The Chemistry of Exoplanetary Atmospheres

The Effects of Non-equilibrium Chemistry

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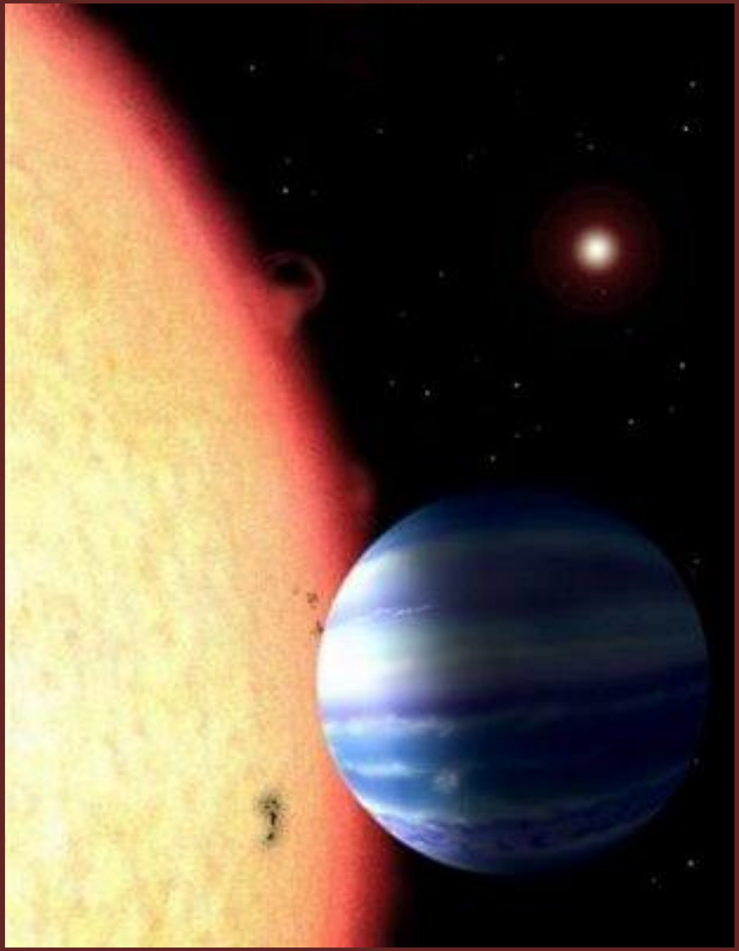
Outline

- Introduction
- Exoplanetary atmospheres
- Results
  - Zero-metallicity
  - C, N, O chemistry
  - Initial conditions
- Further work
- Summary



