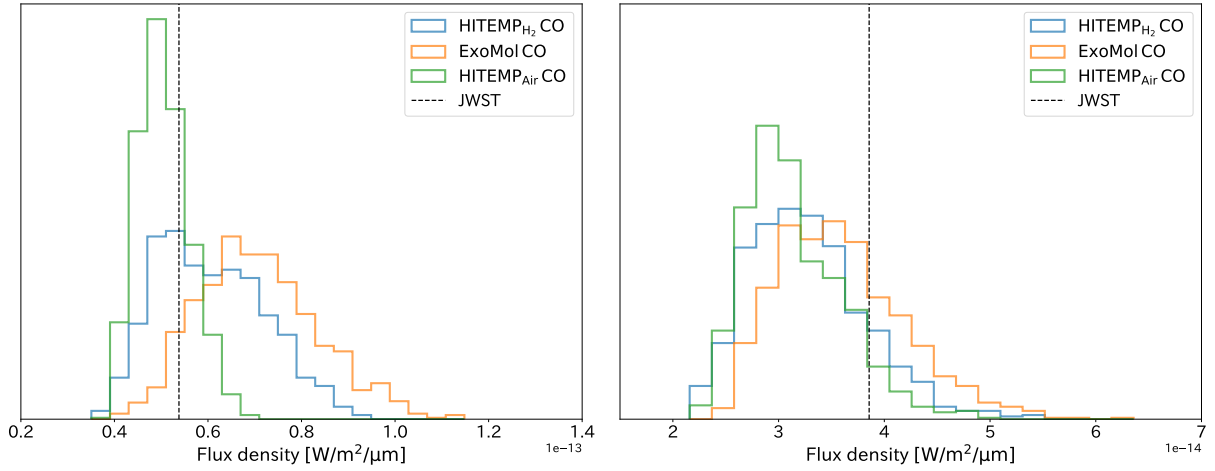


Figure 3.5: Comparison between the observed JWST medium-resolution flux density (vertical dashed lines) at the central wavelength of chip 1 ($2.30 \mu\text{m}$) and the model predictions based on different CO line lists (histograms). The model flux densities are converted from ExoJAX emergent fluxes to JWST units using Eq. 3.27. (Left) Luhman 16A. (Right) Luhman 16B.

Impact of Photometric Variability in Luhman 16B

Luhman 16A shows $> 2\%$ variability over a 7-hr baseline (Biller et al., 2024), and Luhman 16B exhibits $\sim 3\%$ variability over 5 hr (Crossfield et al., 2014) and up to $\sim 6\%$ over 7 hr (Biller et al., 2024). Such variability, common among L/T transition brown dwarfs including Luhman 16AB, is often attributed to heterogeneous silicate/iron clouds whose evolving rotational modulation produces temporal brightness changes (Radigan, 2014; Crossfield et al., 2014; Chen et al., 2024; Saumon & Marley, 2008). The CRIRES time series used here comprise 14 spectra (~ 5 hr) for each component (Crossfield et al., 2014) and show comparable normalized flux variability: 2.3% for A and 3.2% for B.

Our baseline retrieval assumes a horizontally homogeneous (i.e., effectively averaged) atmosphere, neglecting cloud patchiness. To assess potential systematics on C/O and cloud - top pressure from this assumption, we performed independent retrievals for each epoch of Luhman 16B using HITEMP_{H₂} CO. We find no statistically significant differences relative to the stacked - spectrum results in C/O or cloud deck pressure (Figure 3.6); quantitatively, the epoch-by-epoch C/O values agree with the stacked value (HITEMP_{H₂} CO) to within at most 1.3σ , and the cloud deck pressures to within at most 2.6σ . Hence, for the present data, the impact of ignoring cloud inhomogeneity appears subdominant to systematics associated with the line lists. This conclusion is consistent with the analysis of the *J*-band VLT/CRIRES⁺ spectrum by de Regt et al. (2025), who found that a patchy-cloud model is only weakly preferred for Luhman 16B and that the

retrieval outcomes are largely insensitive to the inclusion of patchiness.

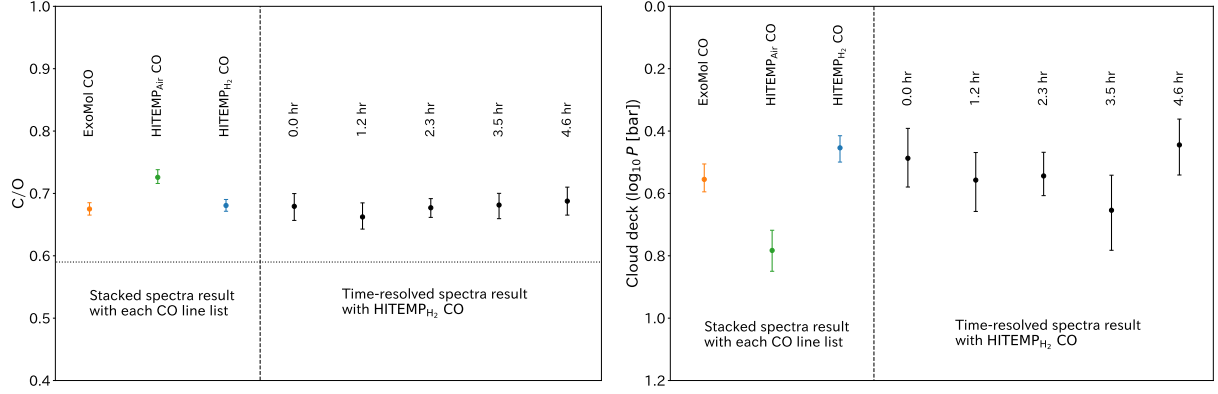


Figure 3.6: C/O and cloud deck pressure for Luhman 16B from stacked and time-resolved spectra. Left: C/O. Right: cloud deck pressure. In each panel, the region left of the vertical dashed line shows results from stacked spectra using three CO line lists (orange: ExoMol; green: HITEMP_{Air}; blue: HITEMP_{H₂}). The region right of the dashed line shows epoch-by-epoch (time-resolved) retrievals using HITEMP_{H₂} CO; from the 14 spectra spanning 0.0–5.0 hr we use five representative epochs. Error bars denote 90% credible region. In the left panel, the dotted horizontal line marks the solar C/O (= 0.59; [Asplund et al., 2021](#)).

3.4 Retrievals Using a Flexible Gaussian Process T – P Profile

Some high-resolution retrieval studies of brown-dwarf and exoplanet atmospheres adopt simple parameterizations of the T – P profile, such as a power-law form (e.g., [Kawahara et al., 2022](#); [Kawashima et al., 2025](#); [Kasagi et al., 2025](#)). Although efficient, such profiles can be overly restrictive. More flexible parameterizations have therefore been proposed, including schemes that parameterize the temperature gradient in discrete pressure layers ([Zhang et al., 2023](#)) and P -splines (e.g., [Line et al., 2015](#); [de Regt et al., 2025](#)). However, these approaches still remain tied to specific functional forms and may fail to capture complex structures.

As a potential future extension that takes advantage of the computational efficiency of HMC/NUTS in high-dimensional settings,² [Kawahara et al. \(2022\)](#) proposed a nonparametric T – P profile model based on Gaussian processes (GP, [Aigrain & Foreman-Mackey, 2023](#)). That work, however, did not explore its practical applicability in real retrievals, its sensitivity to other parameters, or its validation through injection–recovery tests. Here we refine the GP-based T – P profile model into a more practical framework and demonstrate its performance through application to the retrieval of Luhman 16AB data.

3.4.1 Formulation of the GP T – P Profile

To flexibly represent temperature–pressure (T – P) structures while maintaining numerical stability, we define the temperature profile as a GP in a whitened and logistically mapped latent space. This approach ensures physically bounded temperatures, reduces parameter correlations during NUTS sampling, and avoids the need for explicit box priors.

We model the temperature at 21 pressure layers, denoted $\mathbf{T}_{\text{GP}}$, as a logistic transformation of a underlying latent variable $\mathbf{u}$:

$$\mathbf{T}_{\text{GP}} = T_{\min} + (T_{\max} - T_{\min}) \sigma(\mathbf{u}), \quad \sigma(\mathbf{u}) = \frac{1}{1 + e^{-\mathbf{u}}}, \quad (3.28)$$

where $T_{\min}$ and $T_{\max}$ are the physically allowed temperature limits, set to 210 K and 3500 K, respectively. This transformation guarantees $T_{\text{GP},i} \in [T_{\min}, T_{\max}]$ by construction. The latent vector $\mathbf{u}$ follows a GP prior with mean function $\mathbf{m}_u$ and covariance matrix

²The convergence time of conventional random Metropolis–Hastings scales as D^2 with D being the number of parameters, whereas HMC scales as $D^{5/4}$ ([Neal, 2011](#)). There are also studies suggesting that NUTS scales as $D^{1/4}$ when initialized in the concentration region of the canonical Gaussian measure ([Bou-Rabee & Oberdörster, 2024](#)).

