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The Detection-vs-Retrieval Challenge: Titan as an Exoplanet

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ABSTRACT

Cassini's observations of Titan's atmosphere are exemplary benchmarks for exoplanet atmospheric studies owing to (1) their precision and (2) our independent knowledge of Titan. Leveraging these observations, we perform retrievals (i.e., analyses) of Titan's transmission spectrum to investigate the strengths/limitations of exoplanet atmospheric retrievals with a particular focus on the underlying assumptions regarding the molecular species included in the retrieval. We find that multiple hydrocarbons can be "retrieved" depending on the selection made ahead of a retrieval. More importantly, we find that the estimates of other parameters such as the abundance of key absorbers like methane can be biased by ∼0.5 dex (by a factor of ∼3) due to such choices. This shows that beyond the possible misidentification of a molecular feature (e.g., current debate surrounding dimethyl sulfide, DMS, in K2-18 b), the implicit molecular detections made pre-retrieval to avoid retrieving for hundreds of molecules at a time can bias a large range of parameters. We thus recommend sensitivity analysis to assess the dependencies of atmospheric inferences on such selections in tandem with complementary information (e.g., chemistry models) to support any pre-retrieval selection. Finally, we introduce an independent path to constrain the dominant atmospheric constituent, even when lacking observable absorption feature (e.g., H_2 and N_2) through the scale height.

Keywords: Transmission Spectroscopy, Titan, Exoplanet

1. INTRODUCTION

Titan hosts a complex and high metallicity atmosphere, blanketed by haze (Kuiper 1944; Hörst 2017). The pervasive haze gives Titan its characteristic orange hue. The Visual and Infrared Mapping Spectrometer (VIMS, Brown et al. 2004) onboard Cassini performed high-fidelity observations of Titan's atmosphere using solar occultations (Robinson et al. 2014). Cassini's observations represent an aspirational precision goal for future exoplanet atmospheric studies. The data hence presents an opportunity to investigate forthcoming roadblocks in interpreting exoplanet atmosphere data from new observatories such as JWST, as data will become more informative, and extracting robust scientific inferences increasingly depends on our ability to build high-fidelity models. When it comes to building a representative transmission model of an atmosphere, there are multiple dimensions to consider. Interpretation of transmission spectroscopy requires building climate models, understanding chemical pathways, characterizing detector performance, to understanding the stellar background - numerous factors that add to our modeling error budgets.

In this study, our primary focus is to leverage Titan's precise transmission spectrum and our existing knowledge of its atmosphere to investigate the strengths/limitations of exoplanet atmospheric retrievals. We focus particularly on the underlying assumptions made regarding what molecules should be retrieved for. This focus is timely owing to existing concerns associated with the possible misinterpretation of molecular features (e.g., with DMS in K2-18, Madhusudhan et al. 2025; Welbanks et al. 2025; Luque et al. 2025) and aims to assess if the impact is limited to inferences associated solely to the spectroscopic feature(s) in question or can lead to a bias on other atmospheric properties.

We present the Cassini data used in Section 2 and the models and retrieval framework in Section 3. The core findings of our retrievals for this application are given in Section 4 with details in the Appendix. We discuss our findings in Section 5 and conclude in Section 6.

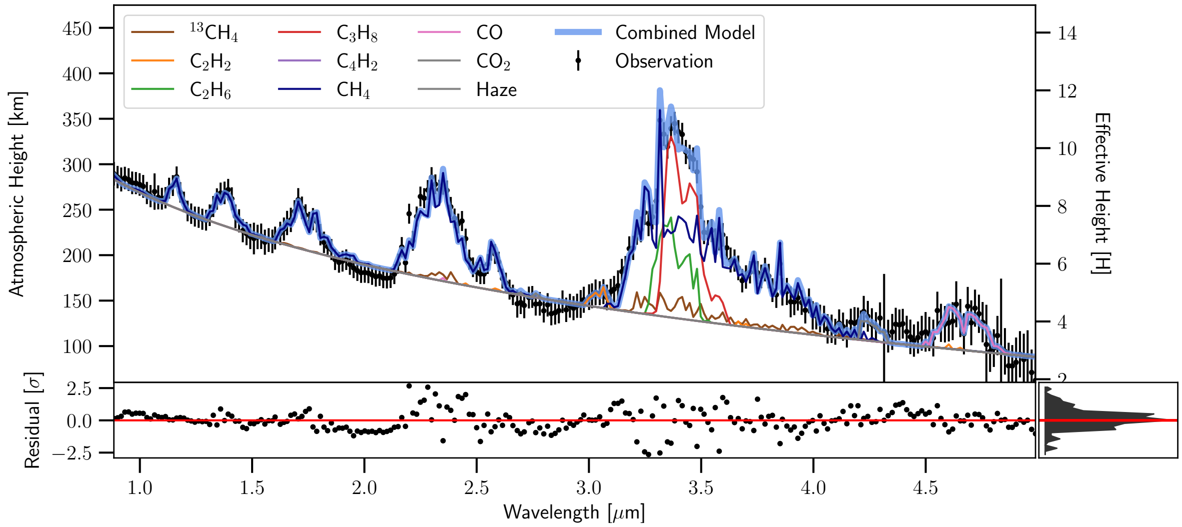

Figure 1. A family portrait of hydrocarbons in Titan's transmission spectrum obtained with Cassini/VIMS. Best fit model (thick blue line) to Titan's spectrum obtained during visit T10 (see Table 1) from Robinson et al. (2014), together with the individual contribution of different absorption molecules (see legend) included in the present retrieval (here, case 25, see Table 3). The best-fit residuals are reported as a function of scaled error together with their distribution in the bottom panels.

2. OBSERVATIONS

Robinson et al. (2014) converted the VIMS observations of attitudinal transmission spanning from 0.88 μm to 5 μm into transmission spectra by numerically integrating over the line of sight. We use these datasets in performing retrievals. However, our retrievals are run individually on four datasets from three visits by Cassini as listed in Table 1.

