7. Non-LTE – basic concepts

LTE vs NLTE

occupation numbers

rate equation

transition probabilities: collisional and radiative

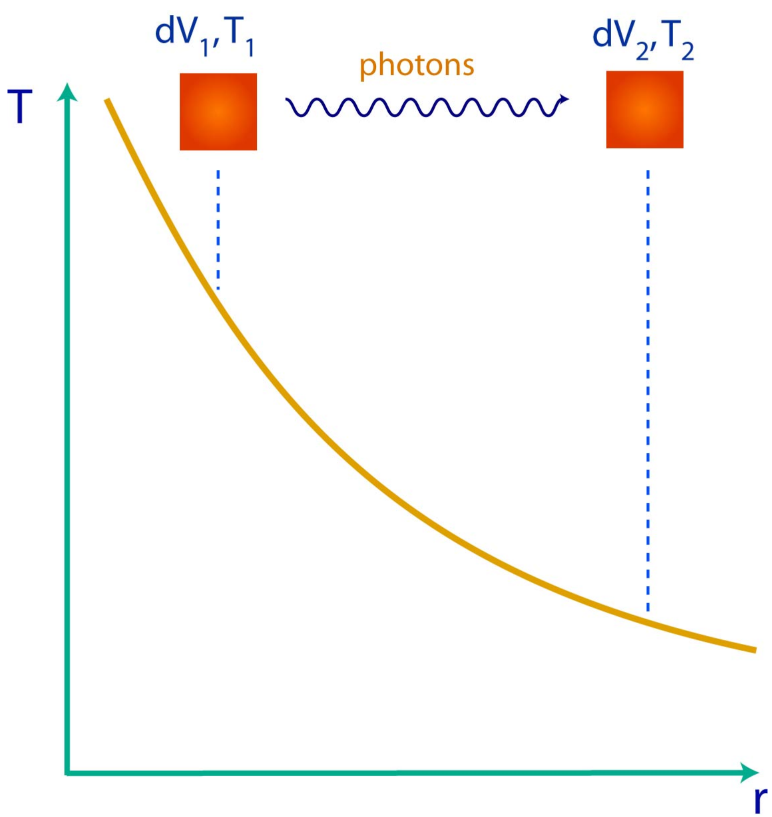
examples: hot stars, A supergiants

Spring 2016

LTE vs NLTE

LTE

each volume element separately in thermodynamic equilibrium at temperature T(r)



1. $f(v)\,dv$ = Maxwellian with $T = T(r)$
2. Saha: $(n_p\, n_e)/n_1 = T^{3/2} \exp(-h\nu_1/kT)$
3. Boltzmann: $n_i / n_1 = g_i / g_1 \exp(-h\nu_{1i}/kT)$

However:

volume elements not closed systems, interactions by photons

➔ LTE non-valid if absorption of photons disrupts equilibrium

Equilibrium: LTE vs NLTE

Processes:

radiative – photoionization, photoexcitation

establish equilibrium if radiation field is Planckian and isotropic

valid in innermost atmosphere

however, if radiation field is non-Planckian these processes drive occupation numbers away from equilibrium, if they dominate

collisional – collisions between electrons and ions (atoms) establish equilibrium if velocity field is Maxwellian

valid in stellar atmosphere

Detailed balance: the rate of each process is balanced by inverse process

LTE vs NLTE

NLTE if

rate of photon absorptions >> rate of electron collisions

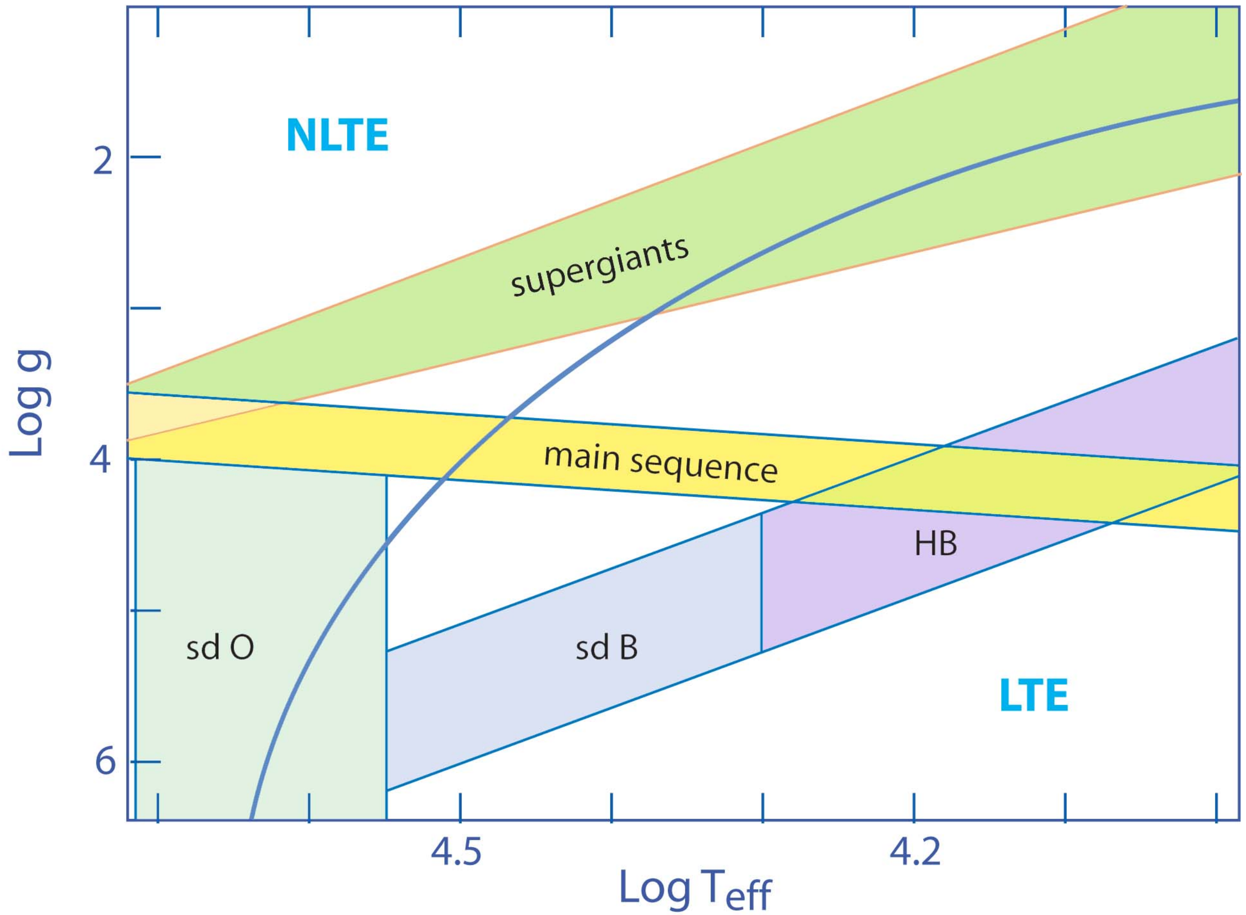
$I_\nu (T)$ » T^α, $\alpha > 1$ » $n_e T^{1/2}$

LTE

valid: low temperatures & high densities

non-valid: high temperatures & low densities

LTE vs NLTE in hot stars



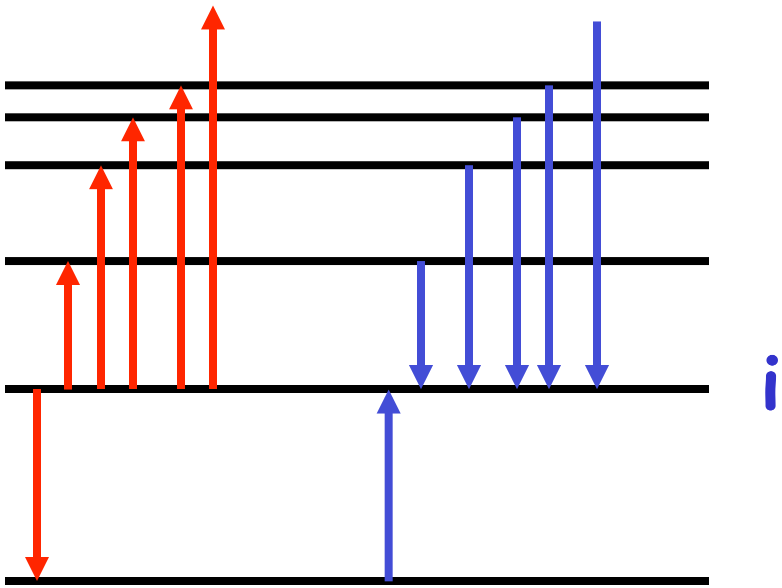
Kudritzki 1978

NLTE

1. f(v) dv remains Maxwellian
2. Boltzmann – Saha replaced by dn_i / dt = 0 (statistical equilibrium)

   for a given level *i* the rate of transitions out = rate of transitions in

rate out = rate in



$$n_i \sum_{j \neq i} P_{ij} = \sum_{j \neq i} n_j P_{ji}$$

rate equations

$P_{i,j}$ transition probabilities

Calculation of occupation numbers

NLTE

1. f(v) dv remains Maxwellian
2. Boltzmann – Saha replaced by $dn_i / dt = 0$ (statistical equilibrium)

   for a given level *i* the rate of transitions **out** = rate of transitions **in**

$$n_i \sum_{j \neq i} P_{ij} = \sum_{j \neq i} n_j P_{ji}$$

$$\underbrace{n_i \sum_{j \neq i} (R_{ij} + C_{ij})}_{\text{lines}} + \underbrace{n_i (R_{ik} + C_{ik})}_{\text{ionization}} = \underbrace{\sum_{j \neq i} n_j (R_{ji} + C_{ji})}_{\text{lines}} + \underbrace{n_p (R_{ki} + C_{ki})}_{\text{recombination}}$$

RATE EQUATIONS

Transition probabilities

radiative

$$R_{ij} = B_{ij} \int_0^\infty \varphi_{ij}(\nu)\ J_\nu\, d\nu$$ absorption

$$R_{ji} = A_{ji} + B_{ji} \int_0^\infty \varphi_{ij}(\nu)\ J_\nu\, d\nu$$ emission

collisional

$$C_{ij} = n_e \int_0^\infty \sigma_{\mathrm{coll}}(v) v f(v) dv$$

$$C_{ji} = g_i / g_j e^{E_{ji}/kT}\ C_{ij}$$

Occupation numbers

can prove that if $C_{ij} \gg R_{ij}$ or $J_\nu \rightarrow B_\nu(T)$: $n_i \rightarrow n_i$ (LTE)

We obtain a system of linear equations for n_i:

$$A \cdot \begin{pmatrix} n_1 \\ n_2 \\ \dots \\ n_p \end{pmatrix} = \mathbf{X}$$

Where matrix A contains terms:

$$\int_0^\infty \varphi_{ij}(\nu) \int_{4\pi} I_\nu(\omega) \frac{d\omega}{4\pi} d\nu$$