Σ_u :

$$\mathbf{u} \sim \mathcal{GP}(\mathbf{m}_u, \Sigma_u). \quad (3.29)$$

The covariance matrix is defined as

$$\Sigma_{u,ij} = K_{u,ij} + \sigma_u^2 \delta_{ij}, \quad (3.30)$$

where we fixed a small jitter term at $\sigma_u = 10^{-6}$ for numerical stability. This negligible value ensures that the term has no physical impact on the retrieved T - P profiles. We adopt the Matérn 3/2 kernel,

$$K_{u,ij} = a_u^2 \left(1 + \frac{\sqrt{3} |\log_{10} P_i - \log_{10} P_j|}{\tau_u} \right) \exp \left[-\frac{\sqrt{3} |\log_{10} P_i - \log_{10} P_j|}{\tau_u} \right], \quad (3.31)$$

with amplitude a_u and correlation length τ_u treated as free hyperparameters with uniform priors on $\log_{10} a_u$ and $\log_{10} \tau_u$. The mean function $\mathbf{m}_u$ is defined as the logit transform of a baseline temperature profile $\mathbf{T}_{\text{mean}}$:

$$\mathbf{m}_u = \log \left(\frac{\mathbf{T}_{\text{mean}} - T_{\min}}{T_{\max} - T_{\min}} \right) - \log \left(1 - \frac{\mathbf{T}_{\text{mean}} - T_{\min}}{T_{\max} - T_{\min}} \right), \quad (3.32)$$

where $\mathbf{T}_{\text{mean}}$ follow a power-law form

$$T_{\text{mean}}(P) = T_{0,m} \left(\frac{P}{1 \text{ bar}} \right)^{\alpha_m}, \quad (3.33)$$

with the parameters $T_{0,m}$ and α_m inferred simultaneously with the GP hyperparameters. For efficient sampling, we adopt the whitened representation:

$$\mathbf{u} = \mathbf{m}_u + \mathbf{L} \mathbf{z}, \quad \mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}), \quad (3.34)$$

where $\mathbf{L}$ is the Cholesky factor of the covariance matrix Σ_u , and $\mathbf{I}$ denotes the identity matrix. The whitened variable $\mathbf{z}$ is directly sampled in the NUTS inference, which improves convergence and decorrelates the GP components. Finally, the temperature vector $\mathbf{T}_{\text{GP}}$ at the 21 layers is interpolated to the 101 layer grid via $\text{IP}(\mathbf{T}_{\text{GP}})$. The joint posterior

is

$$\begin{aligned}
 p(\boldsymbol{\theta}, \mathbf{u}, T_{0,m}, \alpha_m, a_u, \tau_u \mid \mathbf{d}) &\propto \mathcal{L}(\mathbf{d} \mid \boldsymbol{\theta}, \text{IP}(\mathbf{T}_{\text{GP}}(\mathbf{u}))) \\
 &\times p(\boldsymbol{\theta}) \\
 &\times p(\mathbf{u} \mid \mathbf{m}_u(T_{0,m}, \alpha_m), a_u, \tau_u) \\
 &\times p(T_{0,m}, \alpha_m, a_u, \tau_u),
 \end{aligned} \tag{3.35}$$

which we sample using NUTS.

Relative to the GP formulation of Kawahara et al. (2022), our implementation introduces several changes aimed at practical convergence and physical regularization. First, while Kawahara et al. (2022) adopted a RBF kernel, we instead use a Matérn 3/2 kernel. The Matérn kernel is less smooth than the RBF kernel, avoiding the overly smooth behavior inherent to the RBF assumption. In addition, we infer the kernel hyperparameters (the amplitude a_u and correlation length τ_u) jointly with the atmospheric parameters, thereby removing the need to set them manually. Second, instead of adopting a constant mean function as in Kawahara et al. (2022), we use a power-law form characterized by $(T_{0,m}, \alpha_m)$, whose parameters are inferred jointly with the GP. We find that a constant mean tends to force the retrieved profile to flatten toward the average value in the upper and lower layers, as is also hinted in figure 11 Kawahara et al. (2022). The power-law mean model, on the other hand, better reflects the physically expected structure of self-luminous brown dwarfs while allowing the GP to capture deviations from it.

3.4.2 Demonstration

We validate the GP T – P framework using simulated spectra. All physical parameters except those describing the T – P profile are fixed to the posterior medians from our retrieval of the Luhman 16A spectrum with a power-law T – P profile and the HITEMP_{H₂} CO line list (Table 3.2). As the input T – P profile for the simulations, we adopt a Sonora Diamondback model with $T_{\text{eff}} = 1300$ K, $f_{\text{sed}} = 1$, $\log g = 5.0$, $[\text{M}/\text{H}] = 1.0$, and solar C/O. The synthetic data $\mathbf{d}_{\text{sim}}$ are created by evaluating the spectral model $\mathbf{f}(\boldsymbol{\theta})$ at the simulation inputs $\boldsymbol{\theta}_{\text{sim}}$ and adding Gaussian noise with a flux-density uncertainty $\boldsymbol{\sigma}_{\text{sim}}$ matched to the S/N of the Luhman 16A high-resolution data:

$$\mathbf{d}_{\text{sim}} = \mathbf{f}(\boldsymbol{\theta}_{\text{sim}}) + \mathcal{N}(0, \boldsymbol{\sigma}_{\text{sim}}). \tag{3.36}$$

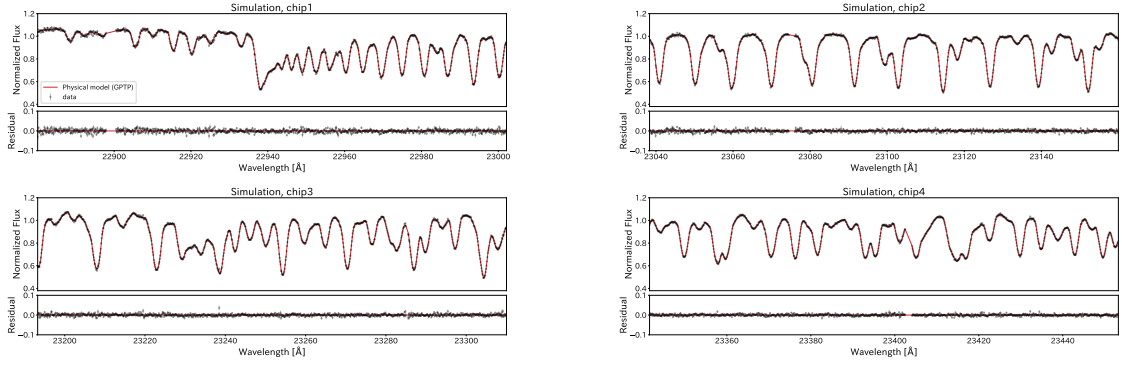


Figure 3.7: Retrieval results for the simulation spectra, modeled with the HITEMP_{H₂} CO line list and a Gaussian process T - P profile. The wavelength coverage is split into four detector segments (chips 1–4) like CRILES. For each chip, the top panel shows the simulated normalized flux data (black points) and the best-fit physical model (red line). The bottom panel shows the residuals (data minus the best-fit model). Each chip is normalized independently.