3. MODELS AND RETRIEVAL FRAMEWORK

We run the publicly available transmission code `tierra` (Niraula et al. (2022) adapted from de Wit & Seager (2013). It uses a 1D formulation of the transmission spectroscopy commonly used in exoplanetary retrievals. Previous work by Robinson et al. (2014) has shown that the impact of the refraction for Titan is minimal. Our retrievals are run with an assumption of an iso-mixture profile with no chemistry constraints. It also assumes an isothermal profile owing to the fact that transmission spectroscopy primarily probes pressure levels beyond 100 mbar corresponding to small temperature changes for objects far from their host star such as Titan. For the system parameters, we fix the mass to 0.0225 $M_\oplus$ and radius to 0.404 $R_\oplus$ adopted from NASA fact sheet[1].

3.1. *Molecular Species*

To assess the effect of *a priori* molecule/model selection on the inferences reached, we perform our study using a series of molecular subsamples. These molecules are selected taking into account the independent knowledge from Titan's atmosphere obtained from higher-resolution data (see Table 2). The 25 sets of molecules are introduced in Table 3. As an example, in case 17 we fit for the abundances of CH_4, CO, CO_2, N_2 (the "Base Combination"), C_2H_6, C_3H_8, and C_2H_2.

3.2. *Opacity cross-sections*

We use HITRAN2020 (Gordon et al. 2022) line lists to calculate absorption cross sections for all molecules of interest except for propane, for which no line-by-line list exists in HITRAN. Thus, following (Cours et al. 2020) we use the pseudo-line list for propane provided by Dr. Geoffrey Toon (JPL NASA)[2], which are based on the high-resolution laboratory measurements of Harrison & Bernath (2010) that span the 3 μm region (i.e., 2560-3280 cm^{-1}). Cross sections for each molecule were calculated for a temperature range of 70 to 400 K with a stepsize of 14 K. As for the pressure, the same grid as (Niraula et al. 2022) was used.

3.3. *Haze opacity model*

Titan has a permanent, though temporally varying, haze layer that prominently impacts transmission spectroscopy (Lavvas et al. 2011; Robinson et al. 2014). Haze not only shrouds the surface, but it also mutes the transmission spectrum (see Figure 1). We use a similar formulation for the haze as in Robinson et al. (2014), as-

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[1] https://nssdc.gsfc.nasa.gov/planetary/factsheet/saturniansatfact.html [2] https://mark4sun.jpl.nasa.gov/pseudo.html

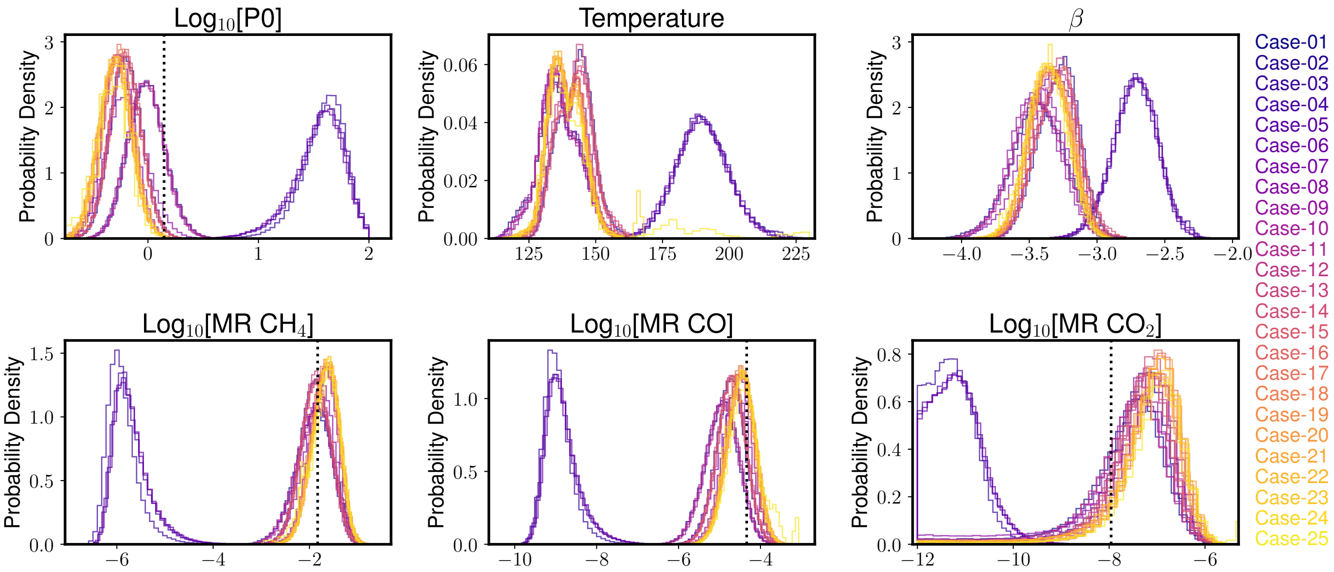

Figure 2. Atmospheric inferences are sensitive to the molecules retrieved for. Posterior distribution of the base atmospheric parameters for an ensemble of 25 "sets", associated with different selections of molecules retrieved (see Table 3). The "truths" reported in Table 2 are shown in the black dotted lines. Except for acetylene and carbon dioxide, the retrieved molecular values are generally consistent within 2σ of previously reported values. Given the precision of the data, some extreme cases can be rejected. This is in particular the case of sets 3, 4, 5, and 6 that do not select a molecule with a sharp absorption feature at the center of the 3.3 μm band forcing large compensations on the abundance of methane and other parameters while still leading exceedingly large structures (~50 km vs ~5 km otherwise) in the residuals (see Figure 6). All other models lead to consistent fits and reveal that biases of ~0.5 dex can be expected on the abundance of dominant absorbers such as methane.

suming a wavelength-dependent power-law which is coupled with the atmosphere through the scale height (H) as $\tau(\lambda) = \tau_0 \cdot (\lambda)^{\beta} \cdot \exp\left(\frac{-z}{H}\right)$, where τ_0 is the normalization factor, λ is the wavelength in microns, β is the power-law coefficient, z is the height of the atmosphere from the reference radius, and H is the atmospheric scale height.

