Modelling and ground-based high-resolution spectroscopic characterisation of magma ocean hosting exoplanets

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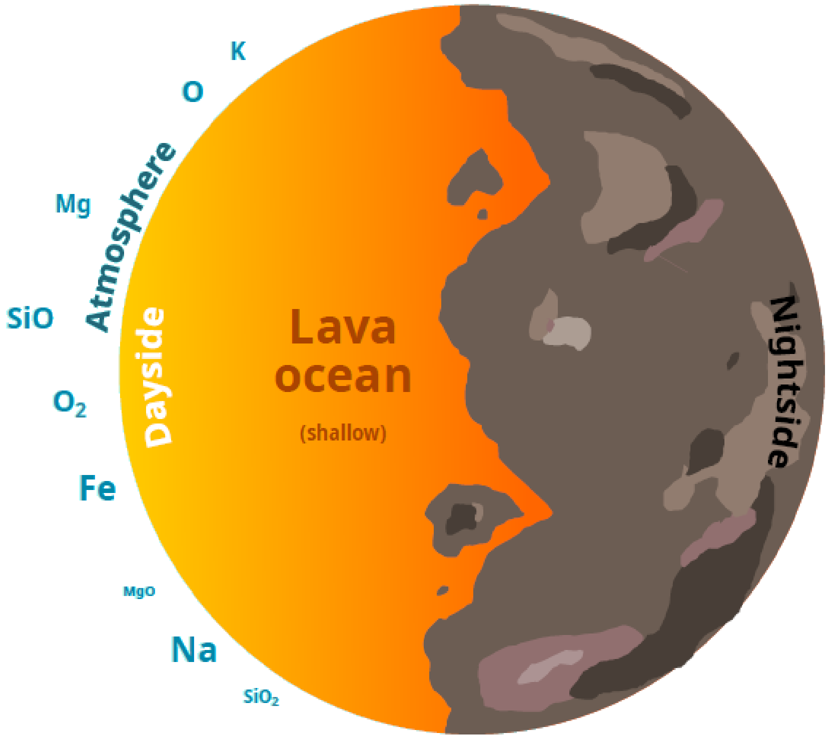
IPGP

Types of exoplanets that could hold magma oceans

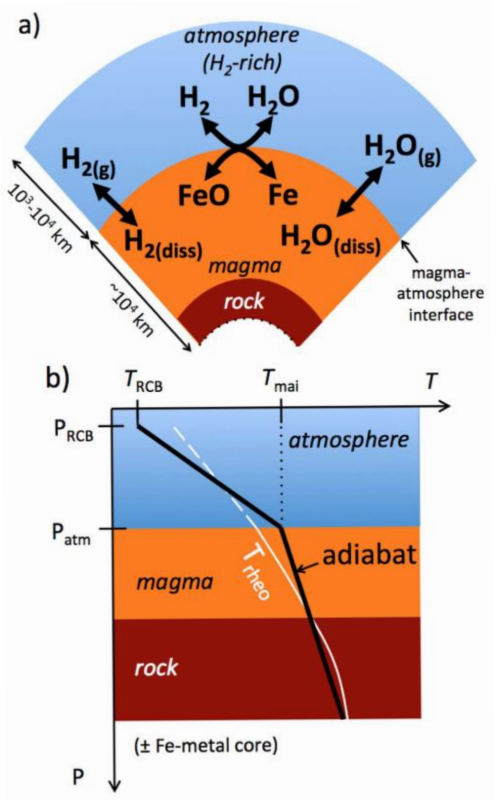
Pressure-Temperature conditions need to be suitable for the upper rocky mantle to melt.

Ultra-short Period rocky exoplanets



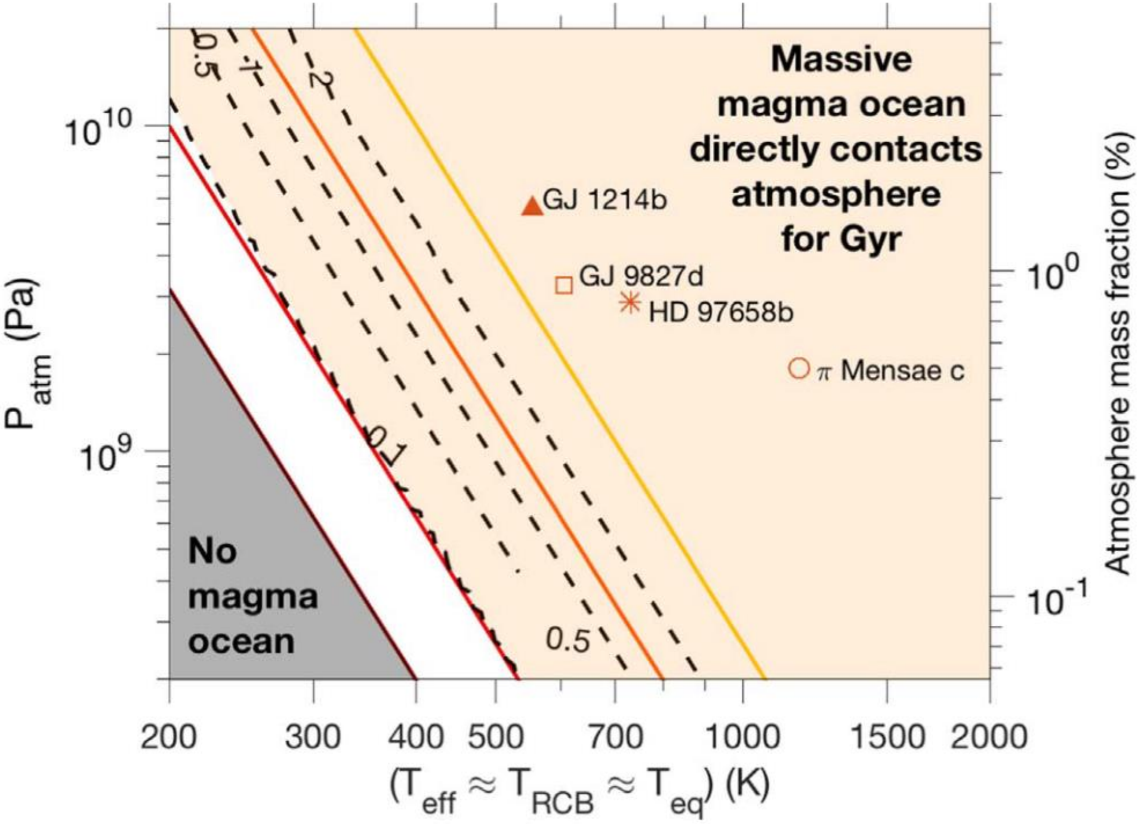
Credits: Fabian Seidler

Puffy super-Earths and sub-Neptunes (?)



Credits: Kite et al. 2020

The case for puffy super-earths and smaller sub-Neptunes



Credits: Kite et al. 2020

1. Most frequently observed exoplanet types (P < 100 days) – Fulton et al. 2017

2. Sample space admitting magma oceans large enough that these exoplanets might harbour the largest amount of long-lived magma oceans in exoplanetary systems

3. Presence of a magma ocean has a massive influence on the atmospheric composition and structure, and hence influence observable spectra (for H-rich exoplanets: Charnoz et al. 2023, Kite et al. 2020, Falco et al. 2024)

Caution: Not all sub-Neptunes might hold magma oceans, especially if the envelope mass fraction is too high or if the atmosphere is high MMW. This can lead to magma ocean solidification and no outgassing in the atmosphere.

See: Breza, Nixon & Kempton 2025

Modelling the interaction: Diverse approaches in literature

Mass-balance and Fugacity-limited regimes

Total mass/number of elements in the system is conserved.

Have to solve for mass balance equilibrium for the total system together with chemical equilibrium (see Charnoz et al 2023, Falco et al 2024, LavAtmos 2.0).