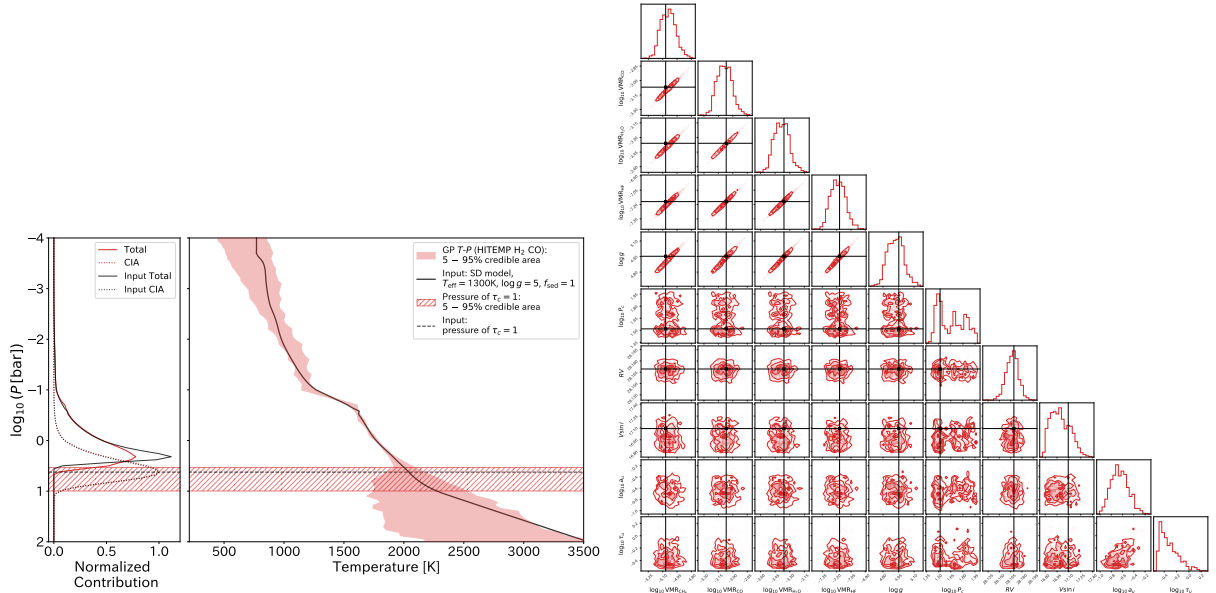


Figure 3.8: (Left) The Sonora diamondback (SD) T - P profile model (black solid line) used to generate the simulation data, and the T - P profile inferred with the GP T - P model (red shaded region). (Right) The corresponding corner plot.

Because noise is drawn independently at each pixel, the likelihood used in the retrieval is

$$\mathcal{L}(\boldsymbol{\theta}) = \prod_{i=1}^n \frac{1}{\sqrt{2\pi\sigma_{\text{sim},i}^2}} \exp \left[-\frac{(d_{\text{sim},i} - f_i(\boldsymbol{\theta}))^2}{2\sigma_{\text{sim},i}^2} \right]. \quad (3.37)$$

Priors for the parameters follow Table 3.1 (shared with Luhman 16A), except for the power-law T - P parameters and the GP for the spectral likelihood.

The simulation spectra and best fit are shown in Figure 3.7. The retrieved T – P profile and posteriors are shown in Figure 3.8. The GP T – P model successfully reproduces input physically parameters as well as non–power-law shape in the input T – P profile at pressures where the contribution function peaks. Conversely, in regions with little or no contribution (e.g., above the photosphere or deep beneath the cloud deck), the temperature uncertainty naturally broadens, reflecting the paucity of information more faithfully than a power-law model. This behavior demonstrates that the GP T – P approach can capture complex thermal structures where the data are informative, while appropriately inflating uncertainties where they are not.

3.4.3 Application to Luhman 16AB

We applied the GP T – P retrieval to the CRIRES data of Luhman 16AB. Best-fit model spectra for both components are shown in Figure 3.9. Corner plots for the selected parameters are shown in Figure 3.10; the retrieved T – P profiles are shown in Figure 3.11 along with the power-law profiles from Section 3.3; the retrieved parameter values are summarized in the rightmost columns of Tables 3.2 and 3.3.

Figure 3.11 shows that the broad trends of the inferred T – P profiles are consistent with those obtained under the power-law parameterization. Consistently, the molecular abundances and C/O ratios agree with the power-law results within uncertainties, indicating that these bulk parameters are robust to the choice of T – P profile. As in the simulation test, the temperature uncertainties increase at pressures where the spectral contribution is small, yielding a more conservative characterization than the power-law model.

At the same time, the GP T – P profiles infer departures from a power-law in the detailed structure. In both components, we find evidence for localized inversions near $\log_{10} P \sim 0.5$ and $\log_{10} P \sim -1$. The feature around $\log_{10} P \sim 0.5$ roughly coincides with the cloud-top pressure inferred in the power-law analysis; an approximately isothermal layer can mimic the behavior of a gray cloud, underscoring that cloud-top inferences are sensitive to the flexibility allowed in the T – P profile. The higher-altitude feature near $\log_{10} P \sim -1$ corresponds to subtle differences in the depths of line cores arising from cooler layers. Whether this structure is physical remains uncertain; possibilities include residual line-list/systematic effects or additional weak condensate/haze opacity at those pressures. Indeed, Sonora models suggest some condensates may be expected in this regime depending on composition and thermal structure. Regardless, the information content from these levels is limited, so any model deficiency there has a negligible impact

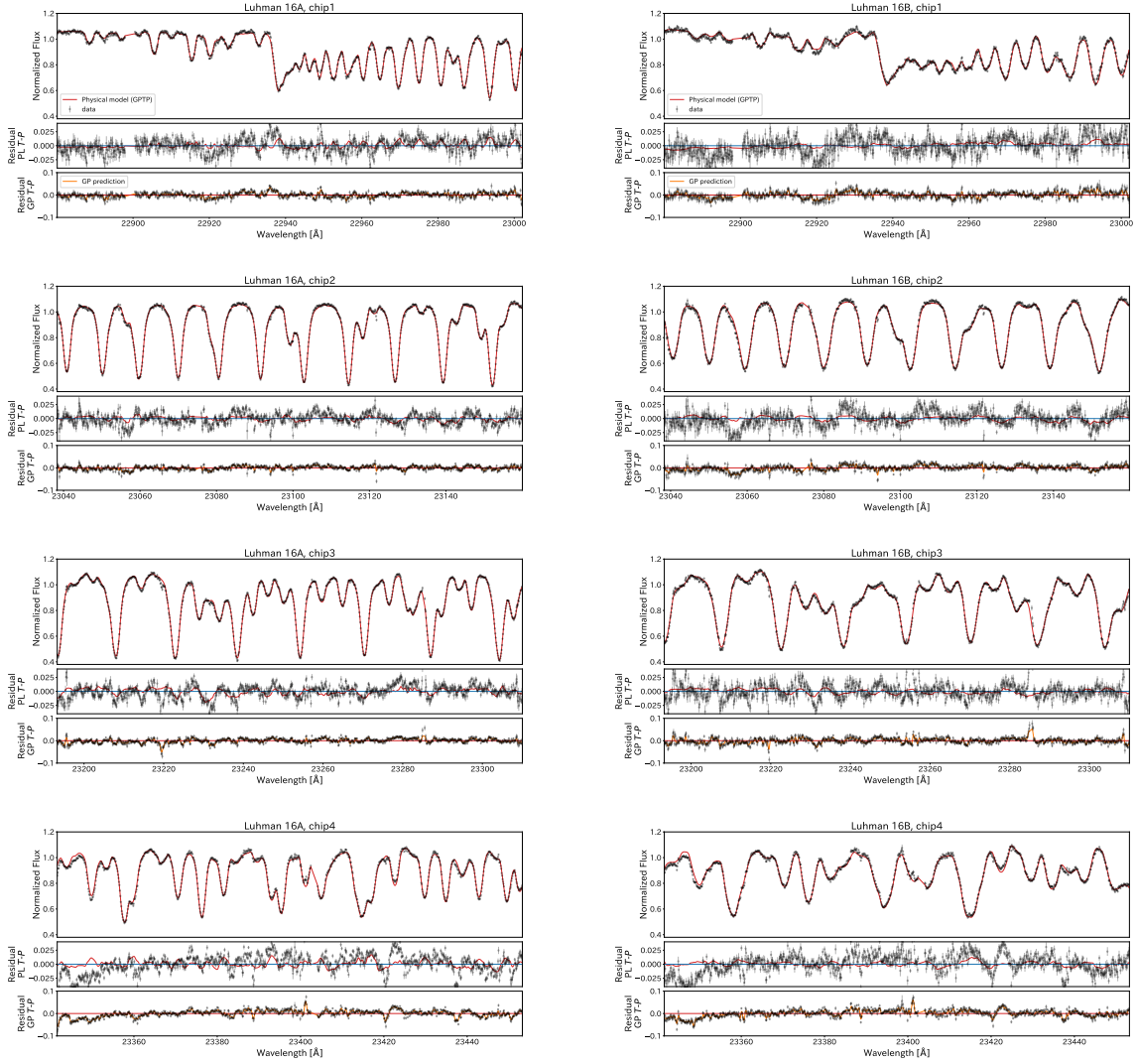


Figure 3.9: Retrieval results for the VLT/CRIRES high-resolution spectra of Luhman 16A (left) and Luhman 16B (right), modeled with the $\text{HITEMP}_{\text{H}_2}$ CO line list and a Gaussian process T - P profile. The wavelength coverage is split into four detector segments (chips 1–4). For each chip, the top panel shows the normalized flux data (black points) and the best-fit physical model (red line). The middle panel shows the residuals relative to the power-law T - P model with the $\text{HITEMP}_{\text{H}_2}$ CO line list (data minus the power-law T - P best-fit model), along with the difference between the GP and power-law T - P best-fit models (red line). The bottom panel shows the residuals relative to the GP T - P model (data minus the GP T - P best-fit model); orange lines indicate the correlated noise predicted by the GP. Each chip is normalized independently.

on global parameters such as C/O for the present data.