Transiting Exoplanets

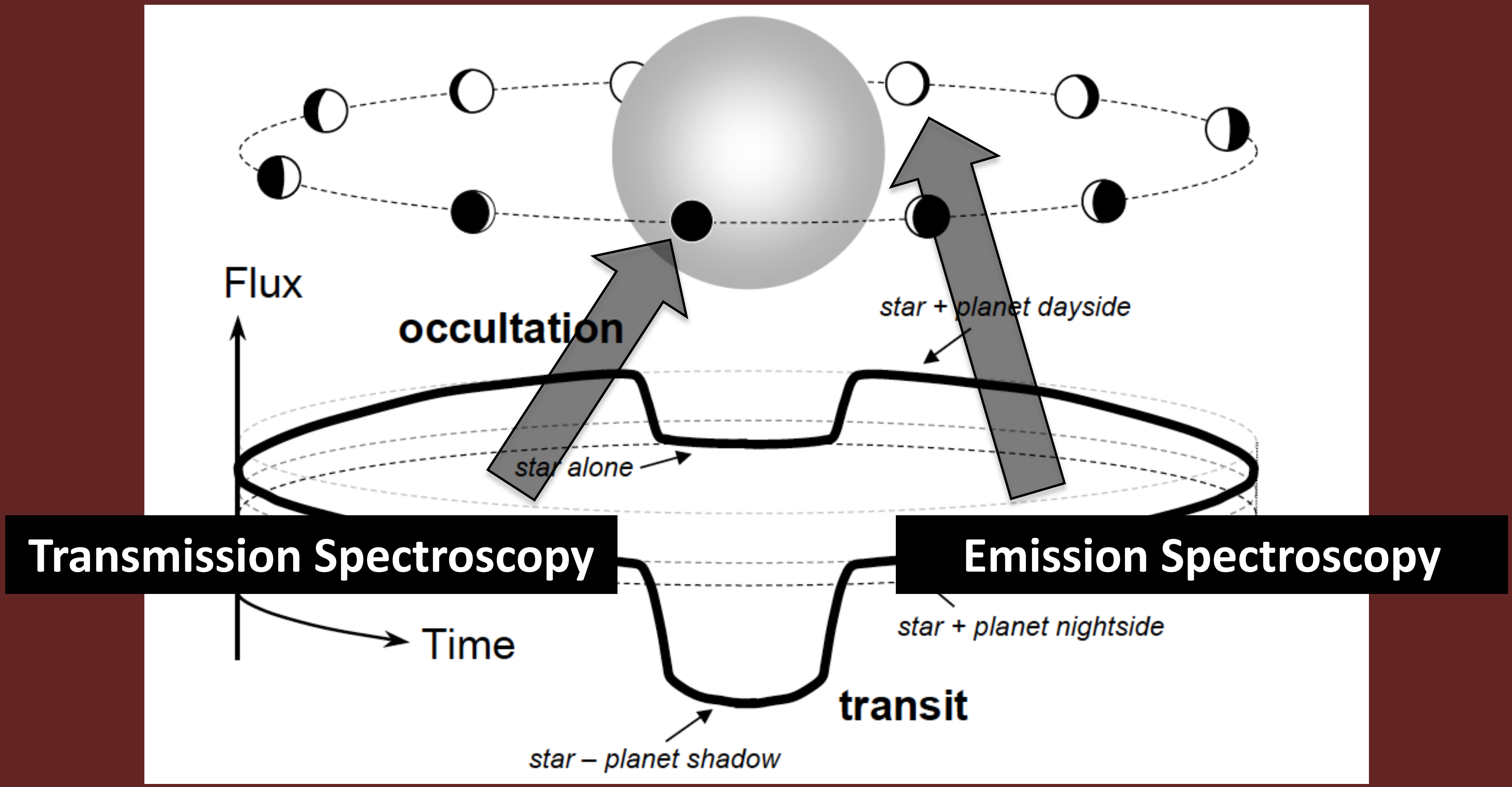


Figure from Winn 2009, in Exoplanets, ed. S. Seager

‘Hot Jupiters’

- **Most transiting planets are ‘Hot Jupiters’**
  - Between < 1 and 10 M_j and < 1 and a few R_j
  - Orbital radius of between 0.01 and 0.1 AU
  - Orbital period on the order of 1 day
  - Heavily irradiated by parent star
  - Tidally locked with a constant night-side and day-side
  - Low Bond albedo i.e. reflectivity
- **Atmospheric chemical composition**
  - Likely molecular hydrogen and helium dominated
  - Trace elements include C, N, O, S, metals
  - Upper day-side atmosphere is heavily irradiated
  - Heat redistribution from day-side to night-side
  - Atmospheric dynamics?
- **Formation mechanisms**
  - Core accretion
  - Disk fragmentation
  - Planetary migration
- **Mass-loss from atmosphere**
  - Evaporation
  - Roche-lobe overflow

