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1. Why phase separation?

- Structure models of interior are designed to fit available observational constraints: mass, radius, gravitational field, rotation rate and atmospheric temperature
- Outcome of modelling efforts: several layers of different composition - gas, ices and rock [1,2,3,4]
- Aim to understand structure requires phase diagrams and equation of state calculations of assumed material and mixtures
- Discrete layers are able to satisfy constraints of magnetic field, and a rather sharp boundary yields the simplest solution to the gravity field [5] and the luminosity of the planet [6]
- Possible explanation for discrete layered structure: immiscibility of major constituents
- Studies on Jupiter and Saturn [7,8,9,10,11,12] suggest H-He phase diagrams agree in predicting demixing of H and He at T around several 1000 K and P of a few Mbar
- Bailey & Stevenson 2021 explore the possibility of H₂-H₂O immiscibility and suggest different states of H₂-H₂O demixing can account for difference in heat fluxes between Uranus and Neptune. Current experimental data on H₂-H₂O shows demixing at pressure of a few GPa, where structure models require a change in composition from H-rich to ice-rich
- Aim to join paths by investigating the possibility of phase separation in the H/He/H₂O system in Uranus and Neptune

2. Phase diagrams

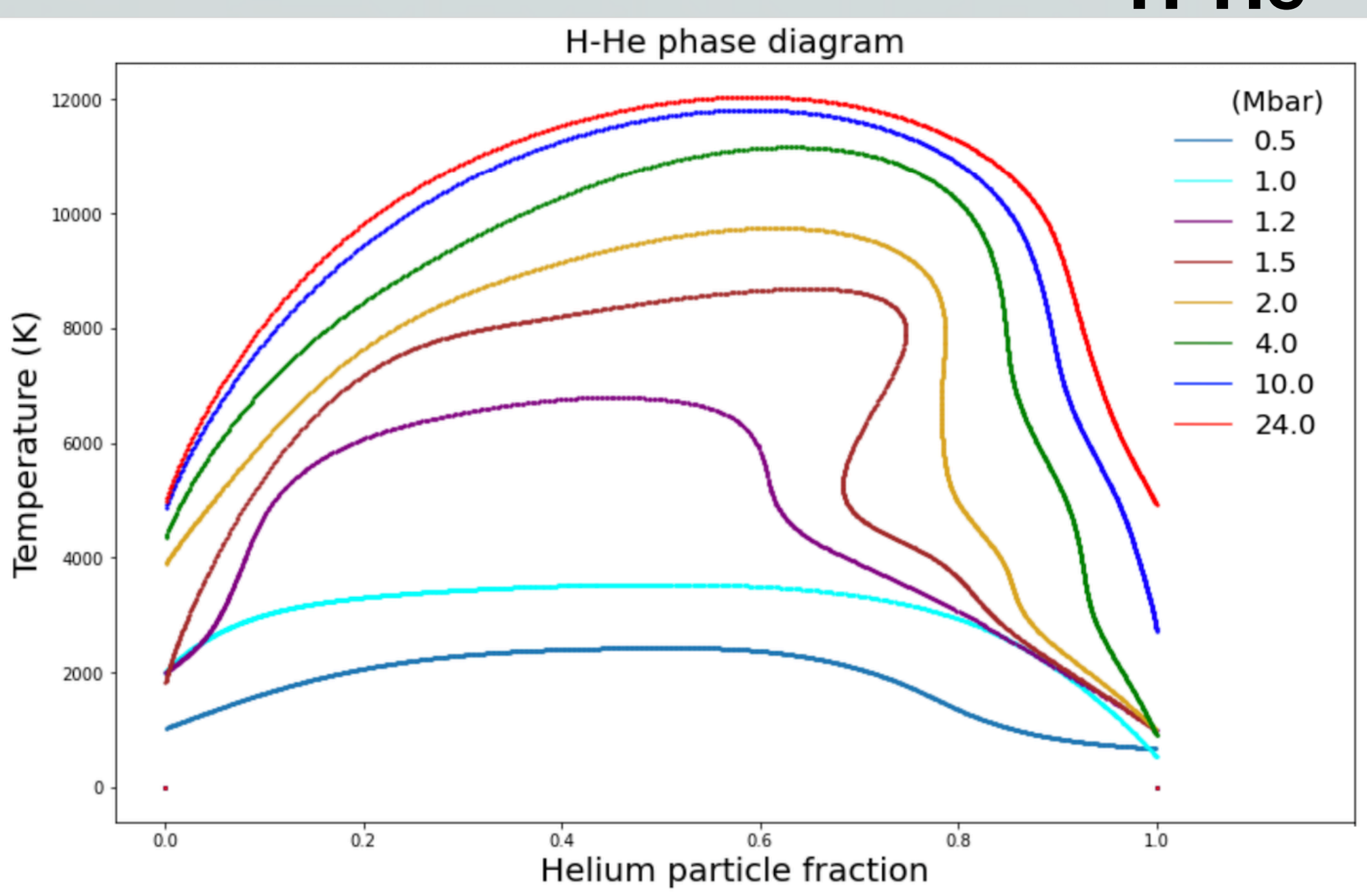


Figure 1: Phase diagram obtained by Schöttler & Redmer 2018 [13] for H-He mixtures in the pressure range 0.5 to 24 Mbar. The vertical straight line shows the protosolar helium particle fraction (0.0866).