3.4. *Retrieval Framework and Uncertainty Budget*

We use the retrieval framework introduced in Niraula et al. (2022) using the *emcee* library. To account for sources of noises/uncertainties beyond the photon noise (e.g. instrumental systematics, imperfections in the opacity model, etc.), our framework maximizes the log of the likelihood (e.g., Carter & Winn 2009).

4. RESULTS

We present the results in this section that pertain to the detection-vs-retrieval challenges. More details on the ensemble of results are provided in the Appendix.

4.1. *What is Detectable Affects What is Retrieved*

As shown in Figure 2, the choice of a subset of atmospheric compounds to be retrieved (i.e., deemed "detectable") has an impact on more than the inference directly associated with them (such as their detection, their abundances, etc.). We find in particular that even the abundance of dominant species such as methane, can be affected by the selection of molecules included in the retrieval as they can jointly contribute to the same spectral range, while the data can be understood to zeroth-order as keeping the sum of their cross-sections constant.

Given the precision of the data, some extreme cases can be rejected. This is in particular the case of cases 3, 4, 5, and 6 that do not select a molecule with a sharp absorption feature at the center of the 3.3 μm band forcing large compensations on the abundance of methane and other parameters while still leading exceedingly large structures (~50 km vs ~5 km otherwise) in the residuals (see Figure 6 in the Appendix).

Yet, among the retrievals that provide equivalent best fits, we find that the abundance of strong absorbers such as methane can be biased by ~0.5 dex (i.e., a factor of 3) and the temperature by up to 20 K.

5. DISCUSSION

5.1. *On the Similarities of Opacity Cross-Sections*

When obtained at high-resolution, high-SNR, and over a wide wavelength range, spectral information (e.g., in the form of cross-sections) can help identify compounds in exoplanet spectra. In the current observations, however, the information content of the 3-3.5 μm band can be associated with hundreds of hydrocarbons as this absorption feature is a consequence of the vibra-

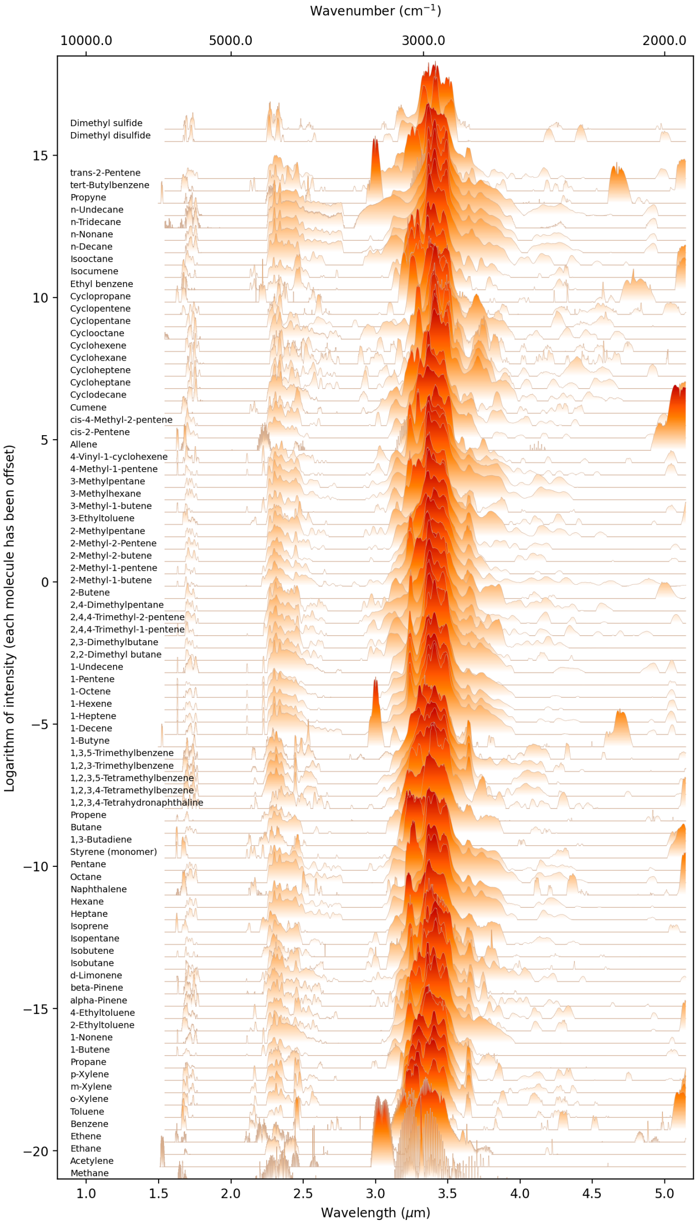

Figure 3. Molecules may have many lookalikes. Overview of the absorption cross sections for hydrocarbons taken from PNNL (Sharpe et al. 2004) and included in HITRAN2024 database (Hargreaves et al. 2025). The y-axis provides the logarithm of intensity, with each absorption cross section offset for display purposes. A minimum intensity of 1.0×10^{-21} cm^2/molecule has been applied for each molecule.

tional mode related to stretch of the C-H bonds. Figure 3 presents infrared absorption cross sections for a set of hydrocarbons (and also dimethyl sulfide and dimethyl disulfide) taken from Pacific Northwest National Laboratory (PNNL) (Sharpe et al. 2004) and now included in HITRAN2024 (Hargreaves et al. 2025) (see further details in Figure 9 in the Appendix). As shown, this selection of molecules mostly provide degenerate absorption features over the spectral range of Figure 1, with additional combination and overtone bands near 2.2-2.6 μm and 1.5-1.7 μm. In addition, these largely align with the signatures of DMS and DMDS due to the C-H bonds of the methyl group.

When molecules can contribute to the same spectral band, one can consider that, to the zeroth order, a retrieval constrains the sum of their absorption. Which molecules are chosen pre-retrieval to contribute to a spectral feature thus affects how much weight (i.e., abundance) is attributed to the others (as pointed out also by Cours et al. 2020), explaining the biases introduced in subsection 4.1.

