

Assessment of Infrared Spectral Data Availability for Carbon Chemistry Detection in Exoplanet Atmospheres

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ABSTRACT: As of February 2025, over five thousand exoplanets have been confirmed, many with carbon-containing atmospheres that remain largely unexplored. Infrared spectroscopy plays a crucial role in identifying carbon signatures. Carbon absorption signatures, key indicators of organic compounds, are prevalent largely in the near to mid-infrared range. This study aims to evaluate the factors limiting the detection of chemical signatures in exoplanetary atmospheric spectra by studying available datasets from the NASA Exoplanet Archive. A quantitative approach is utilized to assess the suitability of infrared spectra to detect and elucidate carbon chemistry in exoplanetary systems. We find that most data have limited spectral resolution, are sampled with fewer than 500 data points per micron, and are insufficient in differentiating specific carbon absorption features. Another key limitation found is the gap in data beyond five microns, largely attributed to engineering difficulties related to budget and technology maintenance. These findings highlight an exigent need for improved detectors and instruments to support the study of the chemistry of exoplanet atmospheres and life beyond Earth.

KEYWORDS: Physics and Astronomy, Atomic, Molecular, and Optical Physics, Spectral Data Processing, Exoplanet Atmospheres, Infrared Spectroscopy, Carbon Chemistry in Space.

■ Introduction

The field of exoplanetary discovery has witnessed a surge in recent years. As of December 2024, the total number of confirmed exoplanets has reached a remarkable 5,811.¹ The atmospheres of these extraterrestrial planets present an intriguing area of study; the composition of these astronomical bodies could uncover many mysteries. Investigations and studies can provide critical insights into planetary composition, formation, and potential habitability. Spectroscopic observations of exoplanets have revealed a diverse array of chemical compositions and processes not previously observed.² Organic molecules, made of carbon, are often referred to as the “molecules of life” as they are recognized as the backbone of life on Earth and are hypothesized to have potentially played a role in the emergence of life. Interestingly, organic molecules are also prevalent in exoplanetary atmospheres,³ so their analysis can uncover vital clues about the processes that drive planetary habitability, offering valuable perspectives on the potential for life beyond Earth.

Carbon is an element that is omnipresent throughout Earth and the universe. Making up approximately 18.5% of the human body,⁴ carbon is one of the few elements known since antiquity.⁵ In space, these molecules tend to persist in the different forms of interstellar carbonaceous grains, such as graphite, nanodiamonds, and polycyclic aromatic hydrocarbons.⁶ Having the maximum number of outer shell electrons capable of covalent bonds, carbon is known to be extremely versatile and can exist in various forms. Carbon-carbon single bonds are extremely diverse in nature, having been observed in hydrocarbons with lengths up to 1.71 angstroms.⁷ On the other hand, carbon-carbon double bonds are shorter and more rig-

id, influencing the molecular shape and reactivity, while triple bonds are even shorter and stronger. Carbon-hydrogen bonds create a chemical species collectively known as hydrocarbons, which are prevalent in space, particularly in the polycyclic aromatic form. These molecules then go through various chemical reactions influenced by environmental conditions, creating a diverse spectrum of organic molecules.⁸

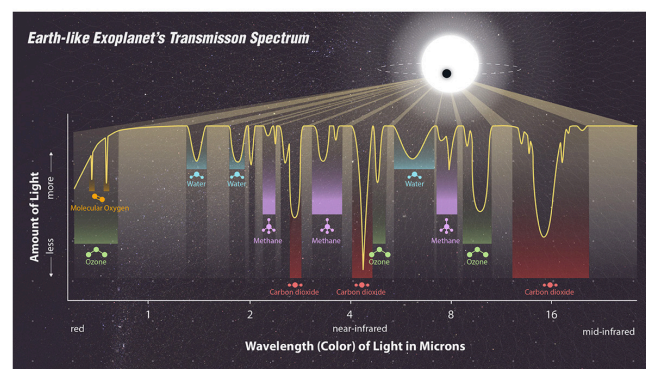


Figure 1: A simulated mid-infrared transmission spectrum of an Earth-like exoplanet as it transits its host star. The dips in the yellow curve indicate the wavelengths where molecules like oxygen, ozone, water, methane, and carbon dioxide absorb starlight. These features demonstrate how different molecules absorb starlight at specific wavelengths, allowing astronomers to identify different chemical signatures in exoplanet atmospheres. Figure credited to J. Olmsted.⁹