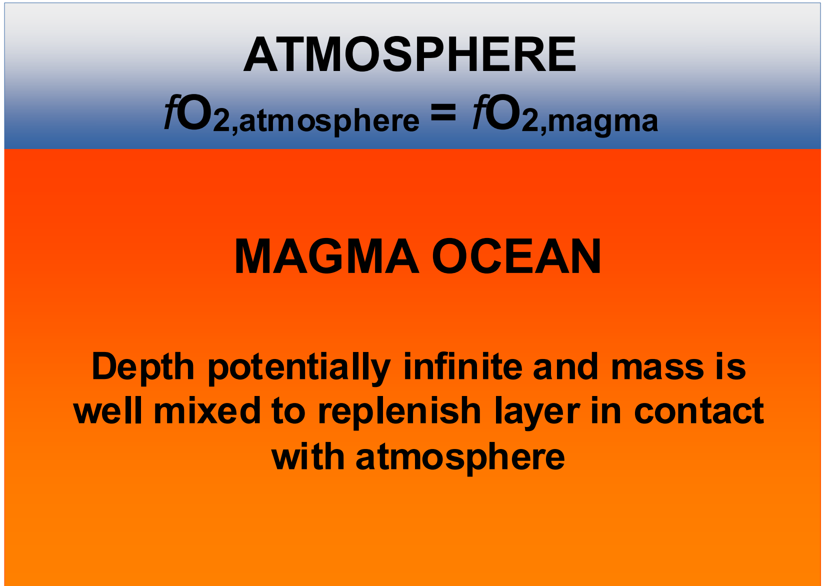
ATMOSPHERE

$$N_{\mathrm{el,atmosphere}} + N_{\mathrm{el,magma}} = N_{\mathrm{el,Total}}$$

MAGMA OCEAN

The depth of the magma reservoir is potentially infinite, or greater than the amount required to buffer the atmosphere. Buffer is always well mixed. The atmosphere is driven to chemical equilibrium with the magma melt.

Atmosphere has the same fugacity as the surface magma melt as determined by a redox buffer equation (see Seidler et al 2024, 2025).



ATMOSPHERE

$$fO_{2,\mathrm{atmosphere}} = fO_{2,\mathrm{magma}}$$

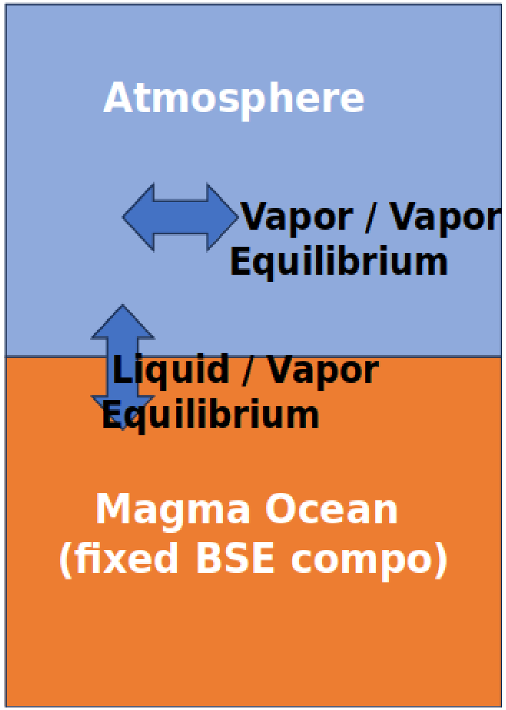
MAGMA OCEAN

Depth potentially infinite and mass is well mixed to replenish layer in contact with atmosphere

MAGMAVOL 2.0

New, will be available on github soon…

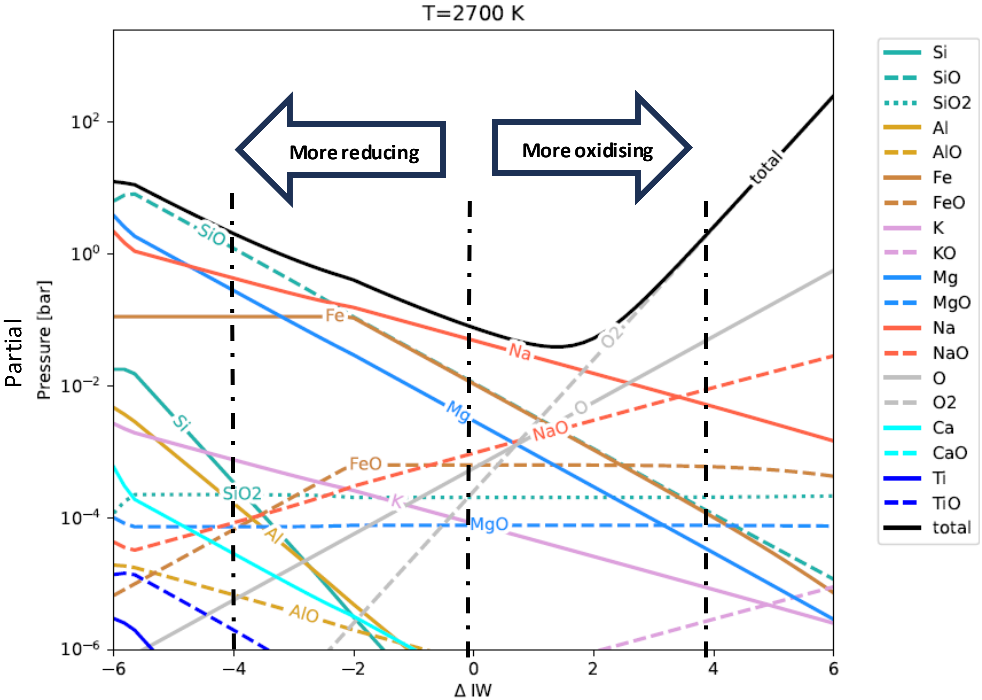
- Base degassing model VapoRock (Wolf et al 2023). Additionally, oxygen fugacity of the magma ocean can now be a free parameter.
- The envelope above the magma ocean is assumed to be mineral or vapour rich (any combination of H, C, N, O, P, S).
- Atmospheric chemistry is solved through FASTCHEM. Reactions proceed both in the mass-balance scenario and fugacity-limited scenario, and is provided as an input parameter.
- An optimisation algorithm is used to find the elemental abundances in the atmospheres which solve for the chemical equilibrium and mass-balance equations simultaneously.
- Dissolution included indirectly - setting initial elemental abundance < final elemental abundance.



Mineral atmospheres: Comparison with MAGMA

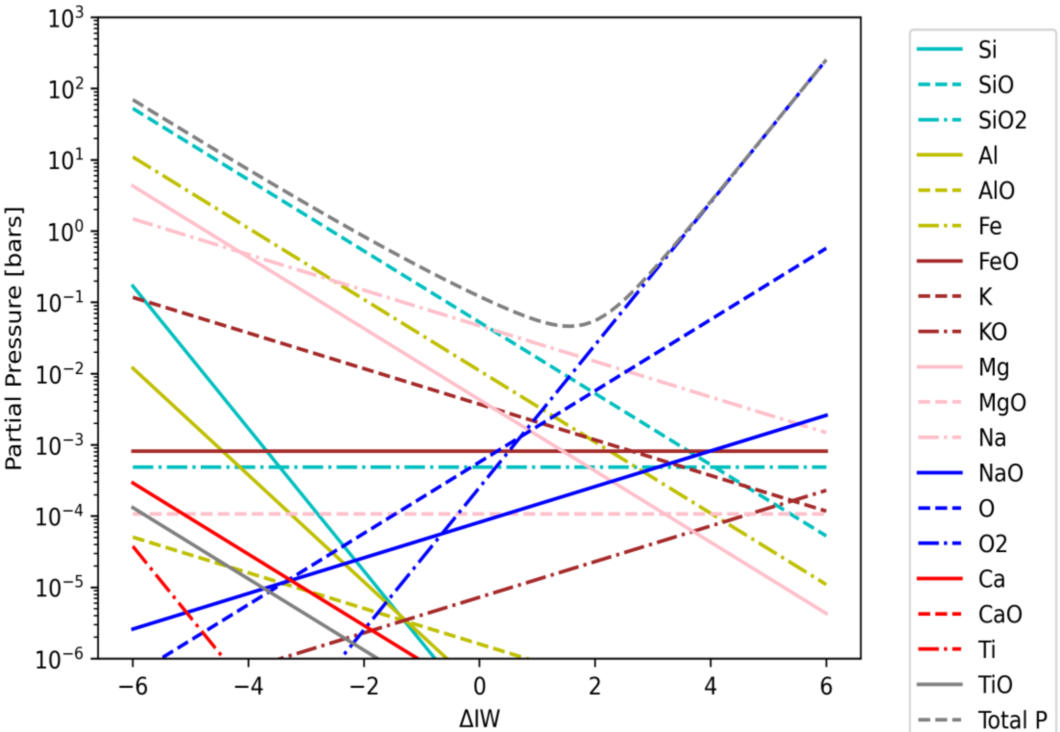
Using BSE (Bulk Silicate Earth) initial abundances for 55 Cnc e

