

Condensation Chemistry and Abundance Measurements in Cloudy Atmospheres

Derek Homeier¹

France Allard¹
Bernd Freytag³

Isabelle Baraffe^{2,1}
Gilles Chabrier^{1,2}

¹CRAL/École Normale Supérieure de Lyon

²University of Exeter

³ Uppsala Universitet



European Research Council
Established by
the European Commission

PEPS



Ultracool atmospheres (M dwarfs, brown dwarfs) are complex — planetary atmospheres are more complex

Low Mass Star

Brown Dwarf



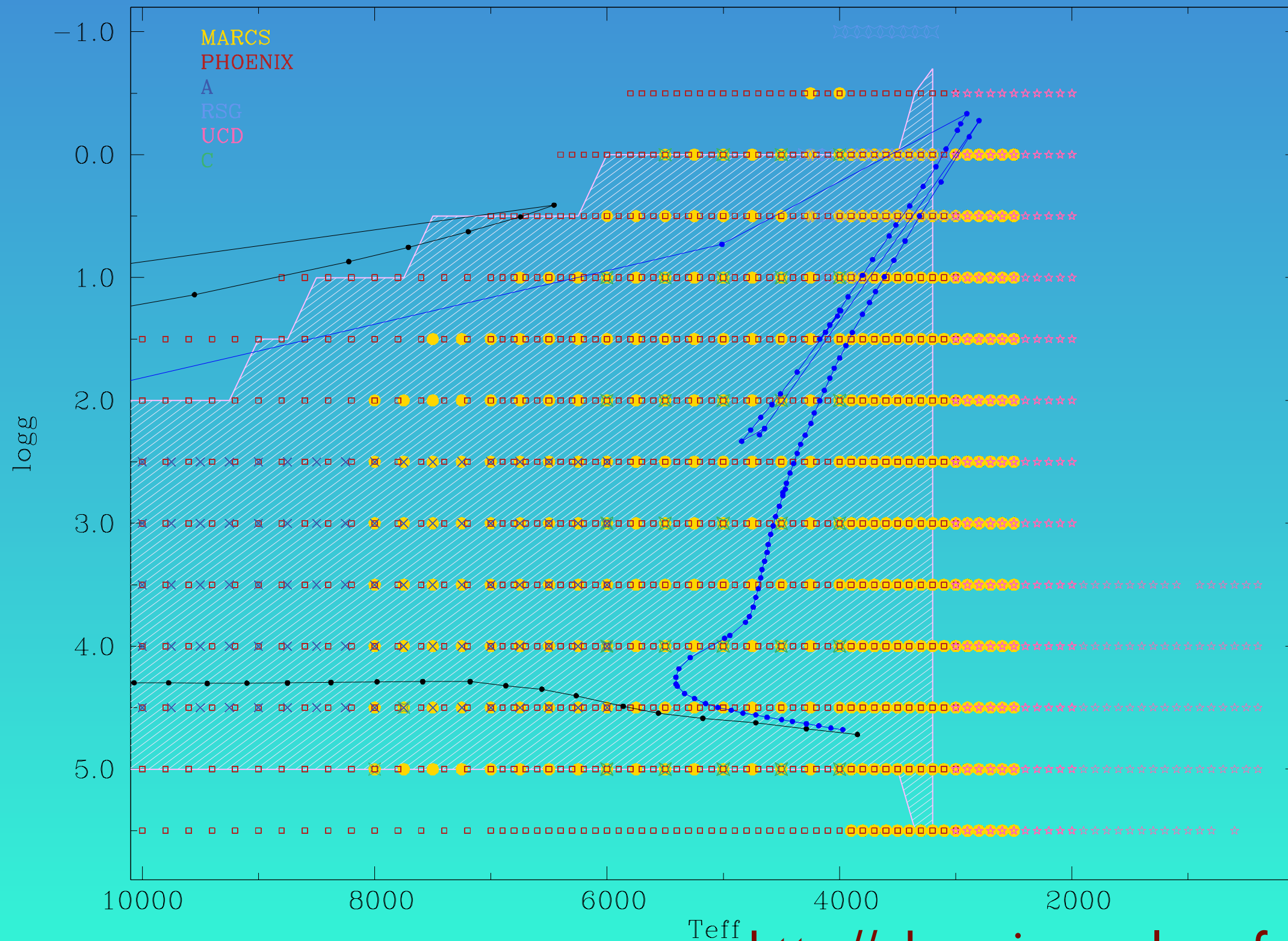
- Irradiation & heat redistribution, rotation
- Greater compositional diversity
- Transmission spectroscopy only sensitive to highest part of atmosphere
- Often few data points to constrain multi-parameter models

Jupiter

Earth

NASA

Atmosphere models from supergiants to brown dwarfs — and beyond



Sordo et al.
2011

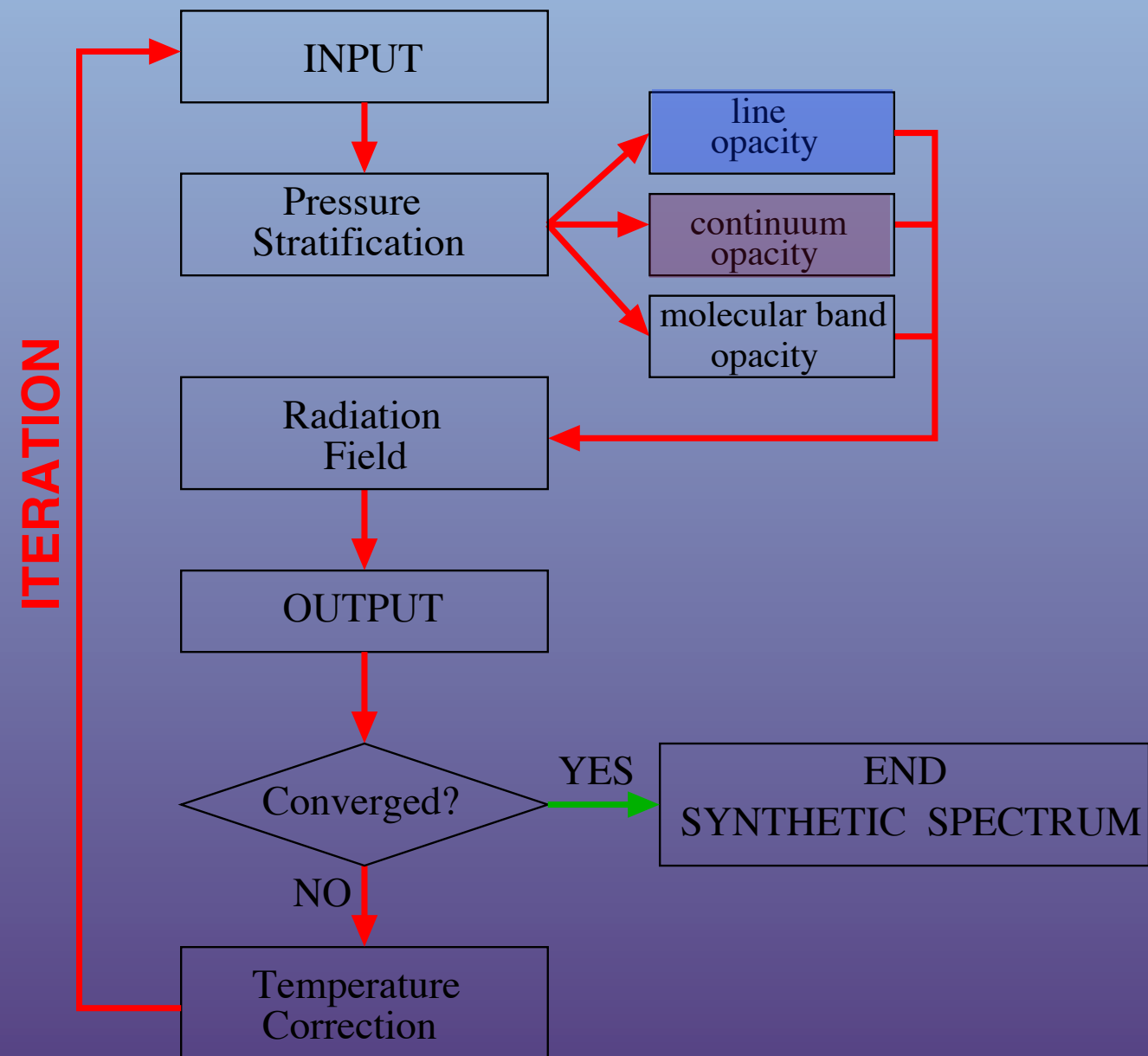
BP/RP and
RVS spectra

<http://phoenix.ens-lyon.fr/fallard/GAIA/>

(Sub-) stellar atmosphere modelling

★ independent Variables (minimal):

- effective temperature T_{eff}
- surface gravity $g(r) = GM/r^2$
- mass M or radius R or luminosity
 $L = 4 \pi R^2 \sigma T_{eff}^4$
- composition ("metallicity")
- convection → (micro-) turbulence & mixing
- rotation
- chemical peculiarities



PHOENIX workflow (P. Hauschildt)

→ self-contained and internally consistent structure in 1D

Molecular Bands — Methane

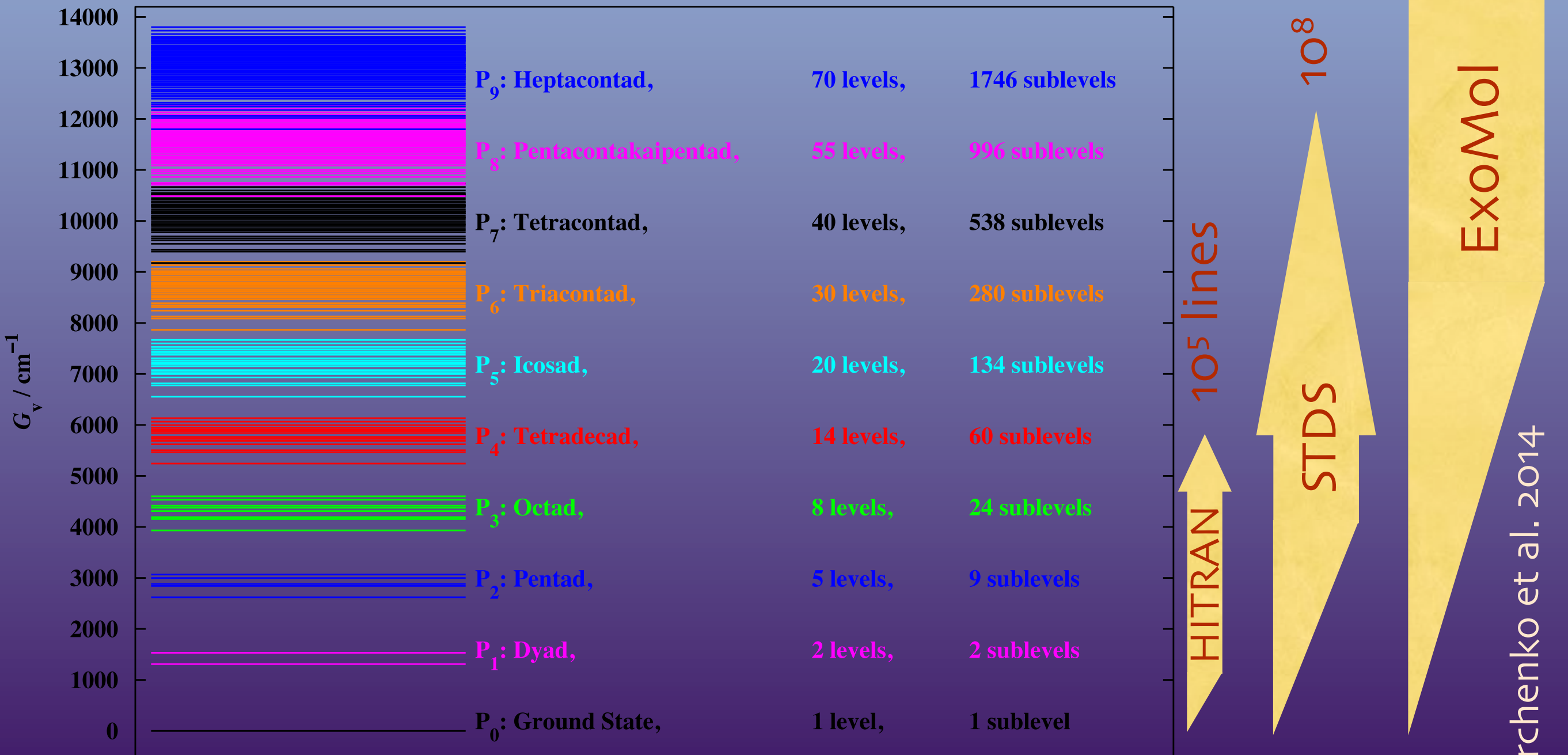
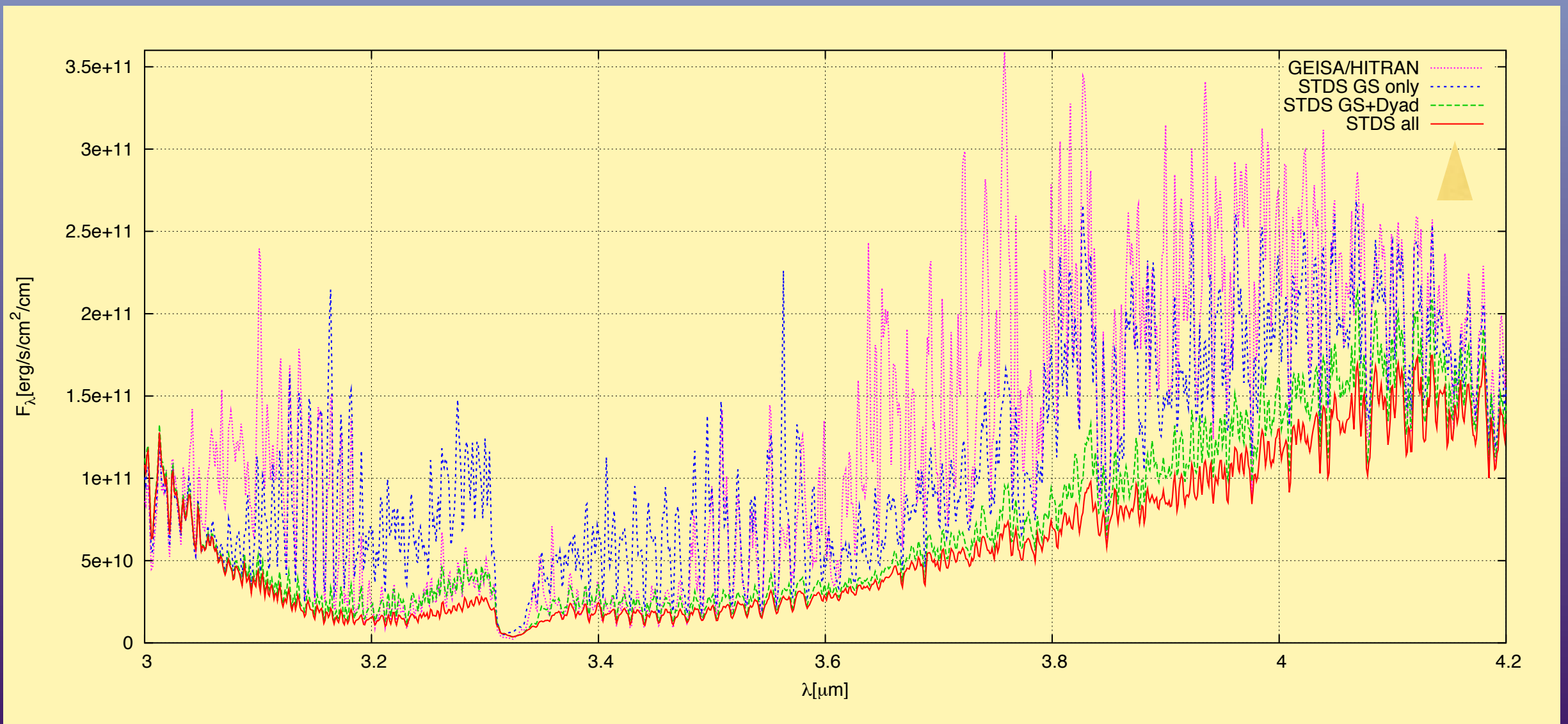