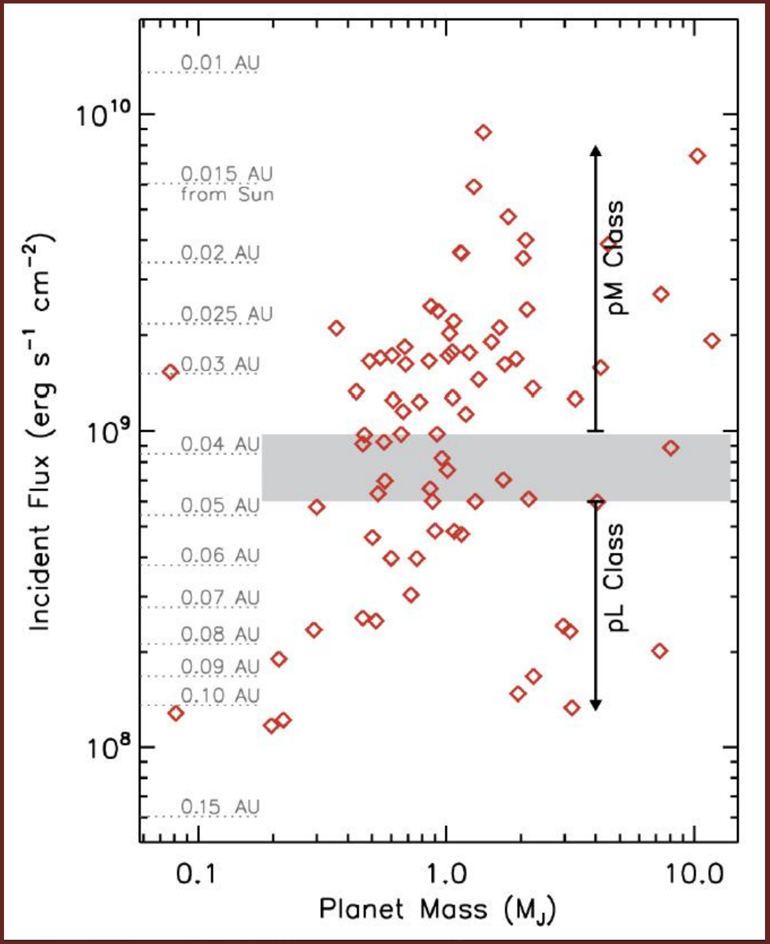


Figure from Fortney et al. 2008, ApJ, 678, 1419

Molecules in Exoplanet Atmospheres

Transmission Spectrum

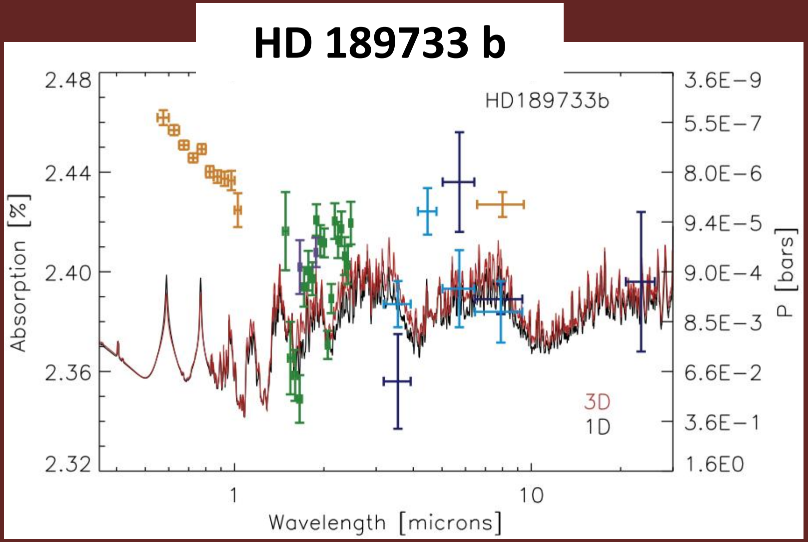


Figure from Fortney et al. 2010 , ApJ, 709, 1396

Emission Spectrum

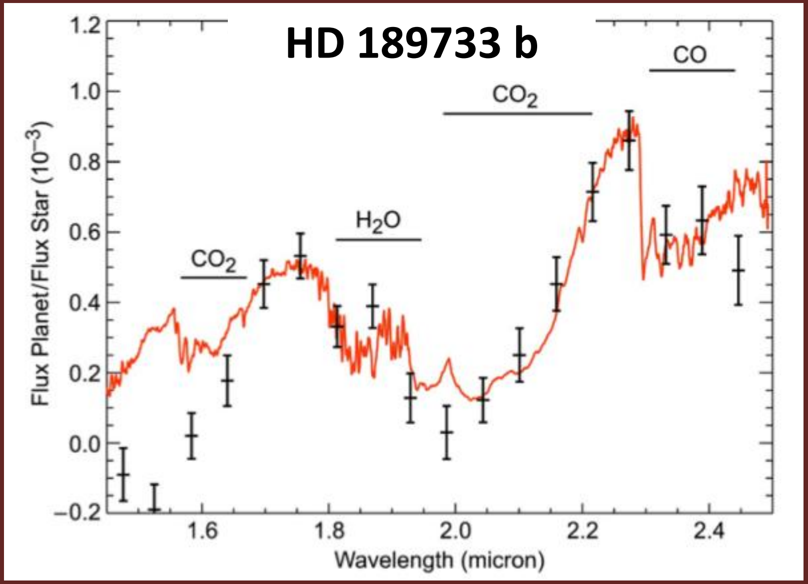


Figure from Swain et al. 2009, ApJ, 690, L114

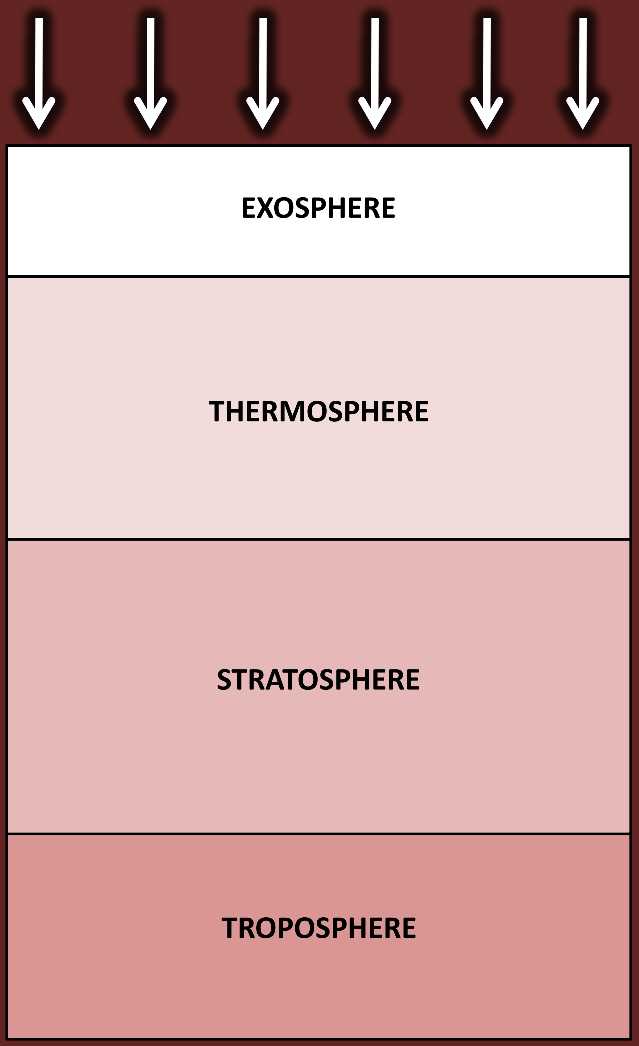
Current forward models struggle to reproduce observed spectra.

Molecules identified using backwards/fitting models. Many free parameters!

Non-equilibrium chemistry, non-LTE effects, temperature inversion?

Building a Model Atmosphere

- **Common assumptions**
  - Plane-parallel geometry