Figure 3.12 shows the comparison with FastChem, analogous to the power-law case. While the overall trends remain similar, the model-predicted ranges broaden owing to the propagated T - P uncertainty. The effect is most pronounced for CH_4 in deeper layers,

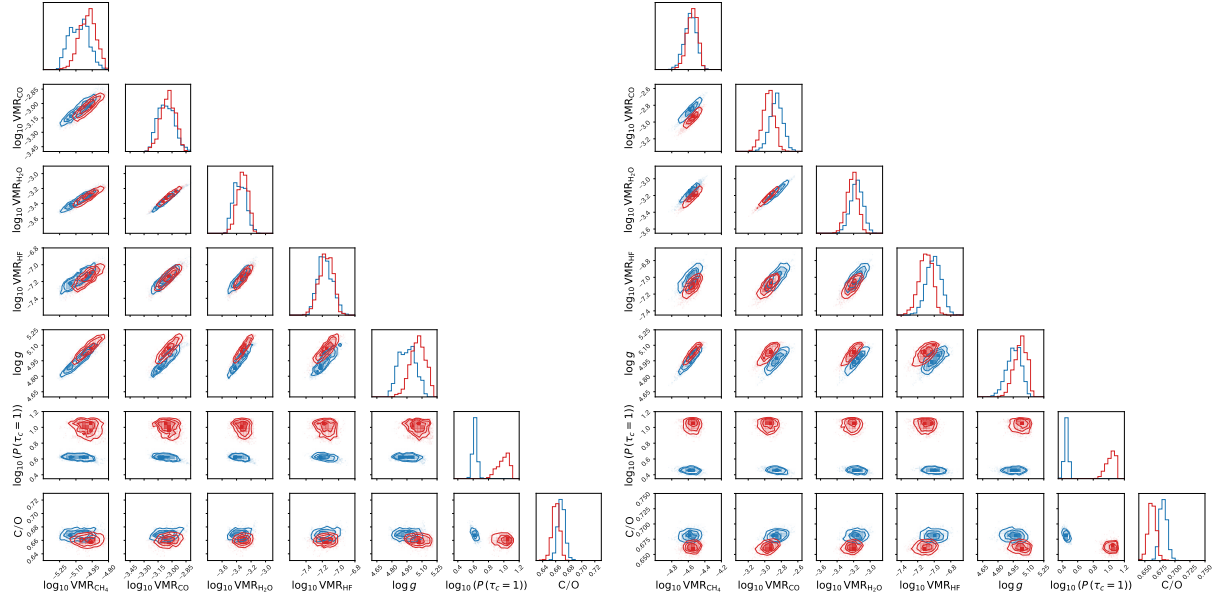


Figure 3.10: Comparison of posteriors obtained with a power-law T – P profile (blue) and with a GP T – P profile (red), both using the HITEMP_{H₂} CO line list. (Left) Luhman 16A. (Right) Luhman 16B.

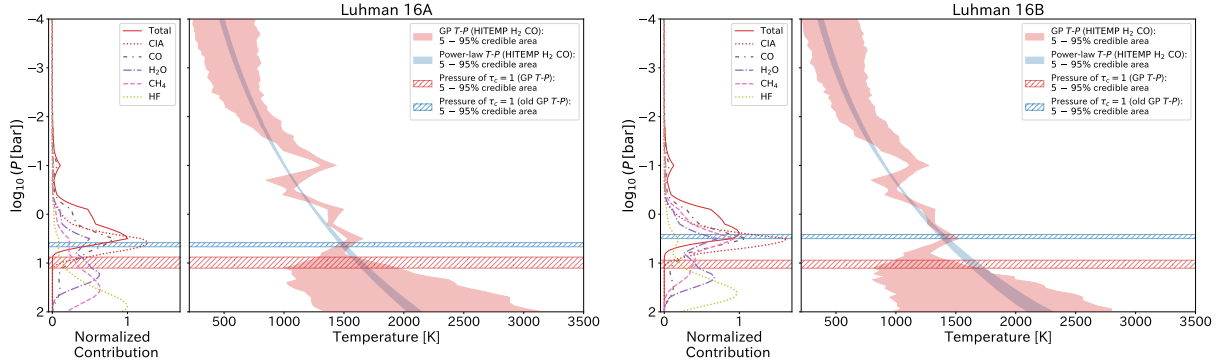


Figure 3.11: Retrieved T – P profiles and contribution functions: GP (red shaded) versus power-law (blue) under the gray-cloud + HITEMP_{H₂} CO configuration. (Left) Luhman 16A. (Right) Luhman 16B.

for which the apparent discrepancy seen under the power-law assumption is no longer compelling once the increased structural uncertainty is accounted for. This highlights that rigorous propagation of T – P shape and uncertainty—including regions with modest contribution—is essential when assessing possible departures from chemical equilibrium. In this regard, the GP T – P profile provides a useful and conservative framework.

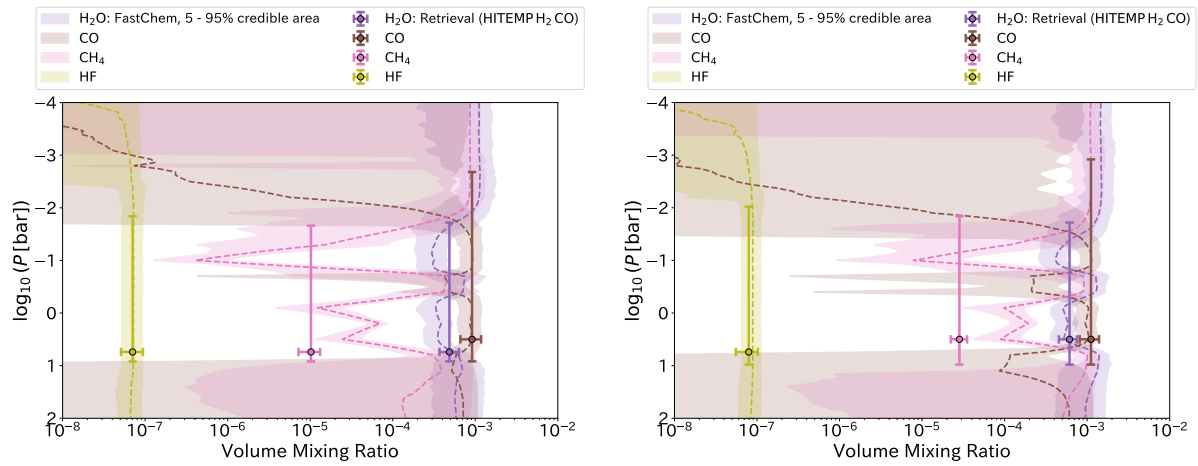


Figure 3.12: Comparison between the retrieved volume mixing ratios and FastChem equilibrium predictions (solar abundances from [Asplund et al. 2021](#)). (Left) Luhman 16A. (Right) Luhman 16B.

3.5 Summary and Discussion

Using ExoJAX, we performed high-resolution retrievals of Luhman 16AB under a gray-cloud assumption and inferred elemental abundance ratios. Taking the HITEMP_{H₂} CO line list and a power-law T – P parameterization as a baseline, we then (i) repeated the analysis with alternative CO line lists and (ii) introduced a more flexible T – P description based on GPs to assess the robustness of the inferred parameters.

3.5.1 Comparison with Previous Work

In addition to the present work, several other high-resolution retrieval studies of Luhman 16AB have recently been reported. Since the spectral wavelength ranges and model setups differ across these works, we focus here on comparing the retrieved physical parameters, namely, molecular abundances and cloud parameters.