Fig. 2. Polyad energy-level structure for ¹²CH₄. Boudon et al. 2006

Yurchenko et al. 2014

Molecular line blanketing: Methane

- 30 Mio. lines computed with the STDS program (Université de Bourgogne) — 2013 update: 80 Mio.
- Vibrational and rotational states up to $\sim 8000 \text{ cm}^{-1}$
- Completeness: $\sim 50\%$ (mid-IR) - 10% (H-band) - 0% (Y/J)



Molecular Line Profiles - Data

- Molecular line data for stellar atmosphere calculations:
 - Extensive data available from spectroscopy line lists (HITRAN and others)
 - Often damping widths and shifts included, sometimes temperature dependence
- Challenges:
 - Most data for Earth and outer planets' atmosphere studies
 - line lists complete only at 296 K
 - damping constants at low temperatures
 - Most experimental measurements for N₂ and O₂ as perturbers
 - Generalisation for large theoretical line lists required

Non-equilibrium Chemistry

- Nitrogen- and Carbon chemistry is inhibited by slow reaction steps breaking up the C=O and N≡N bonds:

- $\text{N}_2 \longleftrightarrow \text{NH}_3$: limited by $\text{N}_2 + \text{H}_2 \rightleftharpoons 2 \text{NH}$

$$K = 8.45 \times 10^{-8} \times e^{(-8151/T)} \quad (\text{Lewis \& Prinn 1980})$$

- $\text{CO} \longleftrightarrow \text{CH}_4$: limited by $\text{H}_2 + \text{CH}_3\text{O} \rightleftharpoons \text{CH}_3\text{OH} + \text{H}$

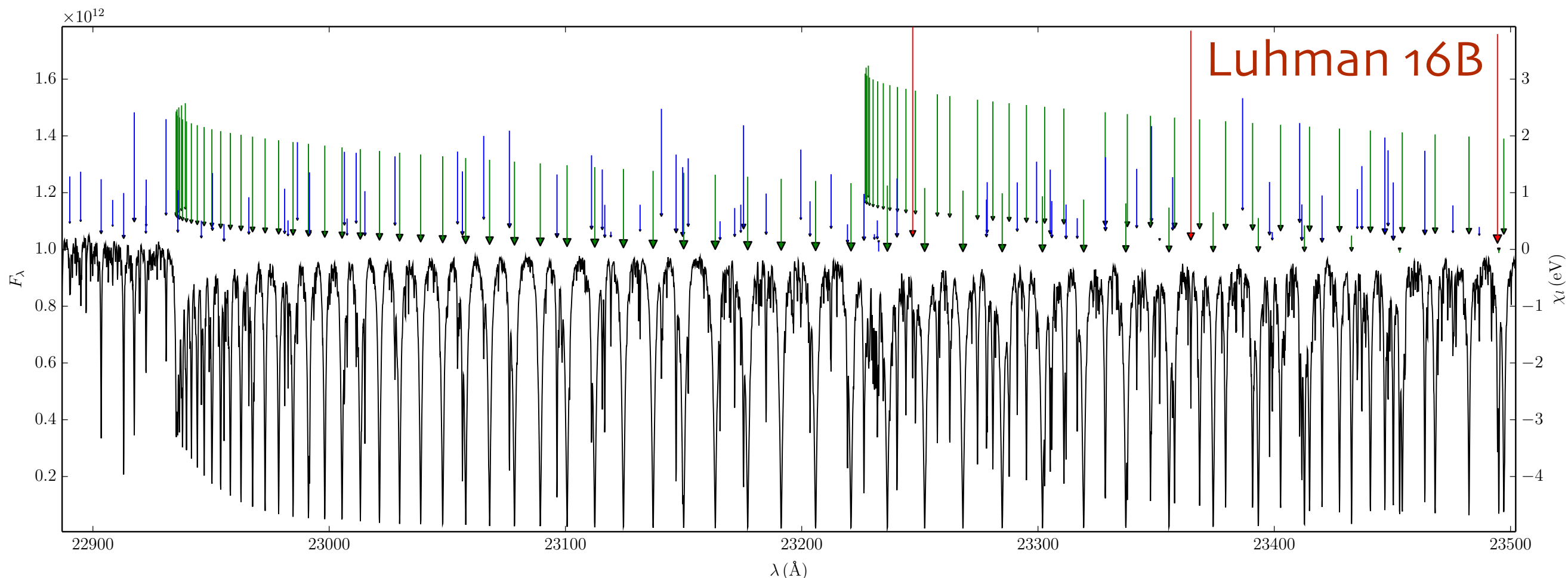
$$K = 1.77 \times 10^{-22} \times T^{-3.09} e^{(-3055/T)} \quad (\text{Visscher, Moses \& Saslow 2010})$$

- $\text{CO} \longleftrightarrow \text{CO}_2$: limited by $\text{CO} + \text{H}_2\text{O} \rightleftharpoons \text{CO}_2 + \text{H}_2$

$$K = 6.44 \times 10^3 \times T^{-3.09} e^{(33889/T)} \quad (\text{Graven \& Long 1954})$$

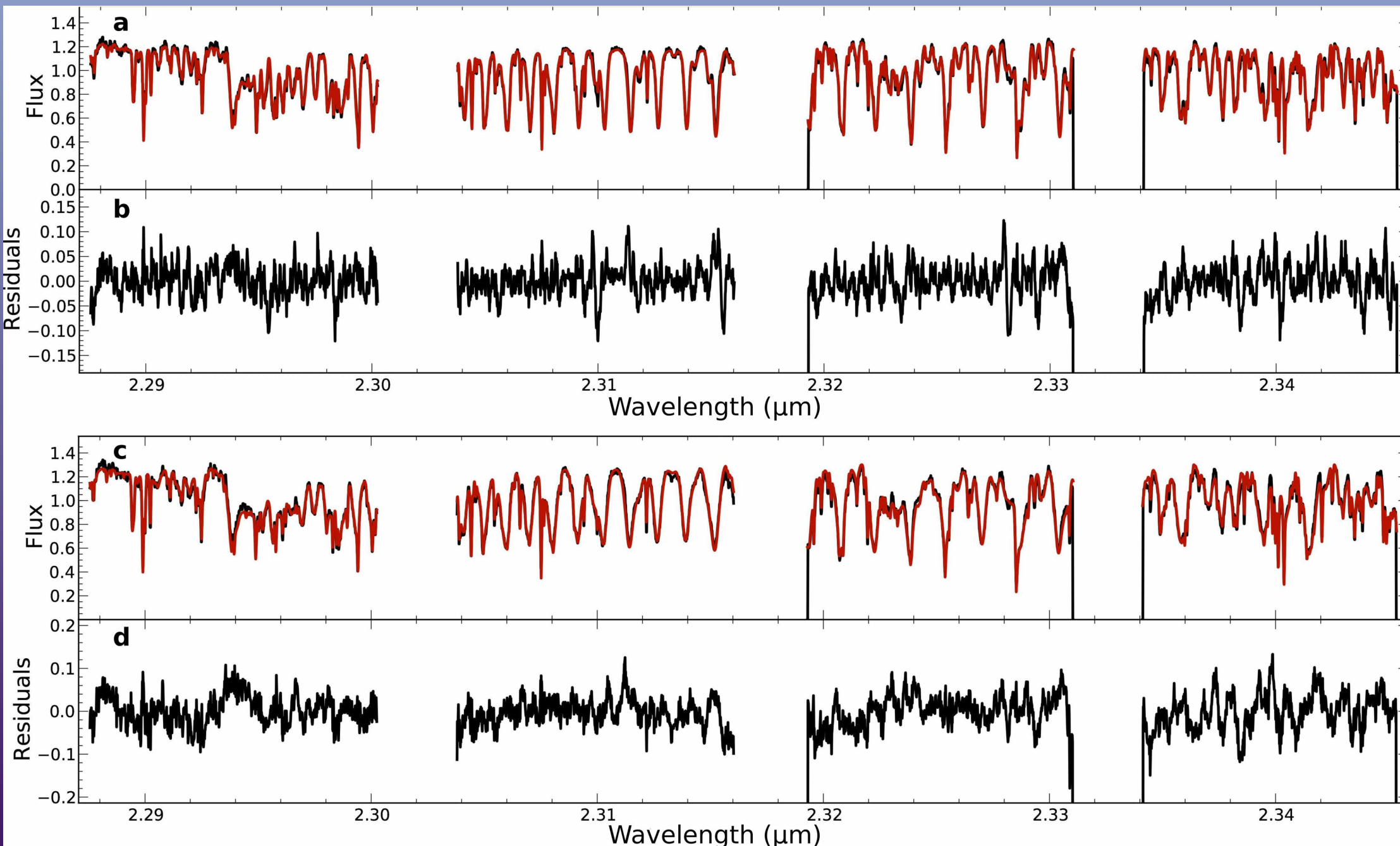
Molecular Line Profiles - Data

- Molecular line data for stellar atmosphere calculations:
 - Extensive data available from spectroscopy line lists (**HITRAN** and others)
 - Often damping widths and shifts included, sometimes temperature dependence



Molecular Line Profiles - Observation

- CO spectrum, testing line positions, strengths, shapes and non-equilibrium chemistry effects