  - Hydrostatic equilibrium
  - Radiative equilibrium
  - Chemical equilibrium
  - Local thermodynamic equilibrium
- **Model Ingredients**
  - Planetary system parameters
  - Chemical elemental composition
  - Absorption cross section data
  - Reaction rate coefficients
- **Complications**
  - Convection
  - Dynamics (e.g. winds)
  - Mixing/diffusion
  - Incomplete opacity line lists
  - Photochemistry
  - Clouds and dust



Radiation from star
Cosmic rays?

Non-LTE
Atmospheric escape?

Photochemistry
Ion-molecule chemistry
Cooling by molecular transitions e.g. H_3^+

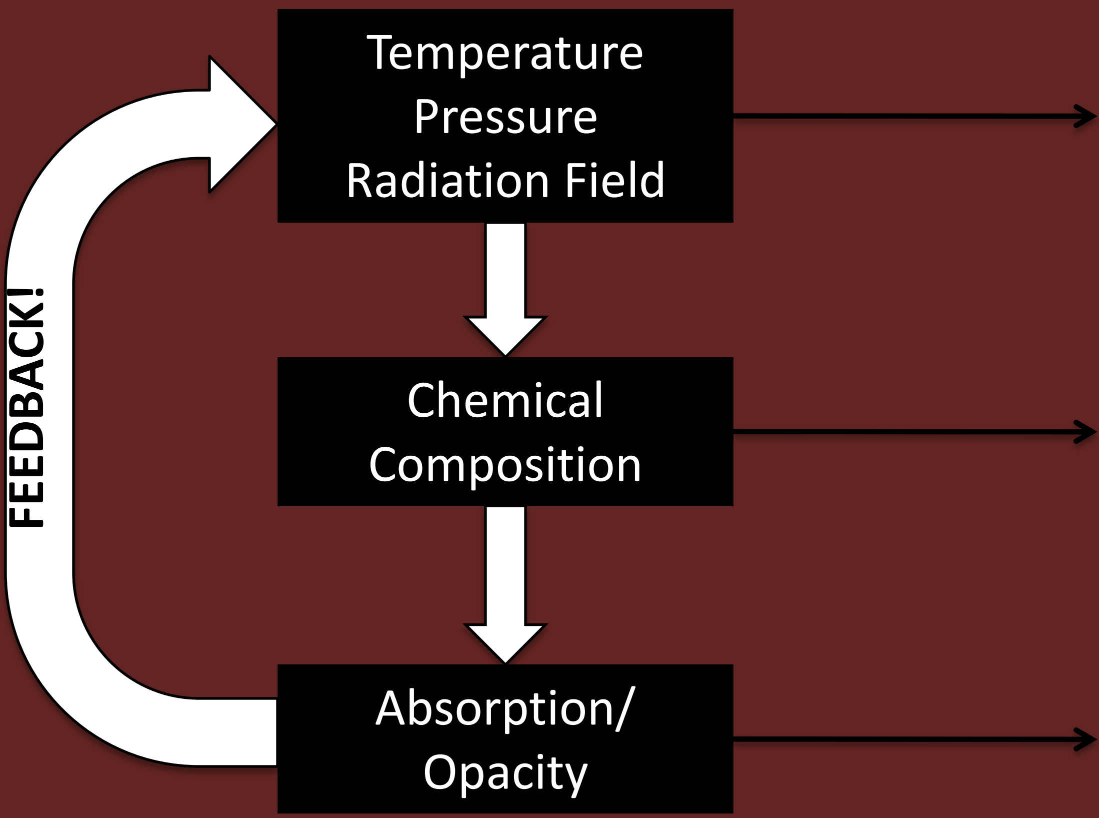
Temperature inversion?
Cloud formation?
Haze?