A careful assessment of the ensemble of molecules matching detected spectral features is thus necessary. Complementary insights (e.g., from atmospheric chemistry) can/should be used to reduce the range of possibilities. Then detailed sensitivity analysis is recommended to assess the dependencies of atmospheric inferences on such selections.

5.2. *A Special Case: Background Gas Identification*

Nitrogen makes up the bulk of Titan's atmosphere and yet does not exhibit prominent absorption features in its spectrum. As a result, the major constituents of Titan's atmosphere were debated for more than a decade, until a mixture of nitrogen and methane was suggested based on arguments of Jean's escape and spectroscopic observations (Hunten 1973). Such conclusions were arrived at through models taking advantage of spatially resolved temperature measurements. Therefore, when it comes to distant terrestrial worlds, identifying the underlying background gas will likely be difficult though not impossible—e.g., through weak collision-based absorption (CIA) features (Kaltenegger et al. 2020).

Fortunately, retrievals from transmission spectra can yield a strong constraint on the atmospheric pressure scale height that, combined with independent constraints on the object's mass and radius, can yield the mean molecular mass as an indicator of the main atmospheric compound. de Wit & Seager (2013) had previously demonstrated that the atmospheric scale height, temperature, and composition can be constrained independently from transmission spectroscopy–which can yield constraints on the planetary mass. Amongst the synthetic scenarios explored, de Wit & Seager (2013) included cases where the dominant atmospheric constituent was a weak absorber (such as H_2 and N_2), yet either their scattering slope or their CIA was detectable because no very hazy cases were explored, leading to a tight constraint on the mean molecular mass.

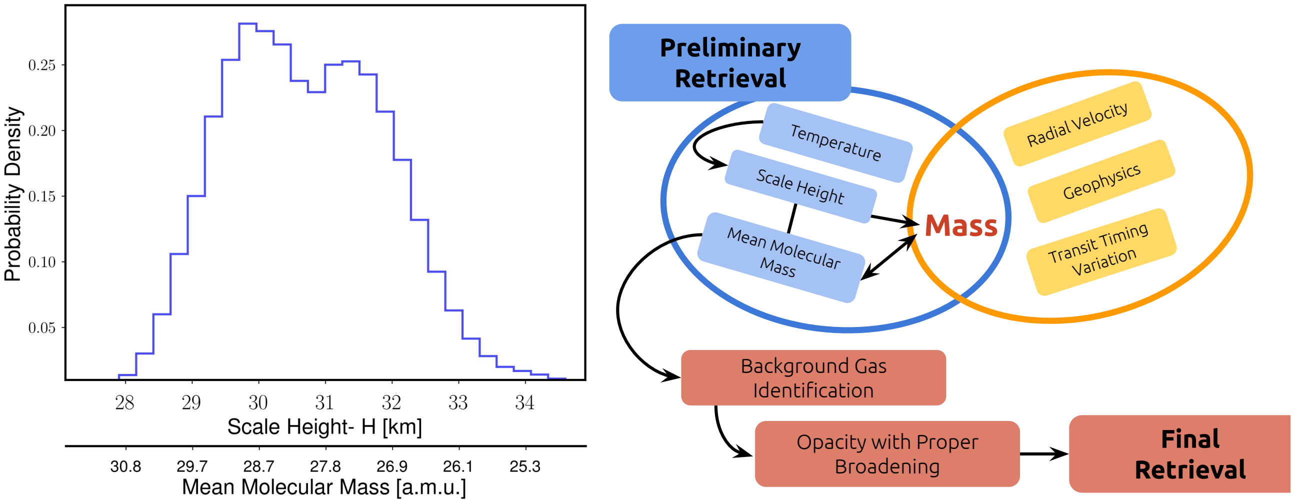

Figure 4. Background gas identification via constraints on the scale height from transmission spectroscopy. **Left:** PPD of Titan's atmospheric scale height yielded by its transmission spectrum (consistent with the stratospheric value). **Right** Framework to yield robust abundances for terrestrial planets using iterative retrievals through identification of background gas.

Our retrievals yield $H = 30.6 \pm 1.6$ km consistent with Titan's stratospheric scale height (Figure 4). Combined with Titan's gravity, this translates into a constraints on a mean atmospheric molecular weight of 27.8 ± 1.8 a.m.u ($\mu = kT/gH$, with k Boltzmann's constant, T the local temperature, g the local gravity, and H the scale height). As none of the strong absorbers identified are dominant compounds (abundances $<<$ 10%), the most likely weak-absorber gas matching the derived molecular weight is nitrogen.

For exoplanet atmospheric studies, we thus suggest following an iterative retrieval process (see Figure 4). This involves first inferring the background gas through scale height (with complementary insights form radial-velocity measurements and/or transit-timing variations were possible), and using the inferred background gas for subsequently generating high(er)-fidelity opacity models (e.g., with adequate broadening parameters, Niraula et al. 2022; Wiesenfeld et al. 2025).

We note that for a large regime of planets, distinguishing between a light (e.g., H_2) and a heavy (e.g., N_2) weakly-absorbing dominant atmospheric component will be possible without independent knowledge on the planetary mass. This is enabled by the fact that their mean molecular weights are one order of magnitude apart. Therefore, for a given scale height constrained via transmission spectroscopy, they each relate to a planetary mass also separated by an order of magnitude – and one of them is likely nonphysical (marked as "Geophysics" in Figure 4). In the present case, without any *apriori* knowledge about Titan's mass, from its atmospheric scale height and temperature alone, one can reject a low-μ atmosphere as it would imply a mass 10 times its actual mass, meaning a density ∼3.5 times Earth's, which is non-physical.

6. CONCLUSION

The high-fidelity data from and independent knowledge of Titan can be used to contextualize characterization frameworks in the new era of exoplanetary data. We found in particular that:

1. The choice of molecules retrieved for in exoplanetary studies can lead to significant biases (0.5-0.75 dex) on the abundance of constituents associated with overlapping absorption features.