Abundance The molecules included in our model, H₂O, CH₄, CO, and HF, have all been detected in the H - and K -band Gemini South/IGRINS high-resolution ($R \sim 28,000$) spectra of Luhman 16AB presented by [Ishikawa et al. \(2025\)](#). Their study compared the spectra against forward models generated with PICASO, which incorporates radiative–convective equilibrium, Sonora Bobcat T – P profiles, VIRGA cloud models, and nonequilibrium chemistry parameterized by a vertical eddy diffusion coefficient K_{zz} . The retrieved volume mixing ratios (VMRs) of the common molecules (their Figure 8) are broadly consistent with ours, but tend to be smaller, likely because they fixed the metallicity to solar whereas we inferred slightly super-solar values. Both H₂O and HF have also been detected in the CRIRES⁺/VLT J -band high-resolution retrieval by [de Regt et al. \(2025\)](#). Their modeling adopted a T – P parameterization based on the temperature gradient at five knots (as in [Zhang et al., 2023](#)), and clouds were treated as gray opacity decreasing with a power-law of pressure from the cloud base upward. Despite these differences, the retrieved molecular abundances are consistent with ours. Neither study provides explicit estimates of the C/O ratio: [Ishikawa et al. \(2025\)](#) fixed the metallicity and C/O to solar, and in the spectral range analyzed by [de Regt et al. \(2025\)](#), no carbon-bearing molecules were detected.

Cloud [Ishikawa et al. \(2025\)](#) also detected H₂ lines. By comparing the inferred H₂ column density with the interstellar gas-to-dust ratio, they suggested that dust clouds may reside deeper than the H₂ absorption layer, located at ~ 3 bar (or $\log_{10} P \sim 0.5$) in both components A and B. Their self-consistent models likewise imply that clouds are

present at similar or deeper pressures relative to the H_2 line-forming region. In the power-law cloud model of [de Regt et al. \(2025\)](#), the cloud opacity is dominated by contributions around $\log_{10} P \sim 0.5\text{--}1$, and this estimate is robust to assumptions about patchiness. In our analysis as well, the inferred cloud top pressures consistently fall within $\log_{10} P \sim 0.5\text{--}1$, broadly agreeing with these results. On the other hand, the quantitative estimates depend on assumptions about the $T\text{--}P$ profile and line lists, which in turn propagate into the inferred C/O ratio as discussed in the next subsection.

3.5.2 C/O Ratios

Figure 3.13 compares CO inferred with each CO line list configuration and with the GP $T\text{--}P$ model (using $\text{HITEMP}_{\text{H}_2}$ CO) to literature values for other brown dwarfs and super Jupiters. For both A and B, the choice of CO line list introduces a systematic offset of $\sim 7\%$ in CO. By contrast, the assumed $T\text{--}P$ profile (power-law versus GP) does not yield a significant difference in CO. An epoch-by-epoch analysis of the Luhman 16B time series likewise reveals no statistically significant impact from cloud-cover variability on the retrieved CO or molecular VMRs (Section 3.3.2). We therefore conclude that, in our framework, the principal systematic on CO arises from the CO line list, whereas the $T\text{--}P$ shape and photometric variability are not dominant. In all cases, the C/O values for components A and B agree within $\approx 2\sigma$, consistent with the expectation that isolated brown dwarfs (and their binaries) form in a star-like manner.

At face value, Figure 3.13 hints that brown dwarfs may exhibit higher CO than super Jupiters. Although this is a collection of inhomogeneous inferences from the literature, our measurements for Luhman 16AB, together with the associated systematic-error budget, reinforce this possibility. While differences in formation pathways (i.e., gravitational instability vs. core accretion) remain a possible explanation, the contrast could also reflect differences in the efficiency of oxygen sequestration by silicate (and other) clouds, as emphasized in previous low-resolution studies (e.g., [Line et al., 2015, 2017](#)): more efficient rainout in field brown dwarfs would raise the gas-phase C/O, whereas weaker sequestration in super Jupiters would leave C/O closer to the stellar value. A decisive test will require a larger, uniformly analyzed sample of both planets and brown dwarfs, so that inter-study systematics are minimized and C/O can be compared on equal footing. Building on such a uniform baseline, joint analyses of high-resolution spectra (to constrain $T\text{--}P$) and JWST coverage (to probe silicate or other cloud composition and vertical structure) can further mitigate cloud- $T\text{--}P$ -chemistry degeneracies, thereby providing a more direct test of the efficiency of oxygen sequestration by rainout. We return

to the prospects and implementation of such joint retrievals in Section 3.5.4.

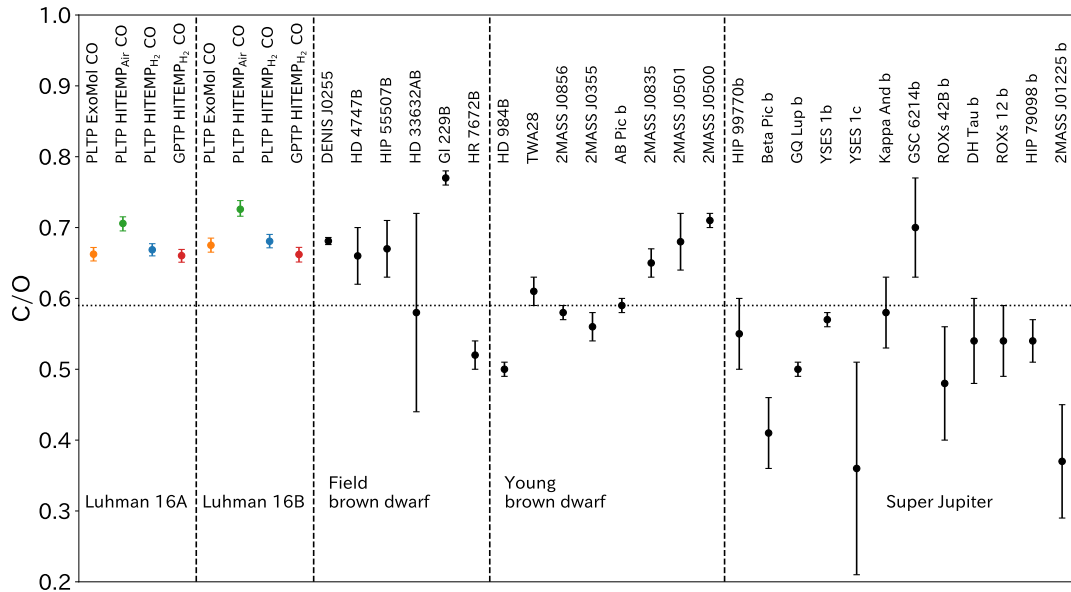


Figure 3.13: Comparison of CO for Luhman 16AB derived in this work with CO values reported for other brown dwarfs and directly-imaged super Jupiters from high-resolution spectroscopic analyses (Table A.1). Abbreviations: PLTP = power-law T - P profile; GPTP = Gaussian-process T - P profile.

3.5.3 Usefulness and Caveats of the GP T - P Model

For both simulations and real data, the GP T - P model captures structures that are more complex than a simple power-law and yields a more faithful assessment of uncertainties. In the present application, these differences have only a modest impact on bulk parameters such as CO. However, as discussed in Section 3.4.3, comparisons between retrieved molecular abundances and chemical-equilibrium predictions are sensitive to how T - P uncertainties are propagated; in this context, the GP framework is important because it enables predictive uncertainties to faithfully reflect the spectra’s information content, remaining conservative where the data are weakly informative. The GP approach is also sensitive to residual model-data mismatches and thus shows promise for diagnosing deficiencies in current models, potentially pointing to additional physics.

On the other hand, as indicated in Section 3.4.3, degeneracies between the T - P shape and cloud opacity can allow nonphysical temperature structures if left unconstrained. Mitigations include imposing weak physical regularization (e.g., monotonicity or stability constraints) on flexible T - P profiles and/or extending the analysis to broader wavelength

coverage where cloud signatures are stronger. The latter strategy can help balance flexibility with physical plausibility; see also Section 3.5.4.