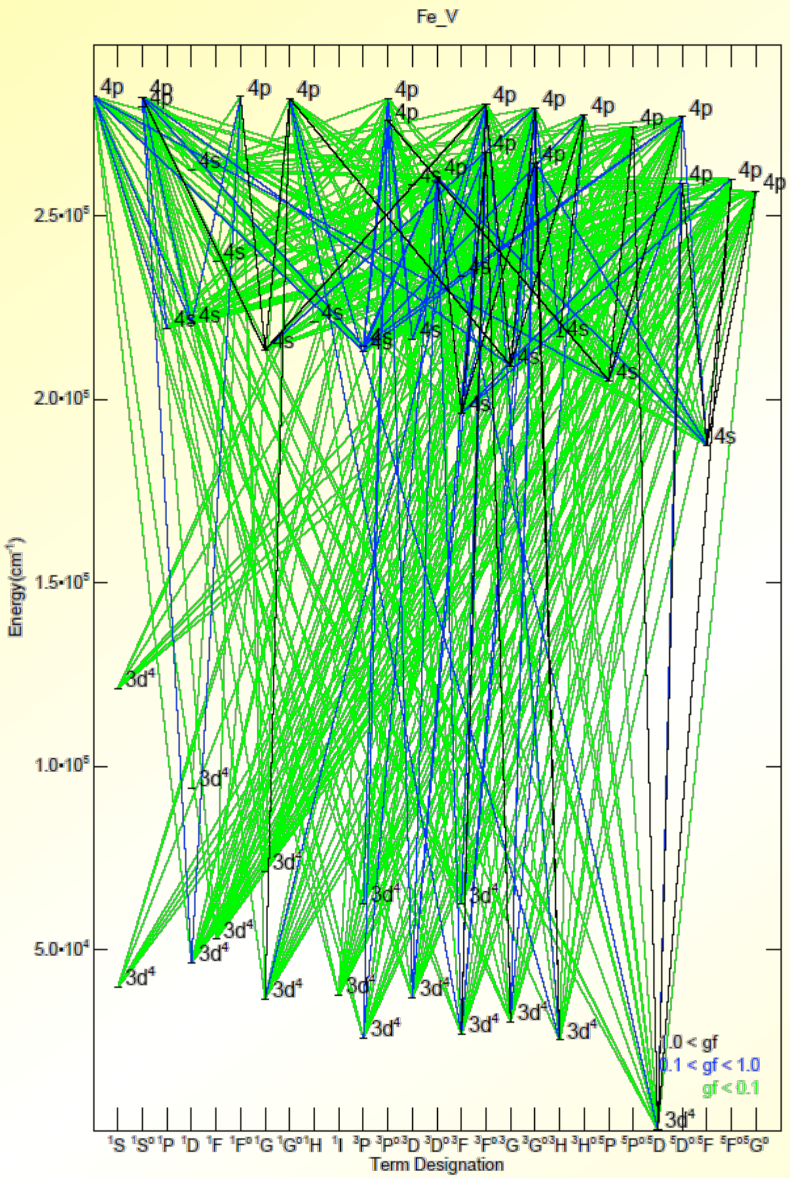
combine with equation of transfer: $\mu \frac{dI_\nu(\omega)}{dr} = -\kappa_\nu I_\nu(\omega) + \epsilon_\nu$

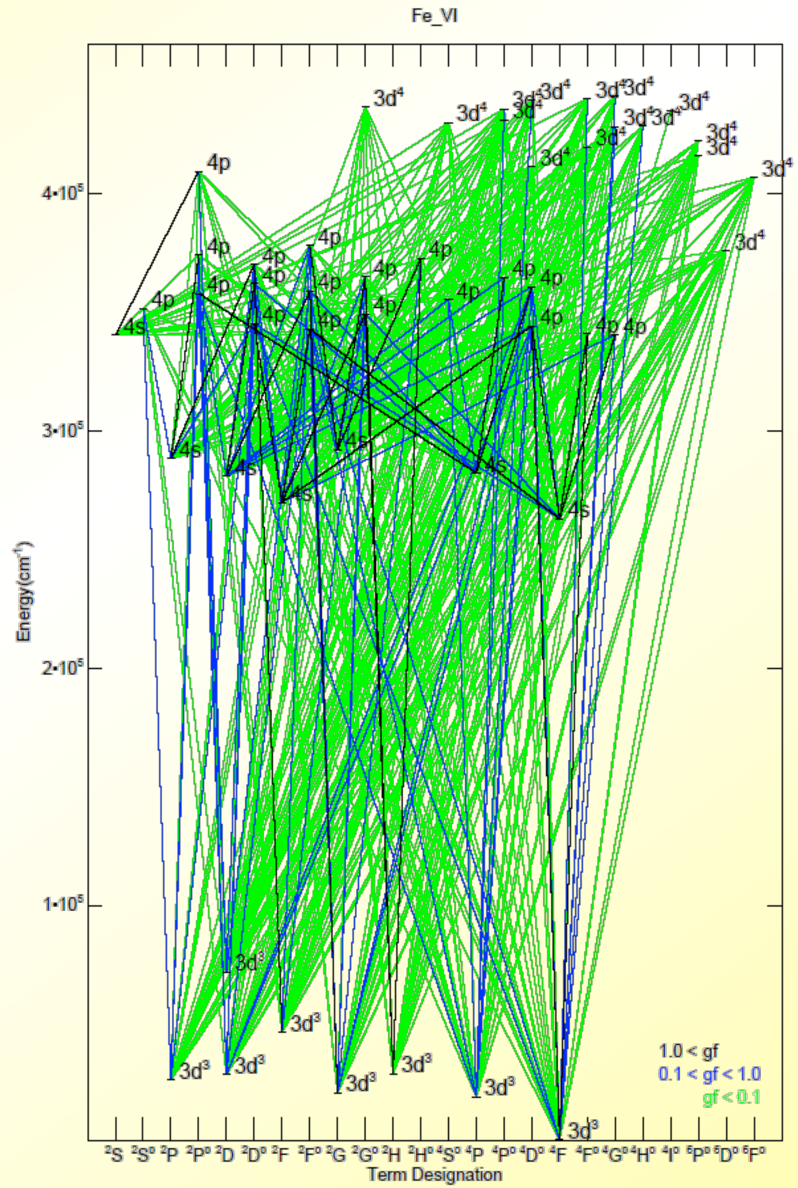
$$\kappa_\nu = \sum_{i=1}^{N} \sum_{j=i+1}^{N} \sigma_{ij}^{\text{line}}(\nu) \left(n_i - \frac{g_i}{g_j} n_j \right) + \sum_{i=1}^{N} \sigma_{ik}(\nu) \left(n_i - n_i^* e^{-h\nu/kT} \right) + n_e n_p \sigma_{kk}(\nu, T) \left(1 - e^{-h\nu/kT} \right) + n_e \sigma_e$$

$$\epsilon_\nu = \dots$$

non-linear system of integro-differential equations

complex atomic models for O-stars (Pauldrach et al., 2001)





Occupation numbers

Iteration required:

radiative processes depend on radiation field

radiation field depends on opacities

opacities depend on occupation numbers

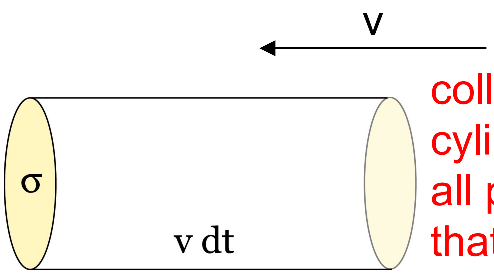
requires database of atomic quantities: energy levels, transitions, cross sections

20...1000 levels per ion – 3-5 ionization stages per species – $\sim$ 30 species

➔ fast algorithm to calculate radiative transfer required

Transition probabilities: collisions

probability of collision between atom/ion (cross section σ) and colliding particles in time dt: $\sim\sigma$ v dt



collision cylinder: all particles in that volume collide with target atom

rate of collisions = flux of colliding particles relative to atom/ion (n_{coll} v) $\times$ cross section σ.

for excitations:

$$C_{ij} = n_{coll} \int_0^\infty \sigma_{ij}^{\mathrm{coll}}(v) v f(v) dv$$

σ^{coll} from complex quantum mechanical calculations

and similarly for de-excitation

Transition probabilities: collisions

in a hot plasma free electrons dominate: $n_{coll} = n_e$

v_{th} = < v > = $(2kT/m)^{1/2}$ is largest for electrons ($v_{th,\,e} \simeq 43\, v_{th,\,p}$)

$$\Rightarrow \quad C_{ij} = n_e \int_0^\infty \sigma_{ij}^{\mathrm{coll}}(v) v f(v) dv = n_e\, q_{ij}$$

f(v) dv is Maxwellian in stellar atmospheres established by fast belastic e-e collisions.

One can show that under these circumstances the collisional transition probabilities for excitation and de-excitation are related by

$$\boxed{C_{ij} = \frac{g_j}{g_i} e^{-E_{ij}/kT} C_{ji}}$$

Transition probabilities: collisions

for bound-free transitions:

collisional recombination (very inefficient 3-particle process) =

$$\boxed{C_{ki} = C_{ik}\, n_e\, \frac{g_i}{g_1^+}\frac{1}{2}\left(\frac{h^2}{2\pi mkT}\right)^{3/2} e^{E_i/kT}}$$

collisional ionization (important at high T)

In LTE:

$$\left(\frac{n_j}{n_i}\right)^* = \frac{g_j}{g_i} e^{-E_{ij}/kT} \qquad \text{Boltzmann}$$

$$\left(\frac{n_1}{n_1^+}\right)^* = n_e \phi_1(T) \qquad \text{Saha}$$

$$\boxed{C_{ij} = \left(\frac{n_j}{n_i}\right)^* C_{ji} \qquad C_{ki} = \left(\frac{n_i}{n_1^+}\right)^* C_{ik}}$$

Transition probabilities: collisions

Approximations for C_{ji}

line transition i → j $$C_{ji} = n_e \frac{8.631 \times 10^{-6}}{T_e^{1/2}} \frac{\Omega_{ji}}{g_j} s^{-1} \qquad \Omega_{ji} \sim \sigma_{ji}$$

Ω_{ji} = collision strength

for *forbidden transitions:* $\Omega_{ji} \simeq 1$

for *allowed transitions*: $\Omega_{ji} = 1.6 \times 10^6 \, (g_i / g_j) \, f_{ij} \, \lambda_{ij} \, \Gamma(E_{ij}/kT)$

Γ: max (g', 0.276 exp(E_{ij}/kT) E_1(E_{ij}/kT)

g' = 0.7 for nl -> nl' =0.3 for nl → n' l'

Transition probabilities: collisions

for ionizations

$$C_{ik} = n_e \frac{1.55 \times 10^{13}}{T_e^{1/2}} g_i' \sigma_{ik}^{\text{phot}}(\nu_{ik}) \frac{e^{-E_i/kT}}{E_i/kT}$$

= 0.1 for Z=1

= 0.2 for Z=2

= 0.3 for Z=3

photoionization cross section at ionization edge

Transition probabilities: radiative processes

Line transitions

absorption $i \rightarrow j$ ($i < j$)

probability for absorption $$dW_{ij} = B_{ij} I_x \frac{d\omega}{4\pi} \varphi(x) dx \qquad x = \frac{\nu - \nu_0}{\Delta\nu_D}$$

integrating over x and dω (dω = 2π dμ)

$$R_{ij} = B_{ij} \bar{J}_{ij} \qquad \bar{J}_{ij}(r) = \frac{1}{2} \int_{-\infty}^{\infty} \int_{-1}^{1} I(x, \mu, r) \varphi(x) d\mu dx$$

emission ($i > j$)

$$R_{ji} = A_{ji} + B_{ji} \bar{J}_{ji}$$

Transition probabilities: radiative processes

Bound-free

photo-ionization i → k

$$R_{ik} = \int_{\nu_{ik}}^{\infty} \underbrace{\sigma_{ik}(\nu)\, c}_{\sigma \times v \text{ for photons}}\, n_{\rm phot}(\nu) d\nu$$

σ × v for photons

$$u_\nu = h\nu\, n_{\rm phot}(\nu) = \frac{4\pi}{c} J_\nu \qquad \text{energy density}$$