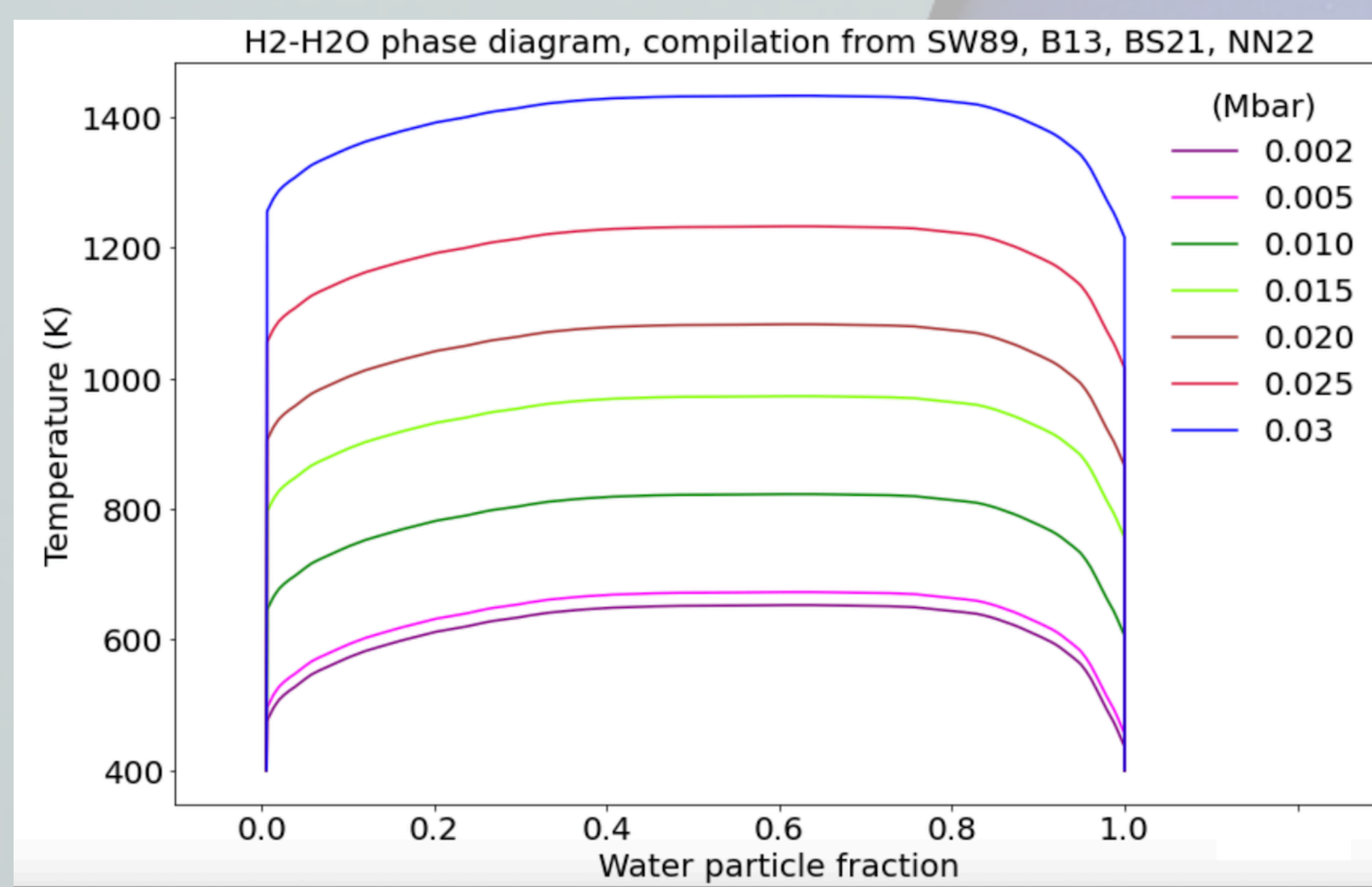
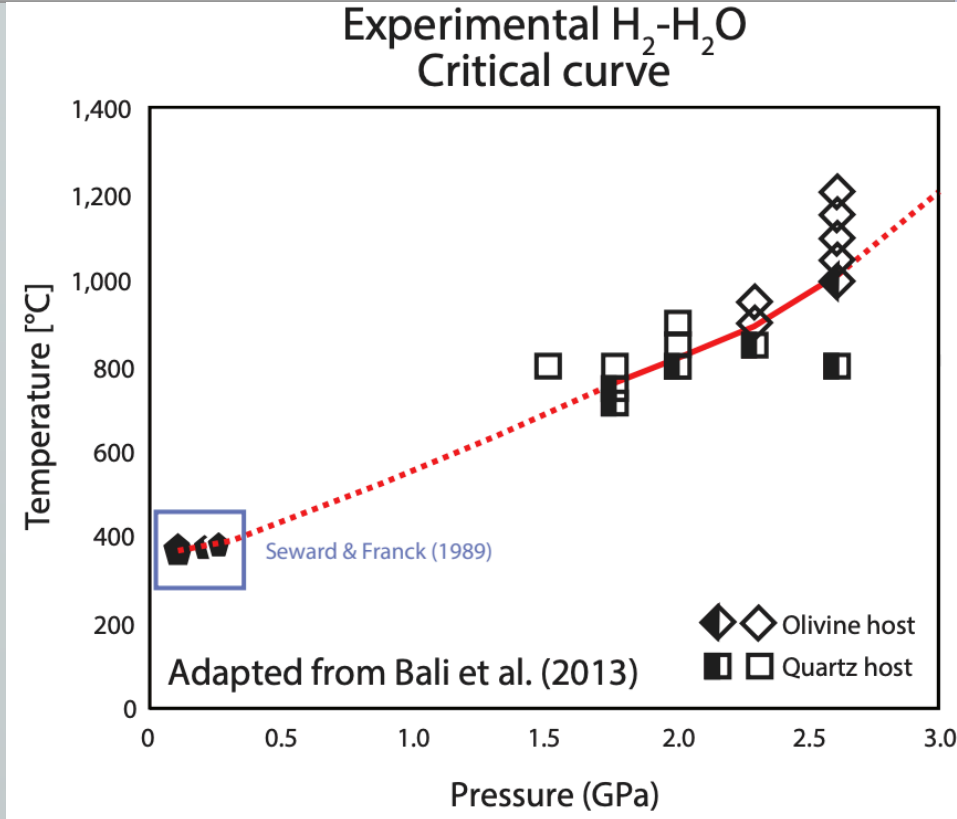