2. Titan's transmission spectrum being anchored (from an information standpoint) by the 3.3 μm feature is a challenge when combined with the fact that hundreds of hydrocarbons (amongst other molecules) has a strong absorption feature in this region.

3. The last point, combined with the limited or scarce opacity data for "heavy" hydrocarbons (heavier than propane), is a bottleneck for performing retrievals in Titan's atmosphere, and will likely be for future exo-Titans.

4. We recommend a careful assessment of the ensemble of molecules matching detected spectral features, while leveraging complementary insights (e.g., from atmospheric chemistry) to reduce the

range of possibilities and, finally, performing a detailed sensitivity analysis to assess the dependencies of atmospheric inferences on the final ensemble of possible molecule/model selections.

5. Still, several molecules (methane, ethane, propane) can be consistently retrieved across four different epochs, and this despite the presence of a strong haze signature.
6. Finally, we show that identifying the dominant atmospheric constituents without relying on absorption features (e.g., for weak absorbers such as nitrogen or hydrogen) can be done through constraints on the scale height (and thus possible mean molecular weights) to support adequate opacity models (e.g., adequate broadening parameters) and a broader understanding of the planetary environment studied.

Facilities: Cassini
Softwares: `tierra`[3], `emcee`

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APPENDIX

A. ADDITIONAL RESULTS & DISCUSSIONS

We present here additional findings that are beyond the primary scope of this Letter and, yet, still of relevance to the community. This includes the visit-to-visit consistency of our findings, the effect and modeling of hazes, and parameter correlations.

A.1. *Findings Across 4 Visits*

Our retrievals specifically lead to detection of multiple hydrocarbons (CH_4, C_2H_6, C_3H_8, and C_2H_2), and CO (Figure 1). As shown in Figure 7, our retrieved parameters are consistent within 2σ with the values reported in the literature (Table 2). Across four different epochs (Table 1), the retrieved parameters yield relatively consistent insights.

The primary differences across visits relates to the haze parameters and the abundances of secondary components such as CO_2. As shown in Figure 5, the contribution of Titan's haze in visit T53 is significantly larger than in visit T10 leading to weaker spectral features (such as CO_2's 4.3 μm feature) to be muted. With the data at hand, we cannot attribute the changes in the abundances of C_3H_8 to variability in the atmosphere across visits or different pressure levels being probed due to the effect of hazes (the changes for C_2H_6 and C_2H_2 are not significant).

As we refer to a possible dependence of our findings to the pressure level probed, we note that acetylene (C_2H_2) is found with an abundance 3σ larger than "truth". We attribute this to the fact that acetylene is photochemically produced in the upper layers of the atmosphere (layers we are particularly sensitive to in transmission), leading to higher than real values when uniformly extrapolated to higher unprobed pressure regimes. Similarly, the abundance of methane is known reach as high as 5.65% ± 0.18% near Titan's surface (Niemann et al. 2010) while stratospheric oscillates around 1.48±0.09% (Hörst 2017) – consistent with our retrievals.

A.2. *Haze Profile*

Our current treatment of the haze profile with a single power law appears adequate for our retrievals. However, if we are to extend the transmission spectroscopy to the far ultraviolet (see Tribbett et al. (2021)), the current single power law fails to capture the opacity trend. Haze has a prominent impact on Titan's transmission spectra. It shows a clear spatiotemporal variation, which can be caused by seasonally varying atmospheric circulation patterns (Rannou et al. 2010). The strong molecular absorption features (such as from methane) are identifiable on the top of the hazes; however, hazes often dominate the absorption continuum, masking any weaker spectral features that could potentially have been observed in between the methane bands (e.g. CO).

A.3. *Correlation Among Parameters*

Figure 8 is a corner plot for Titan for visit T53 for the isothermal model for molecular set 7. A number of parameters show a strong correlation, including the haze normalization factor (τ_0), the power-law coefficient (β), and retrieved temperature (T_0). However, the retrieved molecules are uncorrelated with the hazes, showing that the strong absorbers in these atmospheres can still be characterized by their molecular features despite the presence of atmospheric hazes. The correlation among the abundances of retrieved parameters is driven by their dependency on the scale height (de Wit & Seager 2013; Niraula et al. 2022). The strongest correlation is seen between methane and propane, likely due to their overlapping spectral features. This is expected to be a concern, not just between methane and propane, but across hydrocarbon detections, many of which share spectral features associated with the C-H bond vibration and its overtones (Zhan et al. 2021). High spectral resolutions, combined with complete spectral information for all relevant hydrocarbons, are likely to be required to unambiguously distinguish their individual contributions to Titan's atmosphere, or any future observations of hydrocarbon-rich atmospheres.

B. ADDITIONAL TABLES & FIGURES

Table 1. Cassini/VIMS data adapted from Robinson et al. (2014) used in this work.

Cassini Flyby	**Season**	**Latitude**	**Date**
T10	N Winter	70° South	Jan. 2006
T53	Equinox	1° North	Apr. 2009
T78N1	N Spring	27°	North Sep. 2011
T78N2	N Spring	40°	North Sep. 2011

Table 2. Reported volume mixing ratios for molecules present in the atmosphere of Titan

Molecular Species	Volume Mixing Ratio	Source	Cross-section[§]
Nitrogen [N_2][†]	0.9839	Normalization	H20
Methane [CH_4][†]	0.0148	Niemann et al. (2010)	H20
Methane [$^{13}CH_4$][‡]	1.71×10^{-4}	Nixon et al. (2012)	H20
Carbon Monoxide [CO][†]	4.6×10^{-5}	Maltagliati et al. (2015)	H20
Ethane [C_2H_6][†]	1.5×10^{-5}	Coustenis et al. (2016)	H20
Propane [C_3H_8][‡]	1.5×10^{-6}	Coustenis et al. (2016)	NJPL
Acetylene [C_2H_2][†]	3.0×10^{-6}	Coustenis et al. (2016)	H20
Ethylene [C_2H_4][‡]	1×10^{-7}	Coustenis et al. (2016)	H20
Carbon dioxide [CO_2][‡]	1.1×10^{-8}	Coustenis et al. (2016)	H20
Diacetylene [C_4H_2][‡]	2.0×10^{-9}	Teanby et al. (2009)	H20
Benzene [C_6H_6][‡]	4.0×10^{-10}	Coustenis et al. (2016)	—

[†] Values as reported in Sylvestre et al. (2018)

[§] Where reference codes refer to: H20 – HITRAN2020 (Gordon et al. 2022), NJPL – NASA JPL pseudo-line list based on the measurements of Harrison & Bernath (2010)

Table 3. Sets of molecules used for the retrievals. Base Combination (CH_4+CO+CO_2+N_2).