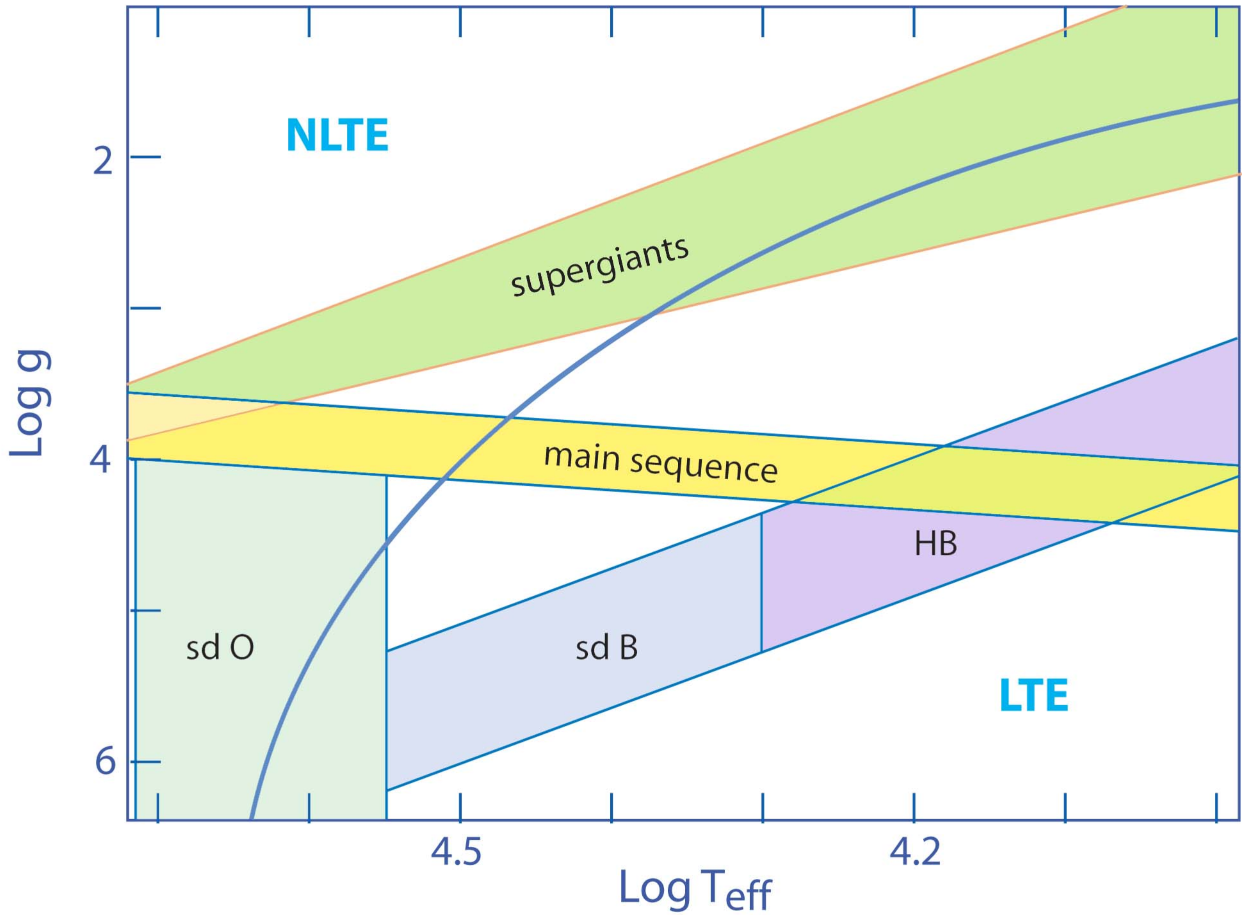
$$\Longrightarrow \quad R_{ik} = 4\pi \int_{\nu_{ik}}^{\infty} \frac{\sigma_{ik}(\nu)}{h\nu} J_\nu d\nu$$

photo-recombination k → i

$$R_{ki} = \left(\frac{n_i}{n_1^+}\right)^* \tilde{R}_{ki}$$

$$\tilde{R}_{ki} = 4\pi \int_{\nu_{ik}}^{\infty} \frac{\sigma_{ik}}{h\nu} \left(\frac{2h\nu^3}{c^2} + J_\nu\right) e^{-h\nu/kT} d\nu$$

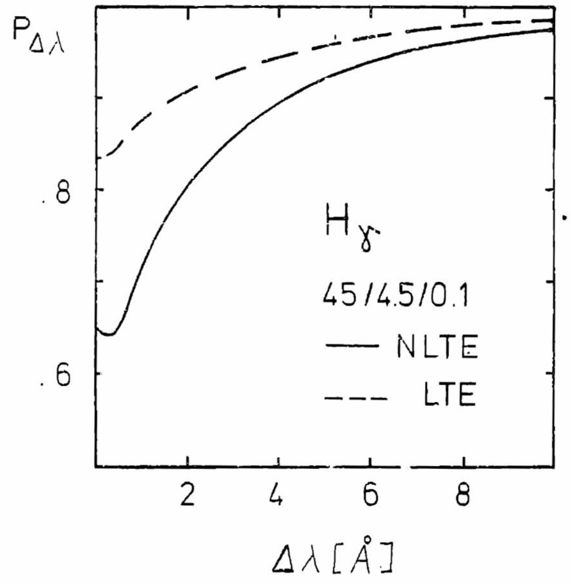
LTE vs NLTE in hot stars



Kudritzki 1979

LTE vs NLTE in hot stars

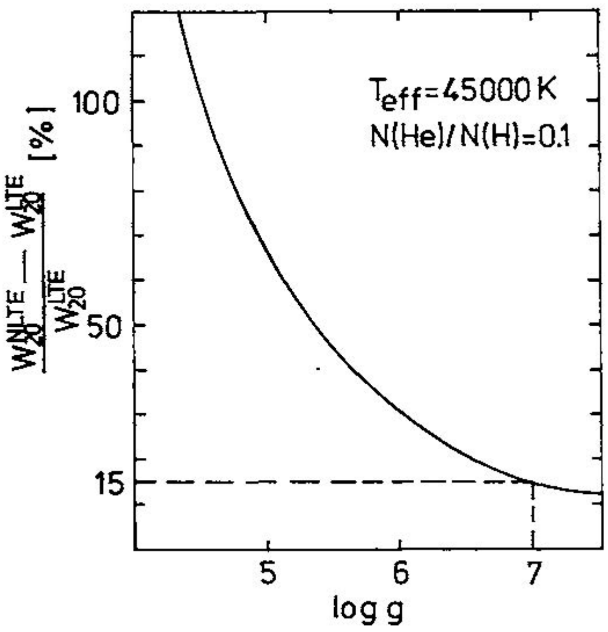
Kudritzki 1979



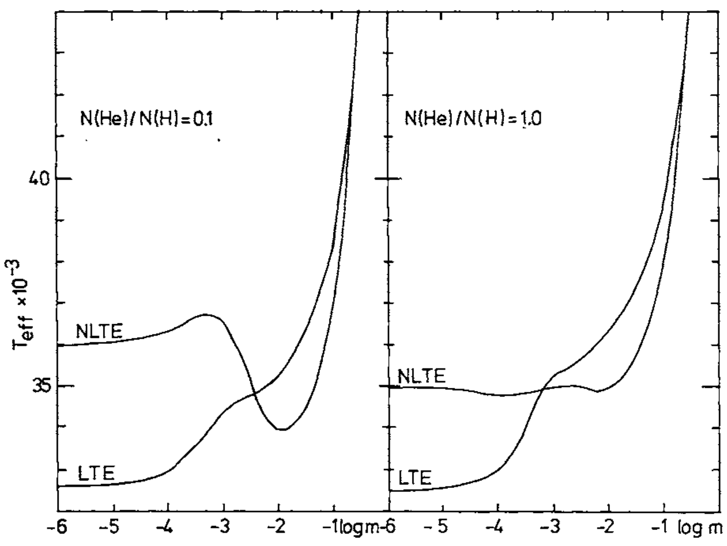
difference between NLTE and LTE in Hγ line profile for an O-star model with Teff = 45000K and log g = 4.5

LTE vs NLTE in hot stars

Kudritzki 1979



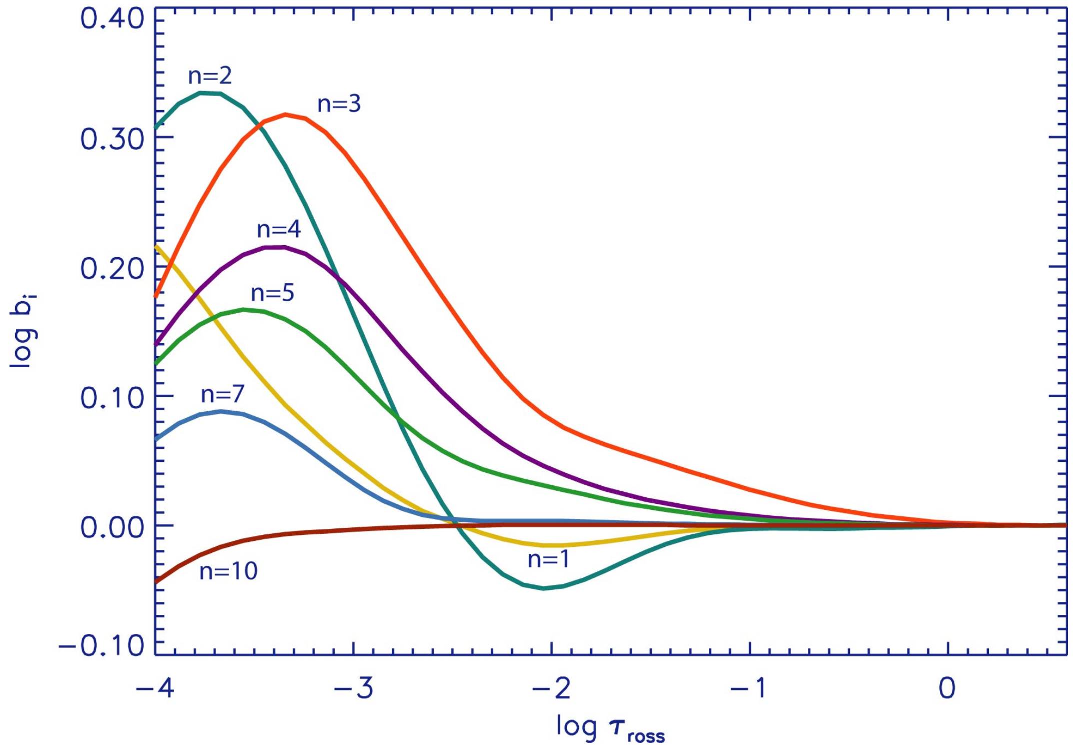
difference between NLTE and LTE Hγ equivalent width as a function of log g for T_{eff} = 45,000 K



NLTE and LTE temperature stratifications for two different Helium abundances at T_{eff} = 45,000 K, log g = 5

LTE vs NLTE: departure coefficients - hydrogen

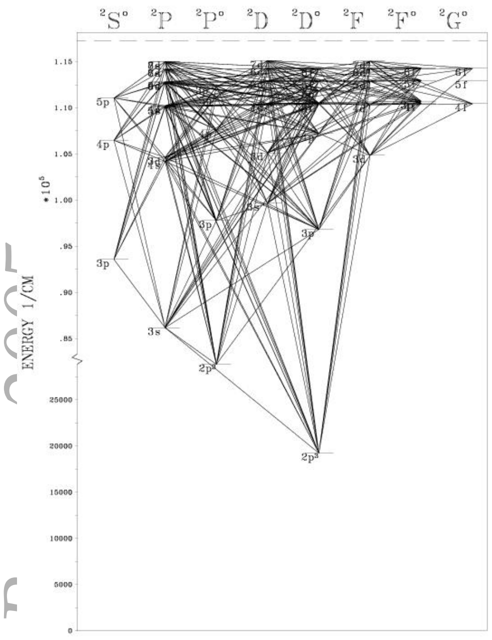
$$b_i = \frac{n_i^{\mathrm{NLTE}}}{n_i^{\mathrm{LTE}}}$$