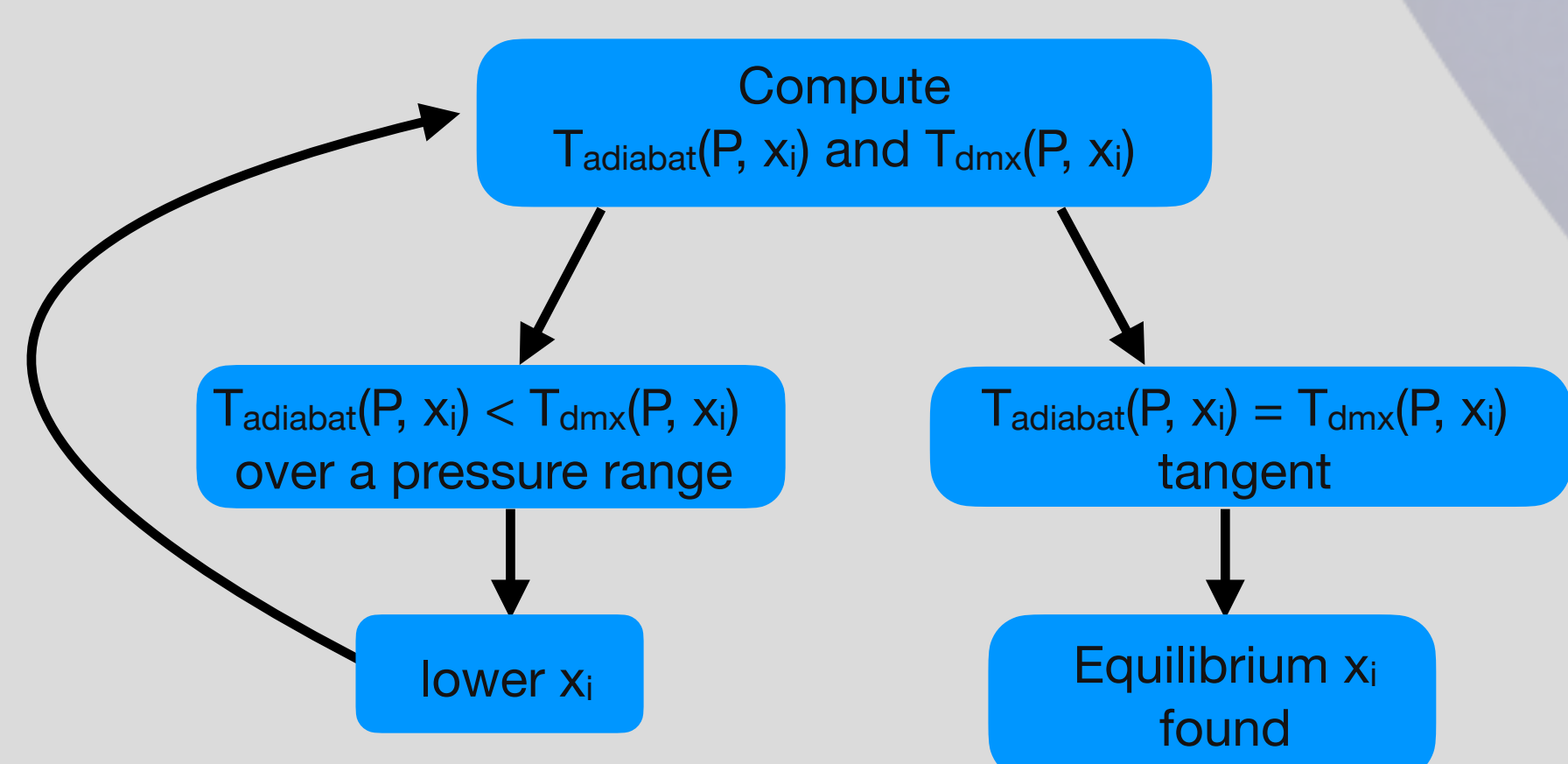


