Assessment of Isoprene as a Possible Biosignature Gas in Exoplanets with Anoxic Atmospheres

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Synopsis:

We study isoprene (C_5H_8) as a potential biosignature gas because it is produced in tremendous quantities, at rates similar to methane (~ 500 Tg yr^{-1}) on Earth. We found that isoprene is widely produced and has no abiotic false positives. Isoprene exist in trace amounts (< 1 pptv) on Earth due to rapid reaction with OH radicals (oxic atmosphere), but given the right condition: an anoxic atmosphere on a habitable exoplanet transiting a M dwarf star, it can accumulate to a detectable amount (> 100 ppmv) that can be observed with the JWST for a TRAPPIST 1e like exoplanet.

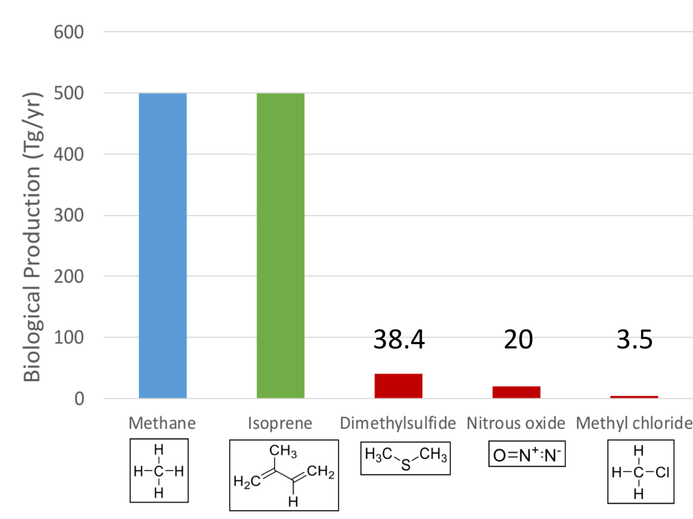

Fig 1: Production rate of biosignature gases on Earth

Introduction and Overview:

Biosignature gas studies thus far:
Simple gases like O_2, CH_4, N_2O, PH_3, CH_3Cl, DMS, etc. (Pilcher 2003; Segura *et al.* 2005; Domagal-Goldman *et al.* 2011; Sousa-Silva et al. 2019, etc.)

However, life produce more than just the simplest gases:
Motivates a systematic study of all small molecules (Seager *et al.* 2016)
Found isoprene as a favorable candidate .

Isoprene on Earth: Not a good biosignature gas
High reactivity with OH and other oxygen containing radicals
However, Earth's atmosphere was anoxic during its initial 2.4 Gyr

In this Work, we assess:
Can isoprene be produced by anaerobic life?
Can it accumulate in anoxic atmospheres?
Does it have distinguishable spectral features that can be detectable?