The measurement of such chemistries in space is not trivial. Chemistry beyond the solar system can be measured in various ways. Many modern Earth-based and satellite-based telescopes are equipped with spectrometers designed for astronomical observations. Spectrometers are instruments that can analyze the

light emitted, absorbed, or scattered by astronomical objects, which can reveal crucial information about their composition, temperature, velocity, and more. These devices collect discrete samples of light across different wavelengths or frequencies, similar to how a prism splits white light into discrete visible base colors.¹⁰⁻¹³ Transmission spectroscopy utilizes spectrometers to analyze the composition of an exoplanet's atmosphere by studying the starlight that passes through the exoplanet's atmosphere during a transit, which is when the planet crosses in front of its star. This process is depicted in Figure 1.

Spectral units are used to quantify and describe the properties of light: wavelength is commonly utilized as the independent variable, and the percentage of transmitted light is measured in response, which is derived from dividing the spectrum in transit by the spectrum out of transit, removing the stellar spectrum and leaving the transmission from just the exoplanet atmosphere. Such atmospheric spectral data can reveal a variety of information about the exoplanet, particularly its chemical composition, which is central to the analysis in this study. This is because spectral bands and lines emerge from the vibrational spectra and atomic structure of a molecule.¹⁴ Figure 2 shows an example spectrum of a molecule, polysaccharide, displaying that different atomic bonds (e.g., the hydrocarbon C-H bond) can vibrate at distinct energies, which are absorbed by the spectral light, resulting in a spectral band related to each molecular fingerprint. Laboratory spectroscopy in the 1-15 micrometer range can help measure atomic spectral lines for organic molecules in astrophysical sources,¹⁵ allowing for accurate observation of the chemical processes within an extraterrestrial atmosphere. In recent times, high-resolution spectroscopy has enabled the better detection of carbon molecules in exoplanetary atmospheres, especially using near-infrared spectroscopy.¹⁶ Therefore, specific carbon bonds can be identified due to their difference in vibration energies, resulting in different spectral bands, which have helped scientists identify many carbon-bearing species in space.¹⁷

There exist numerous databases on the internet containing diverse spectral data of exoplanets; some examples include the Exoplanet Atmospheric Spectral Library (CREATES),¹⁸ Stellar Planet Transmission Spectra Archive,¹⁹ and the Virtual Planetary Laboratory's Spectral Database and Tools.²⁰ These datasets may vary widely in their characteristics, including the wavelengths covered, the number of data points, resolution, and even the type of spectrum recorded. Such variability arises because spectral data can be collected using different instruments, energy ranges, and observational techniques. NASA's Exoplanet Archive is chosen as the focus of this study due to its comprehensiveness, reliability, and integration with other space mission data, widely established as the most extensive repository of exoplanet spectra. However, there exists only a small subset of the data that is relevant to this study. Not all spectrometers are suited for the study of carbon chemistry in space, as carbon bond vibrations are primarily detectable in the infrared.

This study aims to quantitatively analyze and determine how suitable existing astronomical datasets from various in-

frared spectrometers are for the study of carbon chemistry in exoplanet atmospheres. Near to mid-infrared spectral data were obtained from NASA's Exoplanet Archive, loaded and processed using Python, and then classified based on suitability for the study of carbon-related vibrational bonds. The hypothesis is that spectral datasets from exoplanets are limited and not entirely targeted to the study of organic processes in exoplanet atmospheres. This quantitative study aims to identify hypothesized shortcomings of current datasets and guide future instruments of design parameters that are better suited for studies of carbon chemical processes in exoplanet atmospheres.