Convection
Chemical equilibrium
Collisional processes

Exoplanet Atmosphere Model

Physics and chemistry of the atmosphere are intrinsically linked!

Self-consistent solution is required!

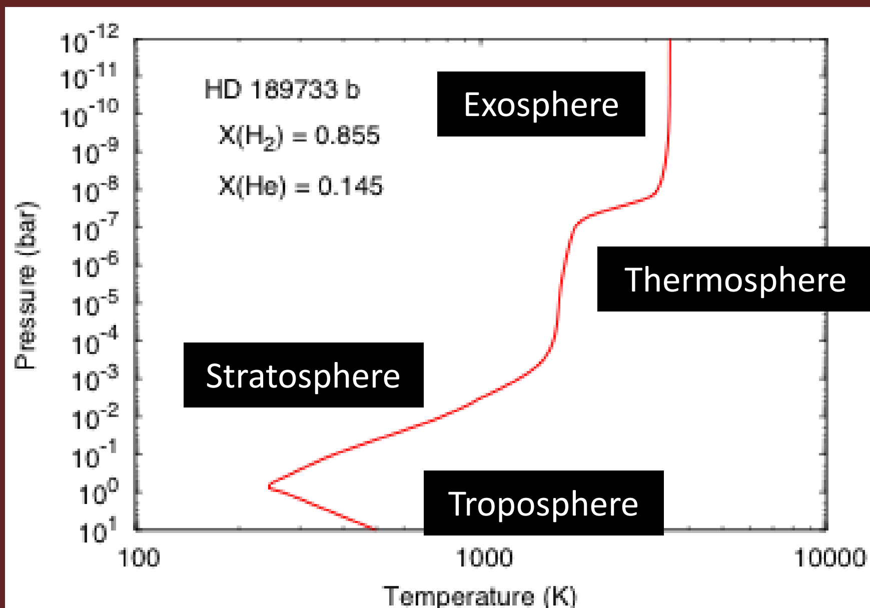


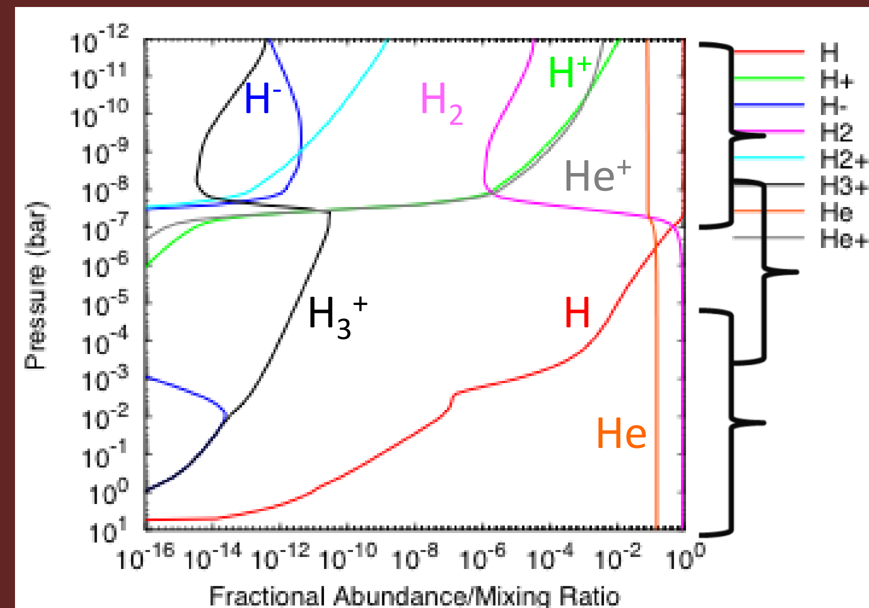
Equation of radiative transfer
Radiative equilibrium
Hydrostatic equilibrium
Ideal gas
Black-body incident radiation