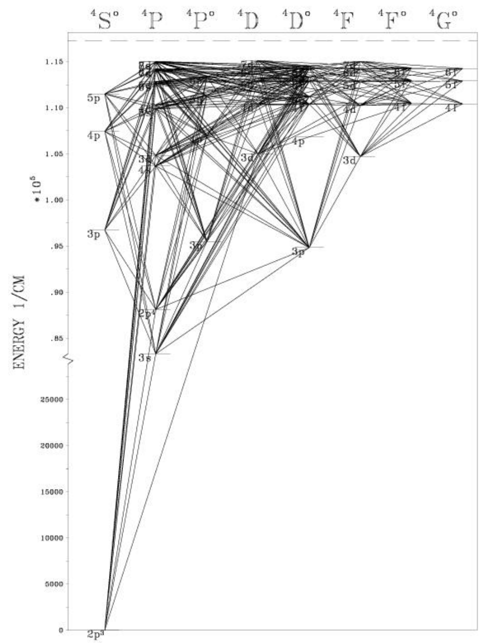


β Orionis (B8 Ia)

T_{eff} = 12,000 K

log g = 1.75 (Przybilla 2003)





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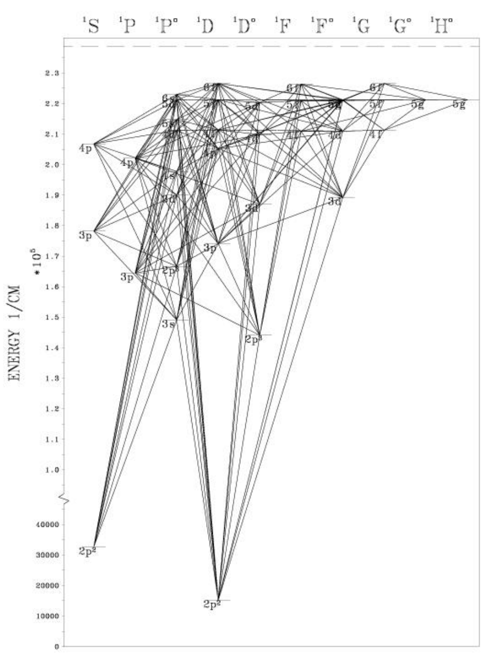
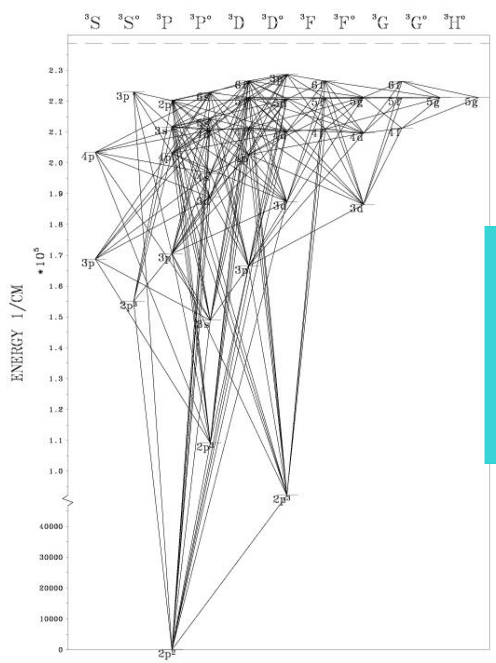


