Spectral Analysis and Atmospheric Retrieval of Terrestrial Exoplanets and Mini-Neptunes Using the TauREx 3 Framework

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Motivation

Biosignature gases — NH_3, PH_3, CH_3Cl, and N_2O — are candidate tracers of atmospheric disequilibrium chemistry and habitability on temperate exoplanets. JWST transmission spectroscopy can, in principle, probe these species, but instrument precision sets a hard floor on what is actually detectable. Any biosignature claim — detection or non-detection — is only as credible as that detectability floor is well characterized.

An initial full atmospheric retrieval for K2-18 b surfaced concerns about the robustness of trace-gas abundance estimates. Before revisiting that retrieval, we address the more fundamental question first: given real JWST noise, at what order of magnitude would NH_3, PH_3, CH_3Cl, and N_2O even become statistically detectable? This poster estimates order-of-magnitude 3σ detectability thresholds for these four gases across three benchmark exoplanets spanning distinct atmospheric regimes — the H_2/He sub-Neptunes K2-18 b (a Hycean-world candidate) and TOI-270 d, and the CO_2-dominated rocky world LHS 475 b — testing how detectability scales with atmospheric composition and mean molecular weight, and providing the necessary foundation for the full retrieval analysis now in preparation.

Methods

Transmission spectra are modeled with the TauREx 3 forward-modeling framework on Guillot (2010) P–T profiles, using system parameters from the literature for each target. Base atmospheric compositions are fixed to published Bayesian retrievals — Madhusudhan et al. (2023) for K2-18 b, Felix et al. (2025) for TOI-270 d, and a CO_2-dominated composition following Lustig-Yaeger, Fu et al. (2023) for LHS 475 b — so the model spectra are built directly on the CH_4/CO_2 abundances these retrievals recovered.

Each biomarker gas is injected on a logarithmic concentration grid (up to 1% for the sub-Neptunes, 10% for LHS 475 b). Model spectra are convolved to instrument resolution and interpolated onto real JWST data bins (NIRISS 0.8–2.8 μm + NIRSpec 2.7–5.2 μm, NASA Exoplanet Archive).

Detectability is quantified with a matched-filter signal-to-noise ratio, $SNR = \sqrt{\Sigma(|\text{model with gas} - \text{base model}| / \sigma)}$, summed over the gas absorption band using real measured JWST uncertainties. The 3σ detection threshold is the concentration at which SNR = 3, found by interpolation between grid points. Each case is repeated across three grey-cloud scenarios — varying cloud-top pressure — to test the robustness of the thresholds to cloud assumptions.

Because the underlying model uses a fixed (non-retrieved) P–T profile and grey-cloud opacity rather than a full retrieval, and thresholds are read off a discrete concentration grid, we report them as order-of-magnitude estimates, quoted to two significant figures rather than as precise detection boundaries.

Results

Table. K2-18 b — order-of-magnitude 3σ detectability thresholds (ppm)

Gas	Less aerosols	Fiducial	More aerosols
NH_3	190	190	280
PH_3	n.d.[1]	n.d.[1]	n.d.[1]
CH_3Cl	1300[2]	1300[2]	1300[2]
N_2O	61	65	110

[1] SNR does not reach 3σ within the tested grid (up to 1% mixing ratio).
[2] Identical across all three cloud scenarios — under verification.

Table. TOI-270 d — order-of-magnitude 3σ detectability thresholds (ppm)

Gas	Less aerosols	Fiducial	More aerosols
NH_3	380	490	790
PH_3	2400[1]	2400[1]	2400[1]
CH_3Cl	930[1]	930[1]	930[1]
N_2O	130	130	160

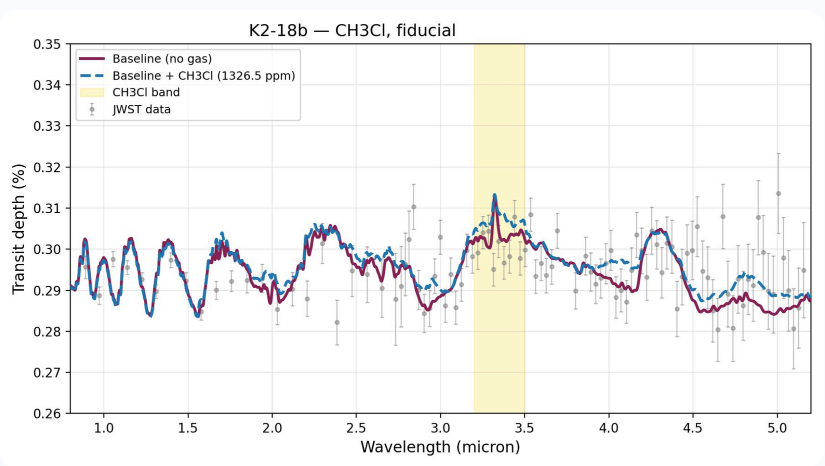
[1] Essentially identical across all three cloud scenarios — same unresolved pattern as K2-18 b CH_3Cl, under verification.