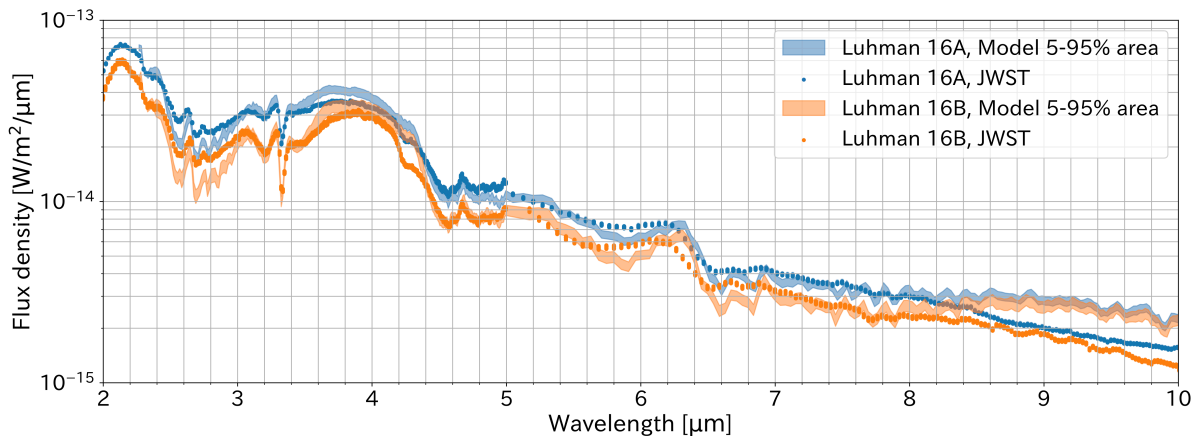


Figure 3.14: Comparison between the medium-resolution spectra predicted by extrapolating our high-resolution retrievals and the JWST observations. Shaded bands show the 90% credible intervals of the predicted spectra computed with the HITEMP_{H₂} CO line list and a power-law T – P profile (blue: Luhman 16A; orange: Luhman 16B). Points show the corresponding JWST medium-resolution spectra from [Biller et al. \(2024\)](#); [Chen et al. \(2025\)](#) (blue: A; orange: B).

3.5.4 Cloud Degeneracies and Joint Analysis with JWST

Throughout this work, we find that the inferred cloud-top pressure is sensitive to assumptions about the T – P profile and the adopted line list. These systematics propagate into the retrieved VMRs and, via absolute flux, into radius inferences. This underscores the value of combining broad wavelength information with high spectral resolution.

In the current era, JWST provides such leverage. In Figure 3.14, we compare the model spectra extrapolated to 10 μ m from our high-resolution analysis (power-law T – P , gray cloud, HITEMP_{H₂} CO) against JWST medium-resolution spectra ([Biller et al., 2024](#); [Chen et al., 2025](#)). Beyond ~ 8.5 μ m the JWST flux densities fall below the extrapolated models, consistent with absorption by silicate particles. Similar features have also been reported in medium-resolution spectra of L dwarfs with the *Spitzer* Space Telescope, linked to the emergence and sedimentation of silicate clouds ([Cushing et al., 2006](#); [Suárez & Metchev, 2022](#)). More recently, JWST has revealed mid-infrared silicate absorption in directly imaged planets: [Hoch et al. \(2025\)](#) report a clear 8.5–11 μ m feature in YSES-1 c, demonstrating that particle size, composition (e.g., Mg silicates and Fe-bearing pyroxenes), vertical distribution, and the T – P profile all shape the mid-infrared continuum and feature morphology. These findings highlight the opportunity to gain a more com-

plete understanding of cloud properties by constraining clouds and the T – P structure simultaneously. Together with the mid-infrared flux deficit relative to our extrapolated models, these comparisons motivate joint retrievals that combine high-resolution ground-based spectra with JWST data. High-resolution spectra exploit the height dependence of individual line formation to tightly constrain the T – P profile, while JWST provides broad coverage to probe cloud composition and vertical structure. Thus, joint retrievals offer a powerful approach to advancing our understanding of cloud physics and composition, fully leveraging the complementary strengths of broad wavelength coverage and high spectral resolution.

Building upon these insights, future work will incorporate more detailed cloud modeling that accounts for realistic particle size distributions, compositions, and vertical structures. While the present analysis adopted a simple gray cloud prescription (Eq. 3.6) to focus on the line list and T – P effects, these developments—particularly when combined with joint retrievals using JWST and high-resolution ground-based spectra—will enable a more comprehensive understanding of cloud formation and evolution in substellar atmospheres.

Chapter 4

Summary and Conclusion

In this thesis, we investigate atmospheric compositions, with a particular focus on the C/O ratio, as key tracers of the formation processes of brown dwarfs and giant exoplanets. Using high-resolution spectroscopy combined with atmospheric retrieval analyses, we perform a detailed characterization of substellar atmospheres. Recent advances in high-resolution spectrographs and analysis techniques have made it possible to resolve individual molecular absorption lines, providing access to atmospheric information that is inaccessible to low-resolution spectroscopy or photometric observations. The primary goal of this work is to assess systematic uncertainties inherent in high-resolution atmospheric retrievals and to use these analyses to constrain the formation origins of brown dwarfs and giant planets.

In Chapter 2, we summarize the radiative transfer framework adopted in this study. We review the definition of optical depth, derive the radiative transfer equation, and describe the principal opacity sources in substellar atmospheres, including molecular absorption, collision-induced absorption, and cloud opacity. Particular emphasis is placed on the intensity-based radiative transfer formalism commonly used in high-resolution retrievals (ExoJAX; Kawahara et al., 2022; Kawahara et al., 2025), as well as on the discretization of the atmosphere into a finite number of layers. These formulations provide the theoretical foundation for the retrieval analyses presented in subsequent chapters.

In Chapter 3, we perform atmospheric retrievals of high-resolution near-infrared spectra of the nearby brown dwarf binary Luhman 16AB obtained with CRIRES on the VLT, and present the first measurements of the C/O ratios for this system. We first adopt models with a power-law temperature–pressure (T – P) profile and compare retrieval results obtained using different CO molecular line lists, namely ExoMol CO, HITEMP_{Air} CO, and HITEMP_{H₂} CO. We find that the choice of CO line list introduces non-negligible systematic differences in the inferred C/O ratios and cloud-deck pressures. In particular,

the C/O ratio is affected by a systematic uncertainty of approximately ($\sim 7\%$), quantitatively demonstrating that molecular line lists represent a major source of systematic uncertainty in high-resolution atmospheric retrievals.

We further introduce a flexible Gaussian-process (GP) representation of the T – P profile as an alternative to simple parametric models. Validation using simulated spectra shows that the GP T – P model is capable of reproducing non-power-law thermal structures predicted by the Sonora Diamondback models. Application to the Luhman 16AB data demonstrates that the GP framework mitigates biases arising from restrictive assumptions about the thermal structure, while enabling robust inference of molecular abundances and C/O ratios. Moreover, we show that comparisons between retrieved molecular abundances and chemical-equilibrium predictions are highly sensitive to how uncertainties in the T – P structure are estimated. In this context, the GP approach is particularly important because it provides conservative, data-driven uncertainty estimates that faithfully reflect the information content of the spectra. At the same time, degeneracies between the shape of the T – P profile and cloud opacity are identified, and we discuss practical considerations when adopting flexible thermal models, including the potential of joint retrievals with JWST medium-resolution spectra to alleviate these degeneracies.

The C/O ratios of Luhman 16AB inferred in this study, including systematic uncertainties, are consistent with the trend that brown dwarfs tend to exhibit higher C/O ratios than directly imaged super-Jupiters reported in the literature. This difference may reflect distinct formation pathways, or alternatively, differences in the efficiency of oxygen sequestration by clouds, as discussed by [Line et al. \(2015, 2017\)](#). Discriminating between these scenarios will require larger and more uniformly analyzed samples of both planets and brown dwarfs, enabling C/O ratios to be compared on a consistent footing.

Overall, the results of this thesis establish Luhman 16AB as an important benchmark system for C/O ratio measurements in substellar objects and demonstrate the utility of flexible T – P modeling in high-resolution atmospheric retrievals. By quantifying the impact of molecular line-list uncertainties on inferred atmospheric properties, this work emphasizes that explicit evaluation of systematic errors is essential when elemental abundance ratios are used as diagnostics of formation processes. These findings provide an important methodological framework for future studies of exoplanets and brown dwarfs.

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Appendix A

Literature C/O Ratios of Brown Dwarfs and Giant Exoplanets

Table A.1 provides the literature values, together with the corresponding references, for the objects shown in Figure 1.5 and 1.6.

Table A.1: Literature C/O ratios and masses for brown dwarfs, super Jupiters, and hot Jupiters.