BSE is the undifferentiated mantle very early during earth's formation with the crust not yet formed



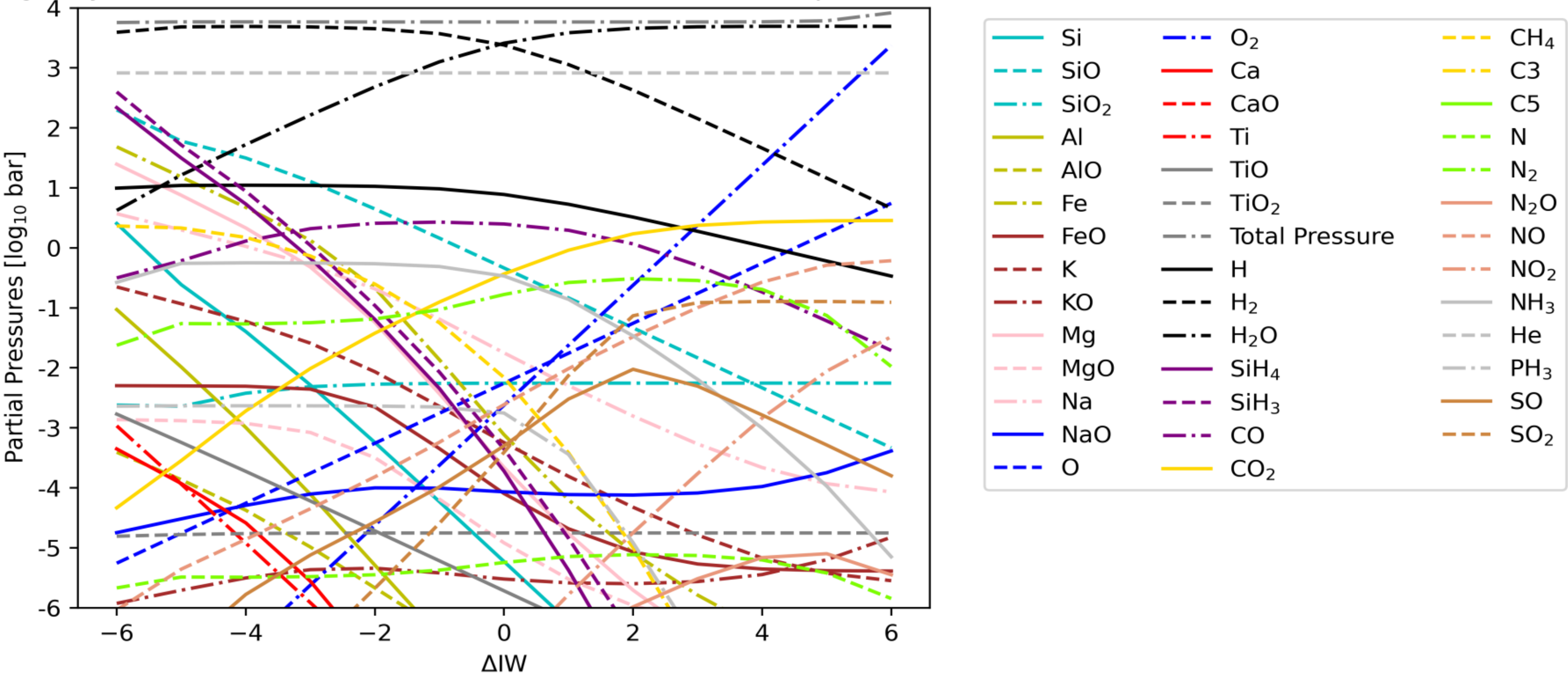
ΔIW is a measure of deviation from *f*(O_2) determined from the temperature alone for an iron-wustite redox buffer.

Credits: Fabian Seidler, using MAGMA



Results using VAPOROCK are similar-ish (difference in very reduced cases, also in K, Ti and their oxides) for mineral atmospheres

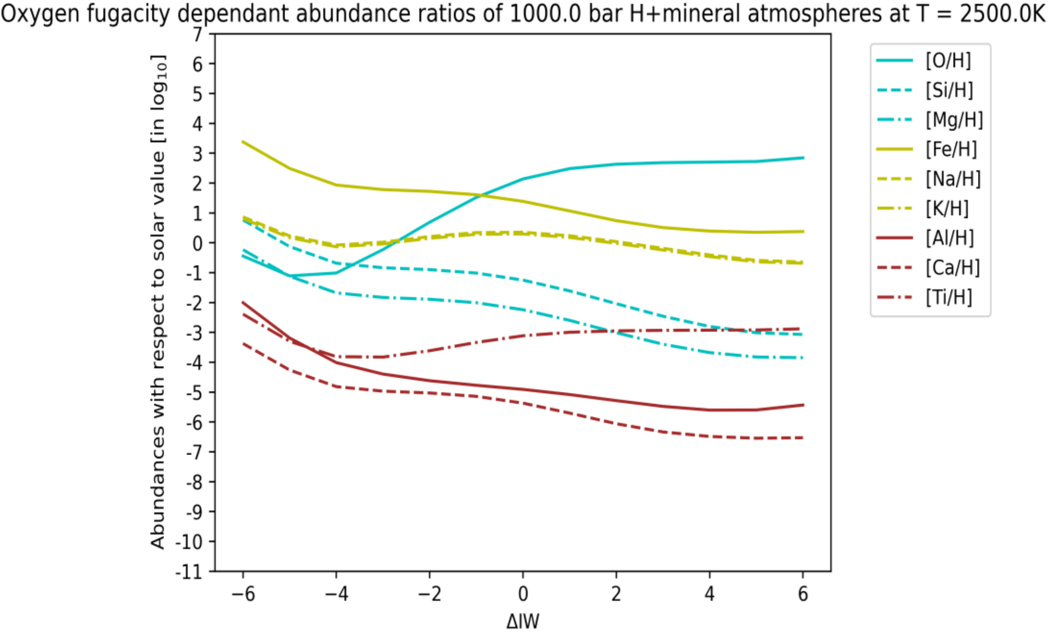
Volatile rich case of solar abundance envelopes (fugacity-limited approach)

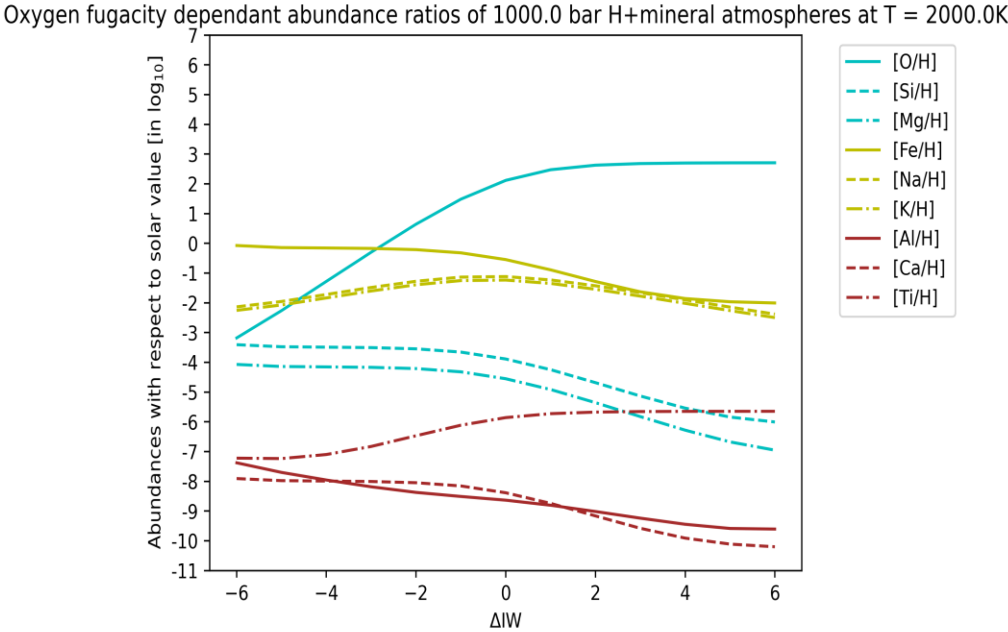


Oxygen fugacity evolution of solar abundance 10000.0 bar atmospheres at T = 3000.0K

H_2O dominates at oxidizing conditions, while H_2 is dominant in reducing conditions (similar to primordial melts early on during planet formation). H_2O in general is still substantial across all kinds of melt oxidation states. Hydrogenated molecules like SiH_4 are strongly limited to atmospheres above reducing melts. CO and CO_2 trends crossover at a more oxidized state. Similar crossover trends also exist for competing oxides of the other volatiles.