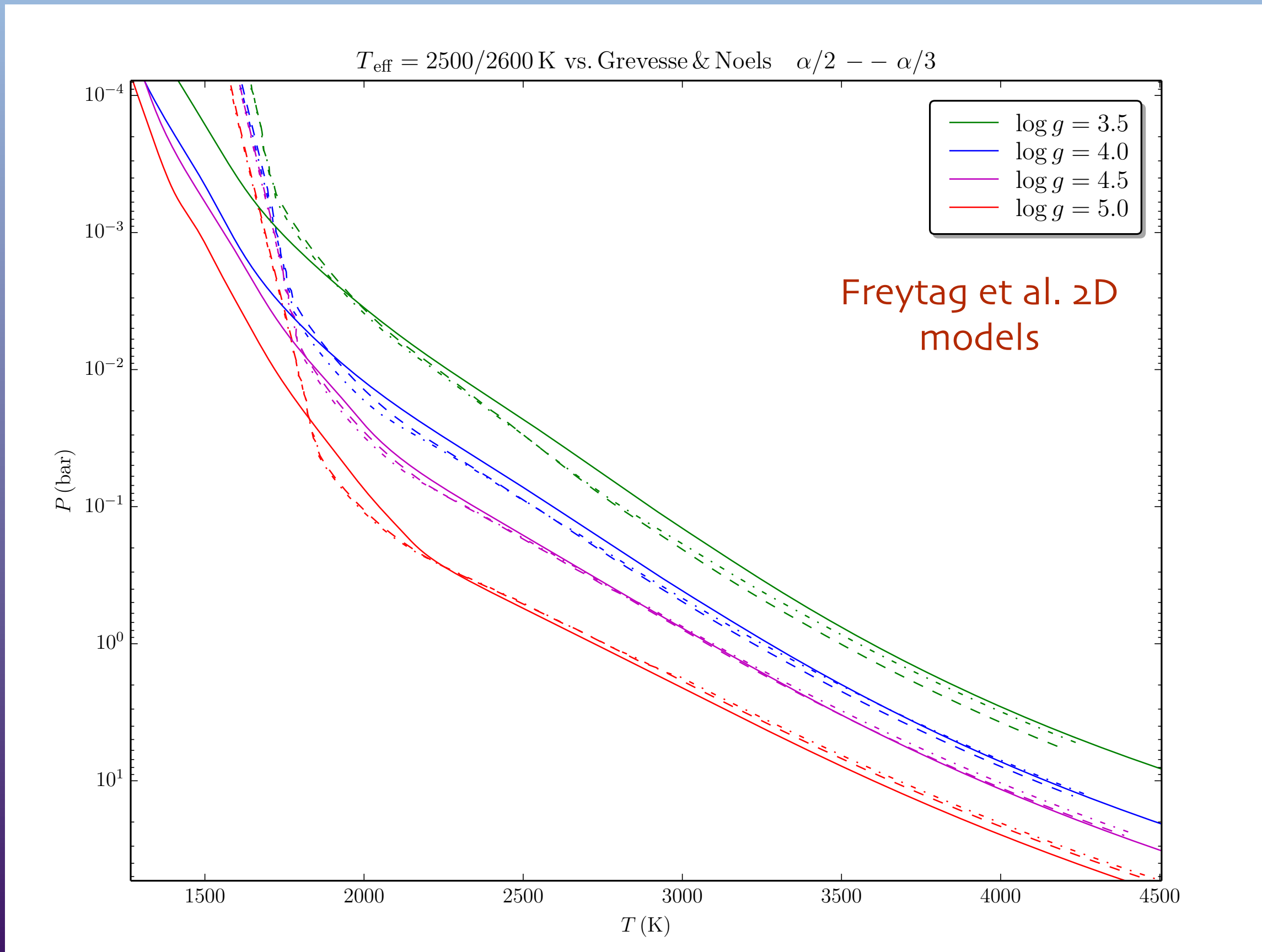
Luhman 16AB
Crossfield
et al. 2014

—
model

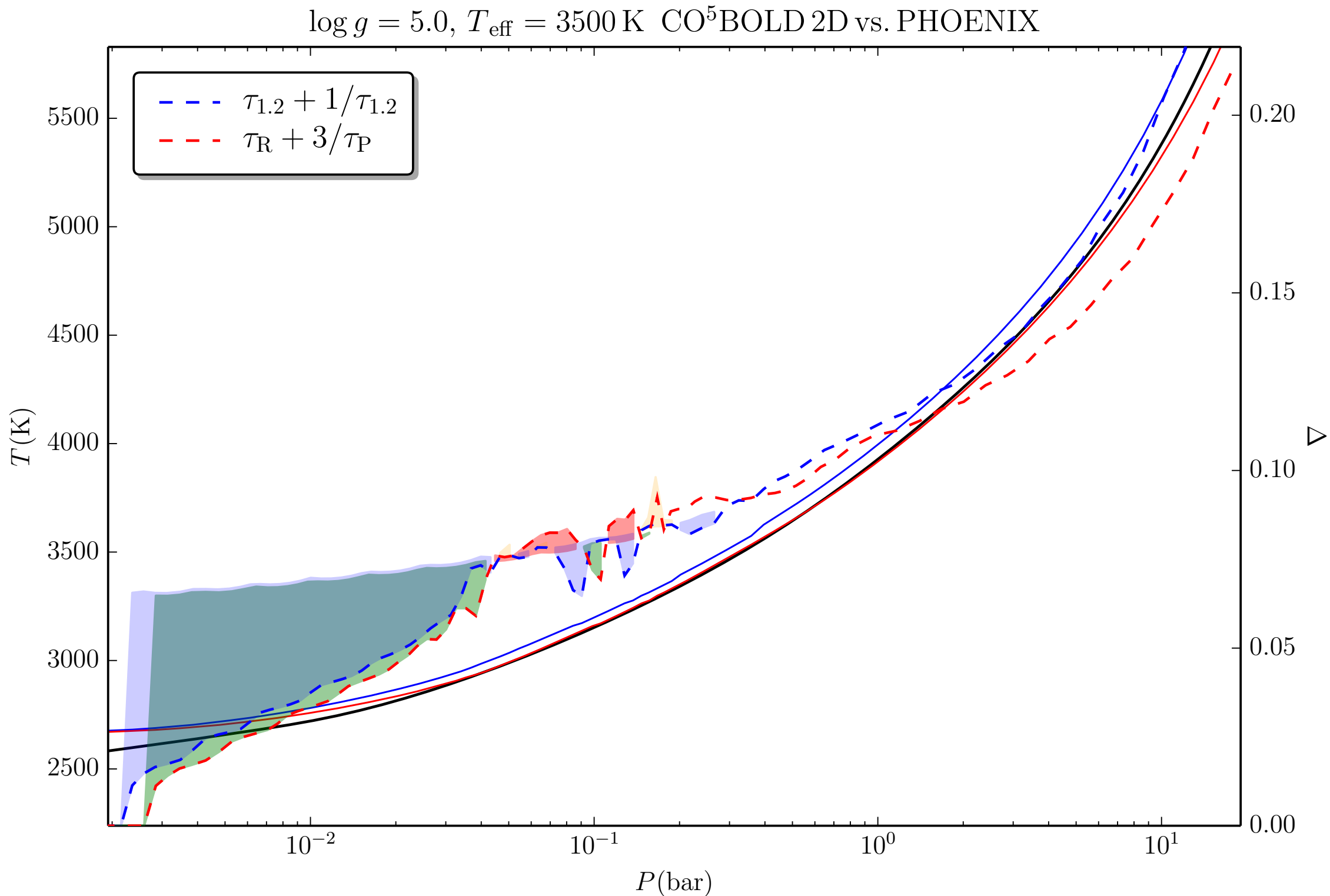
vs.

observation

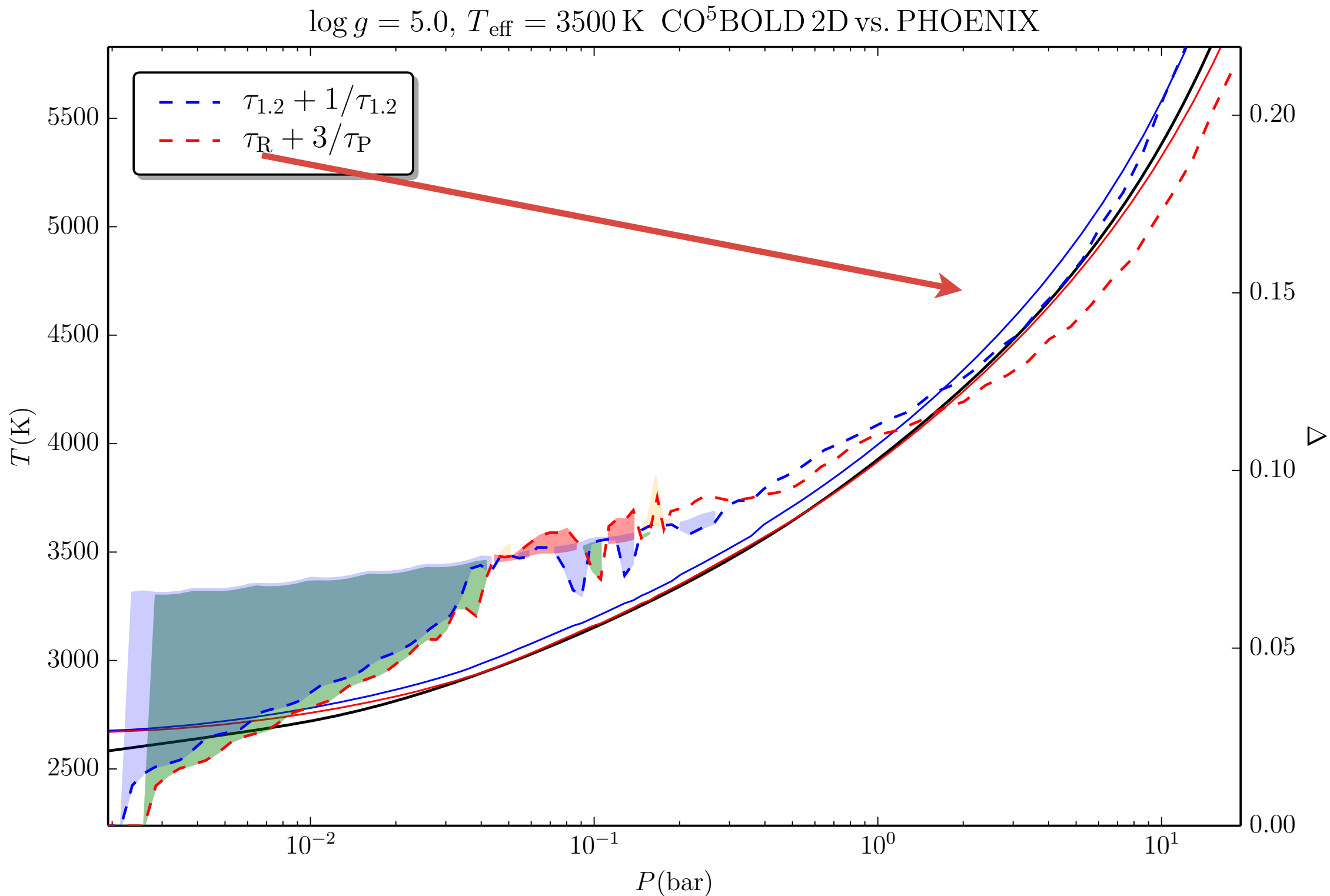
Modelling convection — calibration of MLT