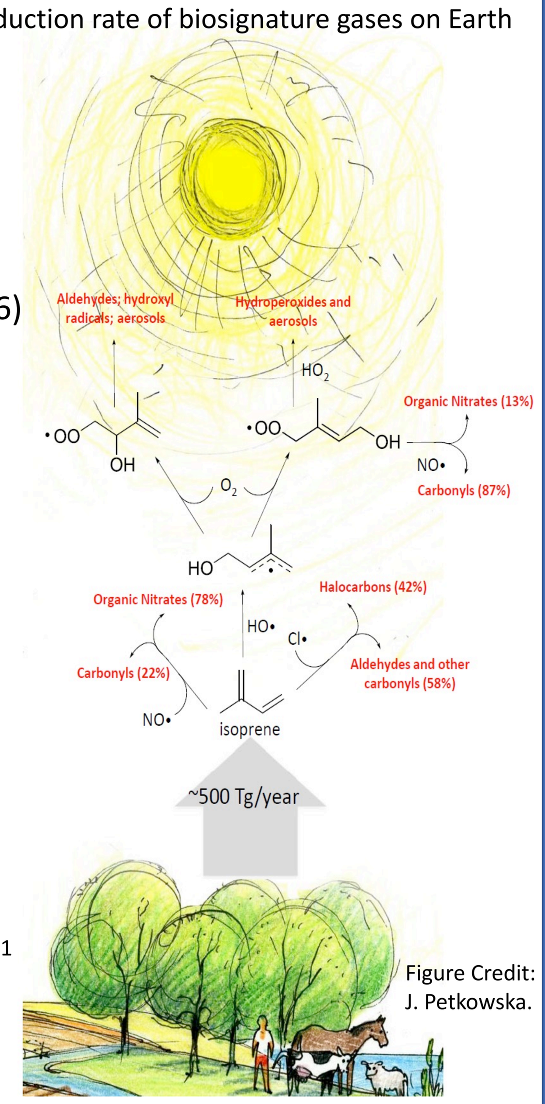

Fig 2: Isoprene destruction pathway on Earth

Molecular Inputs and Atmosphere Simulation:

Isoprene Absorption Cross-Section:
UV-Vis (Dillon et al. 2017): Input for photolysis calculation.
peaks at 218 nm with σ_{peak} = 7.93 ± 0.02 x 10^{-17} cm^{-2} $molecule^{-1}$
Wavelength range: 118 nm to 278 nm
IR (Brauer et al. 2014): Input for detection assessment.
Measured at 298 K, 1 bar with resolution of 1/8 cm^{-1}
Spectral features groups: 3.1-3.6, 5.4-7.5 and 9-12 µm

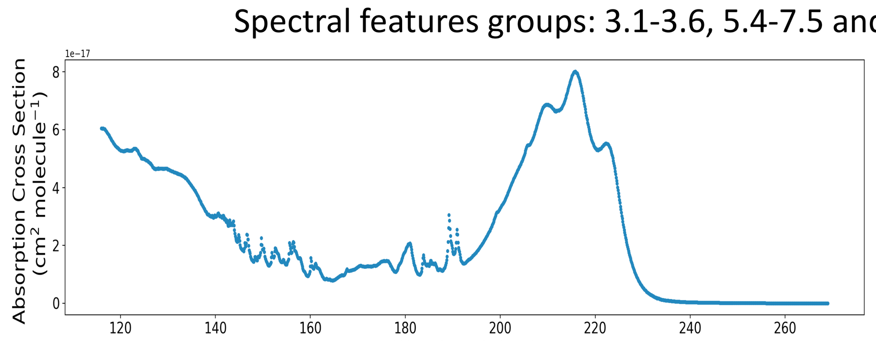

Fig 3: UV-Vis absorption cross-section

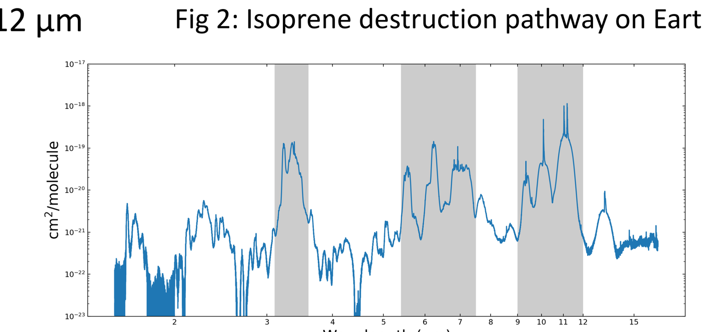

Fig 4: IR absorption cross-section. Grey bars: Isoprene features for detection assessment

Atmosphere Simulation and Observation Parameters:

Star: Sun-like star (5770 K) and M5V star (3000 K)
Planet: 10 M_{Earth} and 1.75 R_{Earth} super-Earth
Target distance: 10 pc
Atmosphere: (Fig 5,6)
H_2-rich (reducing),
N_2-rich (intermediate)
CO_2-rich (weakly-oxidizing)
Transmission and thermal emission model:
in house radiative transfer code
Photochemistry model:
Modification from (Hu *et al.* 2012) to accept isoprene
Instrument: JWST-like (6.5m)
25% quantum efficiency, 50% photon noise,
R=10, maximum observation hours: 100
Detection: 5 σ (Signal-to-noise ratio)