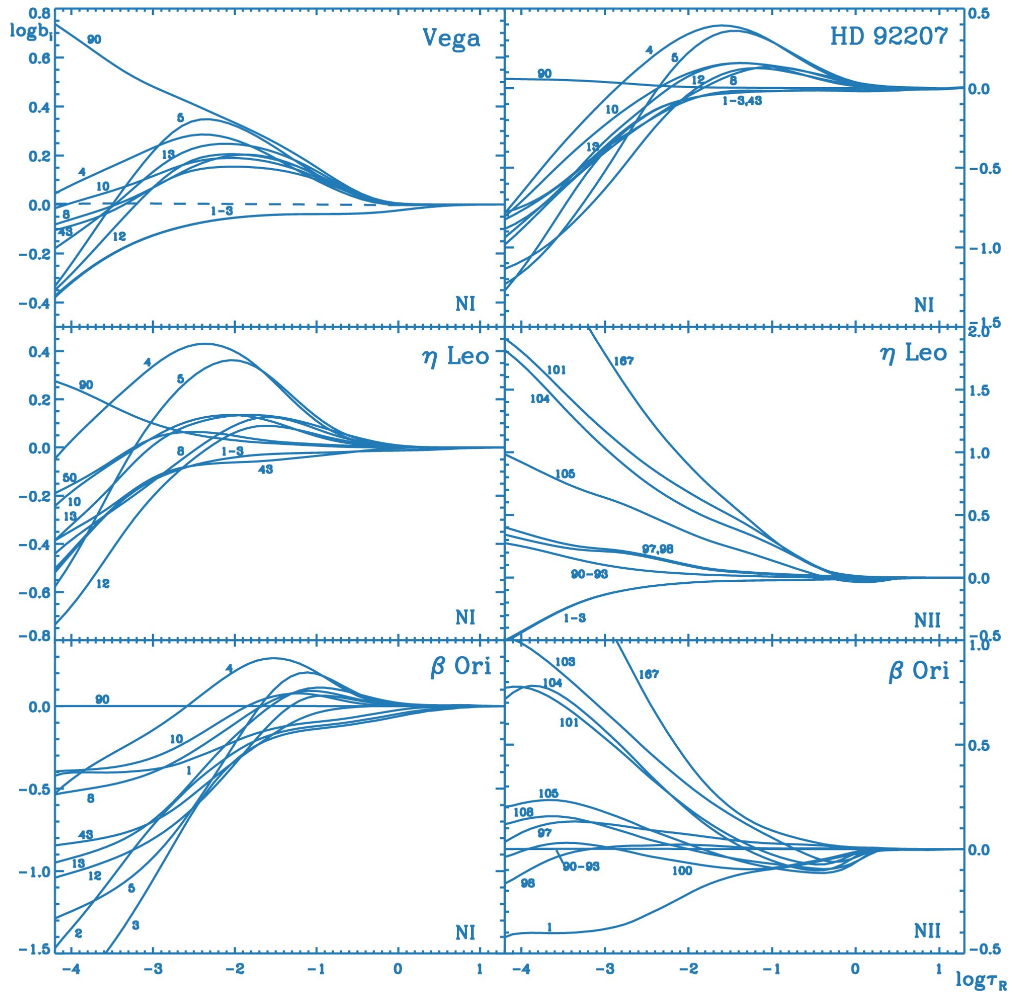


N II

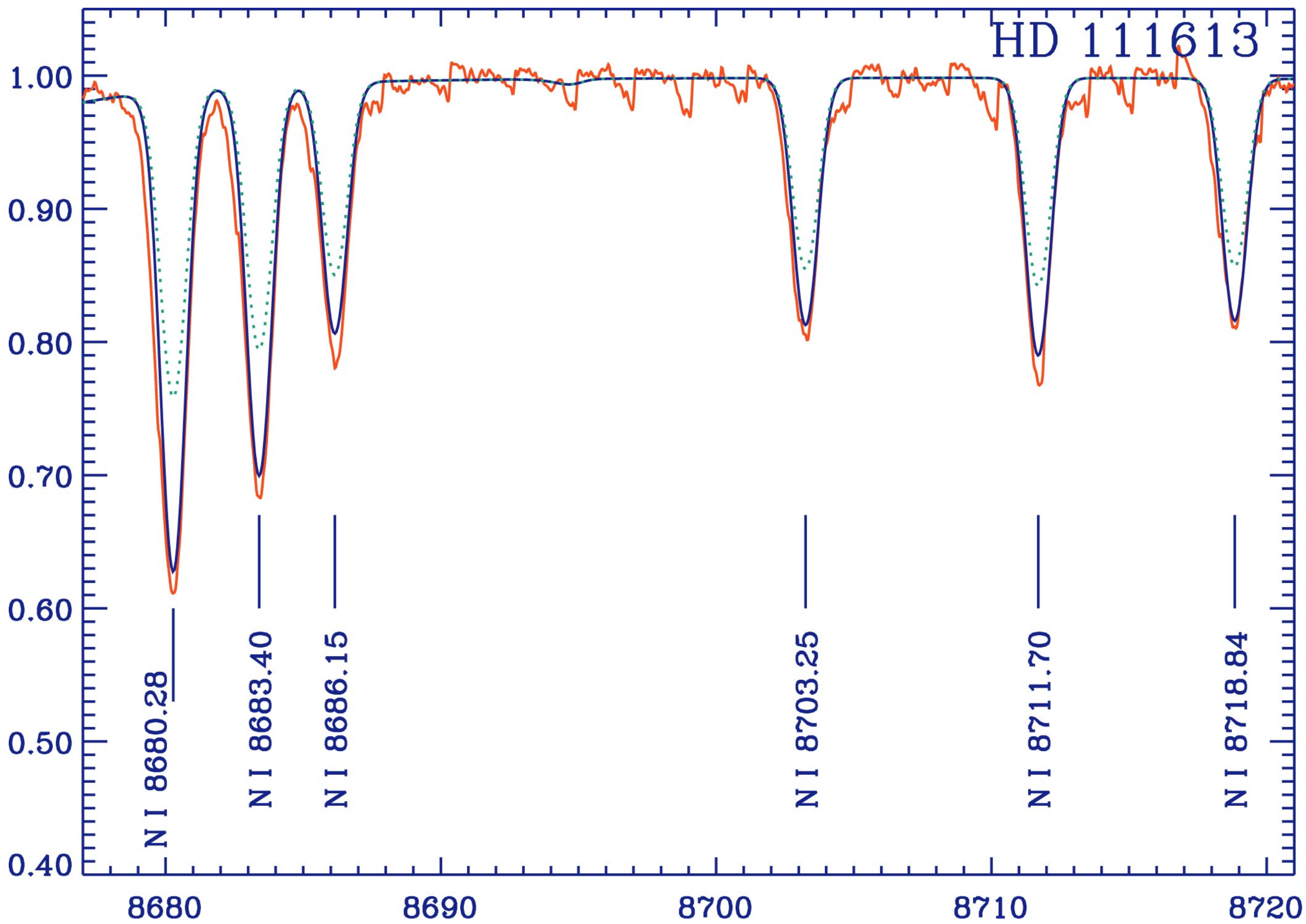
Nitrogen atomic models

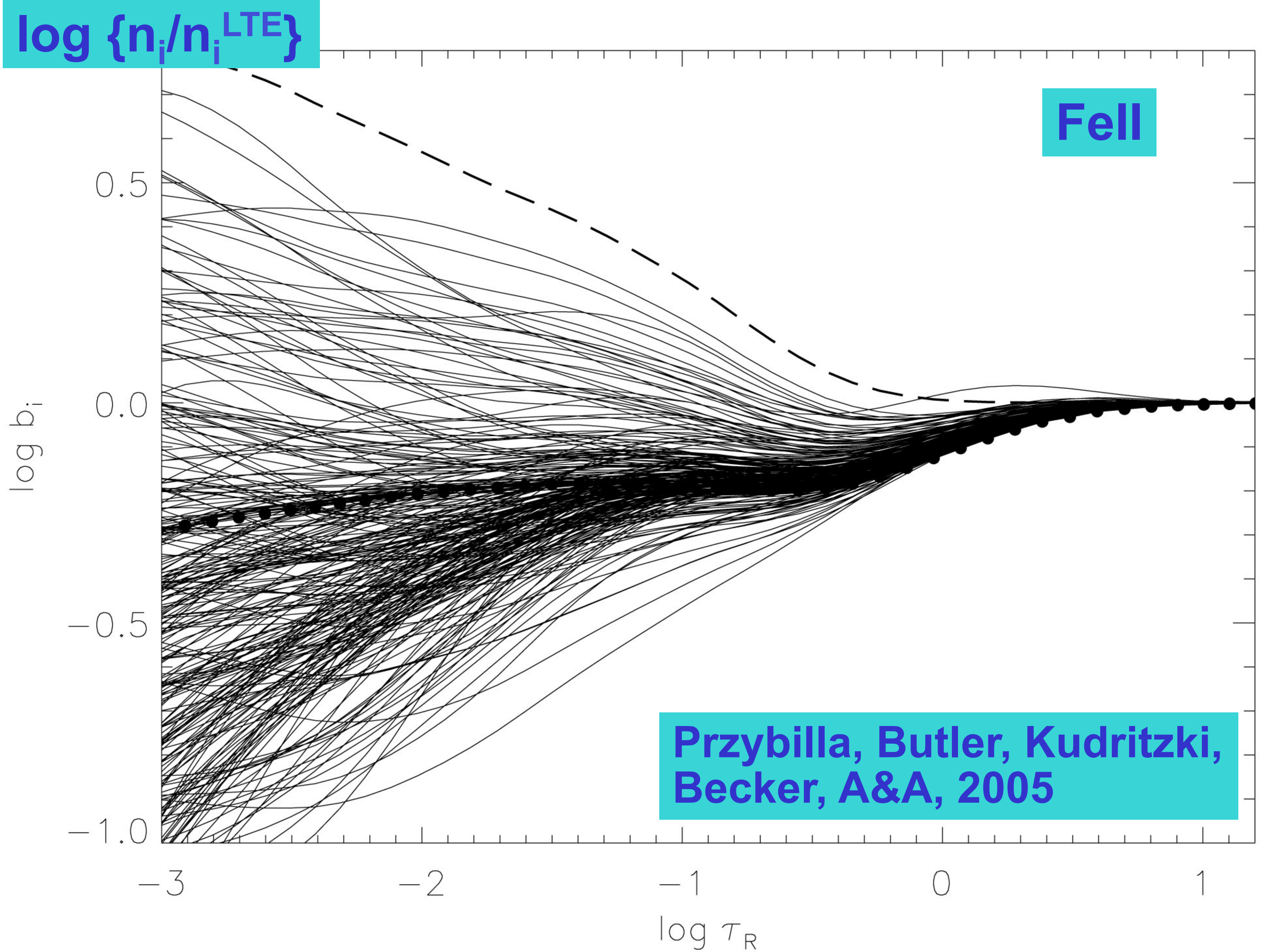
Przybilla, Butler, Kudritzki 2003

LTE vs NLTE: departure coefficients - nitrogen



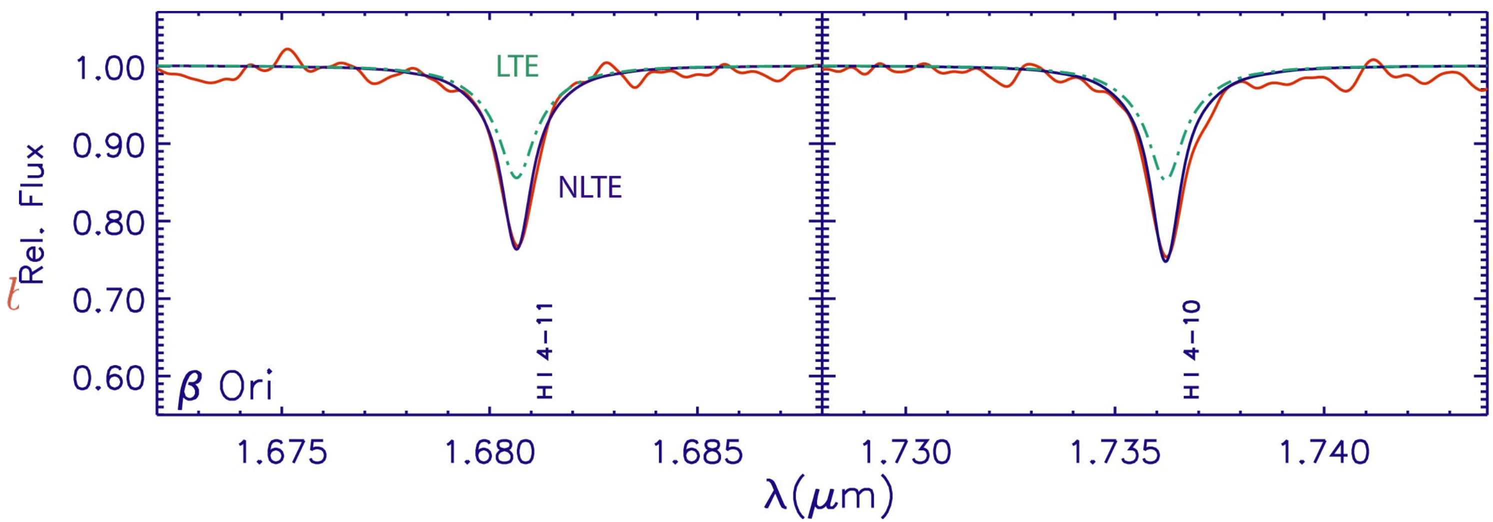
LTE vs NLTE: line fits – nitrogen lines





log {n_i/n_i^{LTE}}
FeII
Przybilla, Butler, Kudritzki, Becker, A&A, 2005
log b_i
log τ_R
0.5
0.0
−0.5
−1.0
−3
−2
−1
0
1