Object	Class ^a	Comp. ^b	C/O	M [M_J]	$T_{\text{eff}}/T_{\text{Day}}$ [K] ^c	Semi-major axis [AU]	Ref.
DENIS J0255	FBD	N	0.681 ± 0.005	45.7 ± 4.4	1554^{+263}_{-53}	—	(1)
HD 4747 B	FBD	Y	0.66 ± 0.04	67.2 ± 1.8	1554^{+128}_{-218}	$10.15^{+0.17}_{-0.16}$	(2),(55)
HIP 55507 B	FBD	Y	0.67 ± 0.04	$88.0^{+3.4}_{-3.2}$	2350 ± 50	38^{+4}_{-3}	(3)
HD 33632 Ab	FBD	Y	0.58 ± 0.14	46 ± 8	1628^{+109}_{-97}	18^{+5}_{-3}	(4),(5)
Gl 229 B ^d	FBD	Y	0.77 ± 0.01	$71.47^{+0.57}_{-0.61}$	850 ± 50	$42.9^{+3.0}_{-2.4}$	(6),(7),(64)
HR 7672 B	FBD	Y	0.52 ± 0.02	$72.84^{+0.71}_{-0.72}$	1806 ± 77	$18.3^{+0.4}_{-0.5}$	(8),(65)
2MASS J0835	FBD	N	0.65 ± 0.02	62.47 ± 15.86	1754 ± 112	—	(9),(10)
2MASS J0501	FBD	N	0.68 ± 0.04	21.45 ± 13.71	1720 ± 55	—	(9),(11)
2MASS J0500	FBD	N	0.71 ± 0.01	63.68 ± 14.44	1793 ± 72	—	(9),(12)
HD 984 B	YBD	Y	0.50 ± 0.01	61 ± 4	2730^{+120}_{-180}	28^{+7}_{-4}	(13),(14),(15)
TWA 28	YBD	N	0.61 ± 0.02	20.9 ± 5.0	2382 ± 42	—	(16),(17),(18)
2MASS J0856	YBD	N	0.58 ± 0.01	14.4 ± 1.4	2380 ± 32	—	(16),(18),(19)
2MASS J0355	YBD	N	0.56 ± 0.02	19^{+7}_{-5}	1527 ± 14	—	(20),(21)
HIP 99770 b	SJ	Y	0.55 ± 0.05	$16.1^{+5.4}_{-5.0}$	1400^{+200}_{-150}	$16.9^{+3.4}_{-1.9}$	(22),(23)
β Pic b	SJ	Y	0.41 ± 0.05	11.9 ± 3.0	1724 ± 15	9.93 ± 0.03	(24),(25),(26)
GQ Lup b	SJ	Y	0.50 ± 0.01	25^{+11}_{-15}	2650 ± 100	117^{+24}_{-23}	(27),(28),(56)
YSES-1 b	SJ	Y	0.57 ± 0.01	21.8 ± 3.0	1893 ± 10	146^{+16}_{-10}	(29),(30),(57)
YSES-1 c	SJ	Y	0.36 ± 0.15	7.2 ± 0.7	958^{+163}_{-76}	320	(29),(30),(58)
κ And b	SJ	Y	0.58 ± 0.05	22 ± 9	1680^{+60}_{-50}	80^{+20}_{-30}	(31),(59)
GSC 6214 b	SJ	Y	0.70 ± 0.07	21 ± 6	1860^{+170}_{-110}	300	(31),(60)
ROXs 42B b	SJ	Y	0.48 ± 0.08	13 ± 5	2270^{+170}_{-140}	140 ± 10	(31),(61)
DH Tau b	SJ	Y	0.54 ± 0.06	12 ± 4	2250^{+120}_{-100}	330^{+90}_{-160}	(31),(59)
ROXs 12 b	SJ	Y	0.54 ± 0.05	19 ± 5	2500 ± 140	210 ± 20	(31),(61)
HIP 79098 b	SJ	Y	0.54 ± 0.03	28 ± 13	2360^{+70}_{-80}	345 ± 6	(31),(62)
2MASS J01225 b	SJ	Y	0.37 ± 0.08	25 ± 12	1710^{+170}_{-160}	52 ± 6	(31),(63)
AB Pic b	SJ	Y	0.59 ± 0.01	30^{+20}_{-18}	2000^{+100}_{-300}	190^{+200}_{-50}	(32),(33),(66)
CoRoT-1 b	HJ	Y	$0.9^{+0.3}_{-0.7}$	1.23 ± 0.10	1924 ± 374	$0.02752^{+0.00022}_{-0.00023}$	(34),(35)
HAT-P-2 b	HJ	Y	$0.5^{+0.3}_{-0.2}$	$8.70^{+0.19}_{-0.20}$	2168 ± 123	$0.06880^{+0.00065}_{-0.00070}$	(34),(35)
HAT-P-7 b	HJ	Y	1.4 ± 0.3	1.806 ± 0.036	2562 ± 253	0.03813 ± 0.00036	(34),(35)
HAT-P-32 b	HJ	Y	1.5 ± 0.3	$0.68^{+0.11}_{-0.10}$	1962 ± 83	$0.03427^{+0.00040}_{-0.00042}$	(34),(36)
HAT-P-41 b	HJ	Y	1.6 ± 0.3	$0.795^{+0.056}_{-0.091}$	2304 ± 169	$0.04258^{+0.00047}_{-0.00048}$	(34),(35)
HAT-P-70 b	HJ	Y	1.00 ± 0.05	6.78	2321 ± 263	$0.04739^{+0.00031}_{-0.00106}$	(34),(37)
HD 189733 b	HJ	Y	$0.8^{+0.1}_{-0.2}$	$1.13^{+0.047}_{-0.045}$	1388 ± 104	$0.03100^{+0.00059}_{-0.00061}$	(34),(38)

Continued on next page

Table A.1: (continued)

Object	Class ^a	Comp. ^b	C/O	M [M _J]	T _{eff} /T _{Day} [K] ^c	Semi-major axis [AU]	Ref.
HD 209458 b ^e	HJ	Y	0.11 ^{+0.06} _{-0.12}	0.682 ^{+0.014} _{-0.015}	1839 ± 21	0.04707 ^{+0.00045} _{-0.00047}	(50),(35)
KELT-1 b	HJ	Y	0.4 ± 0.2	27.38 ± 0.93	2913 ± 300	0.02466 ± 0.00016	(34),(39)
KELT-7 b	HJ	Y	1.6 ± 0.3	1.24 ^{+0.18} _{-0.17}	2480 ± 105	0.0446 ± 0.0013	(34),(40)
KELT-9 b	HJ	Y	1.1 ± 0.6	2.88 ± 0.84	4011 ± 367	0.03462 ^{+0.00110} _{-0.00093}	(34),(41)
Kepler-13 Ab	HJ	Y	0.4 ± 0.2	9.28 ± 0.16	2754 ± 316	0.03641 ± 0.00087	(34),(42)
TrES-3 b	HJ	Y	1.6 ± 0.3	1.801 ^{+0.078} _{-0.083}	1668 ± 114	0.02284 ^{+0.00024} _{-0.00037}	(34),(35)
WASP-4 b	HJ	Y	1.5 ^{+0.3} _{-0.4}	1.170 ± 0.015	1842 ± 265	0.02287 ± 0.00009	(34),(35)
WASP-12 b	HJ	Y	1.0	1.39 ± 0.12	3114 ± 179	0.02312 ^{+0.00094} _{-0.00010}	(34),(35)
WASP-18 b	HJ	Y	0.9	10.20 ^{+0.70} _{-0.72}	2841 ± 174	0.02030 ^{+0.00069} _{-0.00073}	(34),(35)
WASP-19 b	HJ	Y	0.5 ± 0.2	1.157 ^{+0.076} _{-0.078}	2535 ± 221	0.01649 ^{+0.00053} _{-0.00056}	(34),(35)
WASP-33 b	HJ	Y	0.9	2.093 ± 0.139	2600 ± 402	0.02390 ± 0.00063	(34),(43)
WASP-39 b ^e	HJ	Y	0.31 ^{+0.08} _{-0.05}	0.275 ^{+0.042} _{-0.043}	1120 ^f	0.04859 ^{+0.00051} _{-0.00053}	(46),(47),(35)
WASP-43 b	HJ	Y	0.7 ^{+0.01} _{-0.02}	2.050 ^{+0.050} _{-0.052}	1701 ± 54	0.01528 ^{+0.00017} _{-0.00018}	(34),(35)
WASP-74 b	HJ	Y	1.4 ^{+0.4} _{-0.3}	0.944 ^{+0.061} _{-0.059}	2212 ± 101	0.03705 ^{+0.00096} _{-0.00100}	(34),(35)
WASP-76 b	HJ	Y	1.2 ^{+0.4} _{-0.1}	0.92 ± 0.03	2478 ± 159	0.0330 ± 0.0005	(34),(44)
WASP-77 Ab ^e	HJ	Y	0.54 ± 0.12	1.763 ^{+0.055} _{-0.054}	2015 ± 210	0.02405 ± 0.00036	(48),(49),(35)
WASP-79 b	HJ	Y	0.3 ± 0.2	0.843 ^{+0.085} _{-0.080}	1965 ± 219	0.0521 ^{+0.0011} _{-0.0010}	(34),(35)
WASP-80 b ^e	HJ	Y	0.48 ^{+0.06} _{-0.07}	0.54 ^{+0.036} _{-0.035}	859.87 ^{+7.08} _{-9.10}	0.03427 ^{+0.00096} _{-0.00100}	(51),(52),(35)
WASP-96 b ^e	HJ	Y	0.46 ± 0.17	0.490 ^{+0.049} _{-0.047}	1491 ^f	0.0454 ± 0.0013	(53),(54),(35)
WASP-103 b	HJ	Y	1.0	1.455 ^{+0.090} _{-0.091}	2937 ± 129	0.01987 ^{+0.00020} _{-0.00021}	(34),(35)
WASP-121 b	HJ	Y	1.3 ± 0.1	1.157 ± 0.070	2602 ± 53	0.02591 ± 0.00054	(34),(45)

Notes.

a: FBD = field brown dwarf; YBD = young brown dwarf; SJ = super Jupiter; HJ = hot Jupiter.

b: Y = bound to a host star; N = isolated.

c: For hot Jupiters, temperatures correspond to the dayside mean temperature.

d: Gl 229 B may be a binary based on GRAVITY/VLTI and CRIRES⁺ observations (Xuan et al., 2024b).

e: C/O ratios measured with JWST data.

f: Equilibrium temperature.