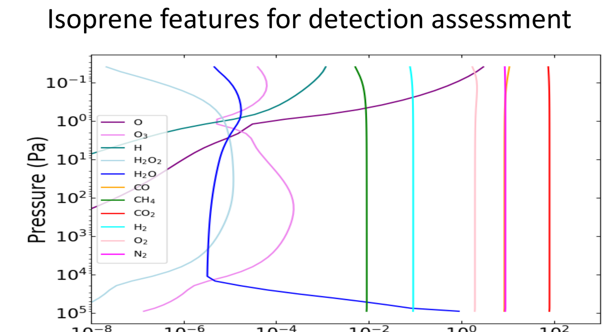

Fig 5: Mixing ratio profile for CO_2-rich atmos. around M5V

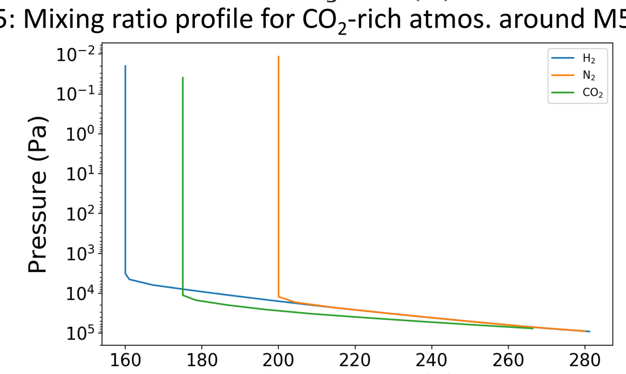

Fig 6: Temperature pressure profile for the 3 atmospheres

Isoprene Main Destruction Pathways

- OH radical: k = 10 ± 1.2 x10^{-11} cm^3 $molecule^{-1}$ s^{-1}
- O radical: k = 3.5 ± 0.6 × 10^{-11} cm^3 $molecule^{-1}$ s^{-1}
- O_2 molecule: k = 2.8 ± 0.7 x 10^{-15} cm^3 $molecule^{-1}$ s^{-1}
- Photolysis: Dependent on stellar UV flux

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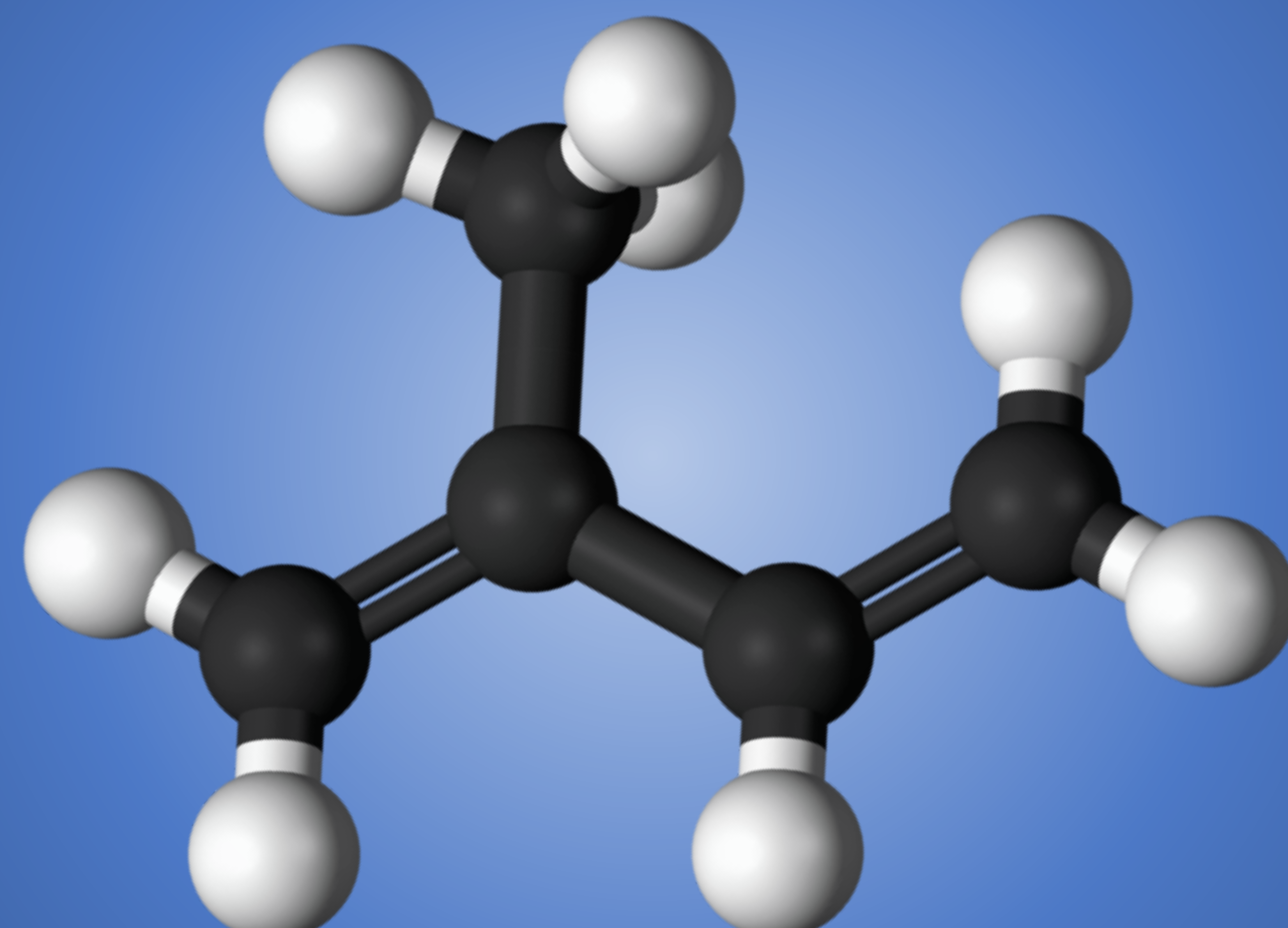
Isoprene, a possible biosignature gas: can accumulate to detectable amounts in anoxic exoplanet atmospheres[1] given similar production rate on Earth.