Modelling convection — calibration of MLT

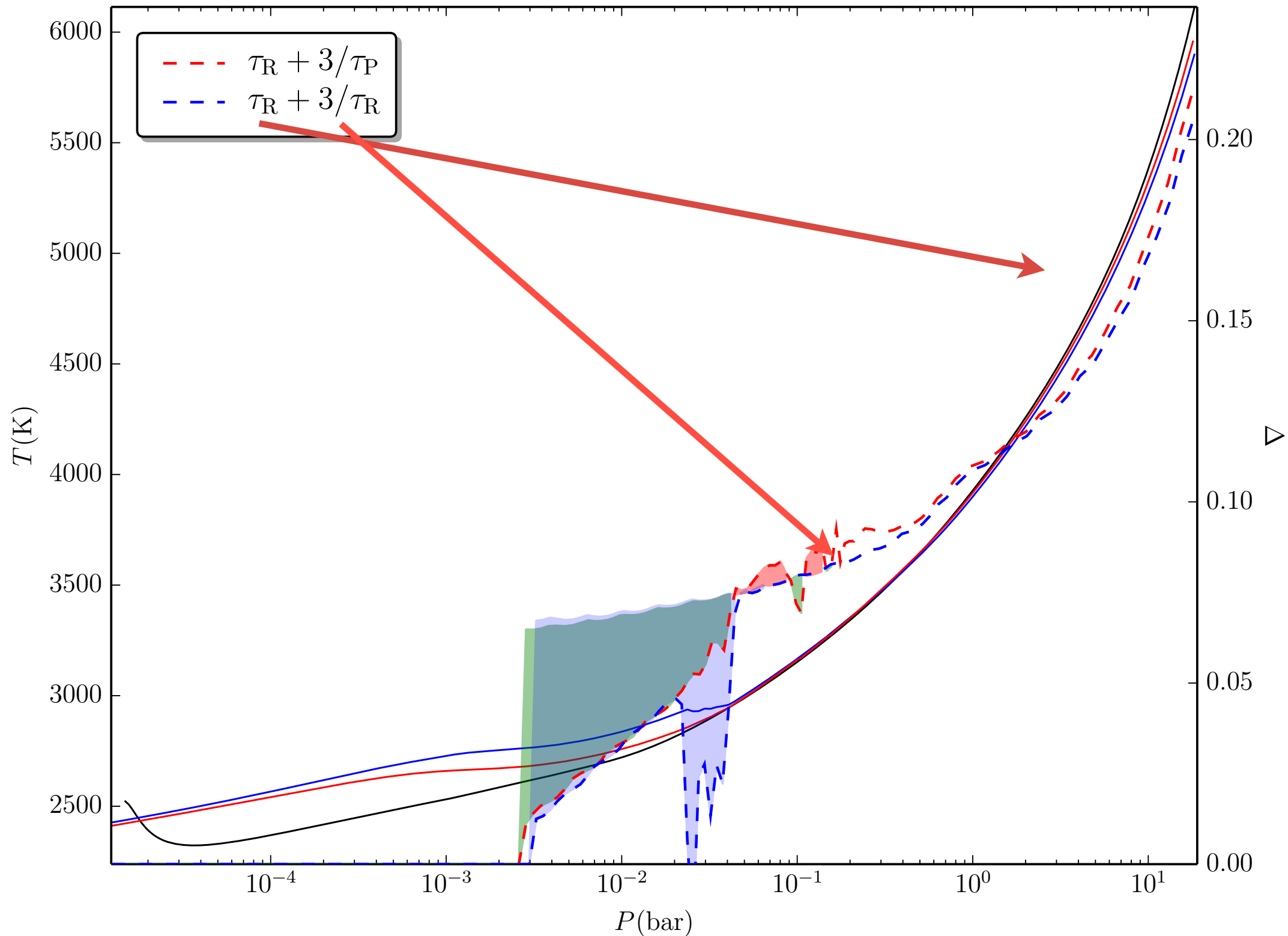


Modelling convection — calibration of MLT



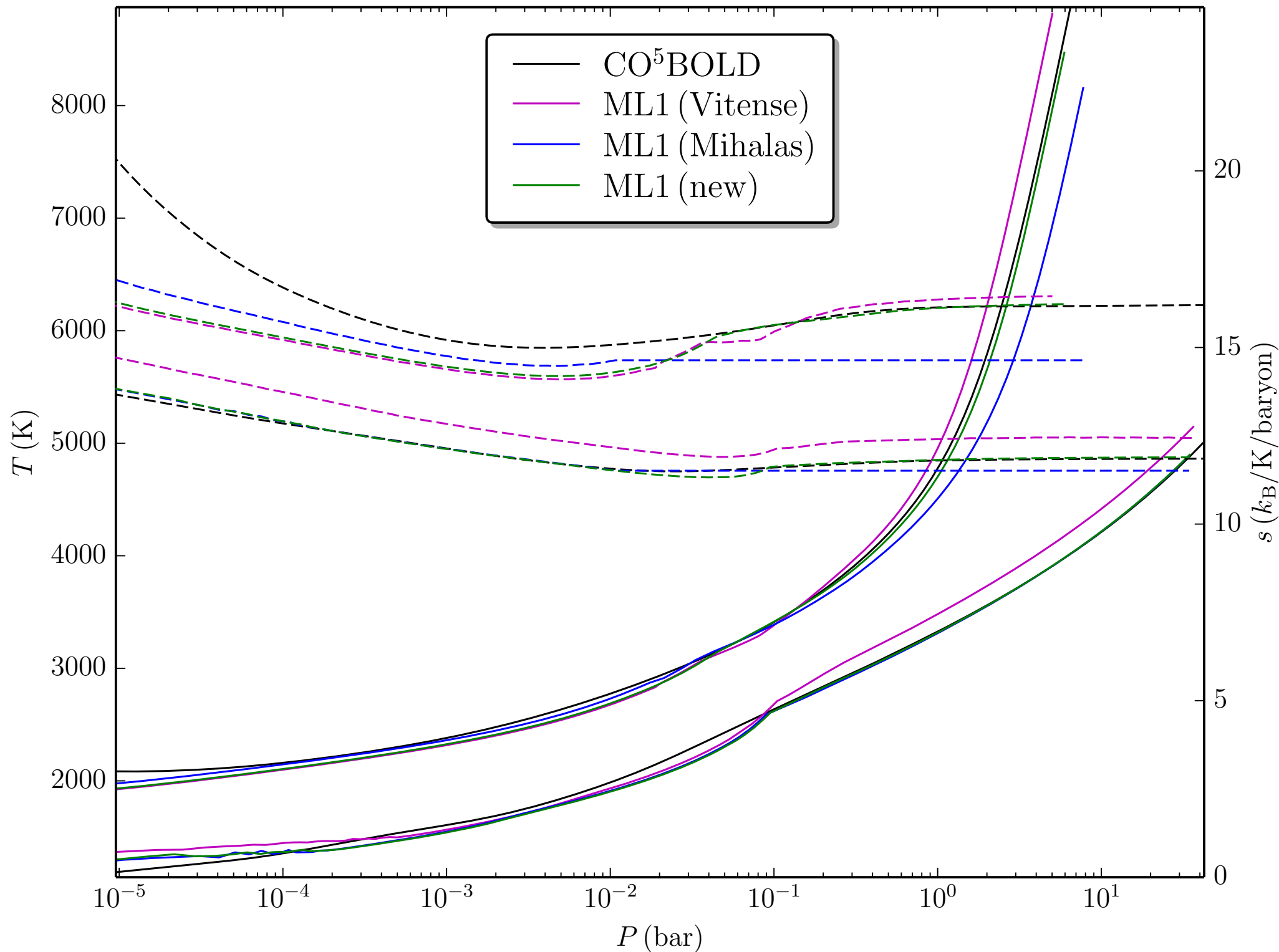
Modelling convection — calibration of MLT

$\log g = 5.0, T_{\text{eff}} = 3500 \text{ K}$ CO⁵BOLD 2D vs. PHOENIX



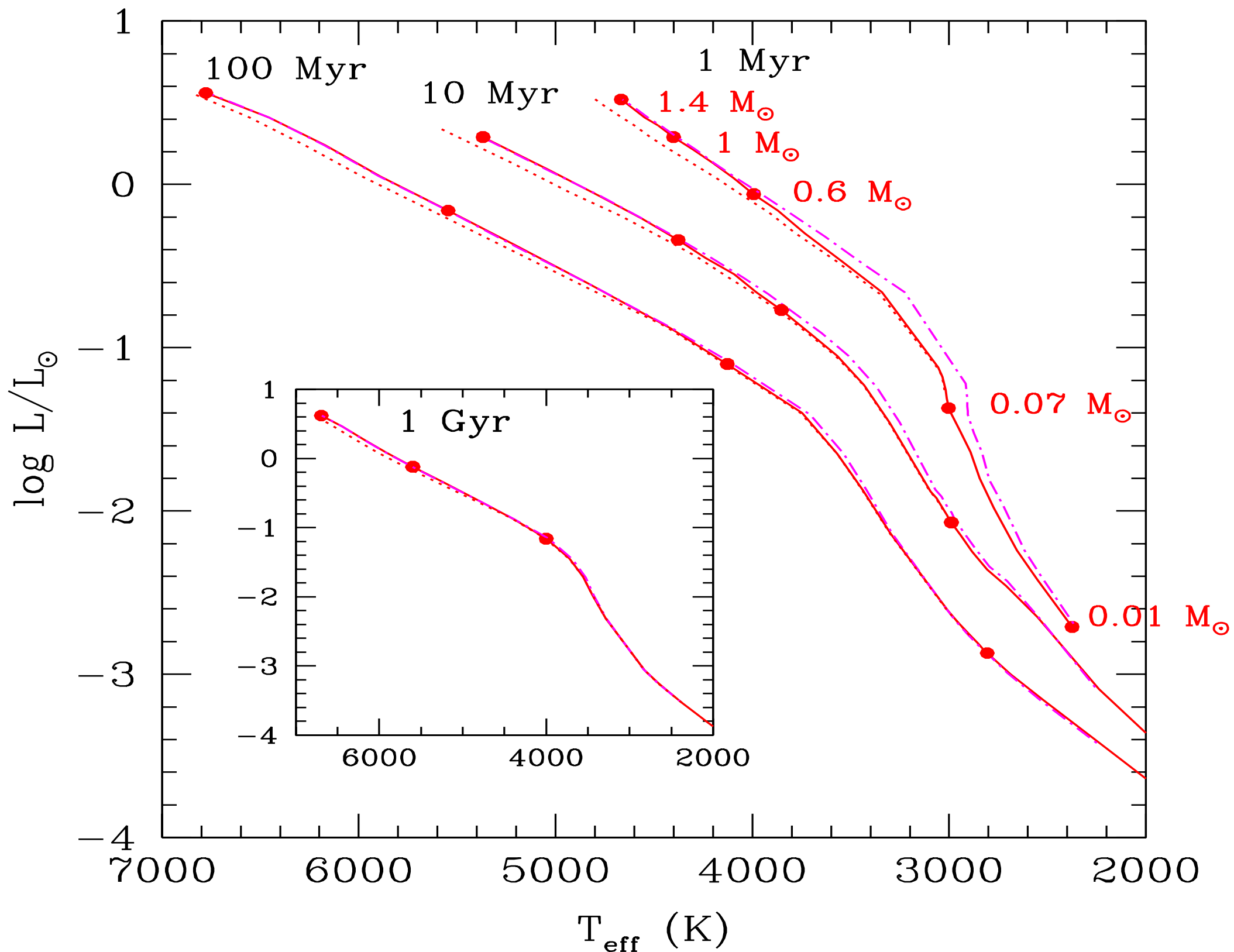
Modelling convection — calibration of MLT

$T - P, s - P : \log g = 4.0, T_{\text{eff}} = 2540 \text{ K}, 3200 \text{ K}$



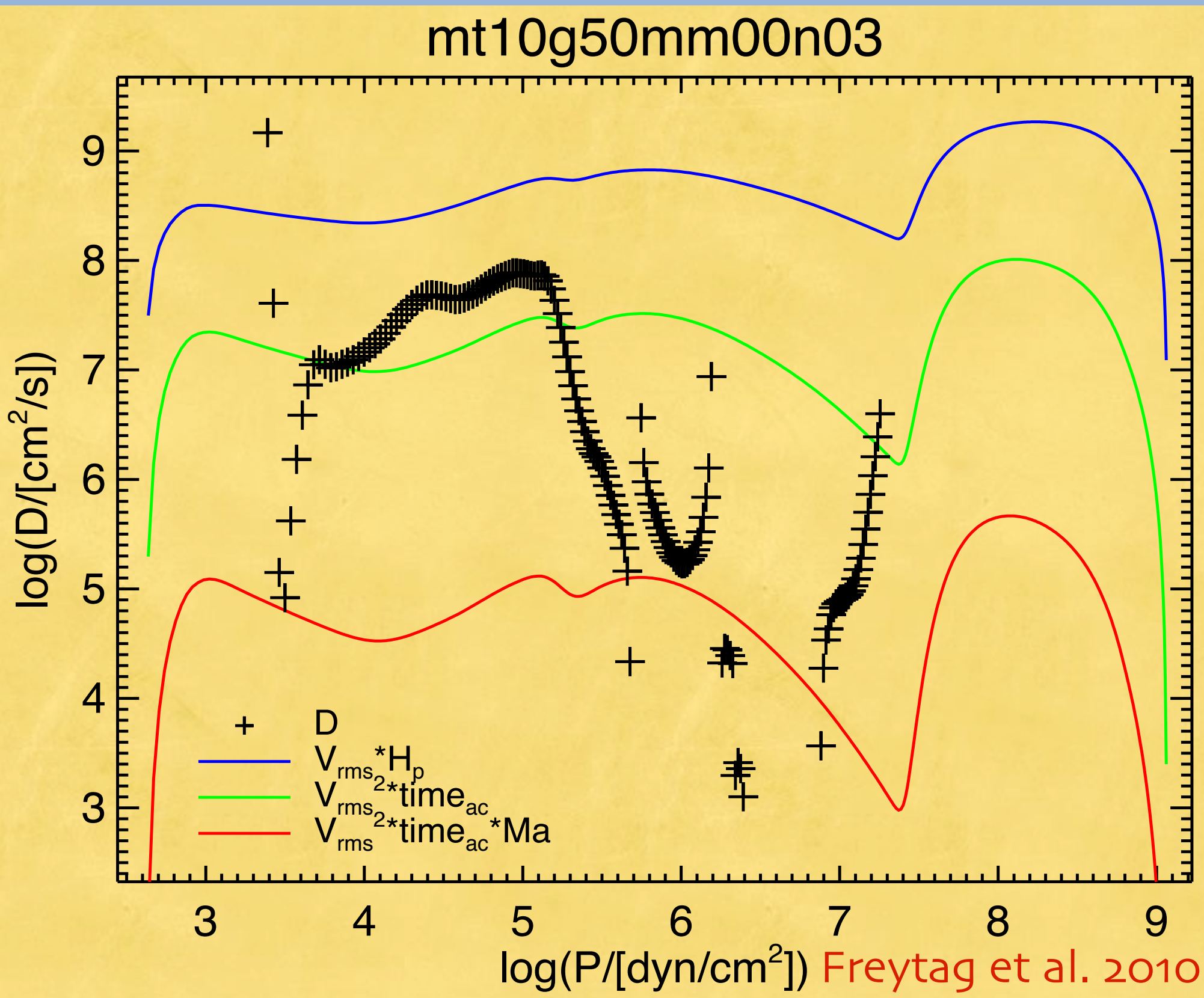
convective
structure
defines deep
thermal profile
→ boundary
condition for
evolution!