Set	**Molecules**	**Set**	**Molecules**	**Set**	**Molecules+ C_2H_6 + C_3H_8**
1.	C_2H_6	9.	$C_2H_6 + C_2H_2$	17.	C_2H_2
2.	C_3H_8	10.	$C_2H_6 + C_2H_4$	18.	C_2H_4
3.	$^{13}CH_4$	11.	$C_2H_6 + C_4H_2$	19.	C_4H_2
4.	C_2H_2	12.	$C_3H_8 + {}^{13}CH_4$	20.	$^{13}CH_4 + C_2H_2$
5.	C_2H_4	13.	$C_3H_8 + C_2H_2$	21.	$^{13}CH_4 + C_2H_4$
6.	C_4H_2	14.	$C_3H_8 + C_2H_4$	22.	$^{13}CH_4 + C_4H_2$
7.	$C_2H_6 + C_3H_8$	15.	$C_3H_8 + C_4H_2$	23.	$^{13}CH_4 + C_2H_2 + C_2H_4$
8.	$C_2H_6 + {}^{13}CH_4$	16.	$C_2H_6 + C_3H_8 + {}^{13}CH_4$	24.	$^{13}CH_4 + C_2H_2 + C_4H_2$
				25.	$^{13}CH_4 + C_2H_2 + C_4H_2 + C_2H_4$

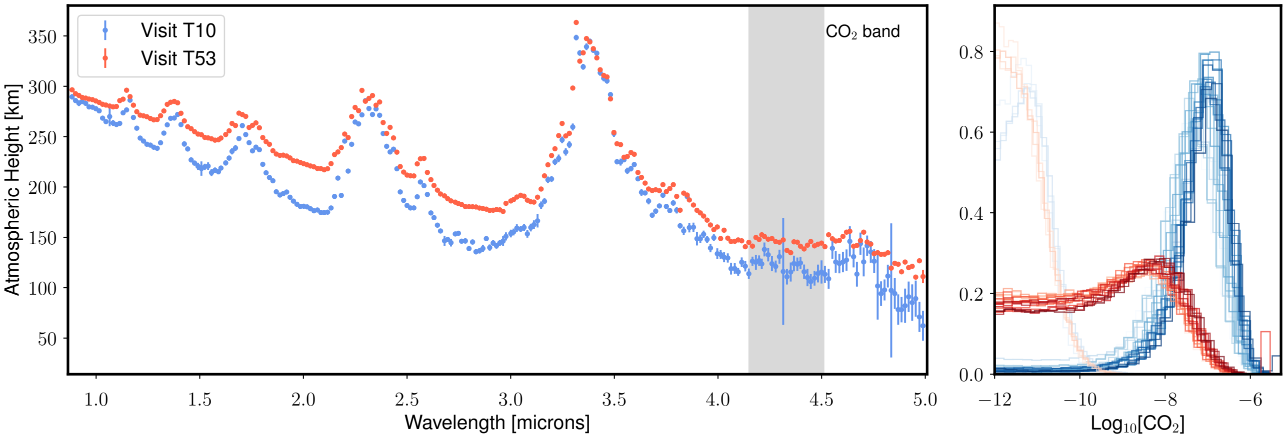

Figure 5. Weak absorption features muted during hazy epochs. **Left:** Titan's Transmission spectrum corresponding to two different visits (T10 and T53, see Table 1). T53 is affected by hazes to such an extent that weak absorption features such as CO$_2$'s at 4.3 μm are mostly muted. **Right:** Retrieved CO$_2$ mixing ratios for T10 and T53 showing that in the latter case the detection of CO$_2$ is significantly less significant due to hazes muting its 4.3 μm band.