Figure 2: Right: Critical curve for H₂-H₂O experimentally derived by Seward & Franck 1989 [14] and Bali et al. 2013 [15]. Obtained from [5]. Above: Phase diagram for H₂-H₂O mixtures based on critical curve.

$$x_i = \frac{N_i}{N_i + N_j}$$



- Phase diagrams provide demixing curves $T_{dmx}(P, x_i)$ i.e. maximum temperature below which phase separation occurs
- Equations of state (EoS) to obtain $T_{adiabat}(P, x_i)$ assuming the volume additive rule:
 - H/He: Chabrier & Debras 2021 [16]
 - H₂/H₂O: AQUA from Haldemann et al. 2020 [17]
- Iterative procedure to obtain converged value of atmospheric equilibrium He and H₂O abundance, yielding the predicted H/He and H₂/H₂O composition in the atmosphere.



3. Adiabats versus demixing curves → equilibrium abundances

H-He

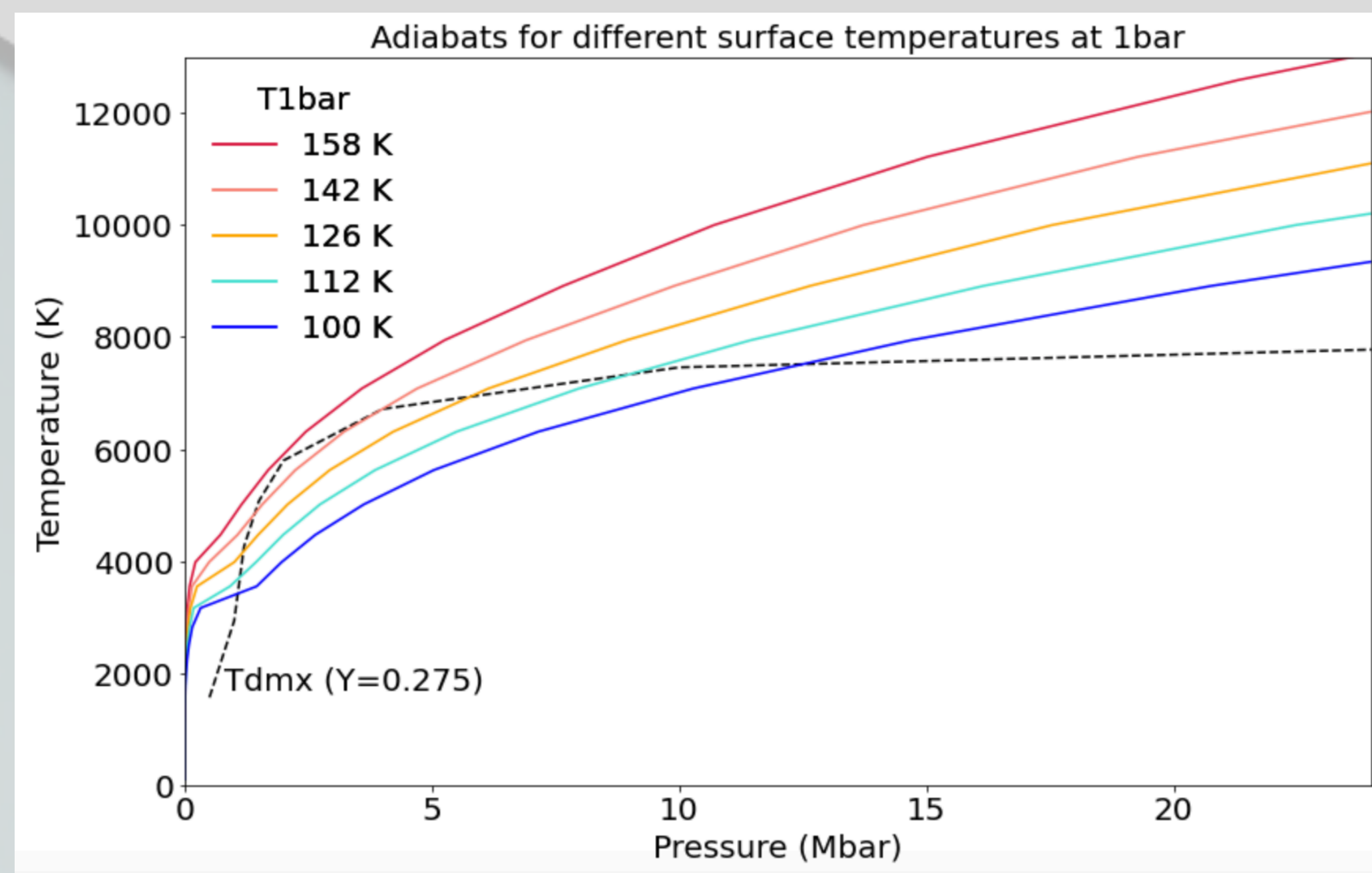
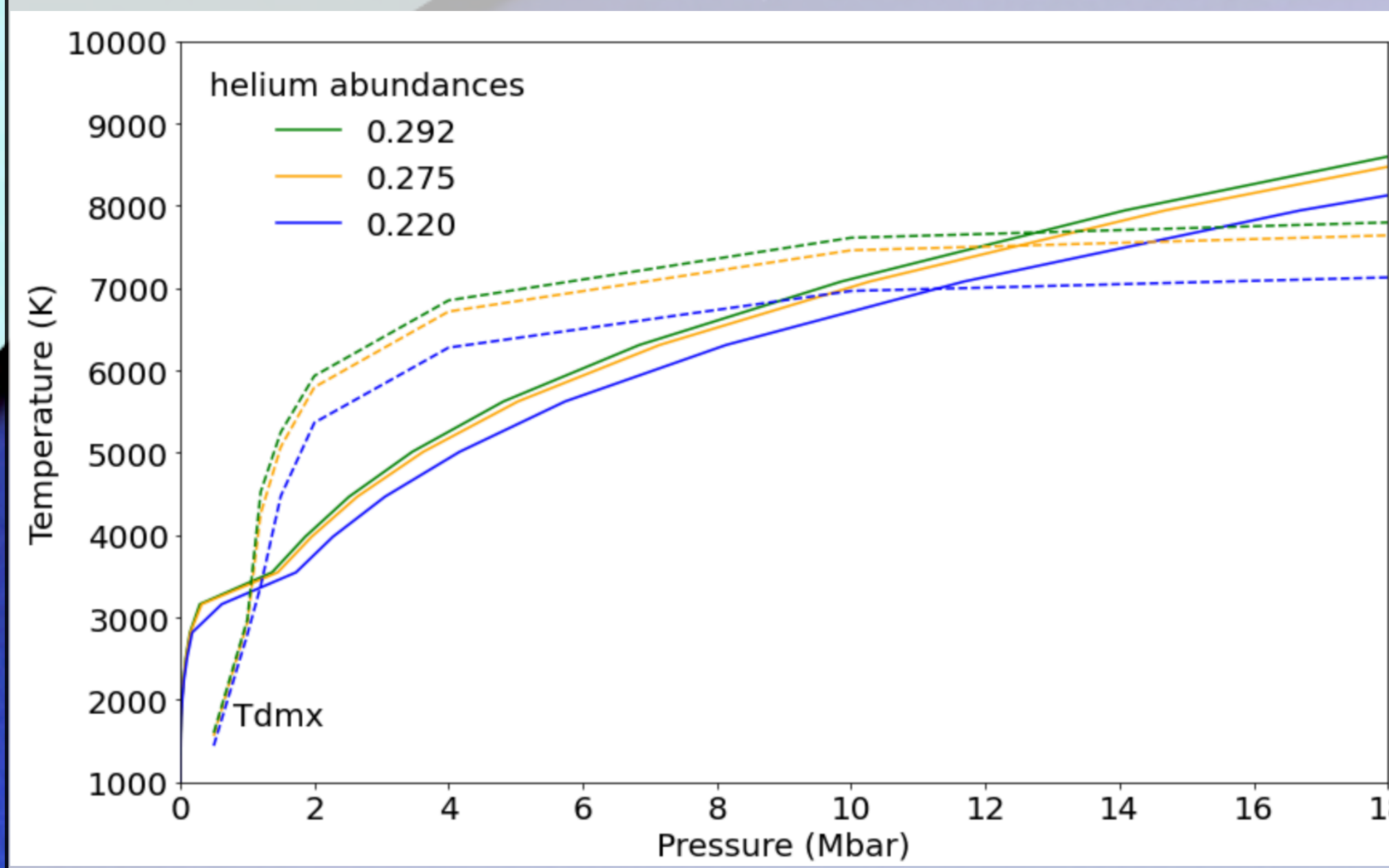