LTE vs NLTE: line fits – hydrogen lines in IR

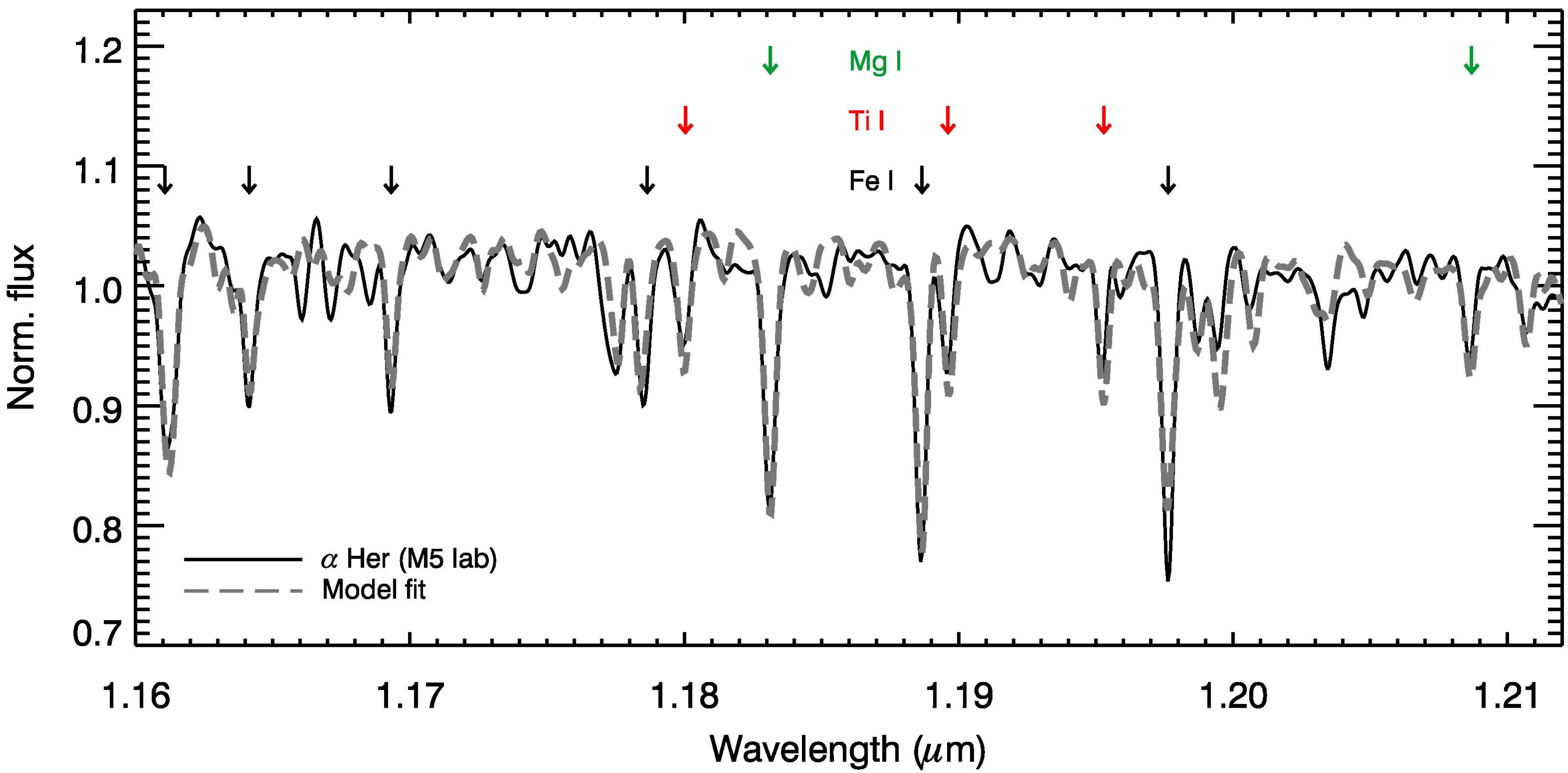


Brackett lines

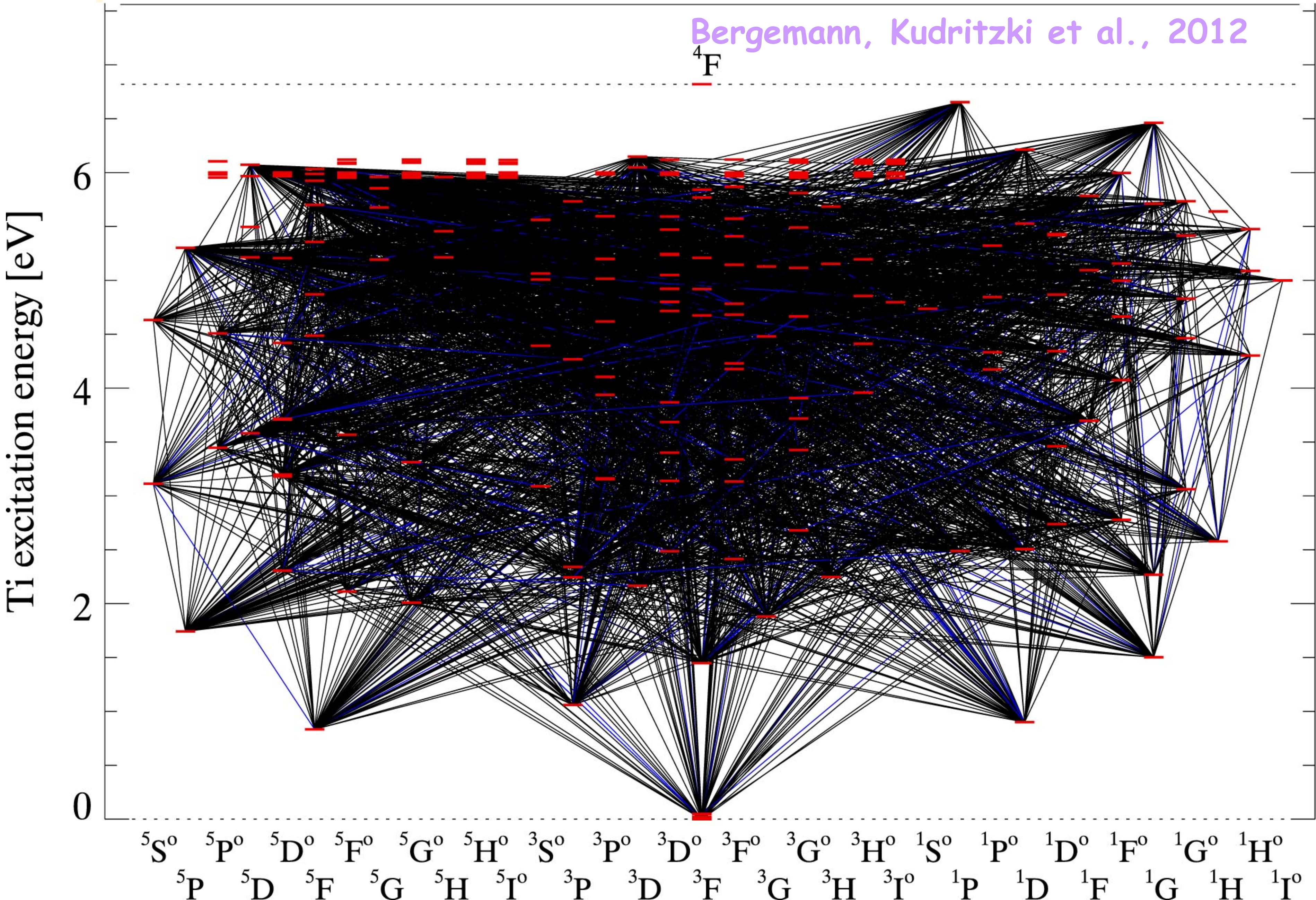
J-band spectroscopy of red supergiants

Cosmic abundance probes out to 70 Mpc distance

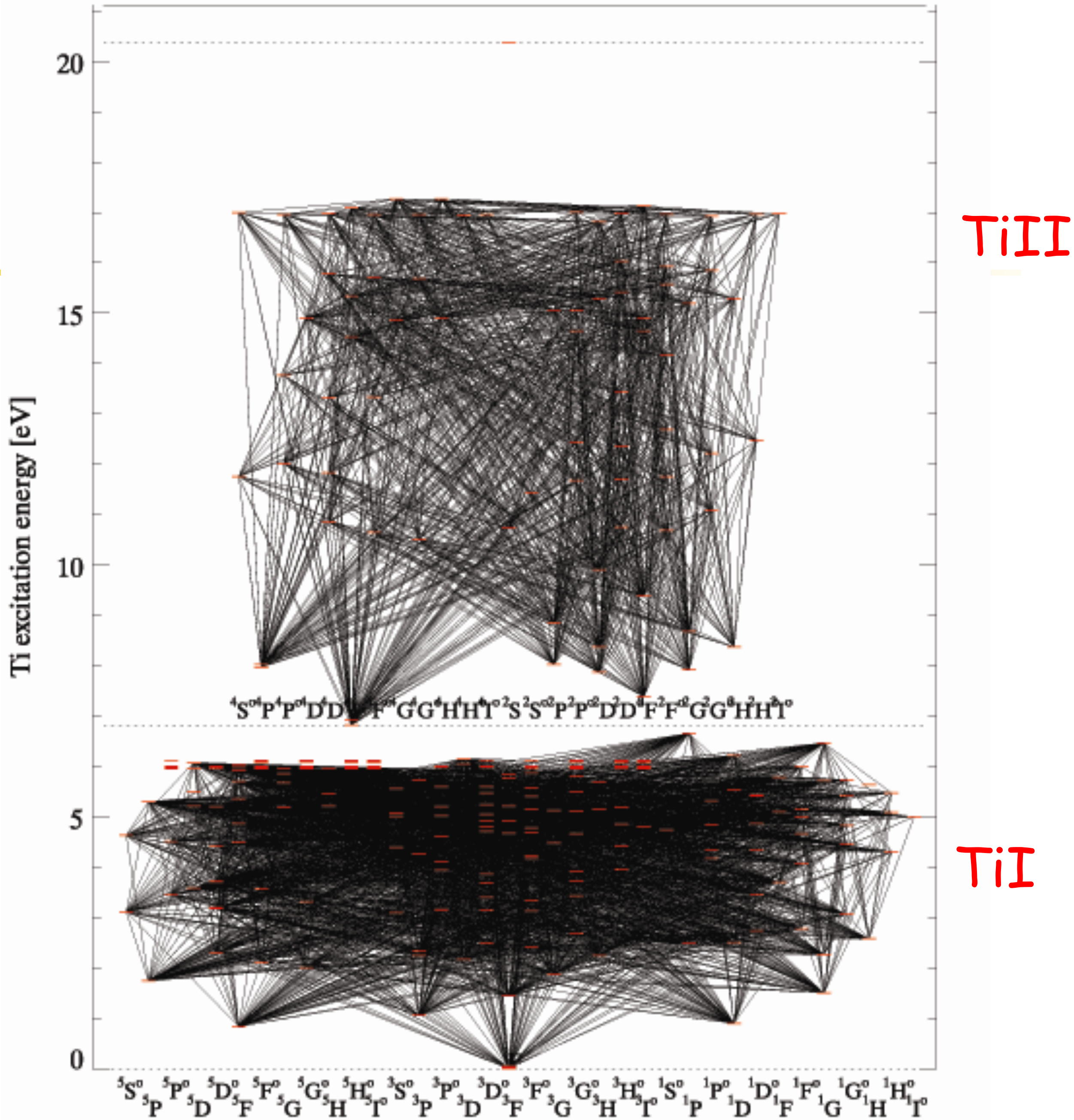
α Her Davies, Kudritzki, Figer, 2010 MNRAS, 407,1203



Red supergiants, NLTE model atom for TiI

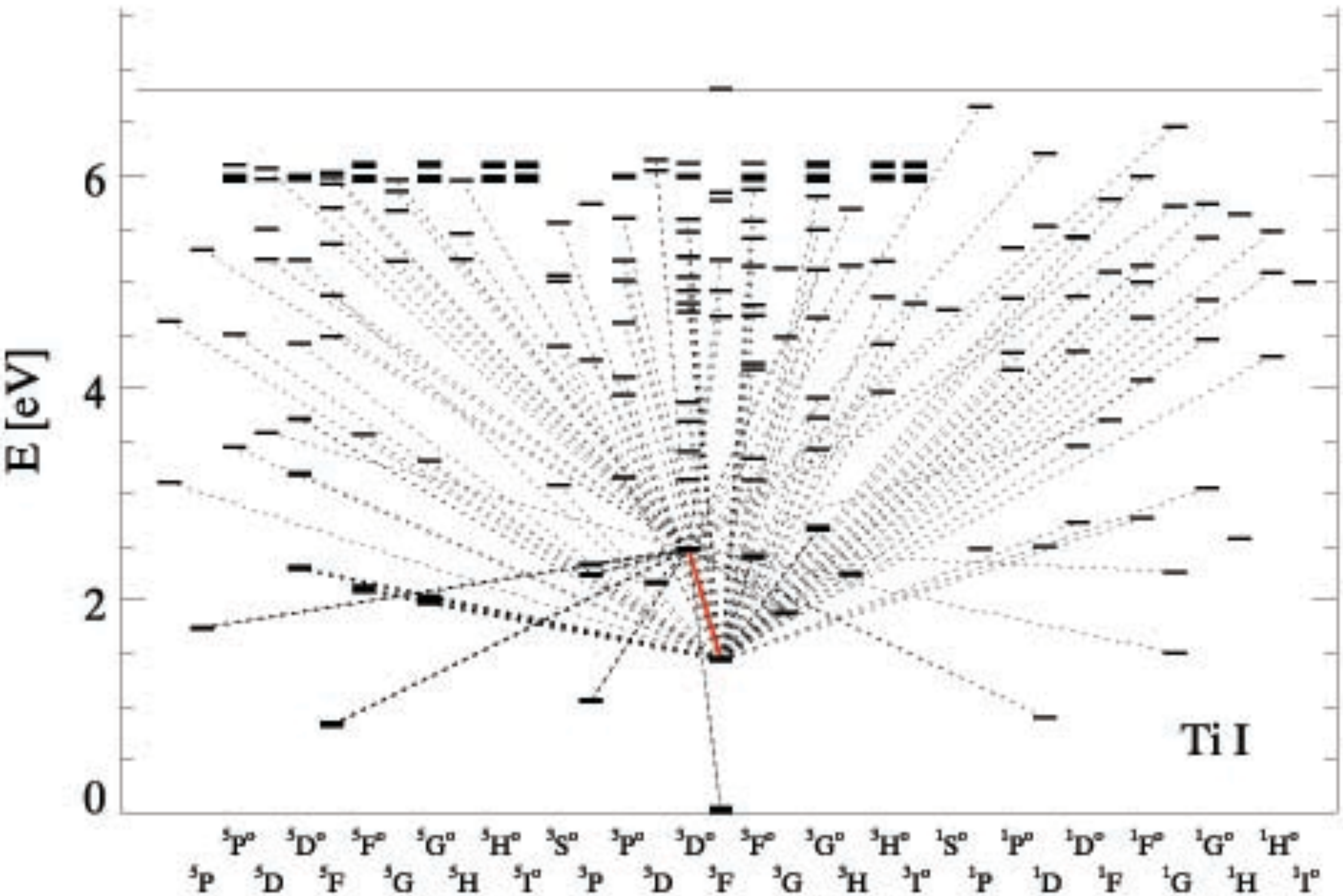


Bergemann, Kudritzki et al., 2012



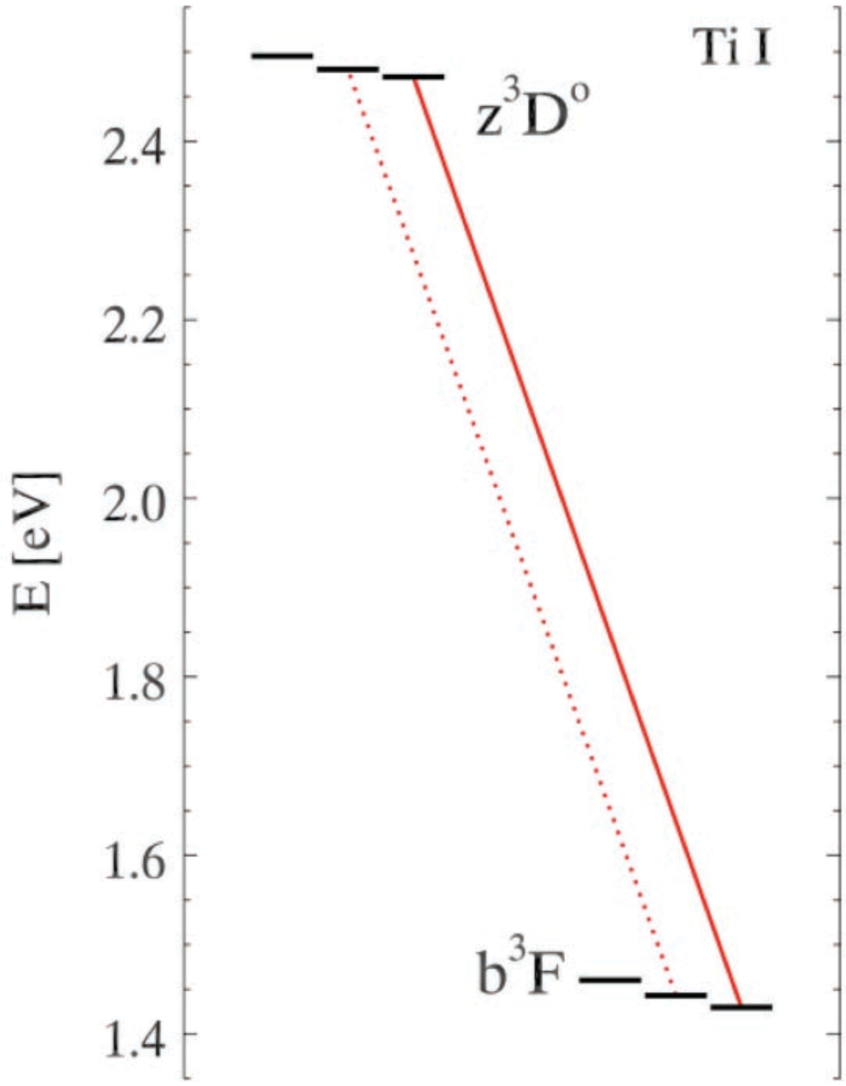
Red supergiants, IR lines and connected transitions for TiI