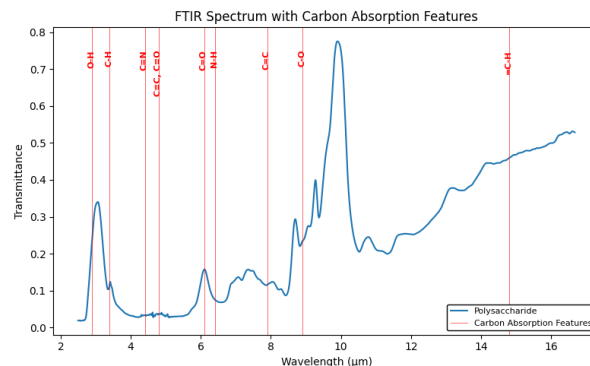


Figure 2: The infrared spectrum of polysaccharides: the most common organic structures in organic chemistry, shows light transmittance as a function of wavelength (μm). The spectrum illustrates the presence of various functional groups associated with the chemical structure of the organic species, providing insights into their chemistry and bonding characteristics. Additionally, the red vertical lines highlight the key carbon bond absorption features. Spectrum credited to Github.²¹

■ Methods

Data Collection:

Spectral data for the analysis were obtained from NASA's Exoplanet Archive, focusing only on exoplanets with publicly available transmission spectra within the infrared (IR) range. Only datasets containing greater than ten significant data points were considered to ensure validity. The near to mid-infrared range (1-15 μm) was selected due to its relevance in detecting chemical bonds, critical to this analysis. The absorption of IR light allows for the identification of the vibrational modes of carbon-based molecules, which are crucial in distinguishing carbon molecules present in exoplanetary atmospheres. A total of 75 spectra were collected for this study, primarily originating from instruments aboard the James Webb Space Telescope (JWST). We note that we did not consider eclipse or direct imaging datasets, but these could be considered in the future.

To confirm the completeness of the datasets, previously mentioned spectral databases like CREATES, the Stellar Planet Transmission Spectra Archive, and the Virtual Planetary Laboratory's Spectral Database were reviewed. No additional infrared spectra relevant to this study were found beyond those available in NASA's Exoplanetary Archive.

Data Loading and Processing:

The data was imported and analyzed using Python, utilizing the Astropy library, supplementing additional astronomy-specific Python packages necessary for data manipulation and analysis. The following preprocessing steps were conducted.

Data Pack Installation: Using Astropy (v6.1.6),²²⁻²⁴ NumPy (v1.26.4),²⁵ and SciPy (v1.13.1),²⁶ the Specutils package (v1.19.0)²⁷ is retrieved and installed. The NumPy library is imported for numerical computations, and the supplemental units module from the Astropy library is imported. Within the Specutils package, the Spectrum1D class is imported specifically to represent 1D spectral data.

Data Standardization: All spectra were carefully calibrated and normalized to consistent units of wavelength and flux density. Wavelengths are set in micrometers (μm) using Astropy's unit handling tools. Flux values, originally provided as transit depth in percentage, were, in this case, converted to a dimensionless form by dividing the values by 100. Transit depth represents the fractional decrease in stellar flux during the transit of a planet. This standardization allows for consistent comparison across datasets from different instruments.

Data statistical analysis:

A reference list of molecular vibrational modes relevant to carbon chemistry in the infrared range was compiled and referenced in Figure 2. These modes were identified based on each molecule's specific characteristic absorption features within the 1-15 μm range. These bands are chosen based on their simplicity and possible correlations with biosignatures. Some vibrational modes include carbon-hydrogen stretching vibrations, carbon-carbon bond stretches, as well as overtones and combinations specific to organic molecules. This list of molecules we find of note includes:

1. Oxygen-Hydrogen (O-H) Stretch - 2.9 μm
2. Carbon-Hydrogen (C-H) Stretch - 3.4 μm
3. Carbon-Nitrogen (C \equiv N) Triple Bond Stretch - 4.4 μm
4. Carbon-Carbon (C \equiv C) and Carbon-Oxygen (C=O) Triple Bond Stretch - 4.8 μm
5. Carbon-Oxygen (C=O) Double Bond Stretch - 6.1 μm
6. Nitrogen-Hydrogen (N-H) Stretch - 6.4 μm
7. Carbon-Carbon (C=C) Double Bond Stretch - 7.9 μm
8. Carbon-Oxygen (C-O) Stretch - 8.9 μm
9. Carbon-Hydrogen (=C-H) Bending Mode - 14.8 μm

This reference was derived from established molecular databases and spectroscopic literature, which are used to identify characteristic absorption features within the spectra. Accordingly, each spectrum was analyzed to identify the presence and intensity of molecular vibrational features corresponding to carbon-based molecules. We determined the number of carbon-related bands of the nine listed above that are covered by the wavelength range of each spectrum in question. Any spectrum whose wavelength range overlaps more than three distinct carbon-related vibrational bands from the reference template, contains greater than ten data points, and exceeds the range threshold of 2.9 microns is noted.