Figure 3: Adiabatic P-T relations for distinct surface temperatures at 1 bar compared with demixing curve (dashed line) for protosolar helium abundance

• Fig. 3 shows how the adiabats depend on surface temperature and how colder adiabats have a wider crossover with the demixing curve for a given helium abundance (here 0.275) and therefore require lower x_{He} values to reach the equilibrium point.

• H-He phase separation will occur in regions of the planets that cool below the P-T curve for the relevant helium mass fraction. An example: Fig. 4 (left) shows that for a protosolar helium abundance, the demixing region will start at $P \sim 1.1$ Mbar until ~ 12 Mbar, after which the mixture will be miscible again

H-He



H2-H2O

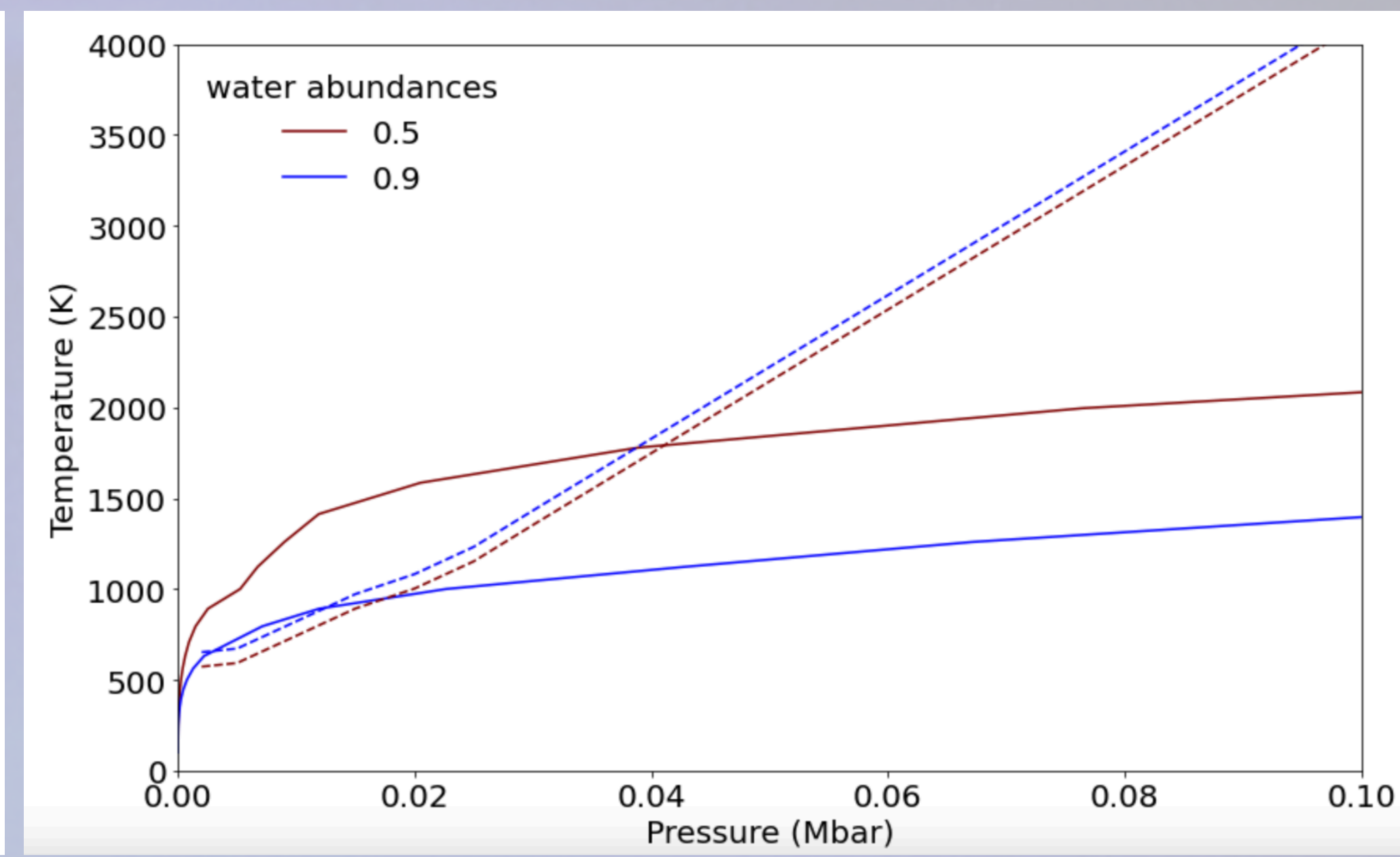


Figure 4: Demixing temperature curves (dashed lines) for helium abundances (left) and water abundances (right) compared with corresponding adiabatic P-T relations for $T_{1bar}=100$ K.