Ion-molecule chemistry
Neutral-neutral chemistry
Collisional processes
Photochemistry

Line absorption
Continuum absorption
Free-free absorption
Collision-induced absorption
Raleigh scattering

Results: Zero Metallicity

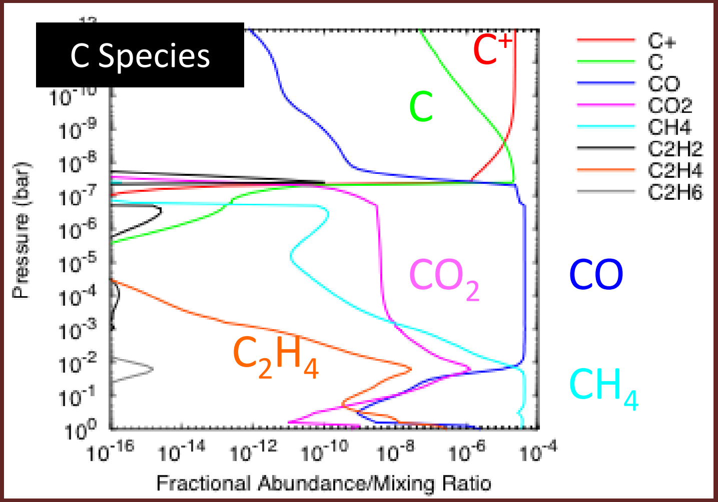


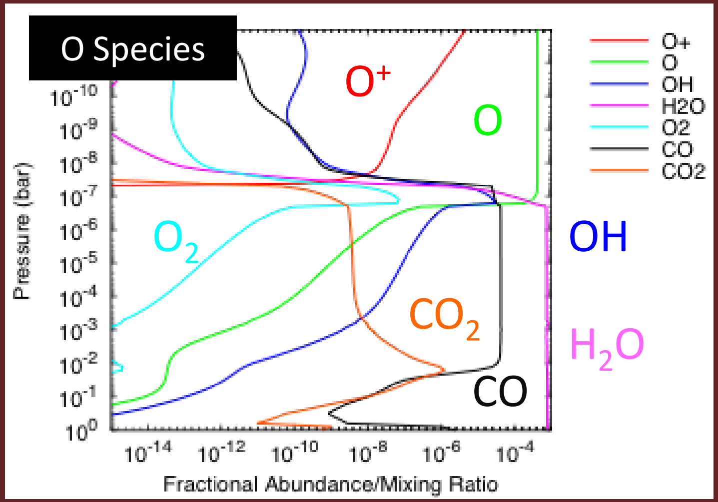


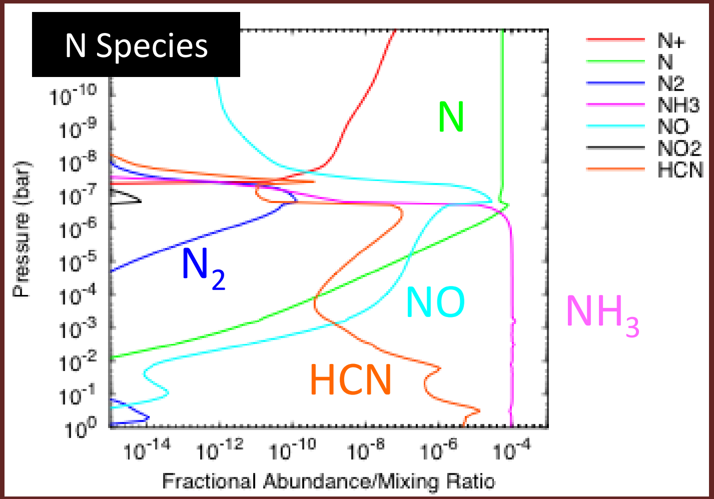
- Model reproduces expected atmospheric structure
- Photochemistry and ion-molecule chemistry lead to chemical stratification and an ionised layer at high altitudes (similar to PDR/PPD)
- Significant abundances of H^- and H_3^+ - both absorb at IR wavelengths!