Link to metallicity in H atmospheres (fugacity limited regime)





H rich atmospheres above reduced melts can have order of magnitudes higher metallicity compared to solar values. Higher temperature melts also lead to higher metallicity due to increased degassing of refractory elements.

Self-consistent atmospheric modelling with ATMO

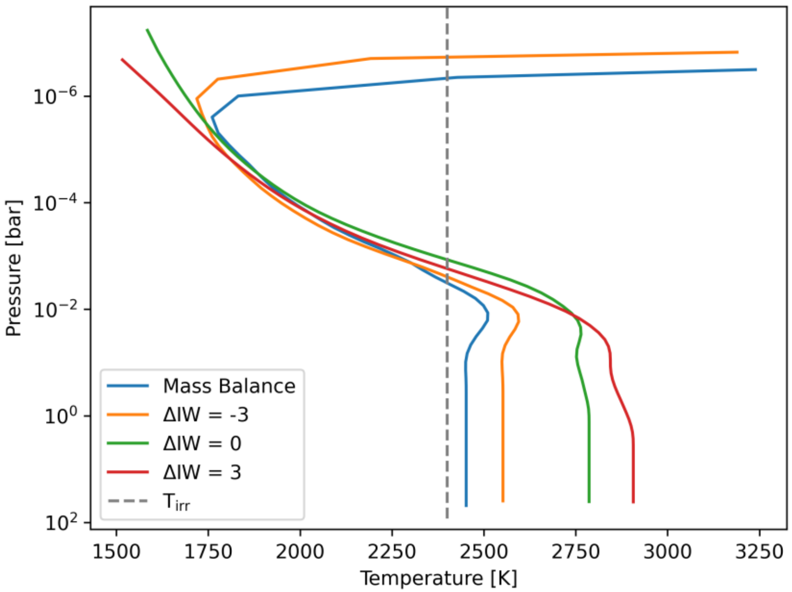
(scheme described in Amundsen et al 2014, Tremblin et al 2015)

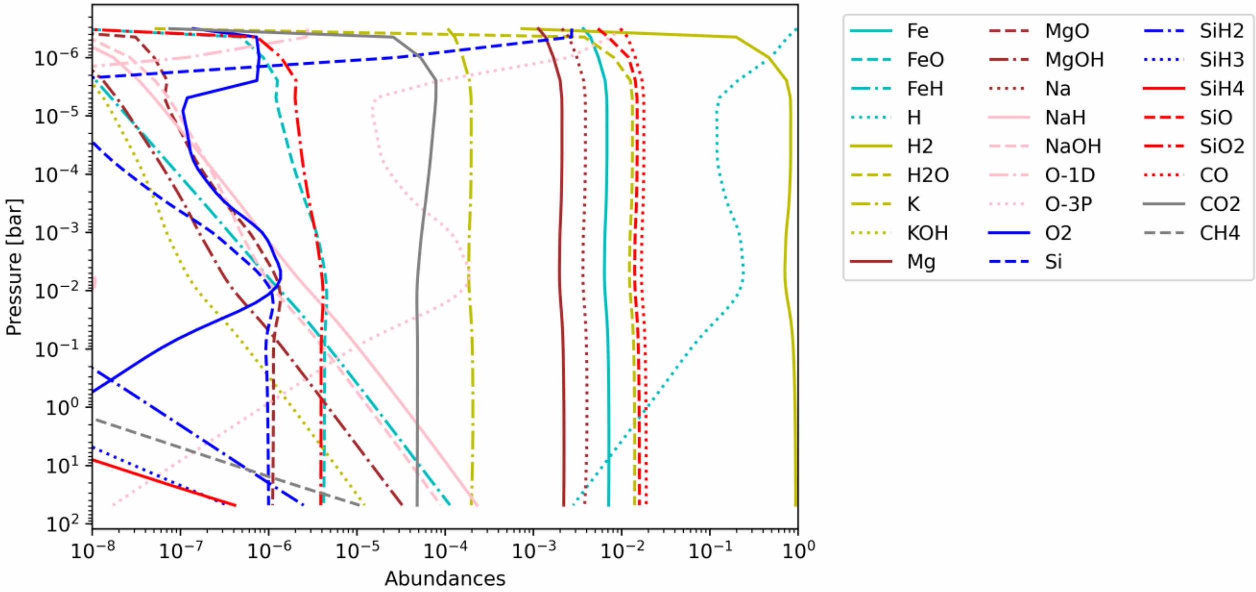
ATMO solves the radiative transfer of the magma ocean and atmosphere together by assuming the presence of a very high opacity ocean layer at the bottom of the atmosphere.

Initial temperature required set by the dayside irradiation temperature with dilution factor (f = 0.25), 55 Cnc e like system assumed.