Results and Discussion

The spectral data were obtained from NASA's Exoplanet Archive and filtered as described in the previous section. Of

the remaining spectra after filtering for those of interest, the only represented instruments are those aboard JWST: Near Infrared Spectrograph (NIRSpec), Near Infrared Imager and Slitless Spectrograph (NIRISS), and Near Infrared Camera (NIRCam). Filtration resulted in only 75 spectra that are viable for this study. This is only 8.23% of the 911 total available spectra within NASA's Exoplanet Archive as of December 2024.

Figure 3a involves a set of 75 spectra, only 39 exist with more than 100 data points, leaving only 52% of the subset applicable to the analysis of carbon features. The greater the resolving power of a spectrum, the more accurate, the more clearly carbon absorption features can be identified, as higher resolution allows sharper and more distinguishable spectral features. Resolving power is defined as:

$$R = \frac{\lambda}{\Delta\lambda}$$

where λ is the central wavelength and $\Delta\lambda$ is the smallest difference in wavelength the instrument can distinguish at that wavelength. This relative measure of resolution is commonly used in spectroscopy to express how precisely an instrument can resolve fine spectral details. In this study, resolving power was estimated by computing the inverse of the median spacing between adjacent wavelength values in each spectrum. Figure 3b demonstrates a highly accurate positive linear correlation, with $R^2=0.884\%$, between the resolving power and the number of data points present in a spectrum. Low resolving power results in the natively narrow spectral features being spread across a wider wavelength range, which results in a shallower absorption depth and more difficult line identification that may cause the signal to dip below background noise levels, or may blend the lines together and make their identification less certain. These carbon vibration bands have many sharp and localized lines at specific wavelengths, making high resolving power optimal for reliable identification. Ultimately, while NASA's exoplanet database includes promising datasets for the study of carbon chemistry, only 39 filtered datasets with high resolution, which lies only a small percentage of the overarching dataset with 911 accessible spectra. This shows only 4.28% of the total datasets are of relevance to the detection of

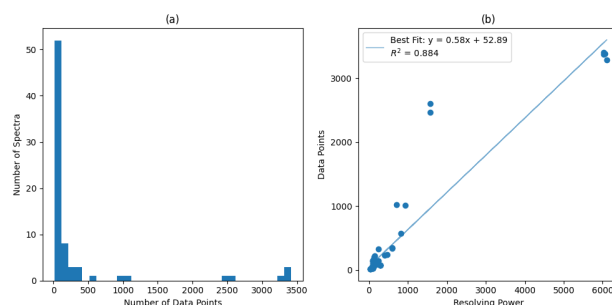


Figure 3: (a) Histogram depicting the distribution of the data points across the dataset, showing that the majority of spectra contain fewer than 500 data points. (b) Scatter plot demonstrating the positive correlation between the resolving power of each spectrum (wavelength/change in wavelength) and the number of data points, with a linear regression fit ($R^2=0.884$) indicating a relatively strong relationship. The high correlation emphasizes the

dependence of spectral resolving power on the quantity of data points, which is crucial for accurate carbon feature identification.

carbon chemistry in exoplanet atmospheres, exemplifying the constraints in current instrumentation.

The NASA Exoplanet Archive comprises data over various energy ranges, and this study focuses on the near to mid-infrared range due to the vibration of carbon bonds. Figure 4 presents a power distribution of the percentage of datasets containing bands in the 2-15 μm wavelength range. The higher the wavelength, the lower the power; therefore, the fewer the spectra containing such power range. The green dotted line represents a cumulative histogram, highlighting a few significant drops in data. By the wavelength of 2.7 microns, approximately 13.33% of the data have been excluded. The most significant drop in the number of datasets is at 5 microns, with only 8.00% remaining. Most carbon bands are outside the range of detection, which emphasizes the exclusiveness of the database, especially for studies based on carbon-bond detection. There are ten useful carbon bands within the 2-15 μm range of detection; these include the O-H band at 2.9 μm , the C-H band at 3.4 μm , C \equiv N at 4.4 μm , C=C and C=O at 4.8 μm , C=O at 6.1 μm , N-H at 6.4 μm , C=C at 7.9 μm , C-O at 8.9 μm , and =C-H at 14.8 μm . The carbon absorption features represented in red demonstrate the specific wavelength ranges in the electromagnetic spectrum that correspond to a specific vibrational mode of a molecular bond. This is crucial because these bonds are key components of complex organic molecules found in interstellar environments. Additionally, the band with the lowest absorption feature is the O-H band, occurring at approximately 2.9 microns. The cumulative histogram reveals that 21.33% of the spectra do not exceed the wavelength of 2.9