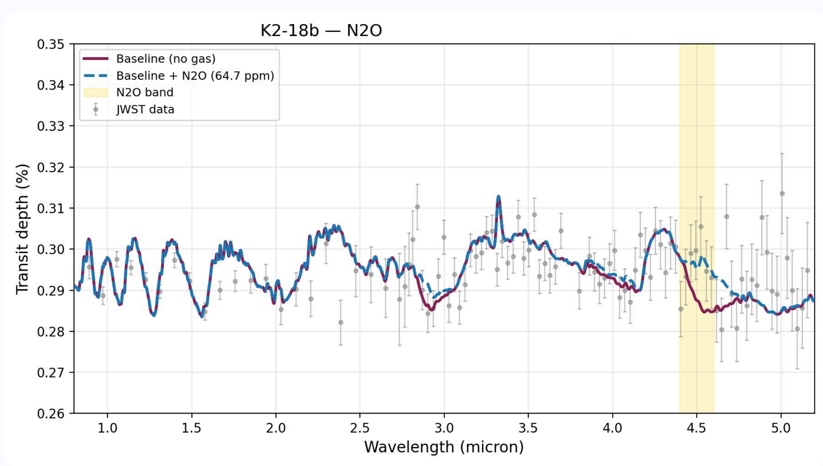
Table. LHS 475 b — order-of-magnitude 3σ detectability thresholds (ppm)

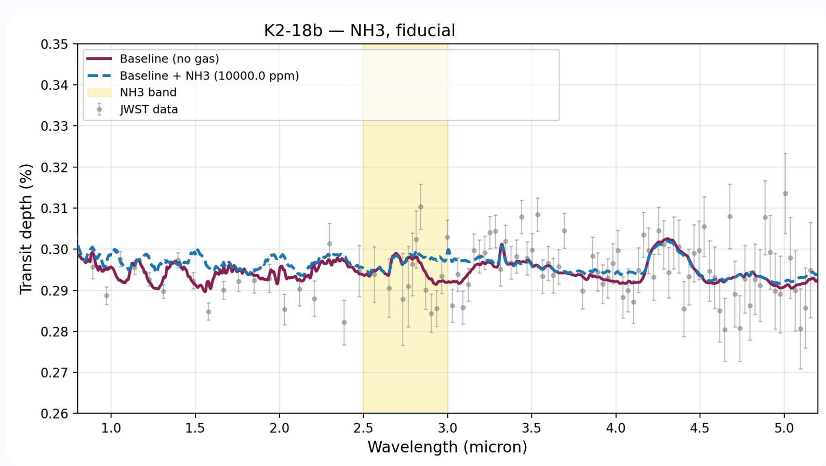
Gas	Less aerosols deep clouds / thin atm.	Fiducial Venus-like clouds, 1 mbar	More aerosols Titan-like haze, 0.01 mbar
NH_3	n.d.	n.d.	n.d.
PH_3	n.d.	n.d.	n.d.
CH_3Cl	61	1700	n.d.[1]
N_2O	n.d.	n.d.	n.d.