Bergemann, Kudritzki et al., 2012



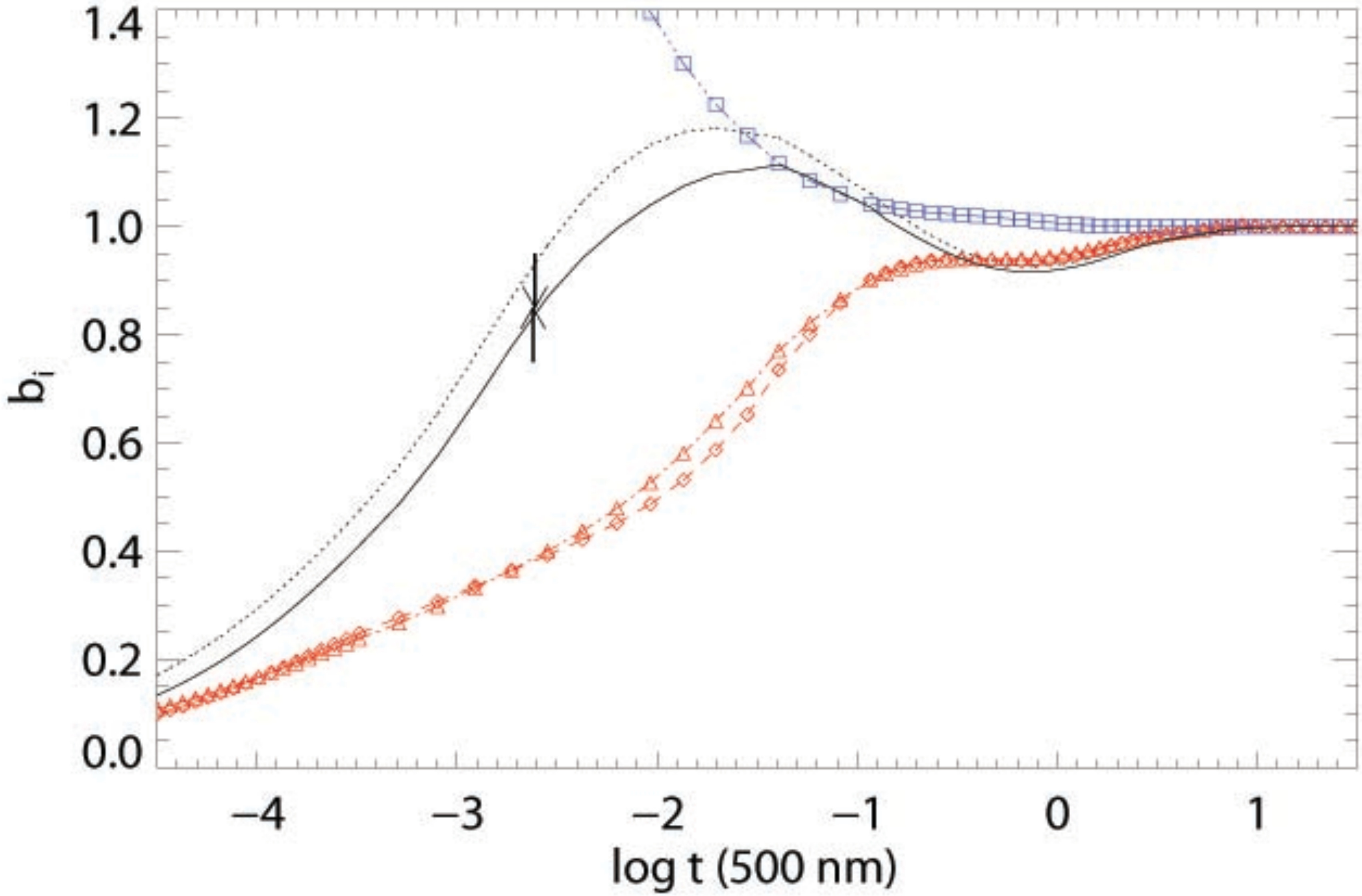
Red supergiants, IR lines fine structure levels for TiI

Bergemann, Kudritzki et al., 2012



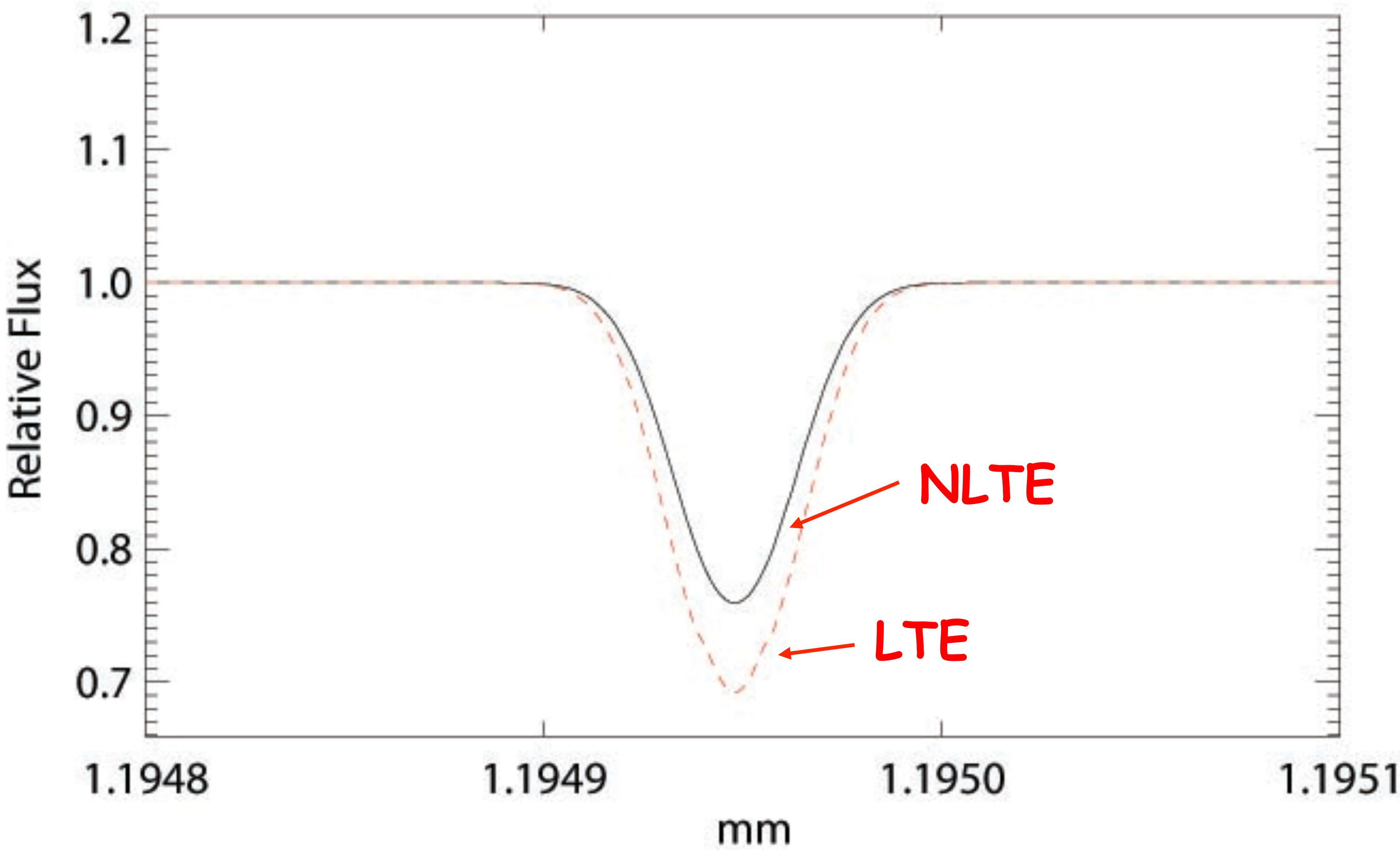
Red supergiants, IR lines departure coefficient for TiI