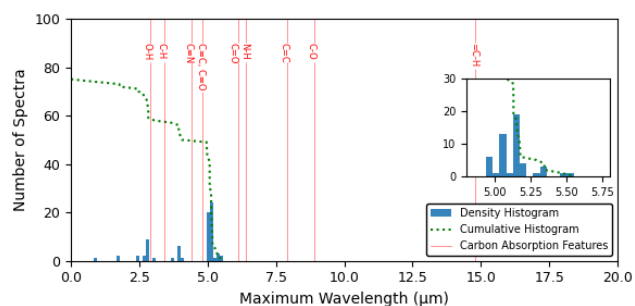


Figure 4: Density histogram of the maximum wavelength of each spectrum, overlaid with a cumulative histogram to illustrate the distribution of spectral coverage. Results indicate that the majority of the spectra are exclusive of wavelengths greater than 5.75 μm . An inset zooms in on the region containing the majority of the data for greater clarity. Red vertical lines indicate key carbon bond absorption features, highlighting the spectral regions relevant to carbon chemistry analysis.²⁰

microns, and are thus useless for carbon band detection.

Based on absorption feature coverage, resolution, and wavelength range, the top datasets from NASA's Exoplanet Archive of Atmospheric Spectra include K2-18b,²⁸ LHS 475 b,²⁹ and WASP-96 b.³⁰ These data all originate from NASA's 6.5-meter JWST, in 2023, though the instrument utilized differs. Therefore, it can be inferred that datasets most suitable for the measurement of carbon chemistry in space originate from more recent studies, especially those from the JWST facility,

due to its highly advanced and specific instruments designed for high-sensitivity infrared observations, enabling the detection of these features in unprecedented detail. Studies in more recent times are becoming more promising for carbon band detection in exoplanet atmospheres due to new space missions, improved telescopes, and new spectroscopy techniques. The JWST has had propitious breakthroughs in its infrared sensitivity with unprecedented resolutions through its Mid-Infrared Instrument (MIRI) and NIRSpec.³¹ The detection of these bands will allow for the analysis and modeling of organic molecules in space. Finally, the limited range of carbon bonds detectable within the energy range offered by the NASA Exoplanet Archive demonstrates its finite relevance to detecting carbon chemistry. We propose that the ideal wavelength range for carbon detection is between 2.9 microns extending past 8.9 microns, which would encompass the spectral features from the bonds considered above. The data presented is sufficient to confirm detections of carbon in exoplanetary environments, but inadequate for the detection of specific carbon species. This is due to the limited resolution of a spectrum. While most of the spectra contain enough data points to reveal the presence of carbon species through the identification of peaks, they often lack the resolving power necessary to distinguish between closely spaced or overlapping spectral features. For example, the detection of two peaks with nearby peak wavelengths is detectable with a relatively lower resolving power. The N-H and C=O features, located at 6.4 and 6.1, respectively, are separated by 0.3 microns. Using the resolving power formula introduced earlier, this yields a required resolving power of approximately $R=21$ to distinguish them. On the other hand, the detection of carbon features that are virtually overlapping would require a resolving power of greater than $R=1,000$ to be distinguished accurately, like that of the C=C and C=O bonds. However, not all instruments considered in this study meet this threshold. The NIRISS/WFSS and NIRSpec/PRISM instruments, for example, have relatively low resolving powers of approximately 150 and 700, respectively. In contrast, instruments such as NIRSpec/M, NIRSpec/H, and NIRCам/WFSS offers significantly higher resolving powers of around 1000, 2700, and 1120-1680, respectively.³² Datasets best suited for the measurement of carbon chemistry would have high resolving power to distinguish closely spaced emission lines, broad spectral range coverage to capture an adequate number of carbon bands, and a high signal-to-noise (SNR) ratio to ensure reliable detection of weak signals.