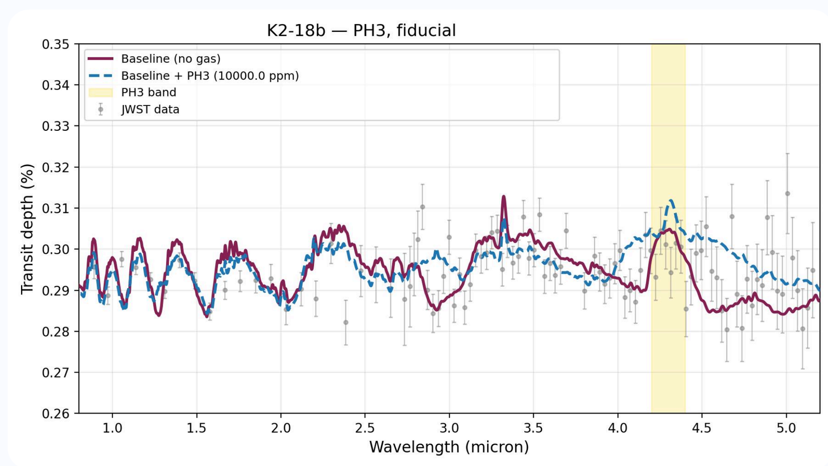
n.d. — SNR does not reach 3σ within the tested grid (up to 10% mixing ratio); base atmosphere is pure CO_2 (Lustig-Yaeger, Fu et al. 2023).
[1] High-altitude opaque haze (0.01 mbar) mutes all spectral features within the tested range.