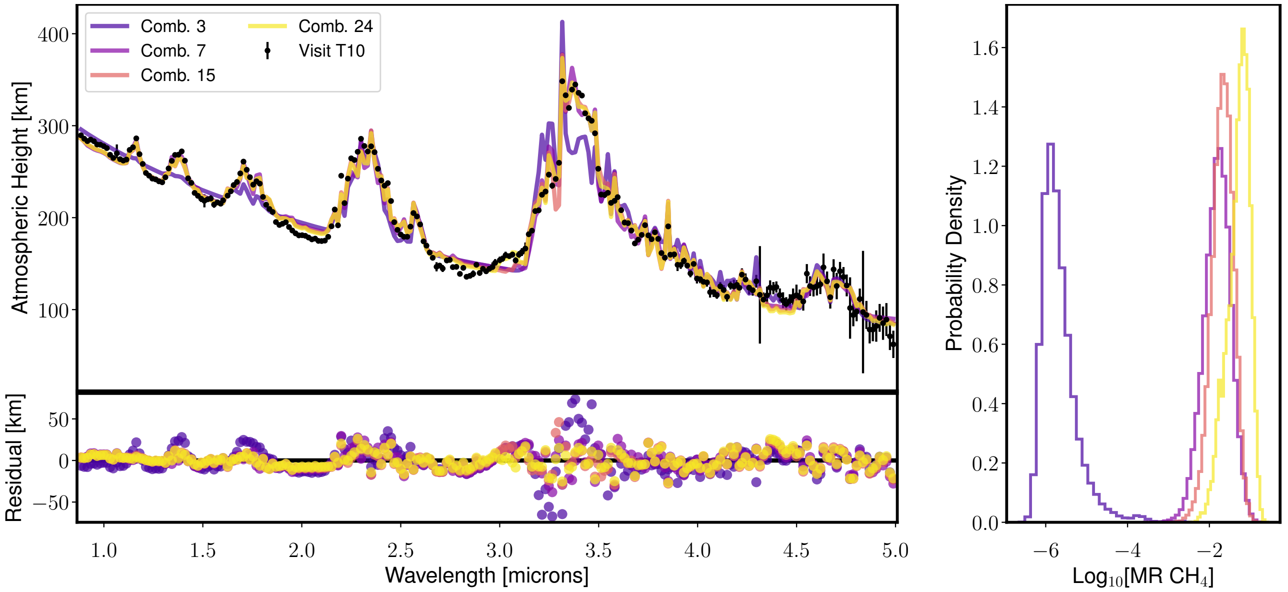

Figure 6. Not all choices of molecule sets yield equally good fits. Fits of four different combinations of models with the corresponding residuals (left) and posterior distribution of methane's mixing ratio (right). Colors indicate the sets of molecules used for each retrieval (see Table 3). Sets of molecules without ethane and/or propane lead to substantially worse fits. All other sets lead comparable fits, yet a range of methane mixing ratio spreading over 0.5-0.75 dex is associated with such pre-retrieval selections.

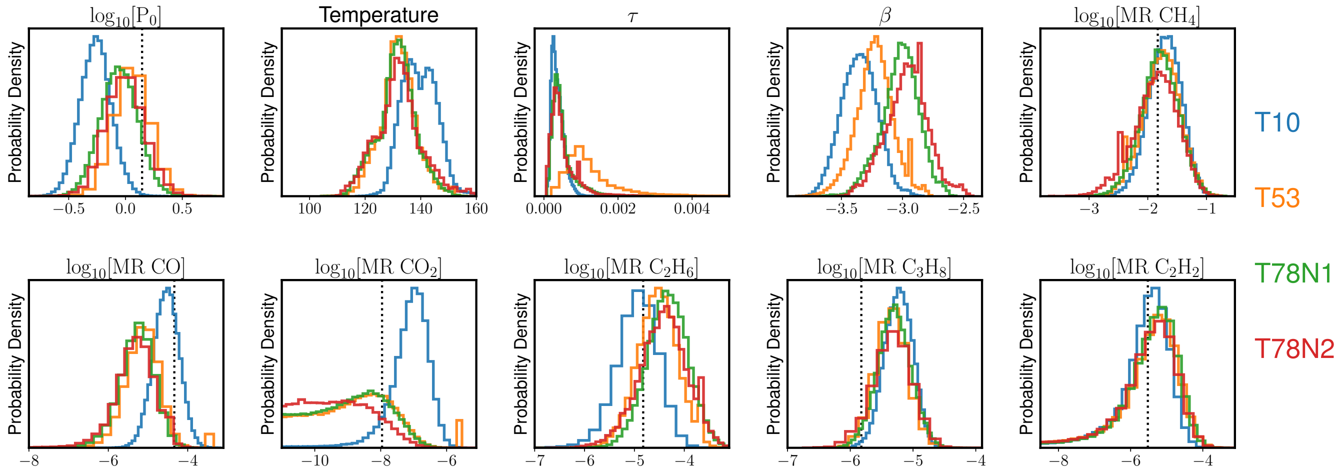

Figure 7. Posterior distribution of different molecules observed for Titan in our retrievals for molecular set 17. The "truths" reported in Table 2 are shown in the black lines. Except for acetylene and carbon dioxide, the retrieved molecular values are generally consistent within 2σ of previously reported values.