100 bars of H + 1 bar of C, T_{irr} = 2400 K

$$T_{irr} = (f(1-A_b))^{1/4}\left(\frac{R_\star}{a}\right)^{1/2} T_{eff},$$



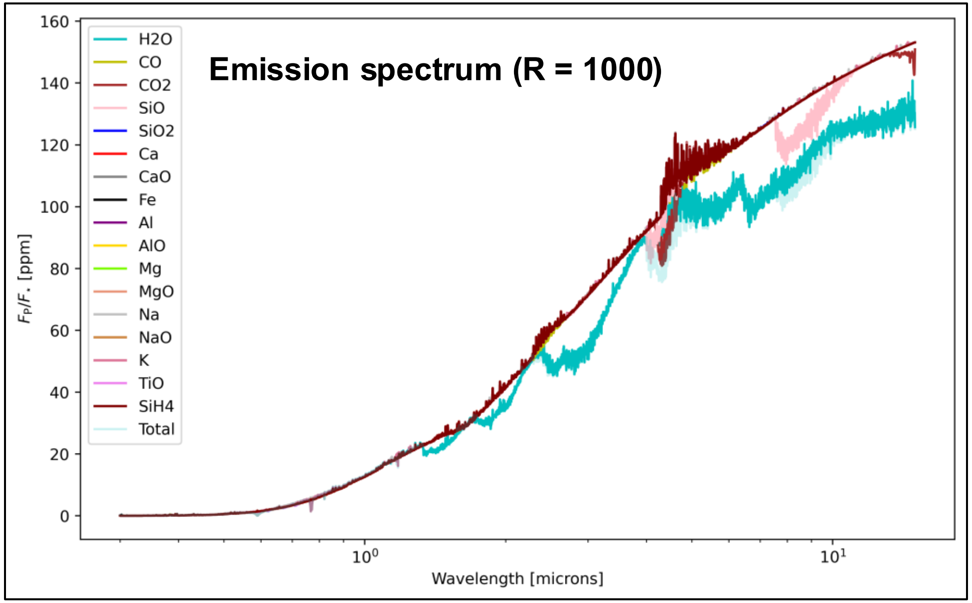


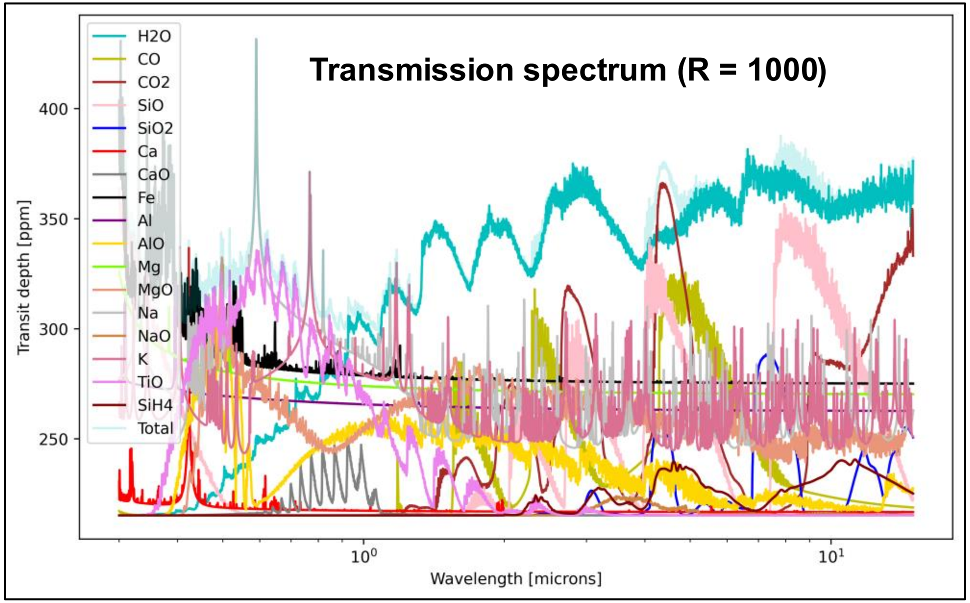
P-T profile varies with fugacity. Mass-balance similar to the reduced fugacity case. All profiles are hotter at base compared to T_{irr} due to greenhouse effect of H_2O, the gaseous abundance of which increases with the fugacity of the melt.

Low-resolution spectra with petitRADTRANS

(described in Molliere et al 2019 and Nasedkin et al 2024)

100 bars of H +1 bar C mass-balance case, Magma ocean temp ~ 2400 K, BSE composition for melt





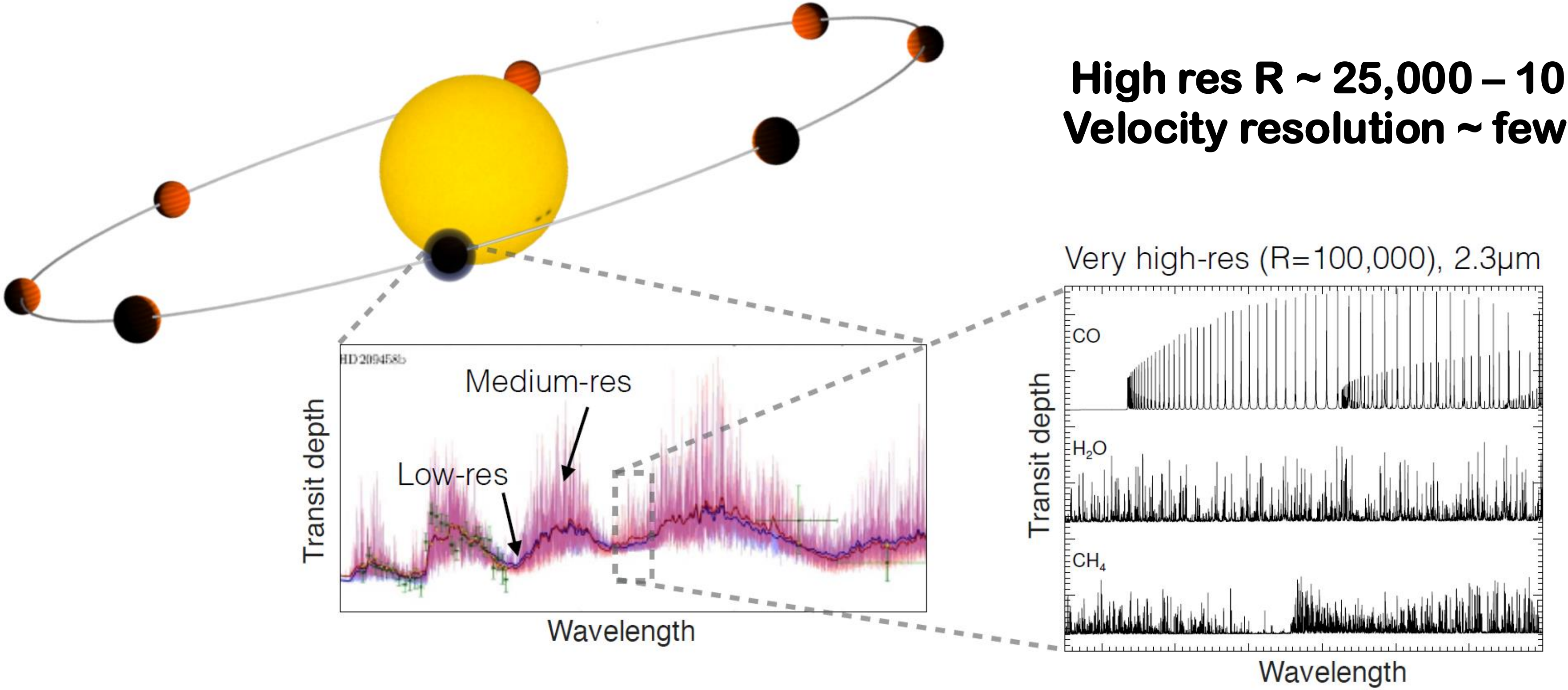
Most absorption features are due to H_2O, but prominent CO_2 feature at 4µm. Strong lines in the optical continue to be due to metals and metallic oxides (Na, K, TiO etc).

Having both refractory elements and their oxides and water in the atmosphere might be an easy indicator about a magma ocean lying at the bottom of an H-rich atmosphere.

What about ground-based high-resolution spectroscopy? This can potentially be used for follow-up and complementary studies.

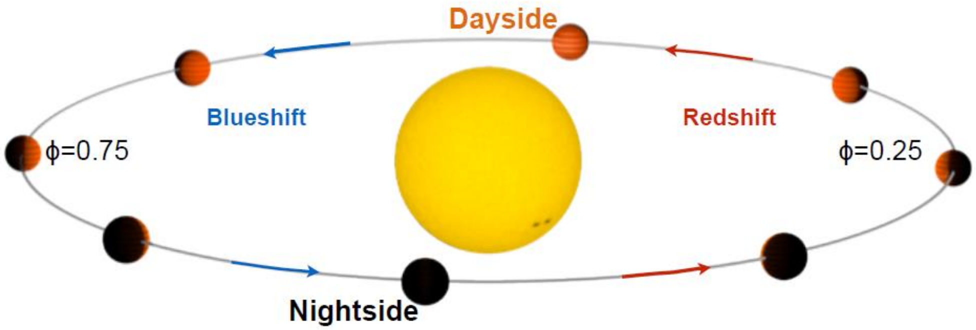
High-resolution spectroscopy

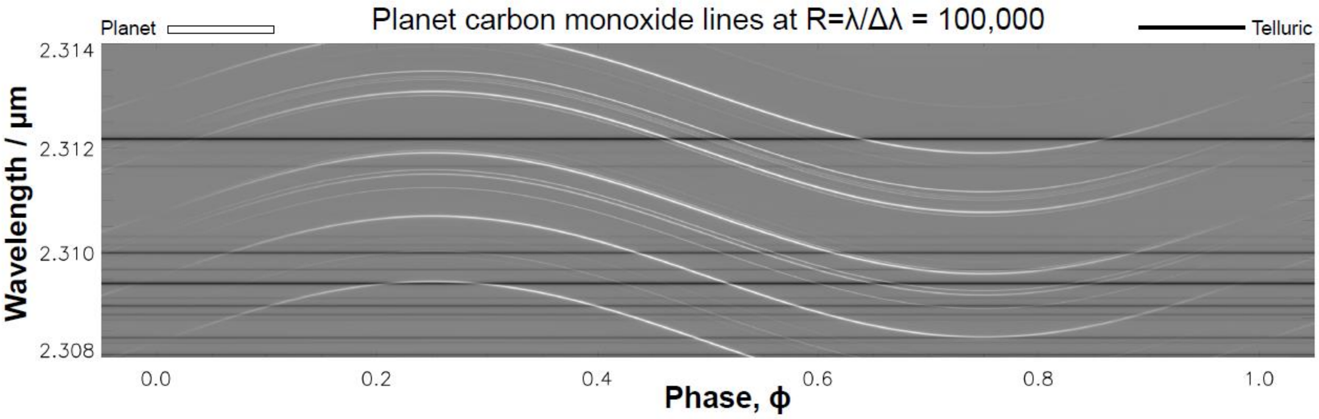
High res R ~ 25,000 – 100,000
Velocity resolution ~ few kms^{-1}