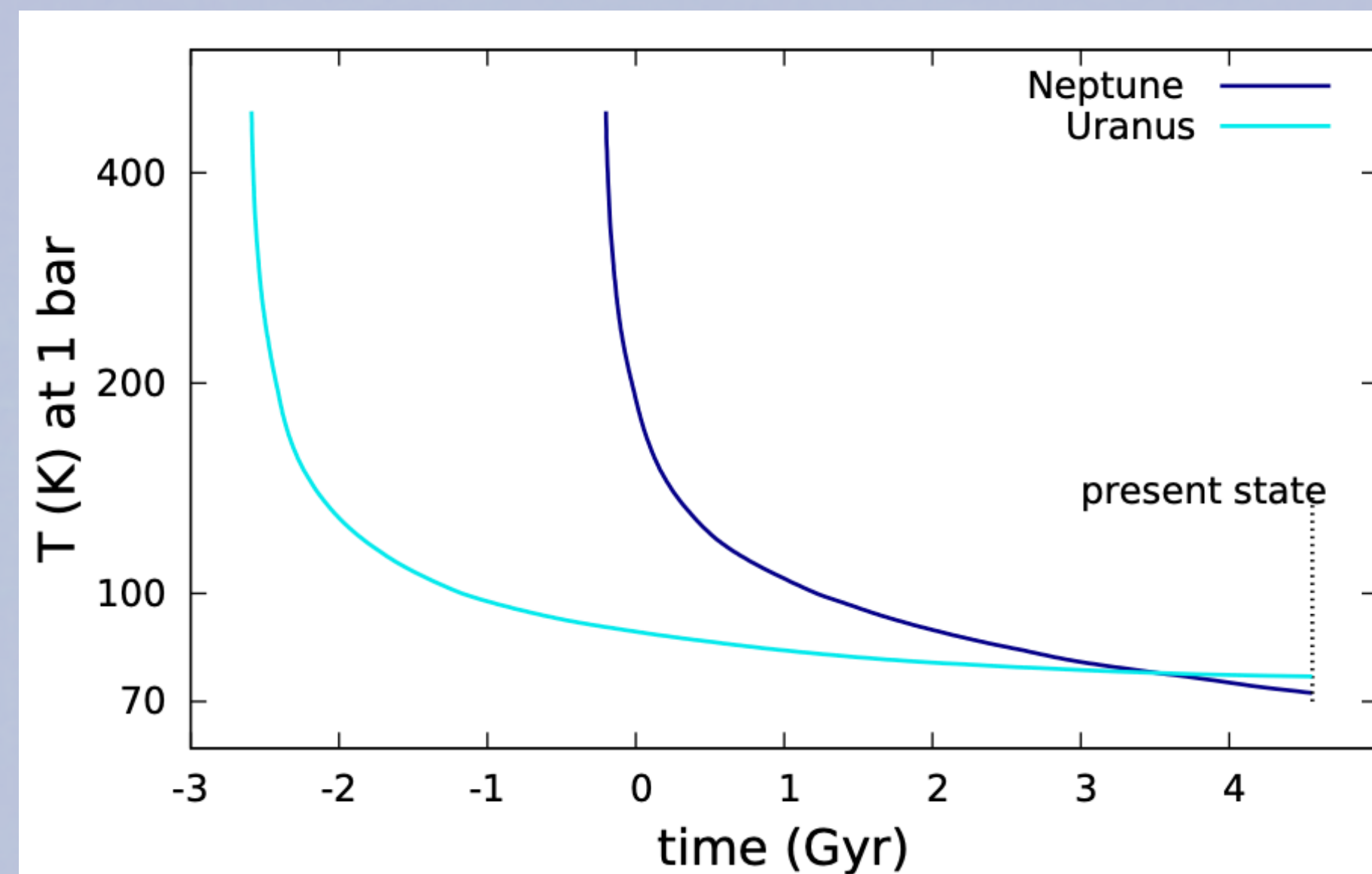
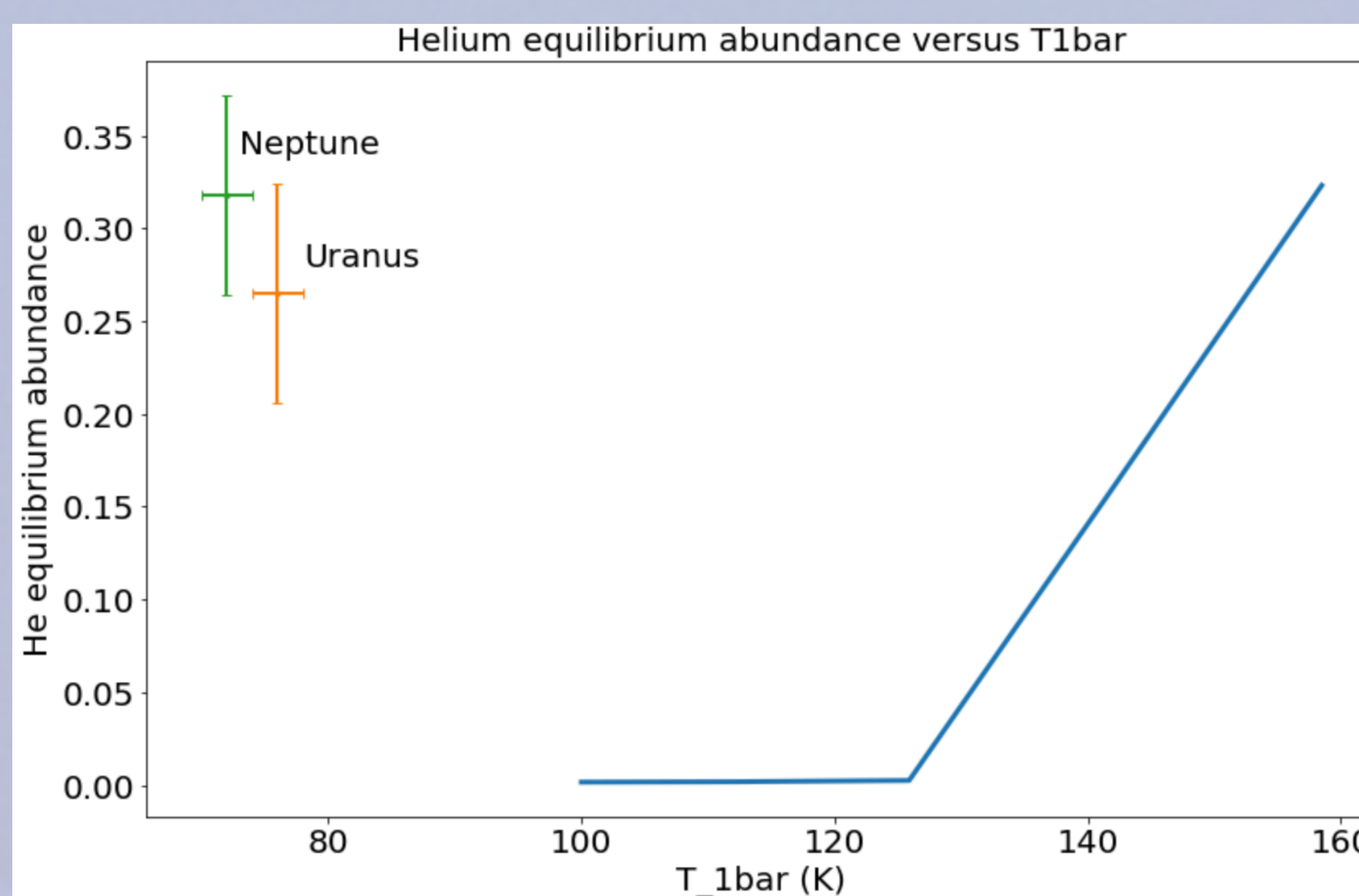


Figure 5: Thermal evolution of Uranus and Neptune to illustrate the cooling of the atmosphere at the 1-bar level over time. Obtained from [18].