Modelling convection — calibration of MLT



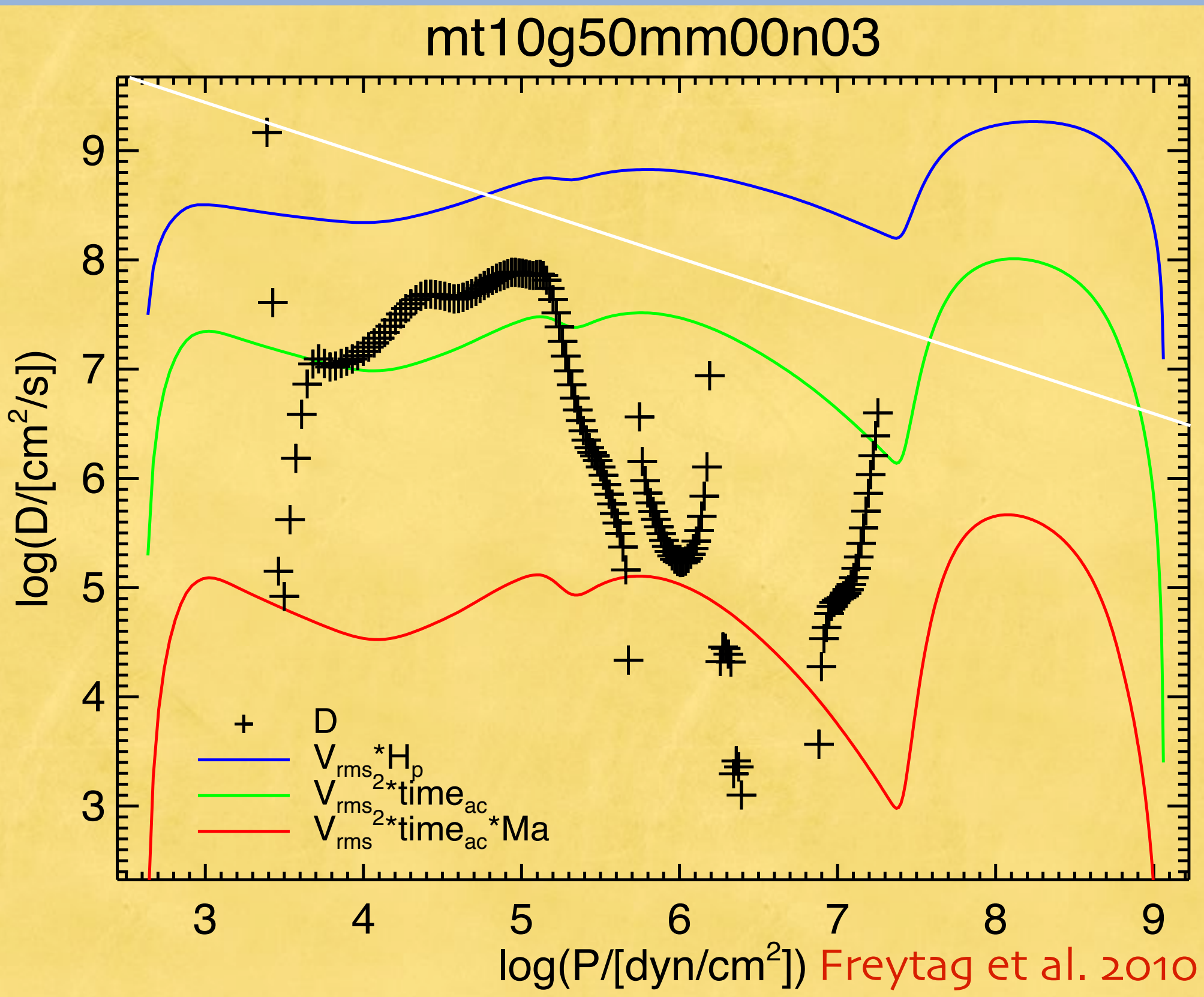
Baraffe et al.
in prep.

Mixing and Diffusion - a closer Look



convective
overshoot and
gravity wave
excitation
dominant in
brown dwarfs

Mixing and Diffusion - a closer Look

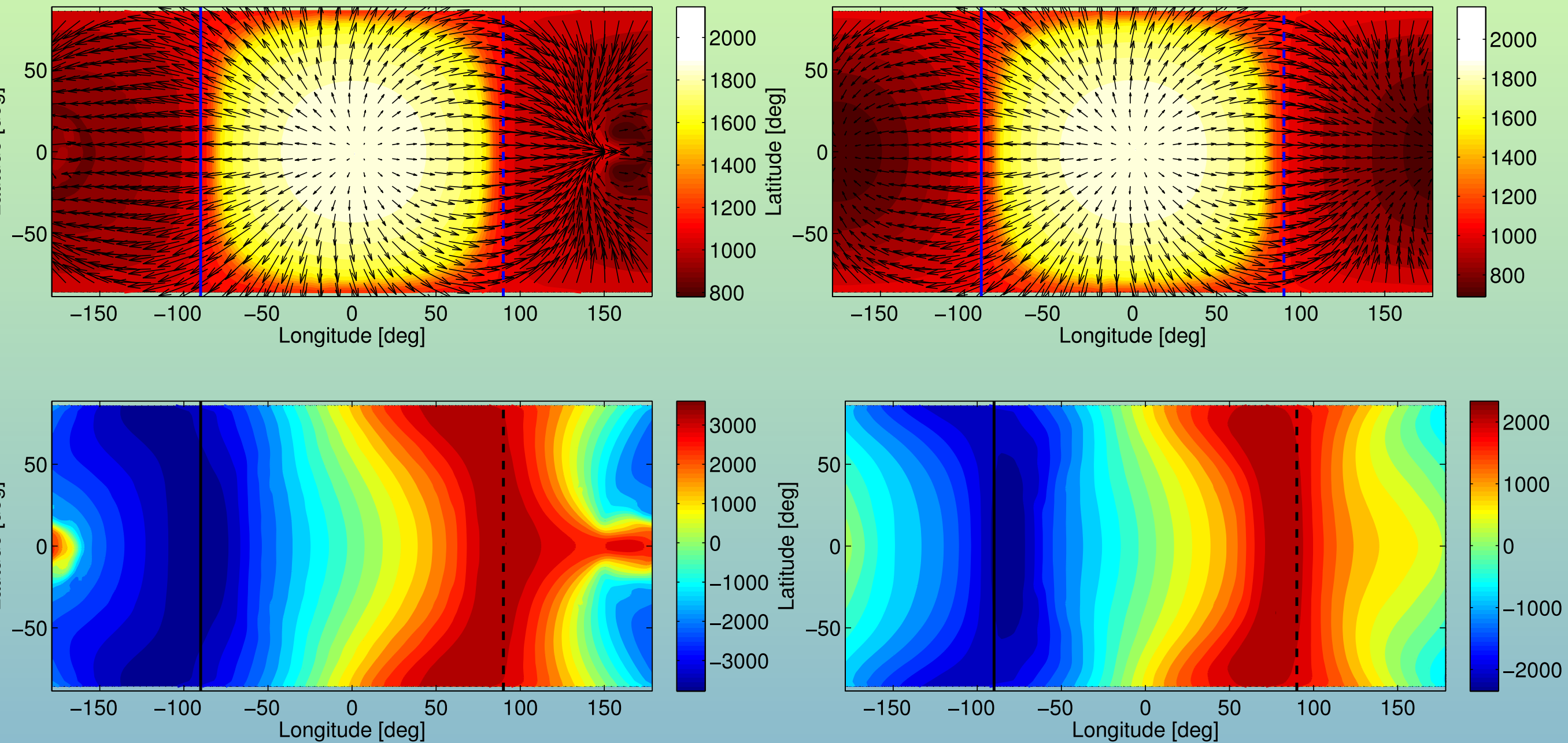


convective overshoot and gravity wave excitation dominant in brown dwarfs — but in planets too inefficient (Schwarzschild boundary @ $\tau \geq 100$)



global circulation important!

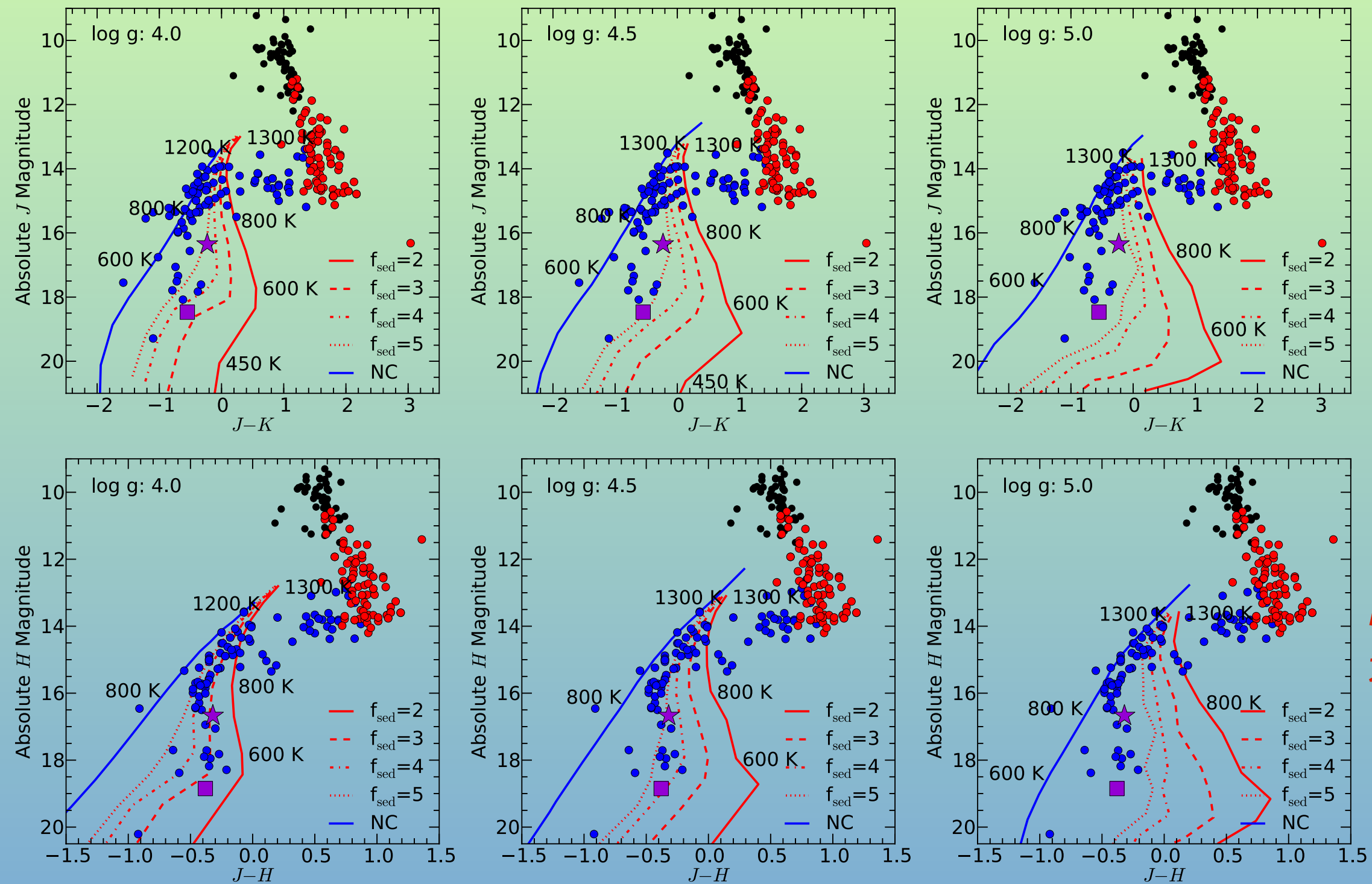
Exoplanets — Irradiation and Circulation



Showman et al. 2013

- Global Circulation models can reproduce temperature redistribution and (observable!) wind patterns
- Strongly non-kartesian (pancake-shaped) grid