K2-18b

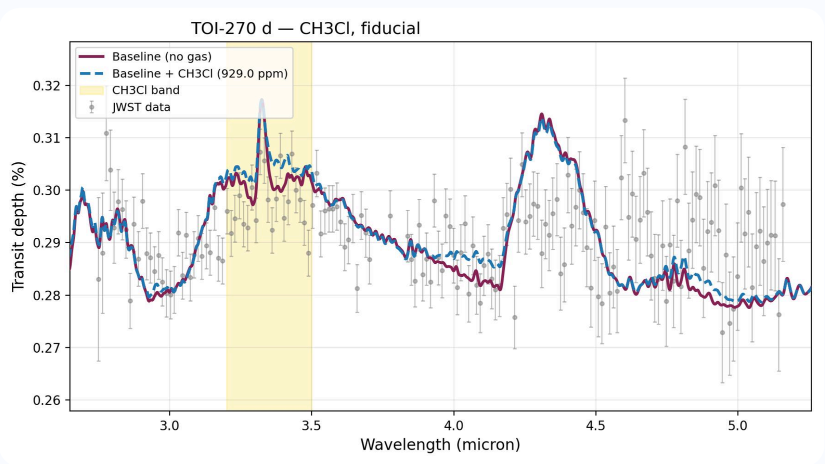


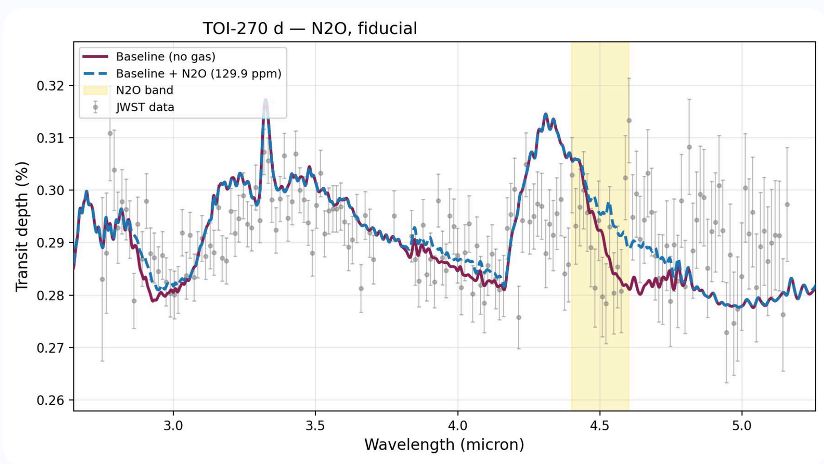


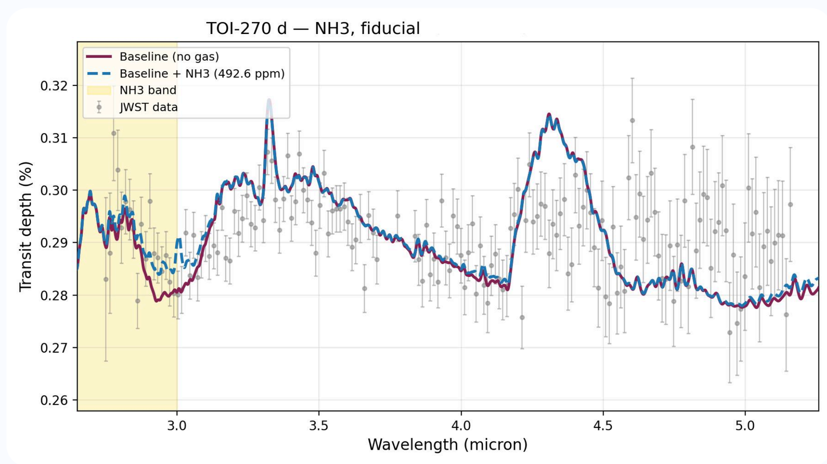


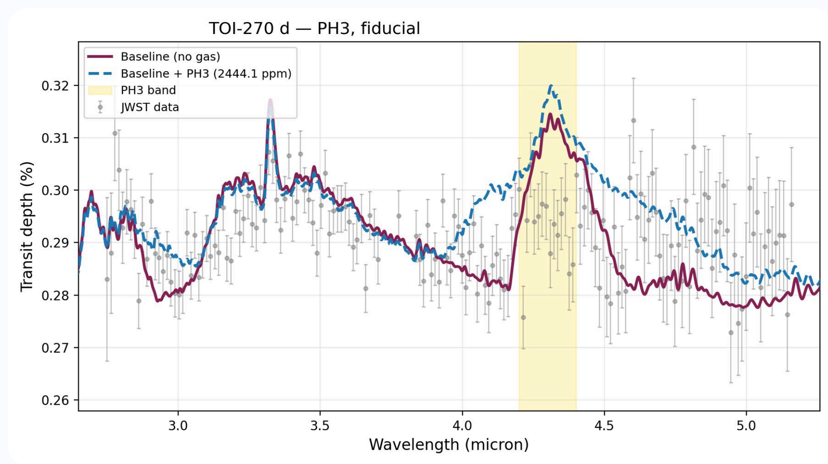


TOI-270d

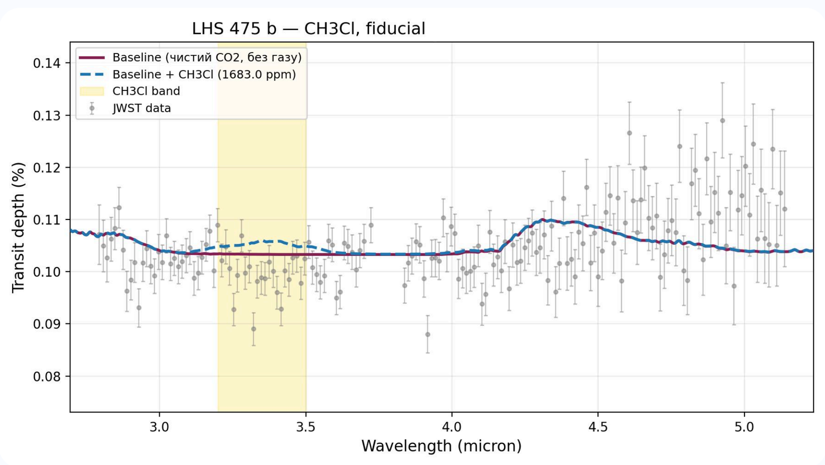


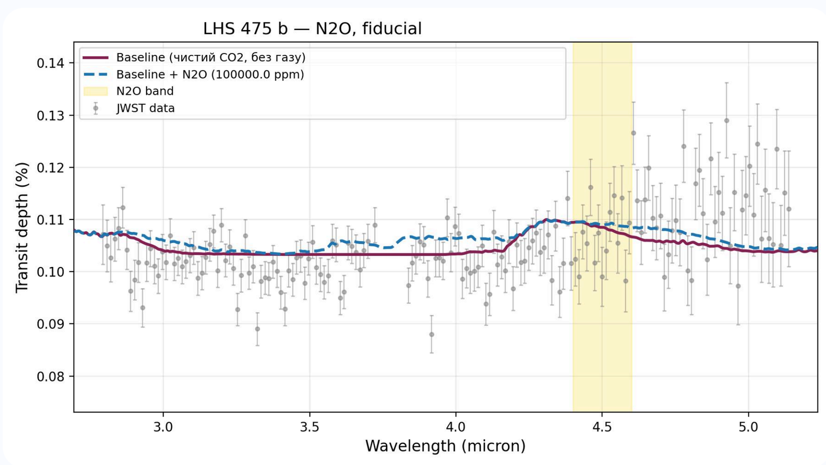


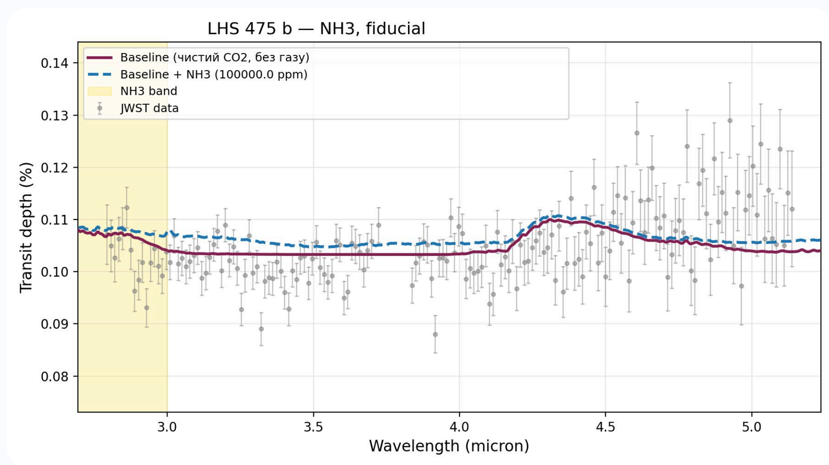


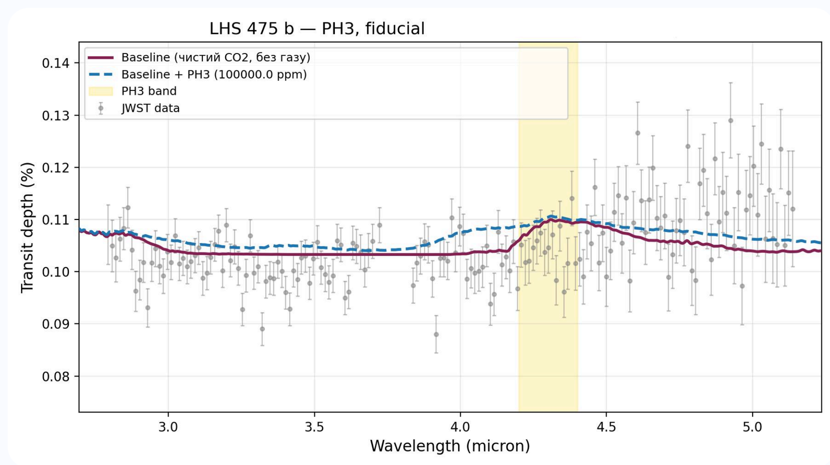


LHS-475b









Conclusions

Detectability is planet-type dependent: the H_2/He sub-Neptunes (K2-18 b, TOI-270 d) allow hundred-to-thousand-ppm 3σ thresholds for most gases, while the CO_2-dominated rocky LHS 475 b suppresses nearly every trace-gas signal.

- Aerosol loading raises most thresholds as expected, but CH_3Cl (K2-18 b) and CH_3Cl/PH_3 (TOI-270 d) show a threshold that is essentially cloud-invariant — likely a mean-molecular-weight effect rather than a band effect, and still under investigation.
- PH_3 is the hardest of the four gases to constrain in this sample; NH_3 is the most consistently tractable, with independent support from a published retrieval (see Validation).
- These order-of-magnitude thresholds provide a practical basis for prioritizing future JWST observing time, and motivate the next step: a full atmospheric retrieval for K2-18 b.

Validation

TOI-270 d's atmosphere has already been characterized by a published Bayesian retrieval (Felix et al. 2025), which finds NH_3 at 148 ppm — though with a wide 1σ uncertainty range of roughly 25–480 ppm, reflecting a marginal detection. Our forward-modeling 3σ detectability threshold for NH_3 on TOI-270 d — 380–790 ppm across grey-cloud scenarios — sits at the upper edge of that published uncertainty range, consistent with the marginal nature of the retrieved detection. This independent agreement supports the reliability of the sensitivity method.

The same pattern holds qualitatively elsewhere: K2-18 b's own retrieval likewise reports a non-detection of NH_3 (Madhusudhan et al. 2023), consistent with a true abundance below our K2-18 b threshold; and LHS 475 b's genuinely featureless spectrum (Lustig-Yaeger, Fu et al. 2023) matches our all-non-detection result for that planet.

References: Madhusudhan et al. 2023 · Felix et al. 2025 · Lustig-Yaeger, Fu et al. 2023 · Al-Refaie et al. 2021 (TauREx 3) · NASA Exoplanet Archive