Results: C, N, O Chemistry

- **HD 189733 b**
  - **M_p = 1.13 M_J**
  - **R_p = 1.14 R_J**
  - **T_{eff} = 4980 K (K1 – K2)**
  - **a = 0.031 AU**
  - **D = 19.3 pc**
- **Solar metallicity (**Anders &Grevesse, 1989)
  - C = 2.455 x 10^{-4}
  - N = 6.026 x 10^{-5}
  - O = 4.571 x 10^{-4}







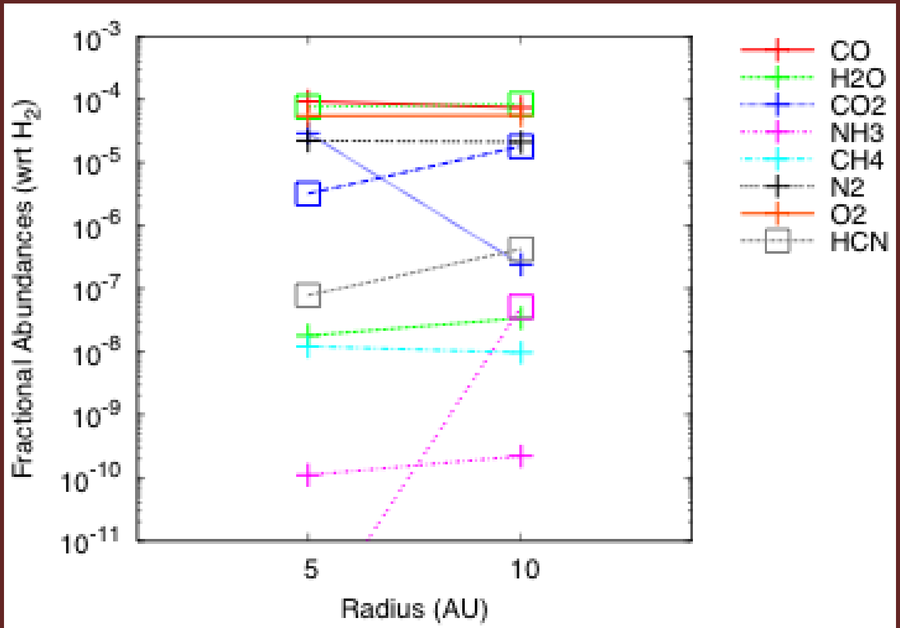
Results: Initial Molecular Abundances

- Link between protoplanetary disk chemical structure and planetary atmosphere composition?

- Gas-giant planet formation
  - Coagulation of icy dust grains in outer disk --->protoplanet
  - Accretion of remnant disk material to form gaseous envelope i.e. core accretion
  - Planet migration from outer disk to inner disk
  - Contamination of atmosphere?

- Generate initial abundances from a protoplanetary disk model?