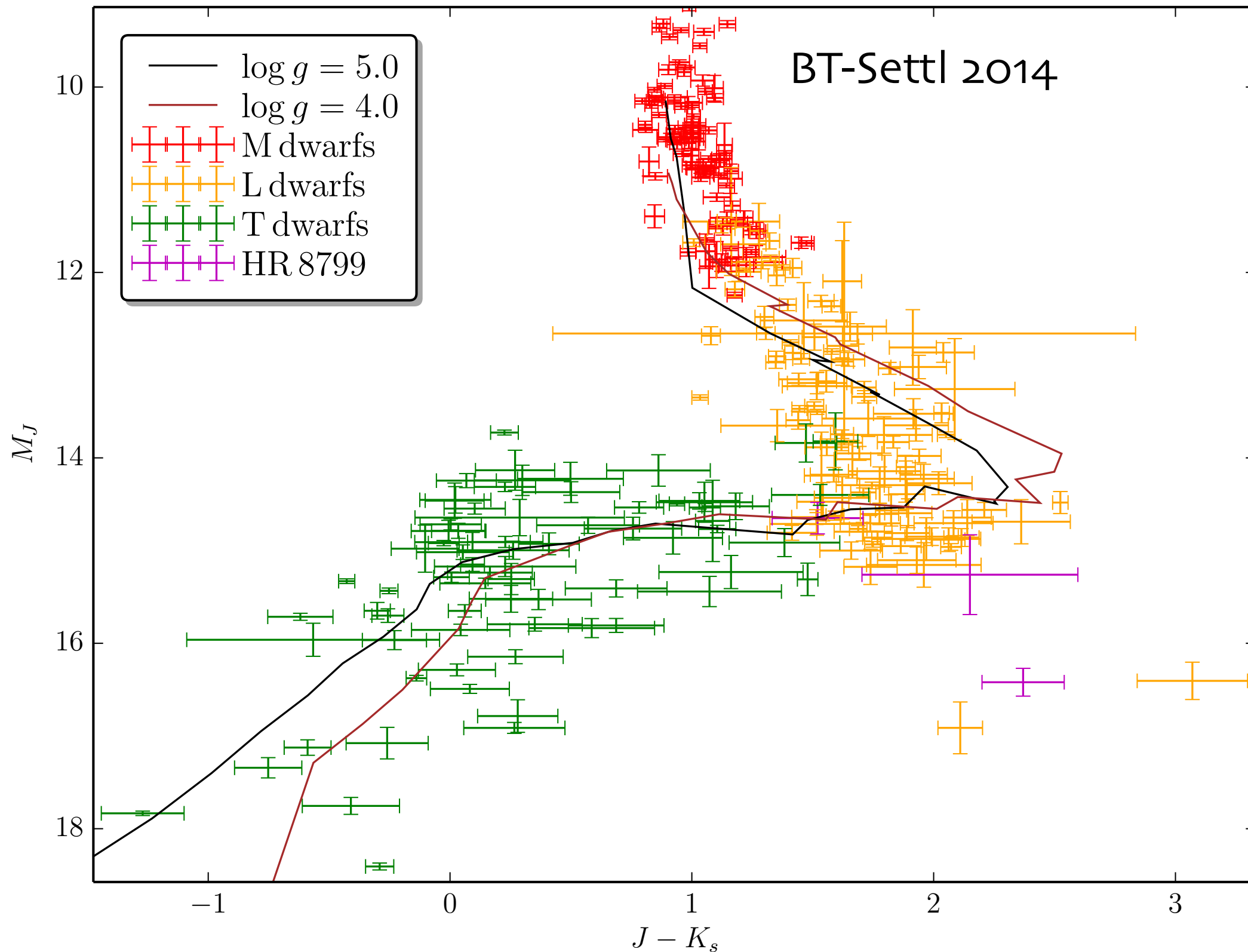
T dwarfs — more clouds



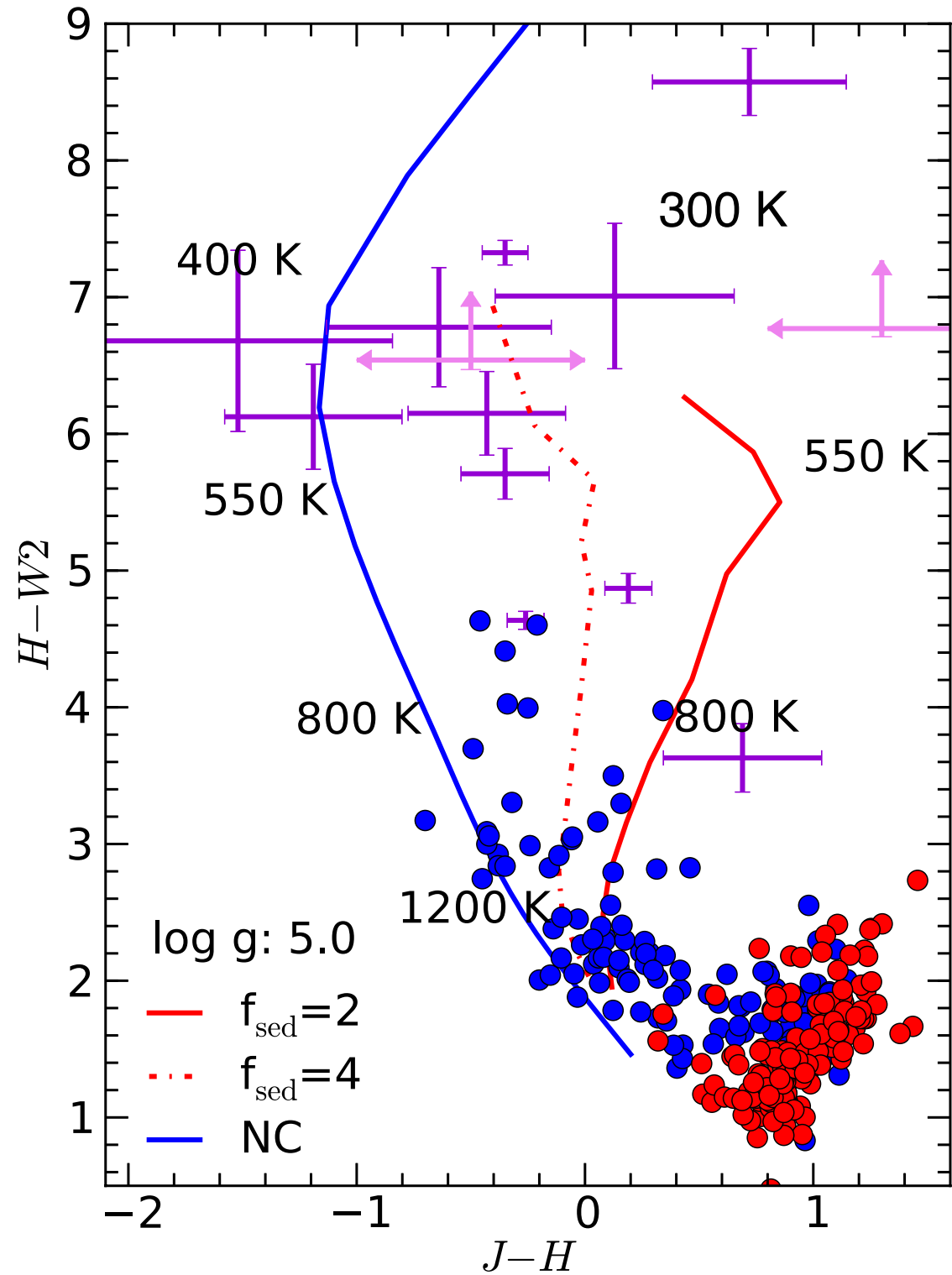
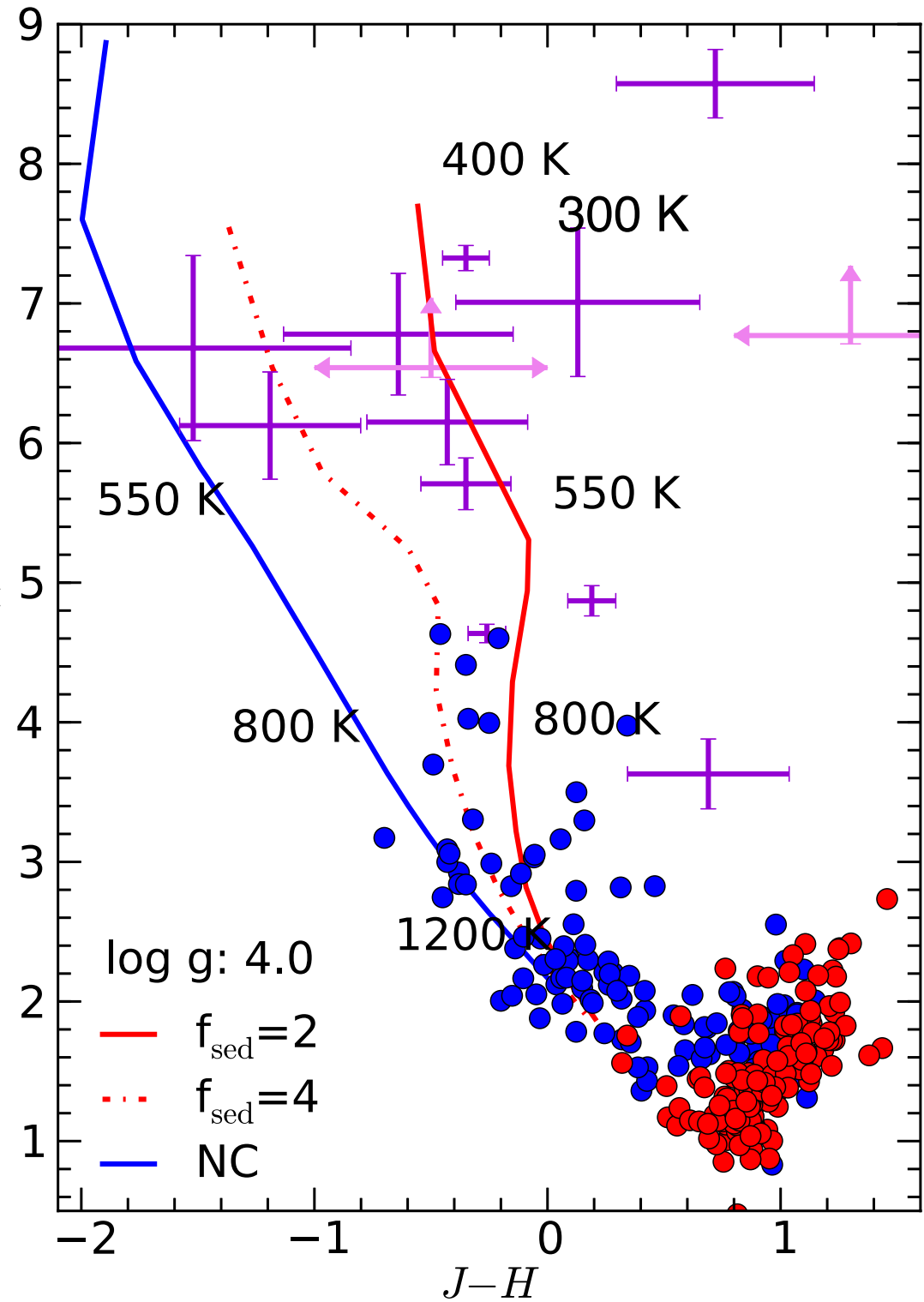
Morley et al.
2012