Ultimately, this research is limited in scope due to its sole coverage of NASA's Exoplanet Archive. Filtering the dataset according to the criteria listed in the Methods section XX results in a small number of spectra out of the full sample, showing the most datasets do not cover the ideal wavelength range we proposed for analyzing carbon chemistry. The required spectral data properties for detecting carbon species include broad wavelength ranges, high SNR, and high resolution. Achieving these data properties remains a significant challenge due to a gap in current instrumentation. The gap between ideal and current detection conditions highlights the

strategies to enrich our current understanding of extrasolar organic molecules. It is crucial to recognize these limitations to underscore the importance of interdisciplinary efforts to refine observational techniques, expand coverage, and improve modeling approaches to ameliorate future research in extrasolar carbon chemistry.

A hypothesis for the limitation of data greater than five microns is mission and telescope constraints. Many telescopes do not have instruments with mid-IR capabilities. Missions may choose to focus on the near-infrared range, as these shorter wavelengths can significantly improve the accuracy and precision of estimations and measurements of data.³³ For example, the Spitzer Space Telescope originally had mid-IR capabilities before its coolant ran out, causing it to operate only in the near-IR range.³⁴ Observing with MIR instruments results in large data volumes due to the nature of the detector readout, which also requires intense computing capabilities and sensitivity to thermal background noise, which then requires intensive cooling. All of these add complexity to operating in the mid-IR. Moreover, another reason for this gap is instrumental limitations. High spectral resolution has not yet been achieved; sending high-resolution spectrometers ($R > 10,000$) into space is not yet possible due to payload weight limitations, and thus these instruments are currently limited to ground-based telescopes. Earth's atmosphere absorbs infrared radiation beyond 5 microns due to the presence of water vapor, carbon dioxide, and other gases, a phenomenon known as telluric absorption.³⁵ This significantly hinders the ability of ground-based telescopes to observe in the MIR, where even locations at high altitudes or dry sites leave deep absorption features that obscure the spectral signals of interest. Another possible reason for this limitation is the relationship between the SNR and the detection wavelength.³⁶ As the detection wavelengths increase, the SNR decreases due to thermal radiation from telescopes, instruments, and even interstellar dust. It is difficult to build and maintain a high-resolution detector due to engineering challenges, heat and thermal noise during data collection, large data volumes and processing power, as well as cost and material constraints. Ultimately, understanding these limitations is crucial for improving observational strategies and instrument design. Potential solutions to bridging this gap include further advancements in space-based infrared telescopes, enhanced cooling mechanisms, and higher-sensitivity detectors. Future missions like the Habitable Planets Observatory,³⁷ the Large Ultraviolet Optical Infrared Surveyor,³⁸ the Origins Space Telescope,³⁹ and next-generation technologies will play a crucial role in expanding our ability to study carbon chemistry in extrasolar environments, allowing us to enhance our understanding of molecular processes and the identification of complex organic compounds in exoplanetary atmospheres.⁴⁰

■ Conclusion

We reviewed the detectability of carbon species in exoplanet transmission spectra by comparing current instrument capabilities to the wavelength coverage and sampling needed. Although SNR is a critical factor in spectral analysis, its impact was not directly investigated in this study. Ultimately, the majority of spectra available on the NASA exoplanet ar-

chive are not of relevance to carbon band detection due to two main constraints: limited wavelength range and low resolving power. We discuss ideal conditions for carbon detection, which would encompass broad and optimal wavelength ranges, high SNR, resolution, and detector sensitivity. Such conditions are arduous due to engineering challenges and budget constraints. Nonetheless, bridging this gap in our detection of carbon-chemistry and its analysis in exoplanets are acute as more and more exoplanets are being detected and analyzed. This study provides valuable insights for the advancement of future spectral detectors, as well as aiding future exploration of extraterrestrial carbon chemical processes. Studying the carbon chemistry in these interstellar environments will allow us to enhance our understanding of Earth-like worlds beyond as well as our own.

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