Credits: Dr. Matteo Brogi

Orbital movement of the exoplanet causes species lines to move



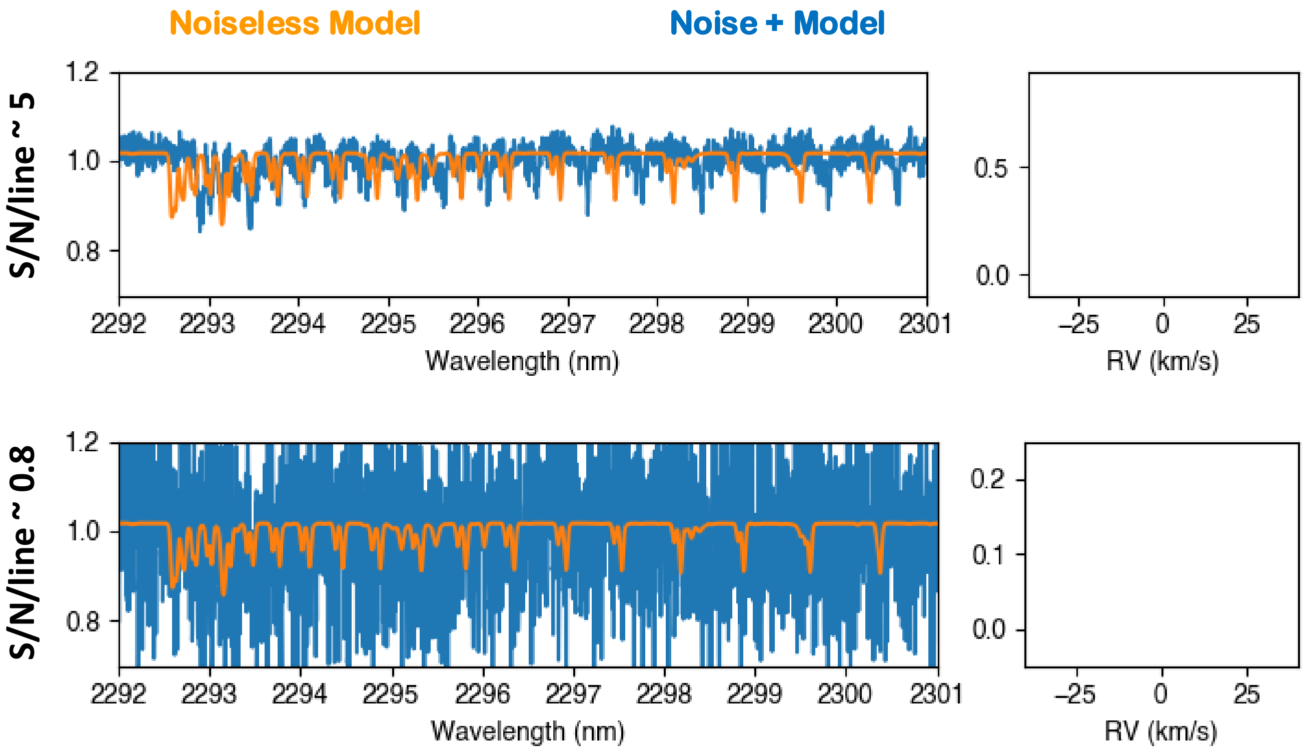


From Birkby 2018

Capturing this exoplanet movement first involves stripping out the information about the continuum, and then trying to remove all telluric (since ground based spectrographs) and stellar contribution to the total flux variation.

We use a SVD/PCA based framework for this as part of our pipeline Upamana.

Cross-correlation



Doppler shift model signal and compare *similarity* with processed data

Gif and picture credits: Dr. Matteo Brogi

$$\left.\frac{S}{N}\right|_{\text{CCF}} \approx \frac{n_{\text{pix}}N_{\gamma,P}}{\sqrt{n_{\text{pix}}N_{\gamma,\star}}} \propto \overset{\text{Just one line}}{\frac{S}{N}}\sqrt{n_{\text{lines}}}$$

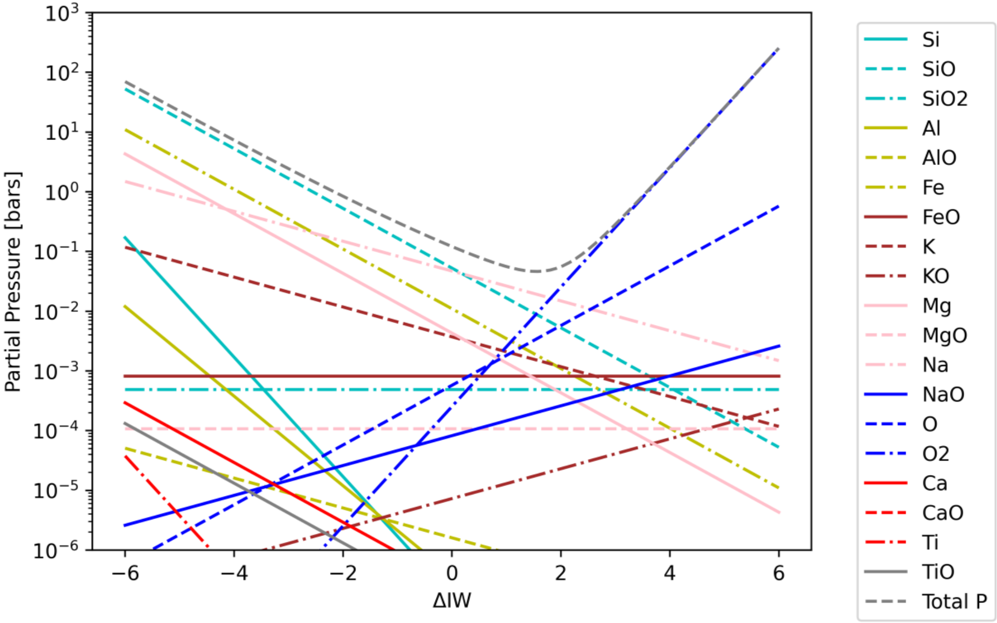
S/N directly proportional to the square root of the number of lines used to compare.

Thus for a template with hundreds of lines, reduced chance of aliasing and the total S/N substantial even though S/N per line is low.

Coming back to mineral atmospheres…

Using BSE (Bulk Silicate Earth) initial abundances for 55 Cnc e

BSE is the undifferentiated mantle very early during earth's formation with the crust not yet formed

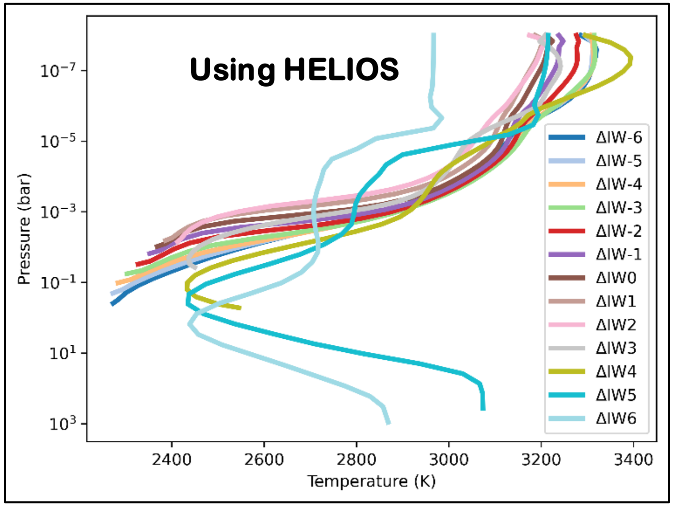


Can we detect and distinguish between these atmospheres using high-resolution cross-correlation spectroscopy? Distinguishing can help us determine melt oxidation state.