- Separate cloud setup for low-temperature condensates

Clouds from L to Y dwarfs in a single model

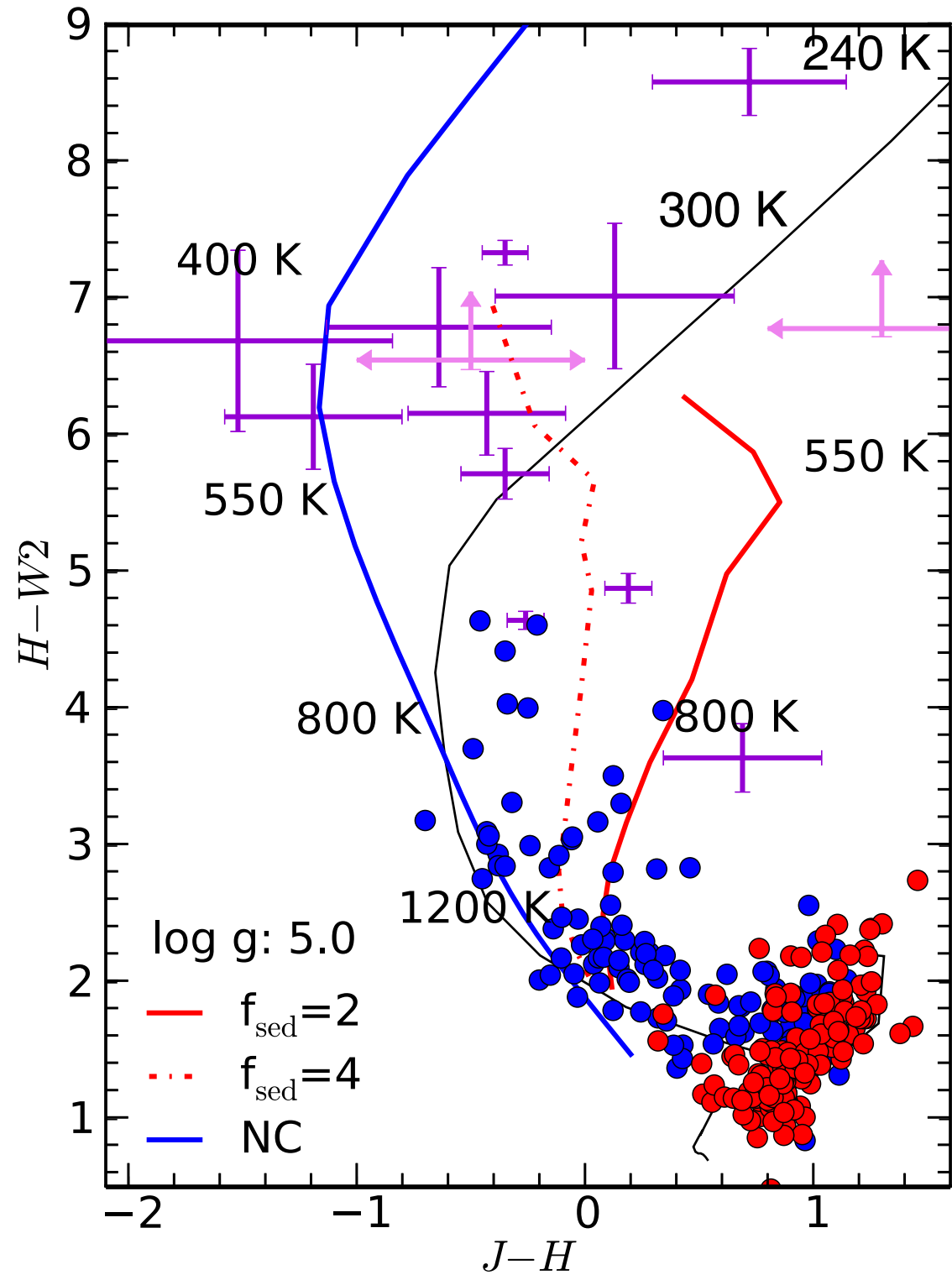
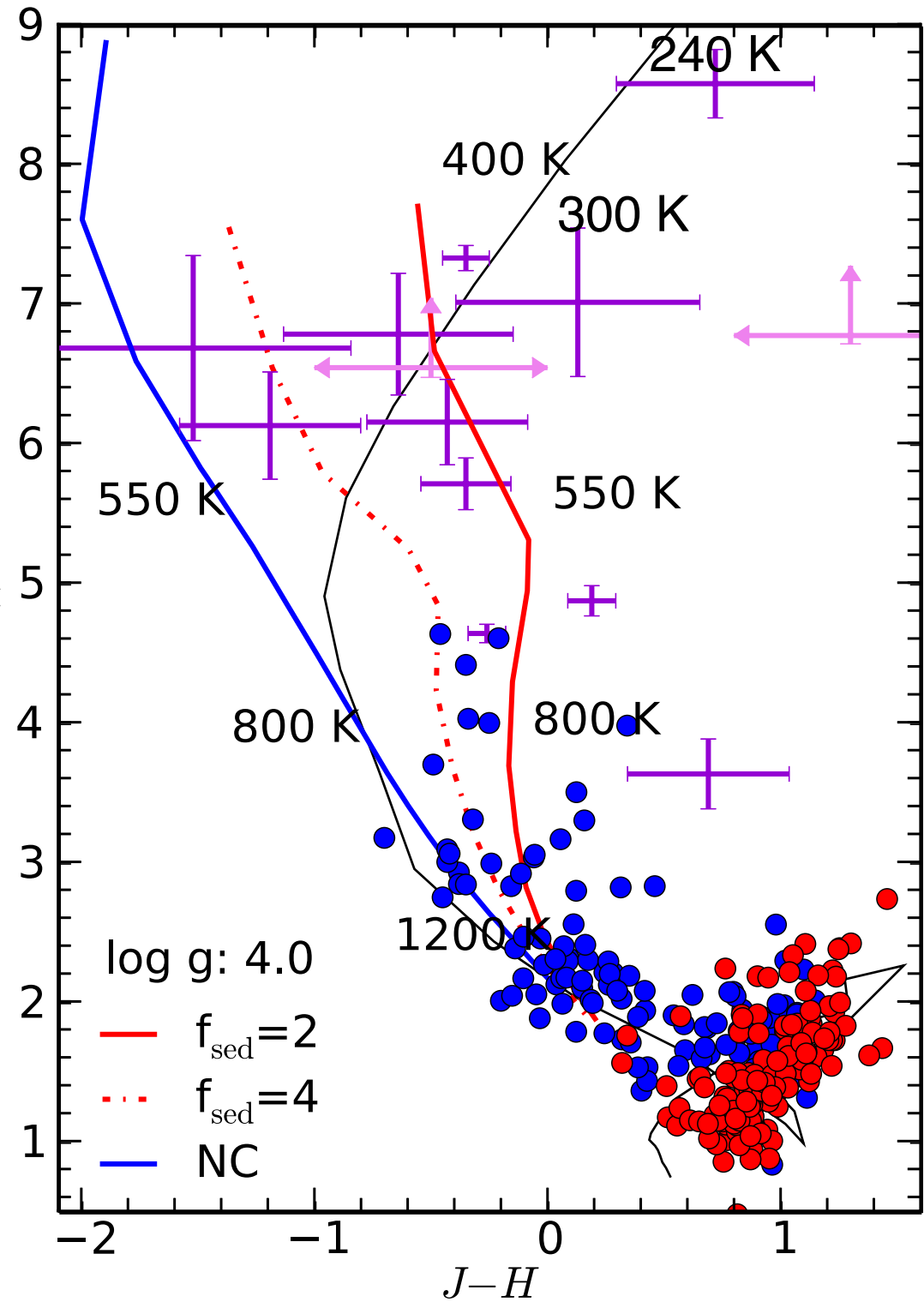


Y dwarfs — yet more clouds



Morley et al. 2012

Y dwarfs — yet more clouds

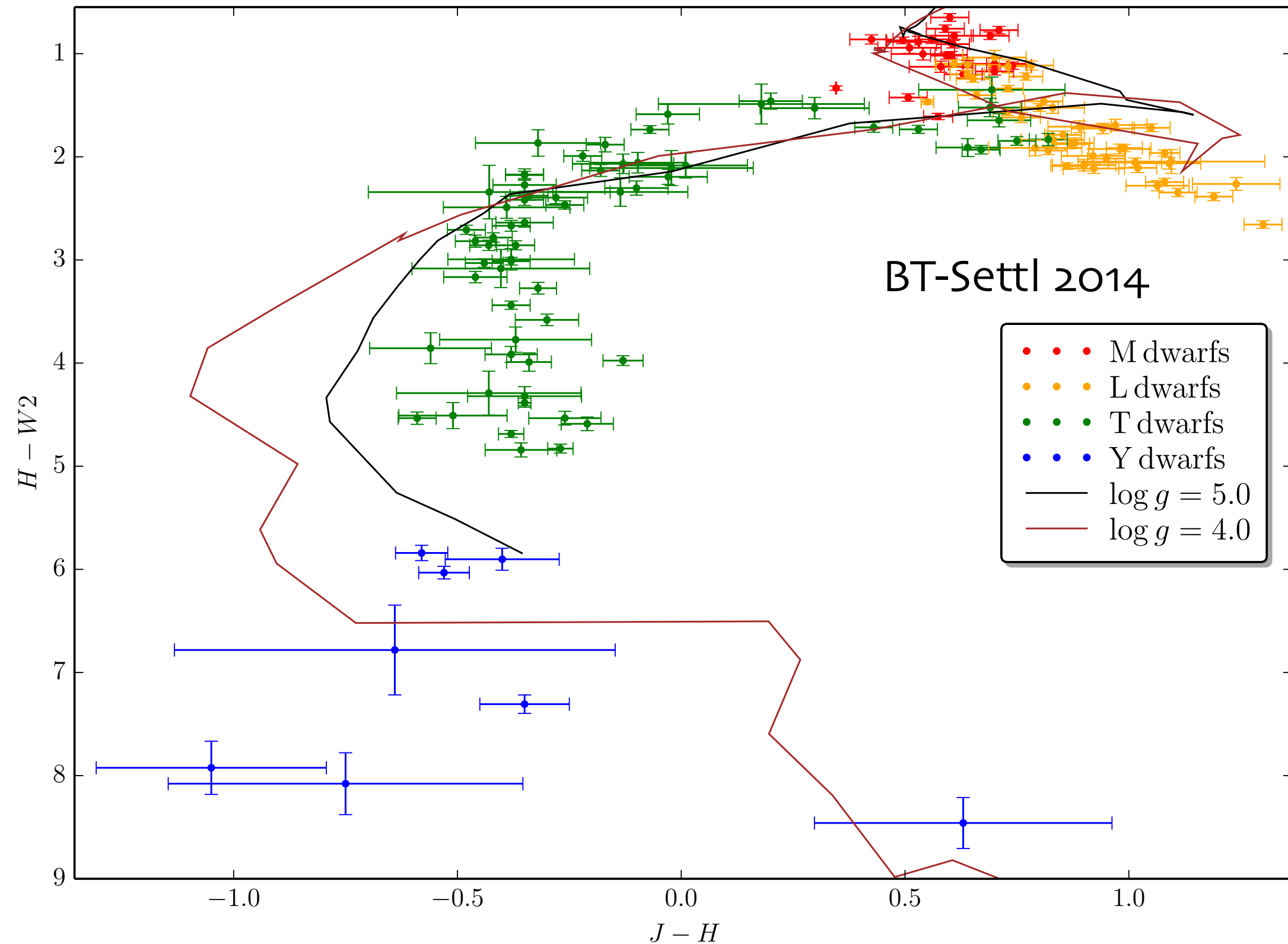


Morley et al. 2012

compared to
BT-Settl 2013

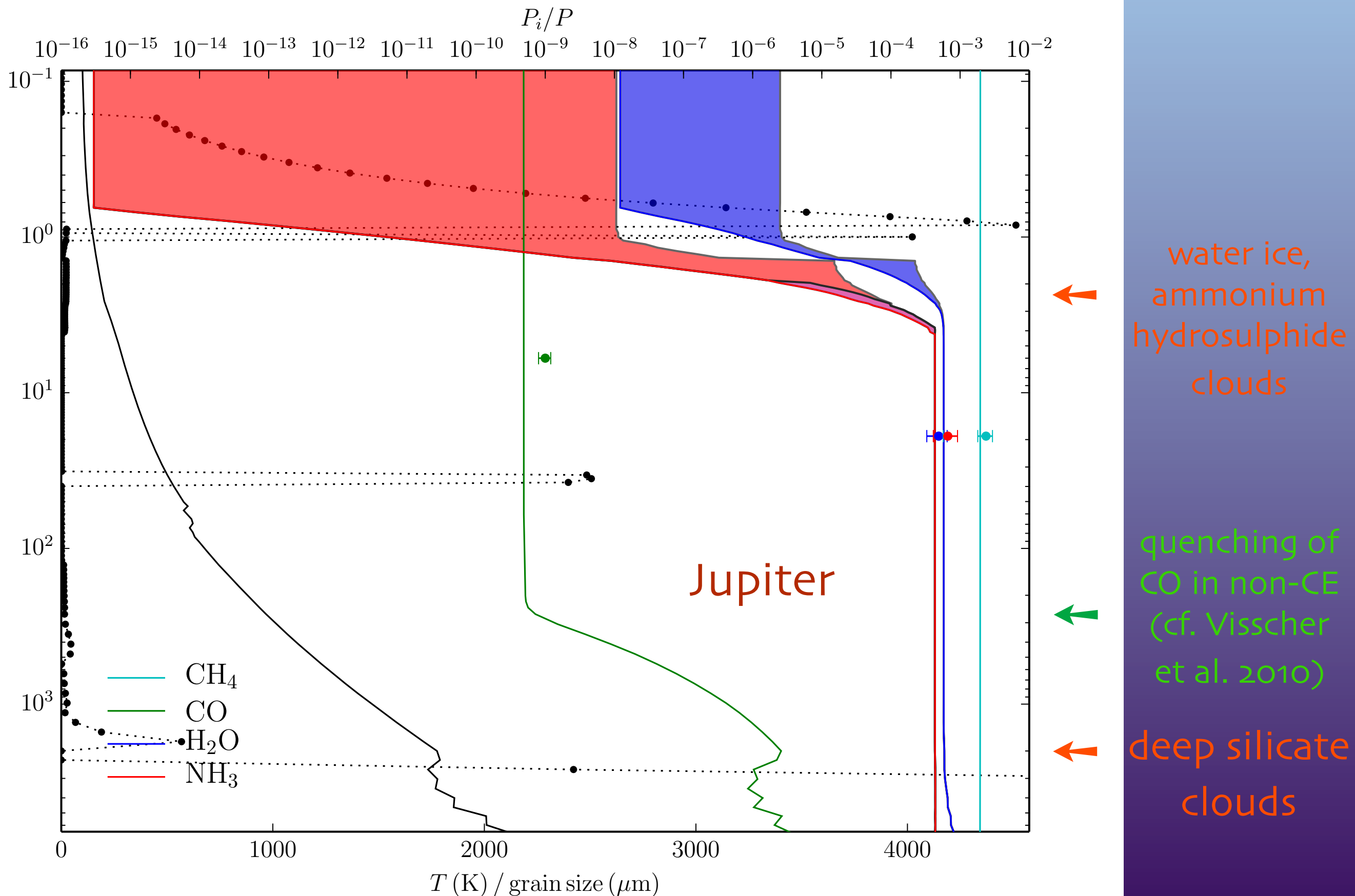
- Water ice clouds appearing between 300 and 400 K