Bergemann, Kudritzki et al., 2012

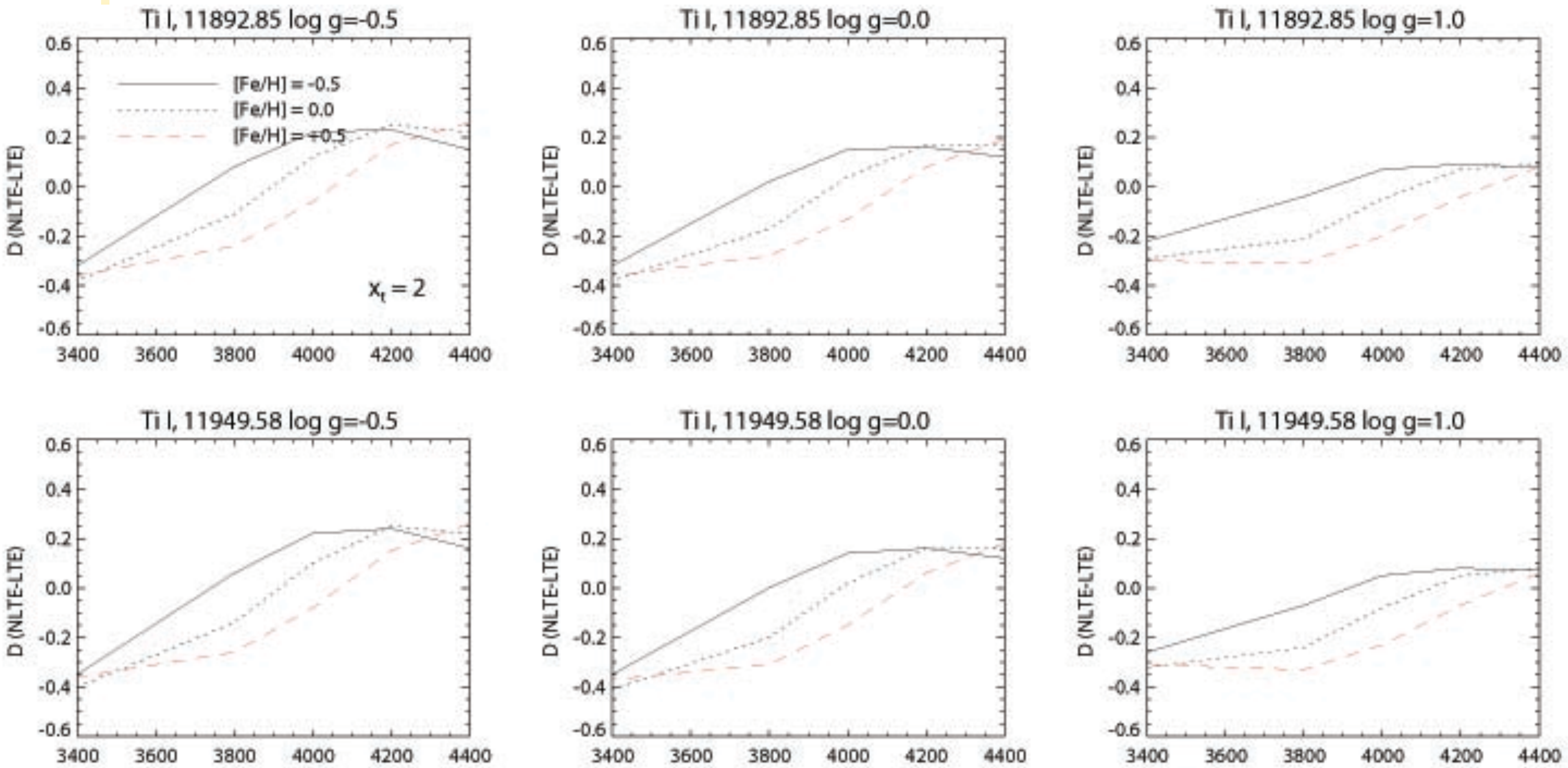


Red supergiants, IR lines for TiI: NLTE vs. LTE

Bergemann, Kudritzki et al., 2012



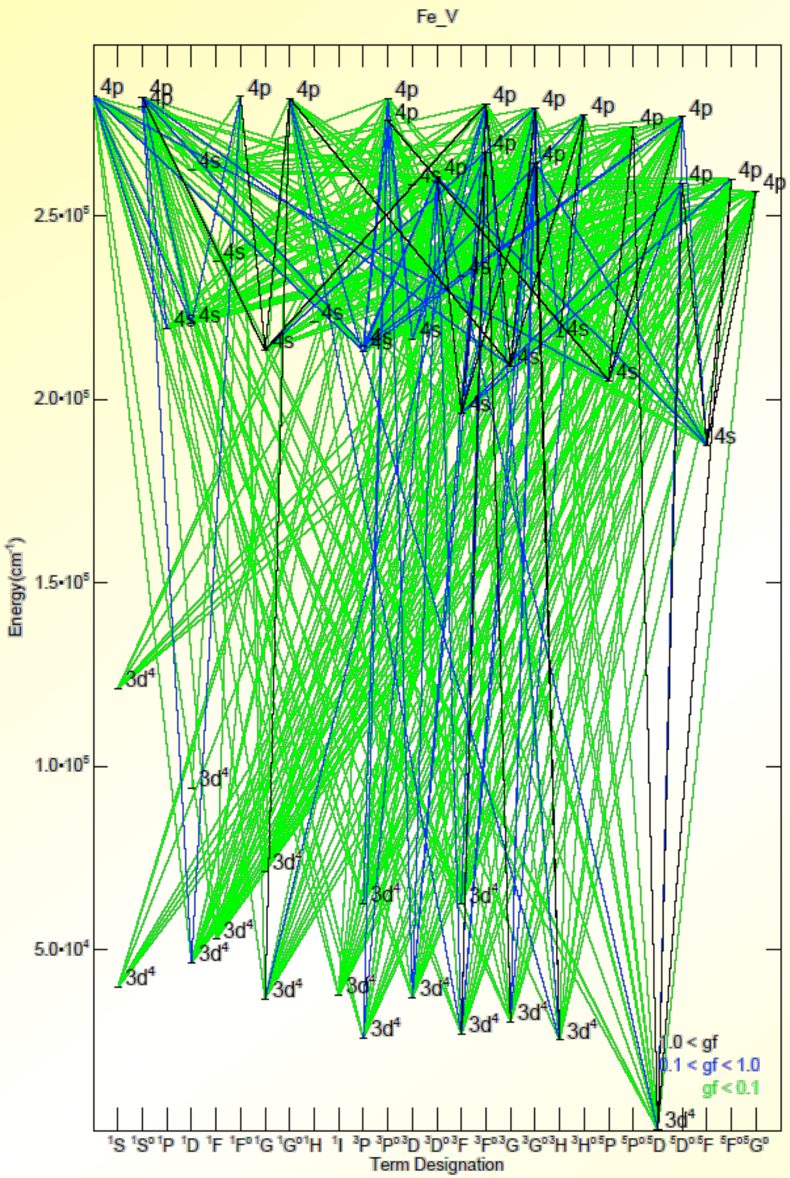
Red supergiants, IR lines NLTE abundance corrections for TiI

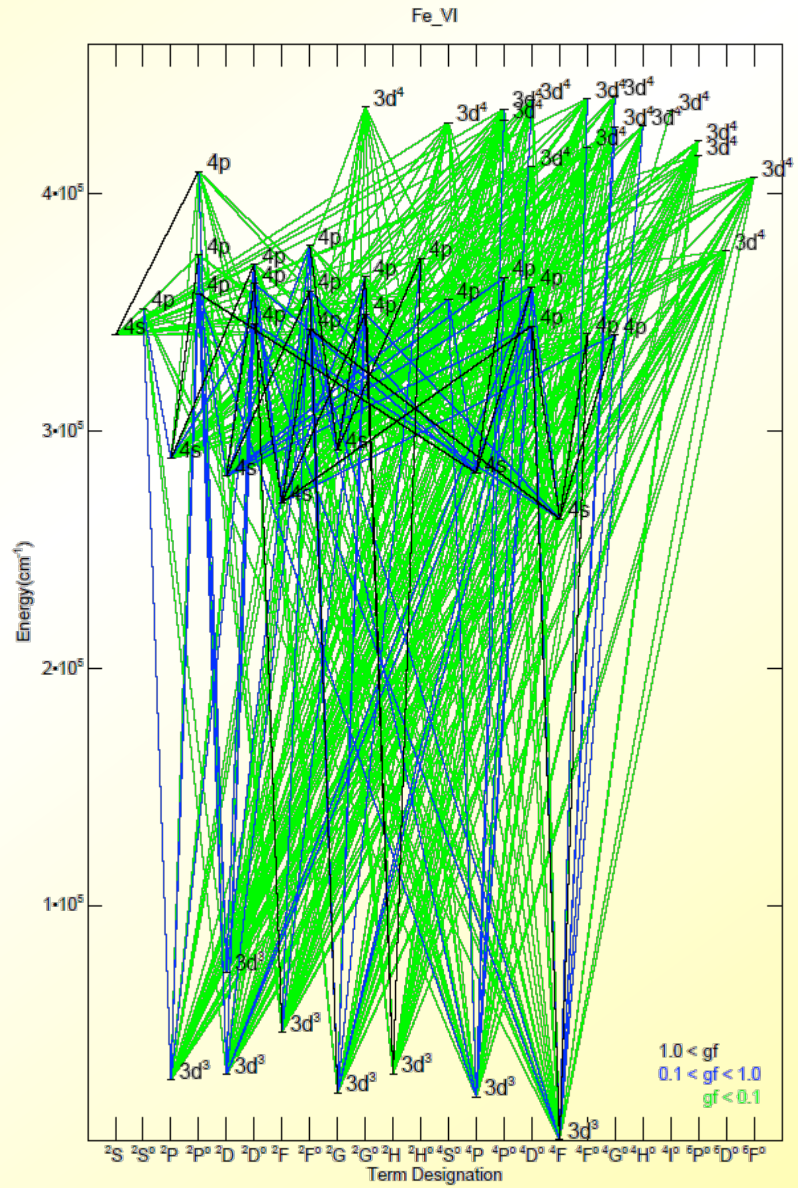


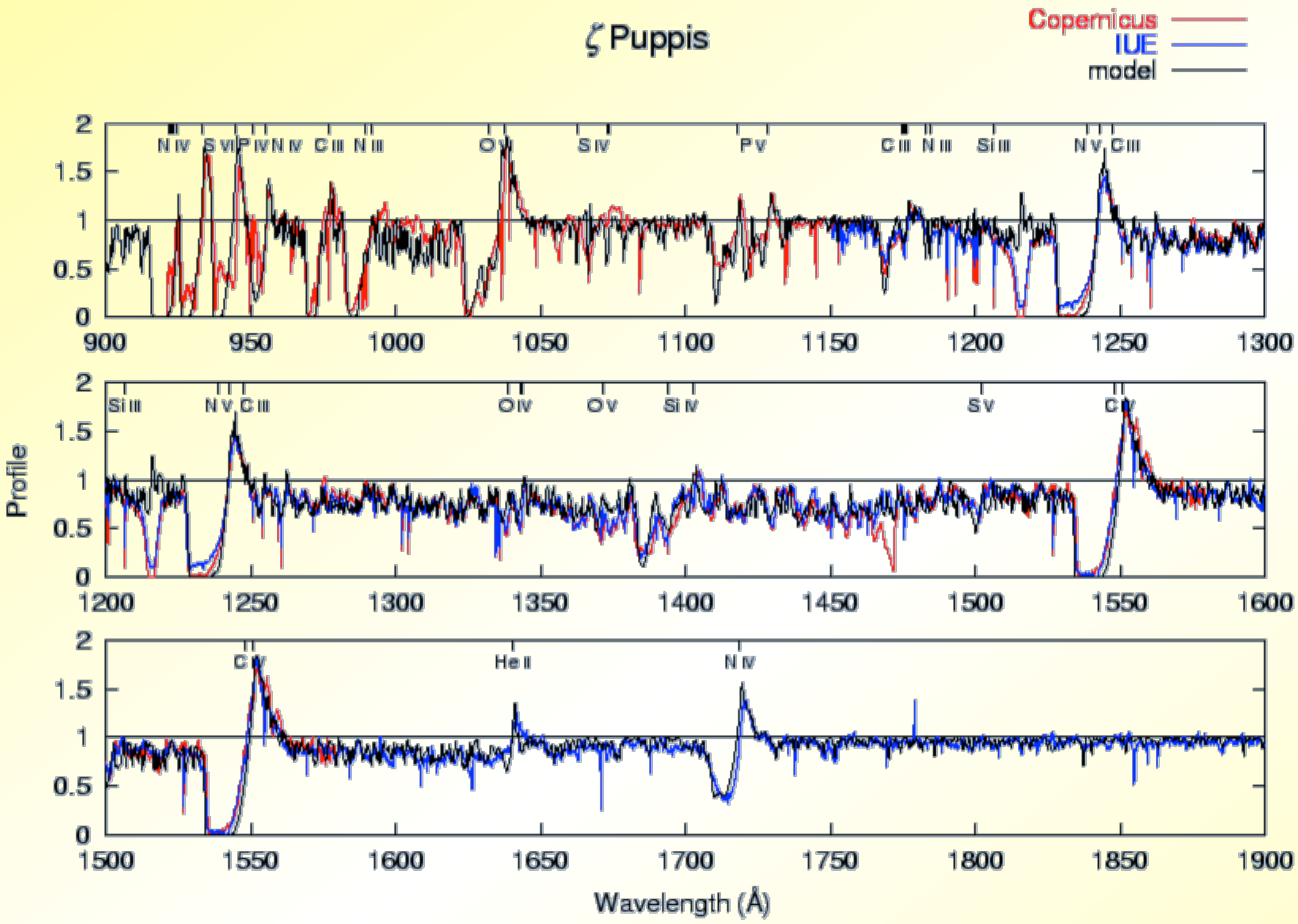
$$D(\mathrm{NLTE-LTE}) = \log\{N(\mathrm{Ti})/N(\mathrm{H})\}_{\mathrm{NLTE}} - \log\{N(\mathrm{Ti})/N(\mathrm{H})\}_{\mathrm{LTE}}$$

Bergemann, Kudritzki et al., 2012

complex atomic models for O-stars (Pauldrach et al., 2001)







Pauldrach, 2003, Reviews in Modern Astronomy, Vol. 16

consistent treatment of expanding atmospheres along with **spectrum synthesis techniques** allow the determination of **stellar parameters, wind parameters, and abundances**