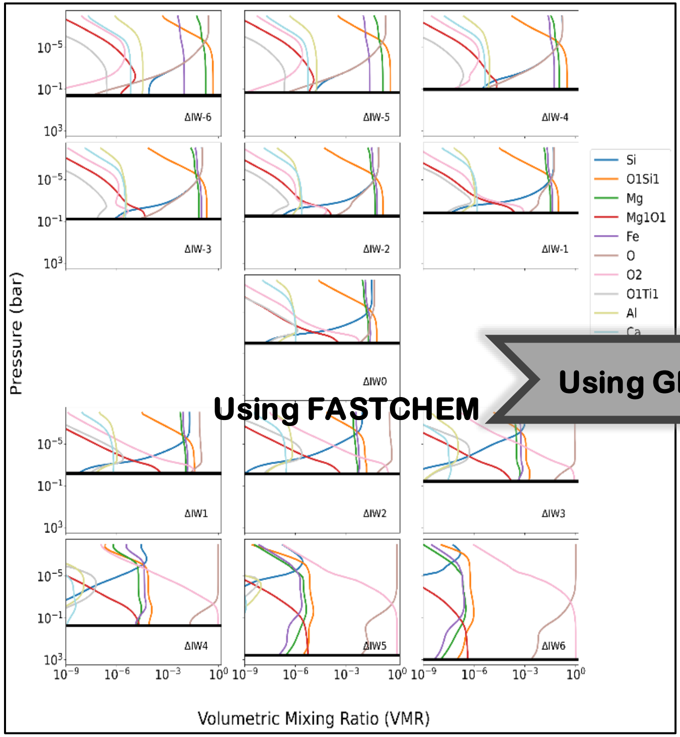
Unique chance to understand surface-atmosphere interaction in hot rocky exoplanets.

Fugacity regimes have observable differences in mineral atmospheric spectra in NIR at high resolution

Produced self-consistently in equilibrium with the surface melt, which is modelled by the code MAGMA.

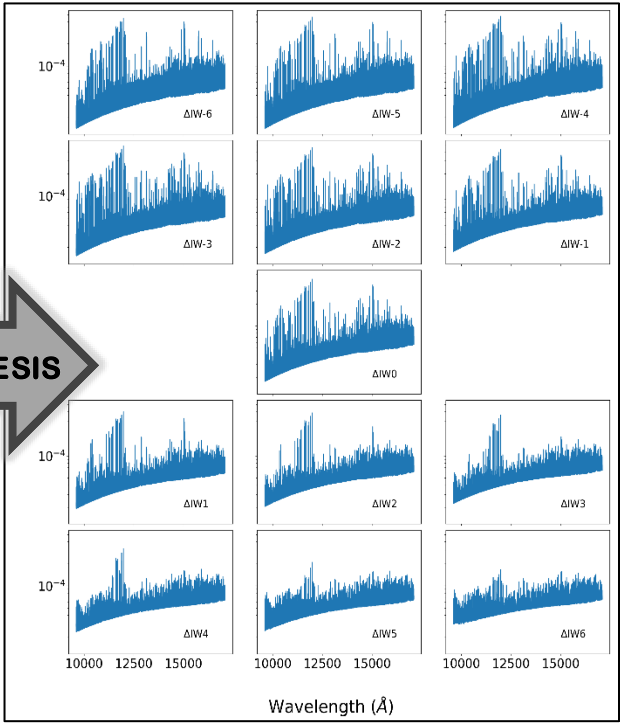


Using HELIOS



Using FASTCHEM

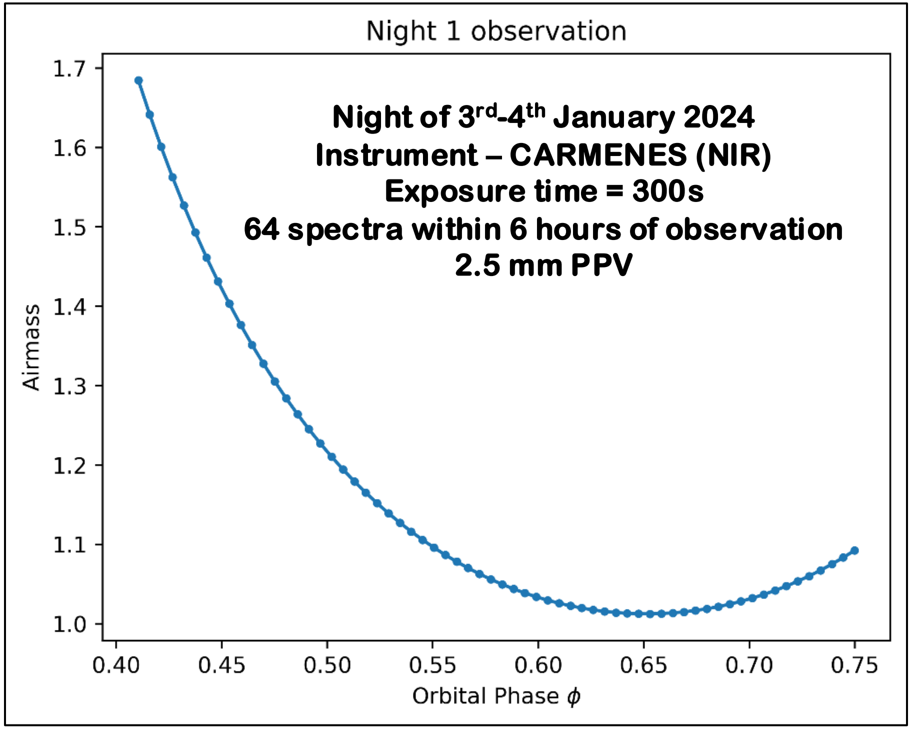
Using GENESIS



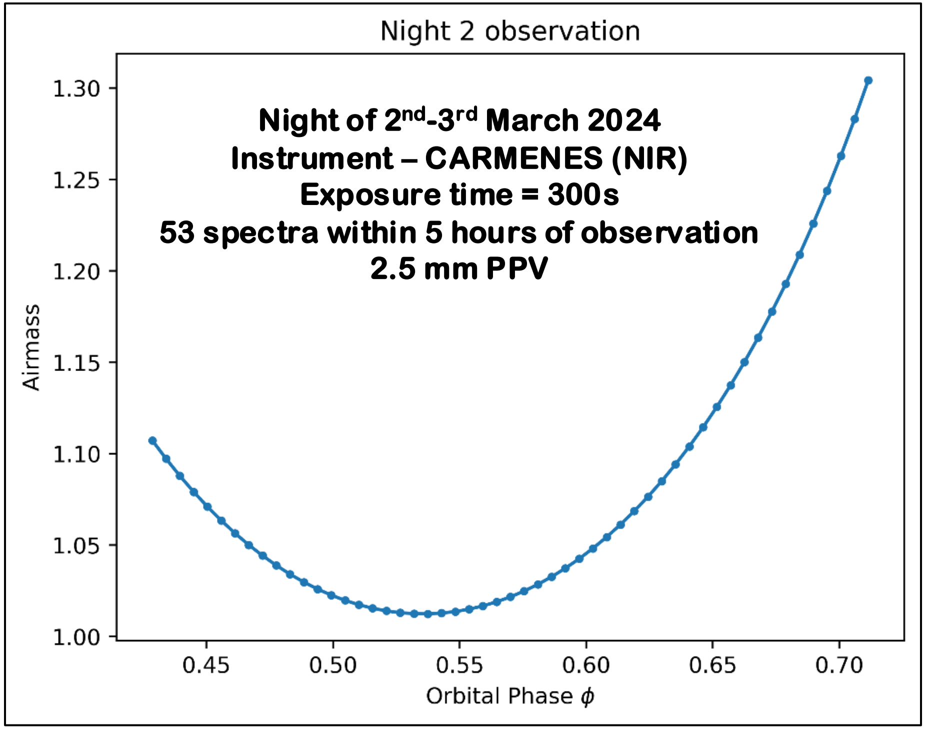
How do we quantitatively check if we can detect and differentiate between these regimes at high resolution? Is it possible using current spectrographs?

Simulated nights with CARMENES using Ratri

CAREMNES is mounted on the 3.5m CAHA telescope at Calar Alto.