H-He



H2-H2O

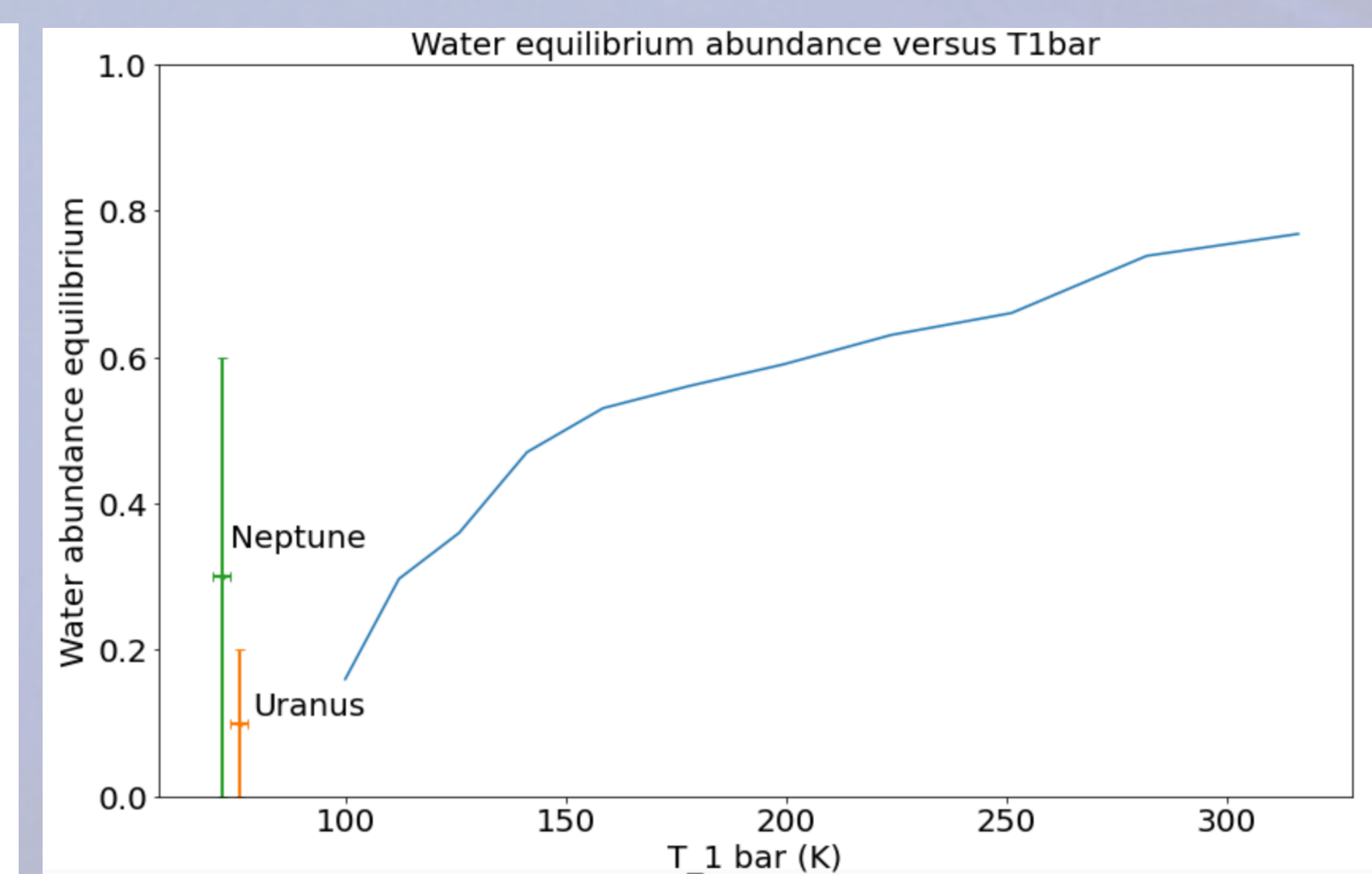


Figure 6: Atmospheric helium abundance (left) and water abundances (right) as a function of T_{1bar} obtained through the iterative process of finding the equilibrium state between adiabatic and demixing curves. Corresponding abundances and error bars are included for Uranus and Neptune obtained from current structure models.

4. Conclusion & Outlook

- Extrapolation of Fig 6. (Right) shows atmospheric water composition found is consistent with outer envelope water abundances from structure models for Uranus and Neptune
- Obtain cooler adiabats for T_{1bar} for Uranus and Neptune ~ 75 K
- Apply phase diagram curve for H₂-H₂O for 4 GPa

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