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et al. (2024); (51) Wiser et al. (2025); (52) Bell et al. (2023); (53) Radica et al. (2023); (54) Taylor et al. (2023); (55) An et al. (2025); (56) Stolker et al. (2021); (57) Roberts et al. (2025); (58) Bohn et al. (2020); (59) Bowler et al. (2020); (60) Ireland et al. (2011); (61) Kraus et al. (2014); (62) Janson et al. (2019); (63) Bowler et al. (2013); (64) Thompson et al. (2025); (65) Crepp et al. (2012); (66) Palma-Bifani et al. (2023).

Appendix B

Atmospheric Retrieval of Luhman 16AB with Cloud-Free Model

We performed atmospheric retrievals using the power-law T - P profile and the HITEMP_{H₂} CO line list described in Section 3.3, adopting a cloud-free atmospheric model. Figure B.1 compares the high-resolution spectra of Luhman 16A and Luhman 16B with the best-fit spectra from the cloud-free and cloudy retrievals. As shown in the residuals in the lower panels, the cloud-free model fails to reproduce the observed spectra for both components, whereas the model including clouds provides a significantly better fit. Although the cloudy model considered here is intentionally simplified—neglecting the wavelength dependence of cloud opacity and adopting a parameterized vertical cloud distribution—it nonetheless indicates that reproducing the VLT/CRIRES high-resolution spectra of Luhman 16AB requires clouds, together with CIA and molecular absorption by CO, H₂O, CH₄, and HF.

Furthermore, a comparison between JWST medium-resolution spectra and model spectra extrapolated from the cloud-free retrieval results shows that the cloud-free model is inconsistent with the observations over most of the wavelength range (Figure B.2). In contrast to this clear mismatch, model spectra extrapolated from the cloudy retrieval results reproduce the JWST spectra reasonably well (Figure 3.14), further supporting the presence of clouds in the atmosphere of Luhman 16AB.

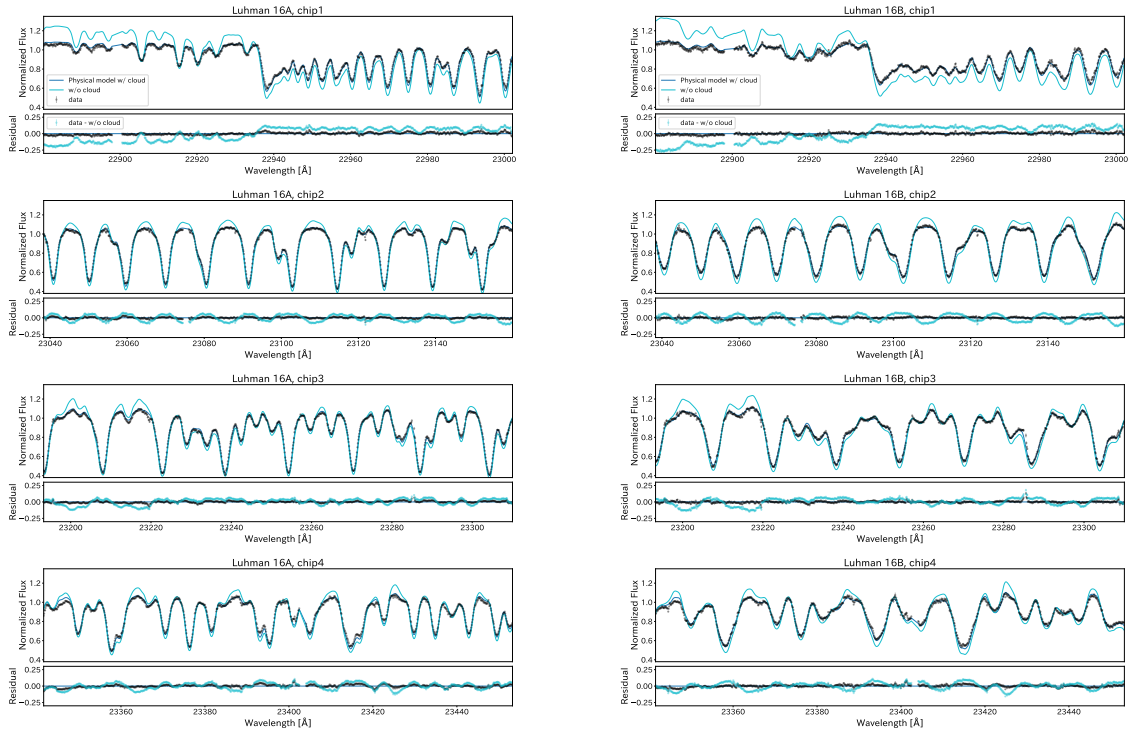


Figure B.1: Retrieval results for the VLT/CRIRES high-resolution spectra of Luhman 16A (left) and Luhman 16B (right), modeled using the $\text{HITEMP}_{\text{H}_2}$ CO line list and a power-law T - P profile without clouds. The wavelength coverage is split into four detector segments (chips 1–4). For each chip, the top panel shows the normalized flux data (black points), the best-fit physical model with clouds (blue line), and the best-fit physical model without clouds (light blue line). The bottom panel shows the residuals (black points; data minus the best-fit physical model with clouds, light blue points; data minus the best-fit physical model without clouds).

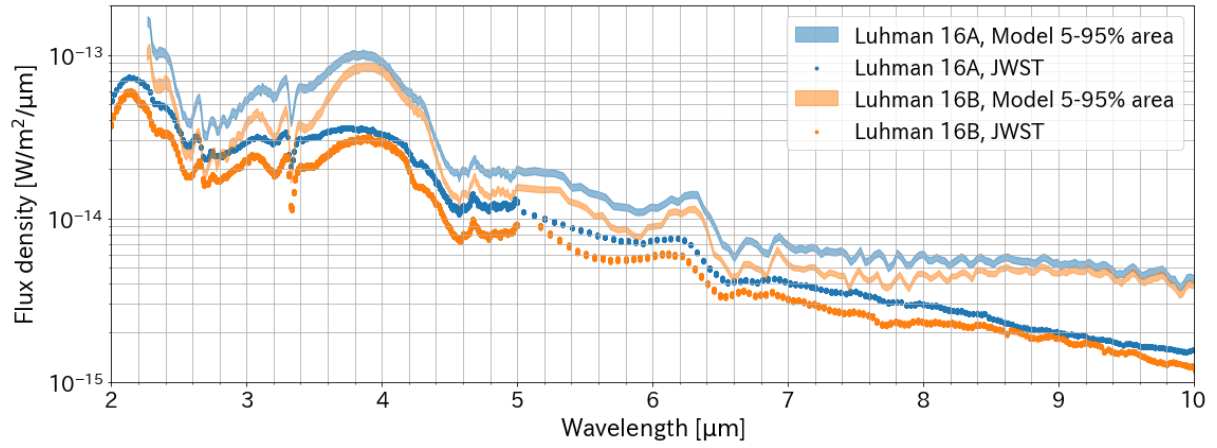


Figure B.2: Comparison between the medium-resolution spectra predicted by extrapolating our high-resolution retrievals using the cloud-free model and the JWST observations. Shaded bands show the 90% credible intervals of the predicted spectra computed using the HITEMP_{H₂} CO line list and a power-law T - P profile without clouds (blue: Luhman 16A; orange: Luhman 16B). Points show the corresponding JWST medium-resolution spectra from [Biller et al. \(2024\)](#); [Chen et al. \(2025\)](#) (blue: A; orange: B).

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