Clouds from L to Y dwarfs



- Water ice clouds appearing between 300 and 400 K

Clouds in Brown Dwarfs and Planets

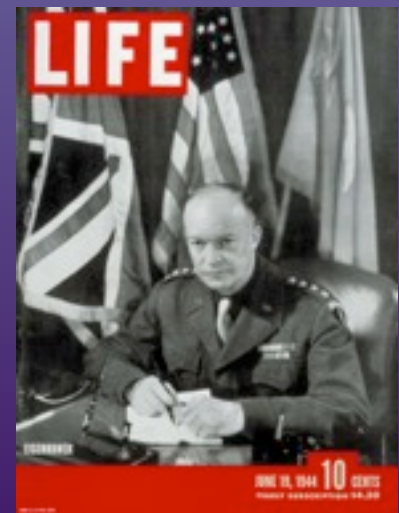


Atmospheric composition

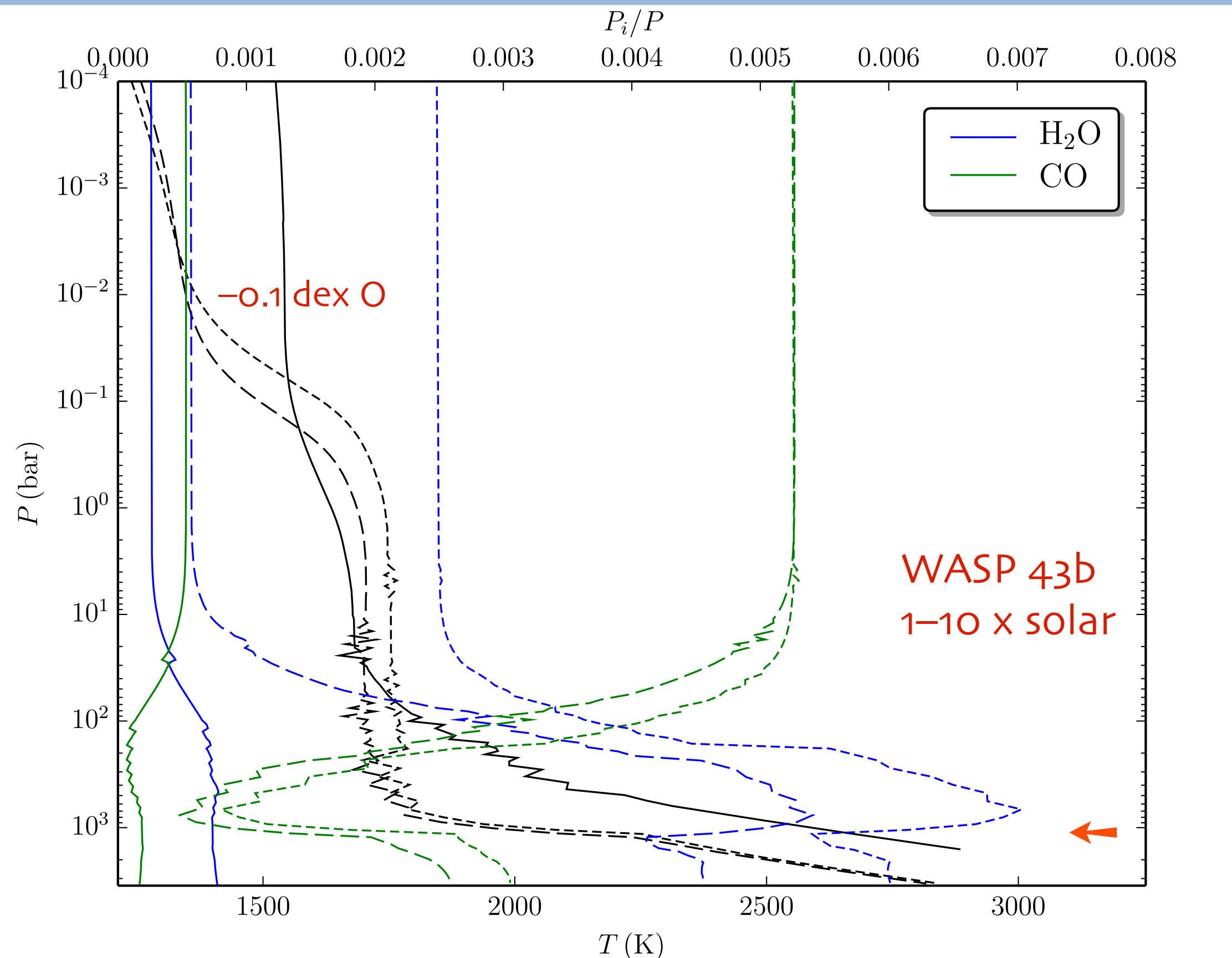
- Metal abundances in general, and carbon and oxygen in particular, can differ from host star
- various degrees of oxygen and carbon depletion can occur depending on location and accretion history in the protoplanetary disk
- “non-solar” C/O, additional impact of cloud condensation
- Ch. Mordasini’s talk;
cf. also Ch. Helling with I. Kamp et al. 2014
(Life, in press)

→ [try arXiv:1403.4420](https://arxiv.org/abs/1403.4420)

?

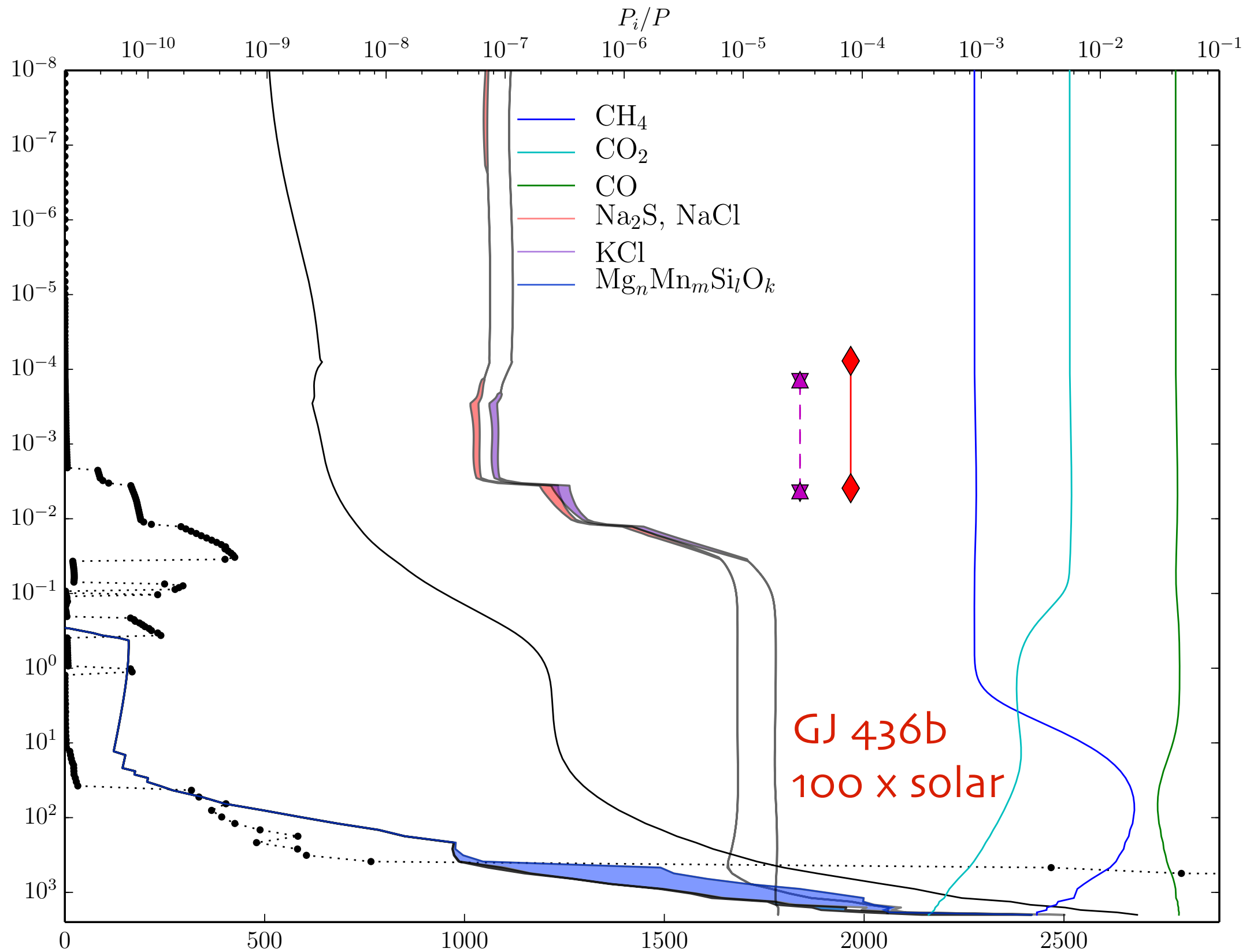


Clouds affect carbon/oxygen chemistry



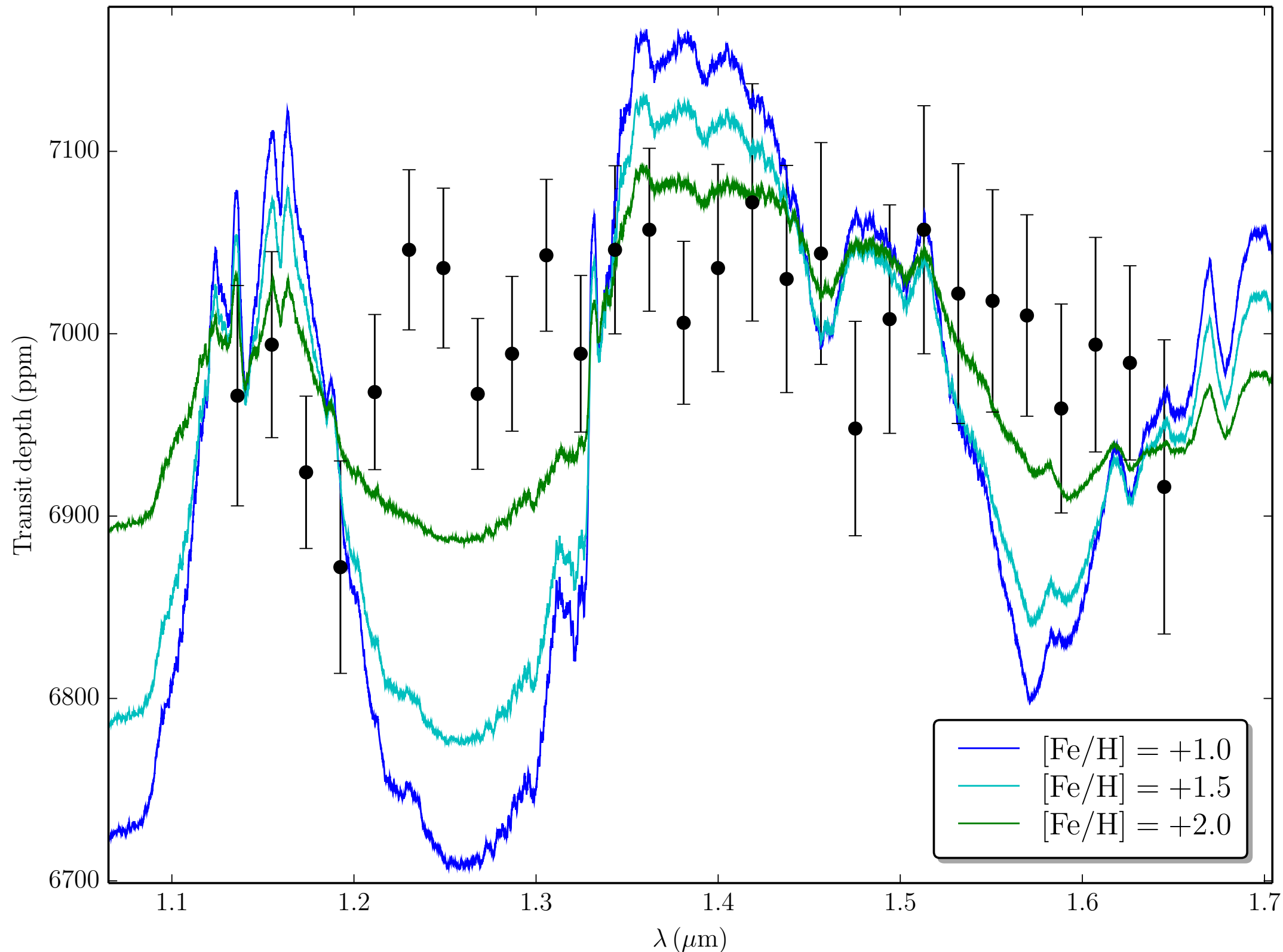
sequestration
of oxygen in
deep silicate
clouds!

Clouds in hot Neptunes and super-Earths



Clouds in hot Neptunes and super-Earths

GJ 436b transit models and WFC3 observations (Knutson et al. 2014)



Conclusions

Low Mass Star

- Cloud modelling successful in brown dwarfs
- Impact also on measured gas phase composition and thermal structure (evolution boundary!)
- Peculiarities of planetary atmospheres (mixing, nucleation processes) yet to be understood
- For mature, irradiated planets connection to circulation models essential

Brown Dwarf

Jupiter

Earth

NASA