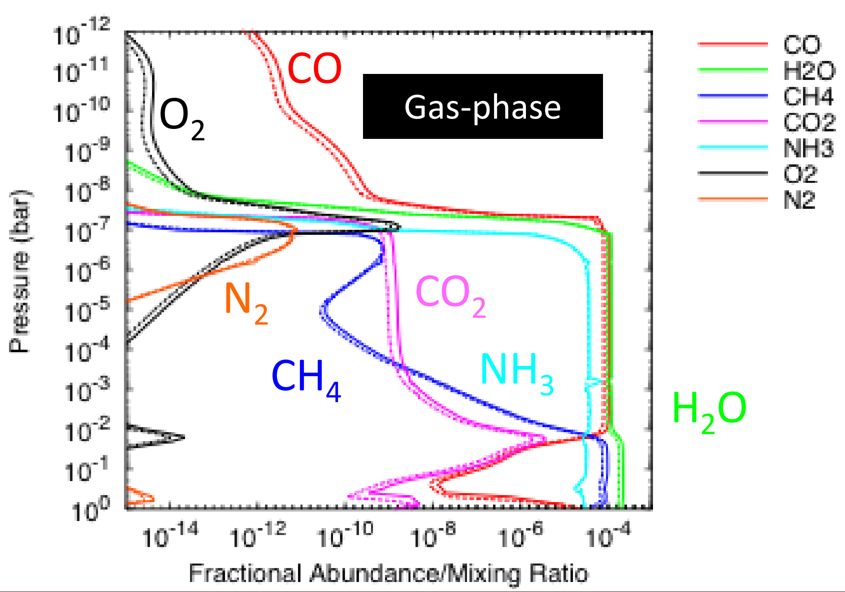
Results: Initial Molecular Abundances



Crosses = gas-phase; Squares = grain-surface
Walsh et al. 2010, 2011

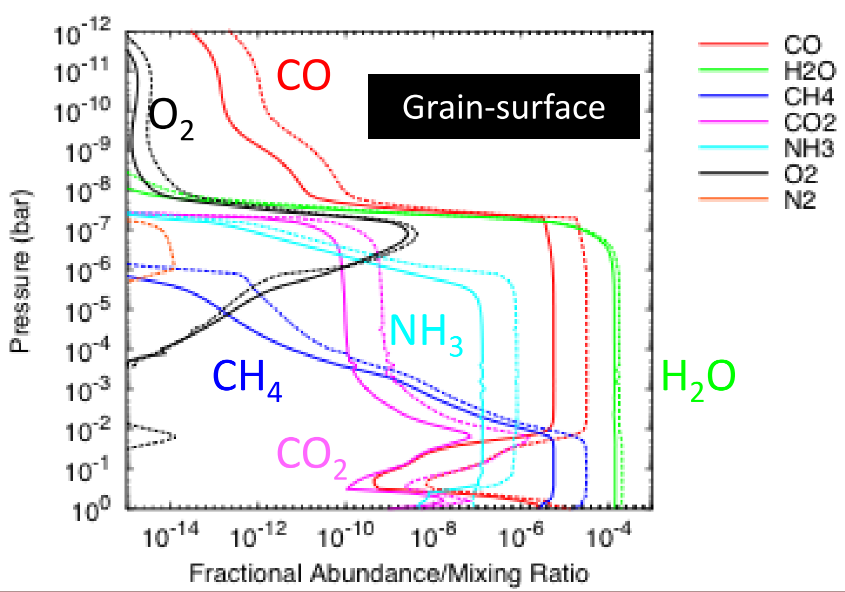
- Planet formation site
- Protoplanetary disk model
  - Gas-phase chemistry
  - Gas-grain interactions
  - Grain-surface chemistry
- Oxygen-rich low-metal initial elemental abundances

Results: Initial Molecular Abundances



Gas-phase initial abundances
Solid lines = 5 AU; Dashed lines = 10 AU

- Major chemical reprocessing in the atmosphere
- Only minor differences in final chemical structure using disk gas-phase initial molecular abundances



Grain-surface initial abundances
Solid lines = 5 AU; Dashed lines = 10 AU

- Larger differences when using grain-surface initial molecular abundances!
- H_2O becomes dominant molecule
- Order of magnitude differences in CO_2, NH_3 and CO/CH_4 at 5 and 10 AU

Further Work

- Immediate
  - Investigate chemical feedback on atmospheric physical structure
  - Addition of trace elements e.g. Na, Mg, Fe, Ti, V
  - Further exploration of initial conditions
  - Generate synthetic emission and transmission spectra to compare with current and future observations
- Future
  - Mixing/diffusion
  - Cloud formation, absorption and scattering
  - Solid particles, aerosols and haze
  - Super-Neptunes, Saturns and Earths
  - Predictions for future missions e.g. JWST

Summary

Self-consistent model of an irradiated exoplanetary atmosphere with non-equilibrium chemistry

- **Zero-metallicity chemistry**
  - Chemical stratification in the atmosphere due to photo- and ion-molecule chemistry
  - Absorption at IR wavelengths by H^- and H_3^+?
  - Impact on physical structure?
- **Carbon, oxygen, nitrogen chemistry**
  - Solar metallicity
  - Chemical stratification due to photo- and ion-molecule chemistry
  - Atomic and molecular regions determined by H/H_2 boundary
  - Dominant molecules in densest region: CO, CH_4, H_2O, NH_3
  - Molecular absorption feedback?
  - Varying metallicities?
- **Initial molecular abundances**
  - Major chemical reprocessing in atmosphere
  - Minor differences in final chemical structure using gas-phase initial abundances
  - Larger differences in relative molecular abundances when using grain-surface/ice abundances
  - Implications on planetary formation theory?