Night of 3rd-4th January 2024
Instrument – CARMENES (NIR)
Exposure time = 300s
64 spectra within 6 hours of observation
2.5 mm PPV

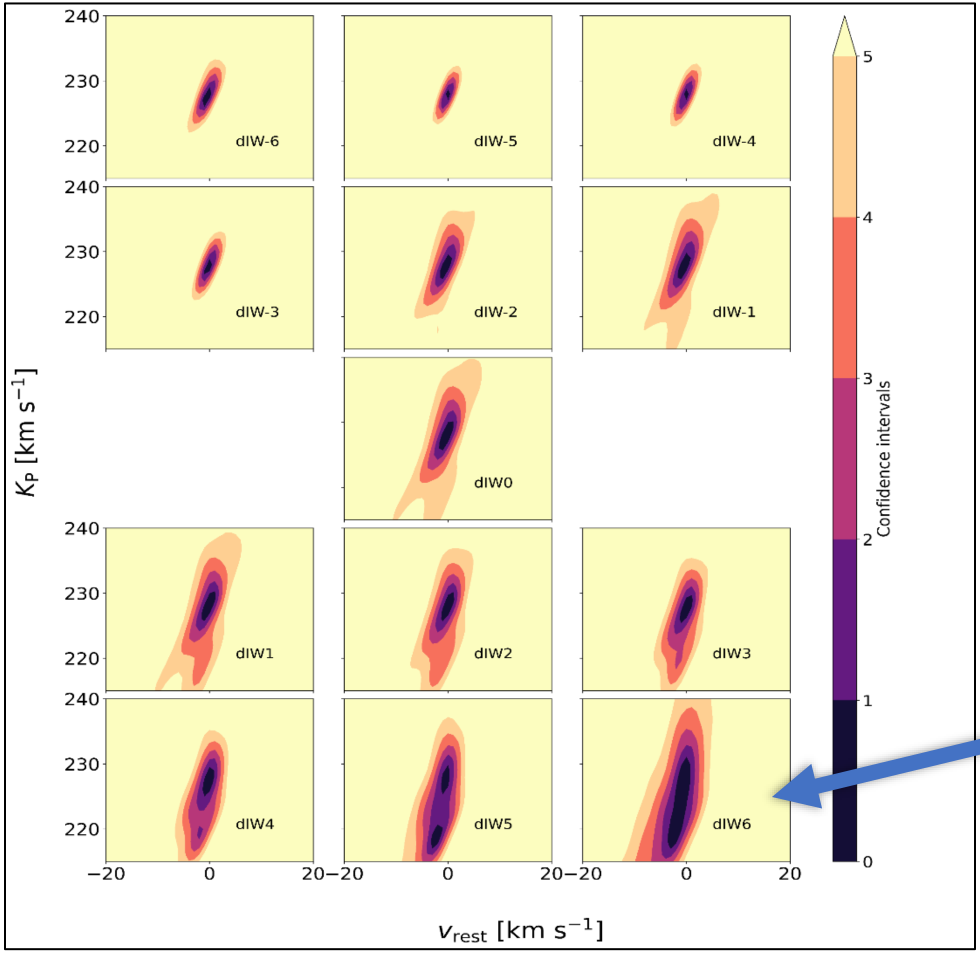


Night of 2nd-3rd March 2024
Instrument – CARMENES (NIR)
Exposure time = 300s
53 spectra within 5 hours of observation
2.5 mm PPV

Total 11 hours of observation of the exoplanet's dayside.

We neglect the effect of occultation as we are concerned only with the total observational time. In a more realistic sense, we would need another night of the same quality as Night 2.

Results from application of Upamana



From Dash et al 2025

All mineral atmospheric models can be detected using the two simulated nights, but the level of detection varies (as expected).

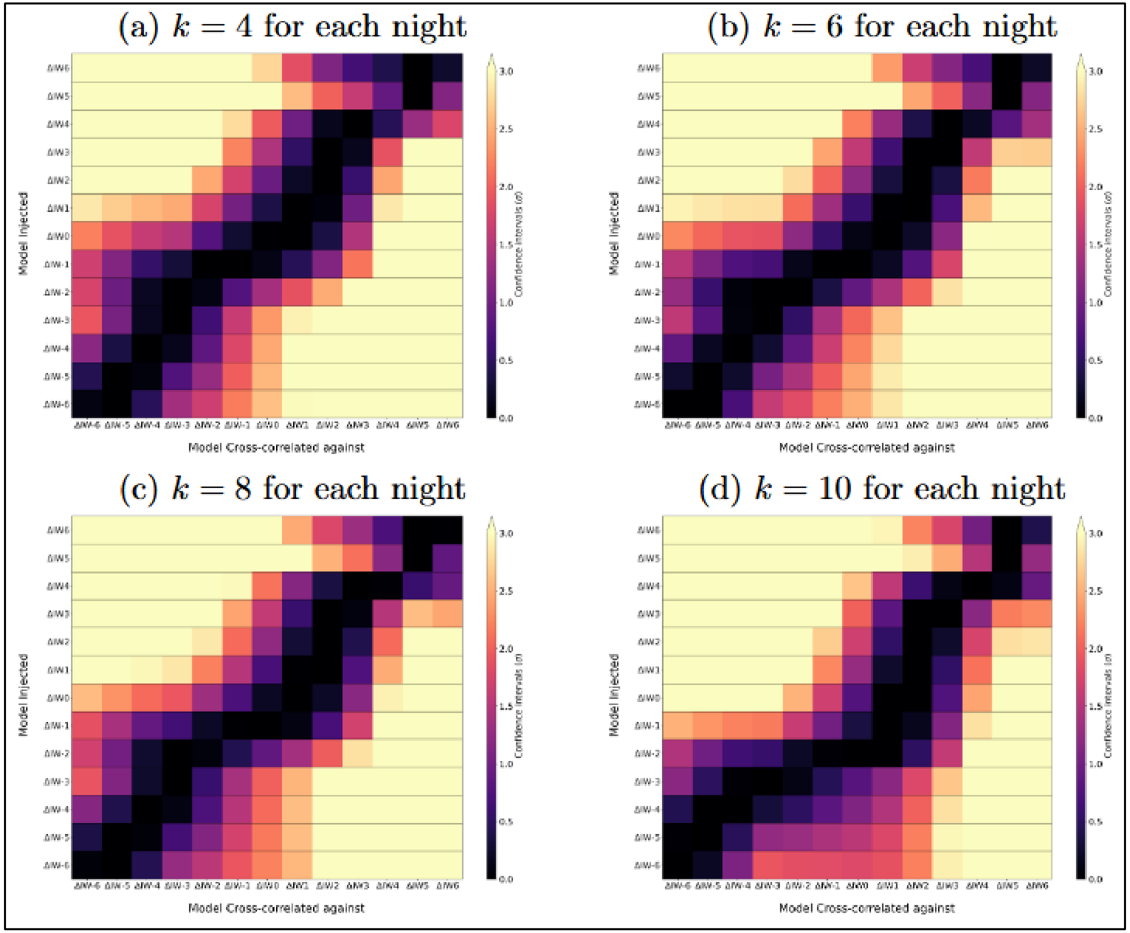
Can these models however be differentiated from each other?

Differences here is due to the maximum likelihood at both nights not overlapping.

Seems like the quality and properties of the night selected can also cause genuine shifts in retrieved properties based on model …

Does it explain similar phenomenon observed in real data?
(Still under investigation)

Model selection on a grid


(a) $k = 4$ for each night

(b) $k = 6$ for each night

(c) $k = 8$ for each night

(d) $k = 10$ for each night

From Dash et al 2025

Models are differentiable at ±1 at about 1.5σ.

Variation in *k* does not change the trend of selection significantly.

Already possible to do this kind of distinguishing using current instruments!

But 55 Cnc e is a special case, as its emission spectrum metric is 6 times larger than the next nearest candidate.

We will need ELT to do comparative exoplanetology for rocky magma ocean worlds.

Future prospects

- We are in the process of extending the high-resolution detectability scenario to volatile rich cases.
- Complementarity to low-resolution space-based studies (like JWST, Ariel, Exoworlds etc) is also essential, since we lose all access to spectral continuum in high-resolution, and complete free retrievals are computationally expensive. Joint retrievals can also provide more precise constraints.
- Primary question that is being worked on is: can we look at some spectrum and be sure that a magma ocean exits at the bottom of the atmosphere/existed at some point of time in the planetary evolution?
- Modelling mixed/secondary atmospheres can also give us a suite of scenarios in exoplanets that we can look forward to detect in the ELT era, especially for super-Earths and terrestrial exoplanets. In our own solar system, many of the terrestrial bodies could have had a magma ocean stage during their early stages of formation.