Why Isoprene?

- High Production Rate[2]: ~ 500 Tg/year
- Ubiquitous Production by All Domain of Life
- No Known or Predicted Abiotic False Positives

Isoprene Formula: C_5H_8 Boiling Point: 34°C Molar Mass: 68.12
IUPAC: 2-Methyl-1,3-butadiene SMILES: CH2=C(CH3)CH=CH2

[1] Habitable super-Earth sized exoplanet transiting a M dwarf star.

[2] Largest source of non-methane hydrocarbon. Biotic Methane Production Rate: 500 Tg/year

Main Results:

1. Isoprene accumulation bifurcated by surface flux "Tipping point". Column average mixing ratio of isoprene drastically increase with increase in isoprene surface flux past 3 x 10^{10} [molecules cm^{-2} s^{-1}] for a CO_2-rich atmosphere and 1 x 10^{11} [molecules cm^{-2} s^{-1}] for a H_2-rich or N_2-rich atmosphere on planet orbiting a M dwarf star.
Past "tipping point": a major gas (10 - 100 ppmv)
Prior "tipping point": a trace gas (<1 ppmv)

P_{iso}	H_2-rich	N_2-rich	CO_2-rich
10^{10}	0.0006	0.0002	0.0016
10^{11}	0.0498	0.0079	6.2207
10^{12}	3.3041	1.9776	635.81
10^{13}	865.41	4426.8	7341.8

Table 1: Isoprene column average mixing ratio [ppmv] for different surface flux [cm^{-2} s^{-1}] in atmospheres around M5V.

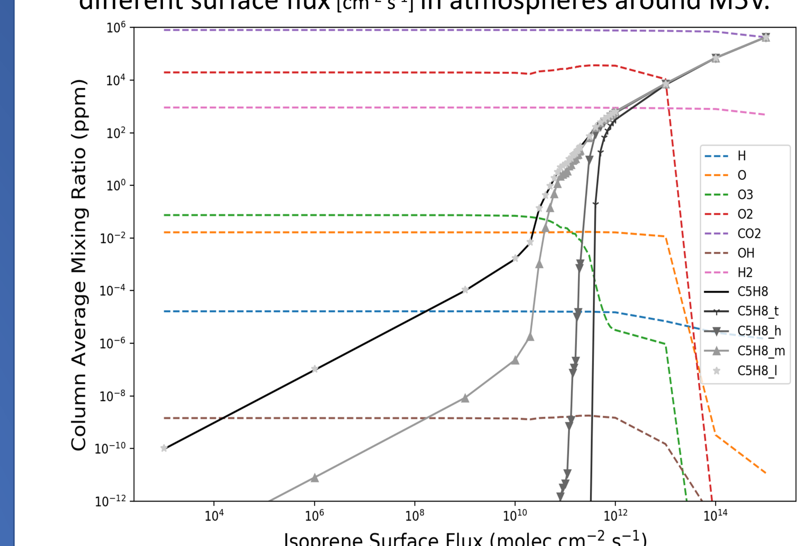


Fig 7: Isoprene volume average mixing ratio vs surface flux for CO_2-rich atmosphere around M5V.