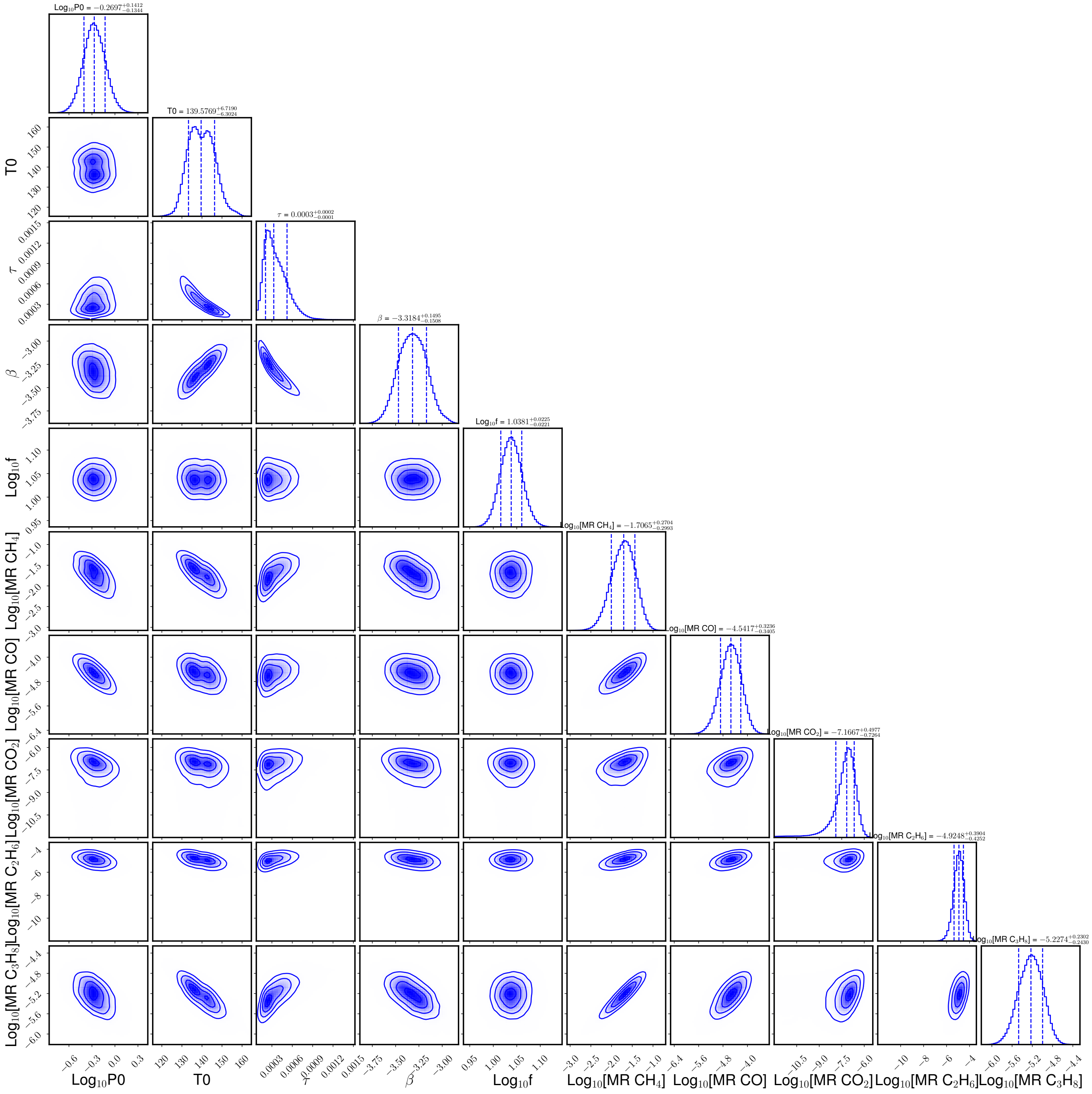

Figure 8. Corner plot showing correlation among different parameters for visit T10 for combination set of 7. A number of parameters, including retrieved abundance of methane and retrieved abundance of propane, show a strong correlation.

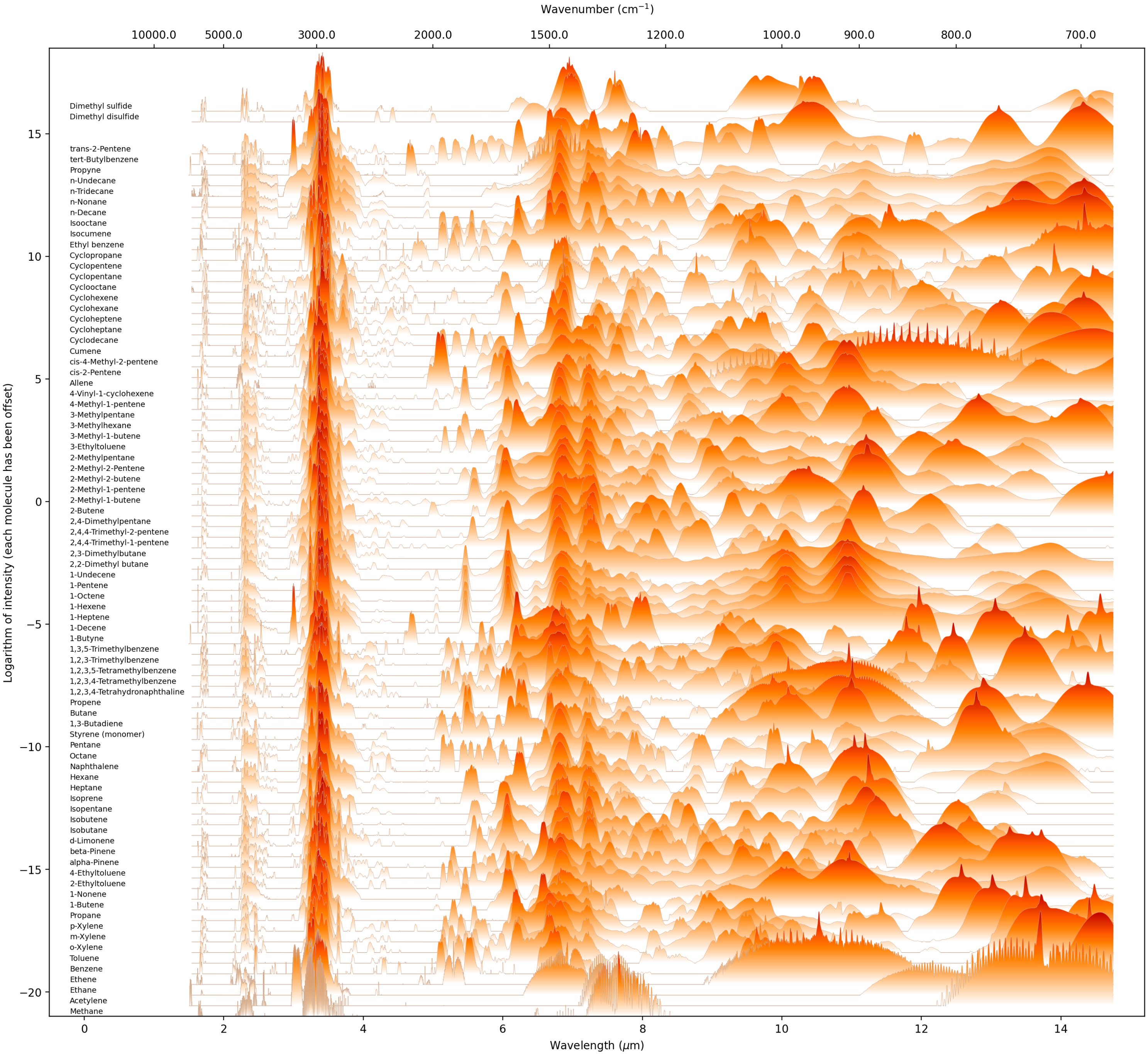

Figure 9. Overview of the absorption cross sections for hydrocarbon molecules, DMS and DMDS, taken from PNNL (Sharpe et al. 2004) and included in HITRAN2024 database (Hargreaves et al. 2025). The y-axis provides the logarithm of intensity and each molecule has been offset for display purposes. A minimum intensity of 1.0×10^{-21} cm^2/molecule has been applied for each molecule. The full spectral range of the underlying PNNL data is presented, showing the degeneracy below 5 μm (also shown in Figure 3). This degeneracy is partially lifted above 5 μm, in the mid- to far-IR, due to the differences in the low frequency vibrational modes of the C-C and C-H bonds.