2. Isoprene is detectable via transmission spectroscopy for some optimistic scenarios with ~10 hr. It is detectable via 2[ndary] eclipse thermal emission spectroscopy but requires near 100 hrs.

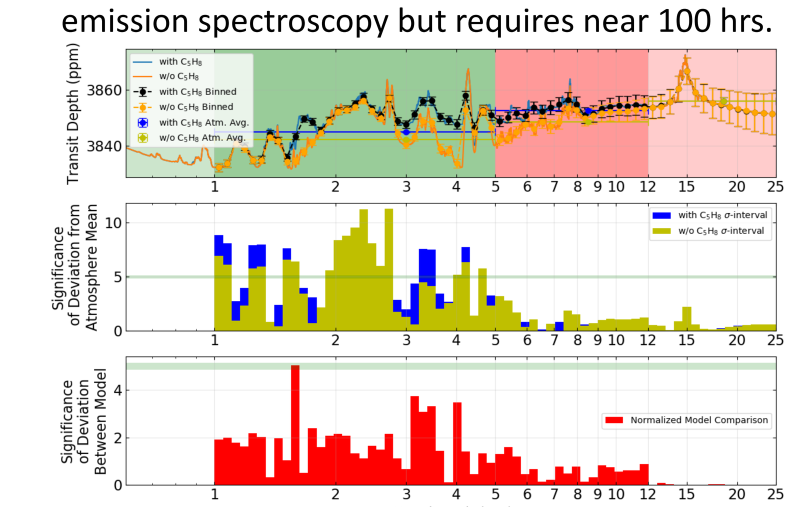


Fig 8: Simulated detection of isoprene in H_2-rich atmosphere given 14.1 hr in-transit with JWST.

3. Isoprene has no abiotic false positives and is thermodynamically disfavored. (Table 2)

Proposed geochemical isoprene formation pathways	ΔG of reaction (kJ/mol)
$5CO_2 + 14H_2 \rightarrow C_5H_8 + 10H_2O$	1670.1
$5CO + 9H_2 \rightarrow C_5H_8 + 5H_2O$	1294.8
$5CH_4 \rightarrow C_5H_8 + 6H_2$	477.7

Discussion:

1. **Current limitations** and lack knowledge of:
   - Lab measured isoprene cross sections in broad T-P space and baseline error correction.
   - Isoprene reaction rate with reducing radicals
   - Isoprene haze production in anoxic atmosphere
2. **Identifying Isoprene** can be complicated by mixture of other hydrocarbons.

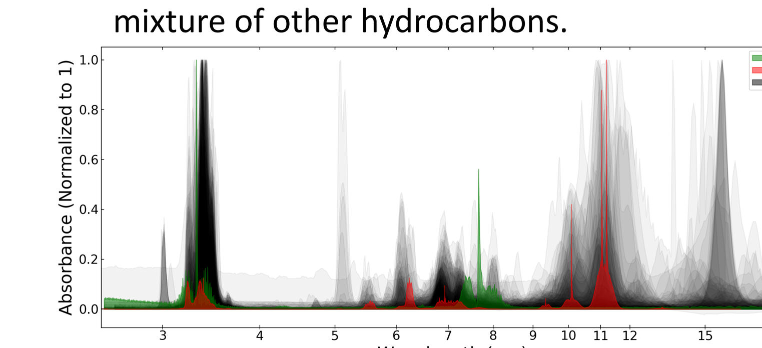


Fig 9: Isoprene (red) vs methane (green) vs other hydrocarbon (black)

3. Isoprene can be considered as a **"biosphere signature"** not only because it is produced in high abundance by life on Earth but also due synthesis of isoprene and many other terpenoids (isoprene polymers), are present in virtually every domain of life on Earth.

Did You Know?

Atmosphere with Enriched Isoprene Smell Like Forests

Isoprene, a possible dabbing gas