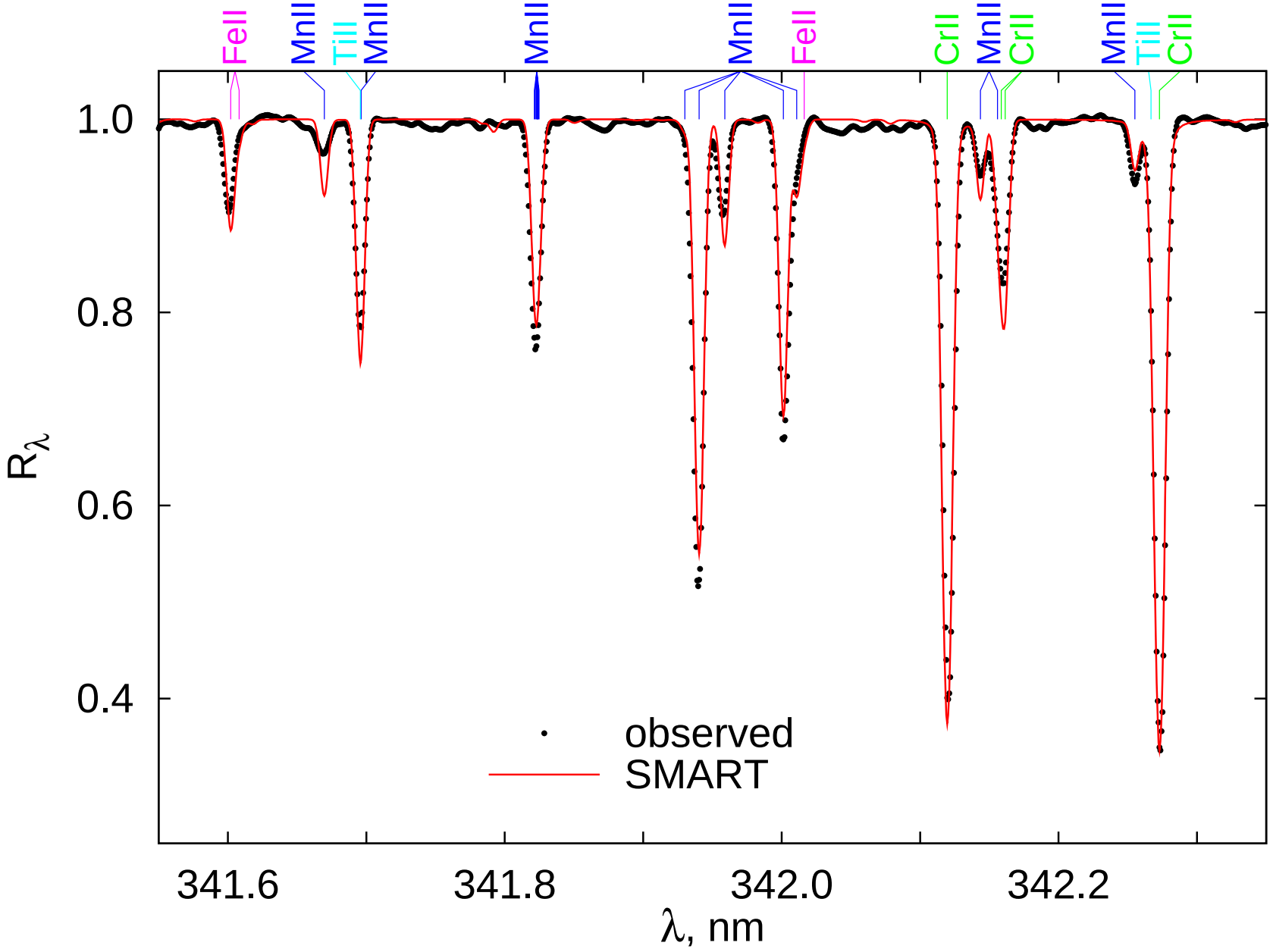
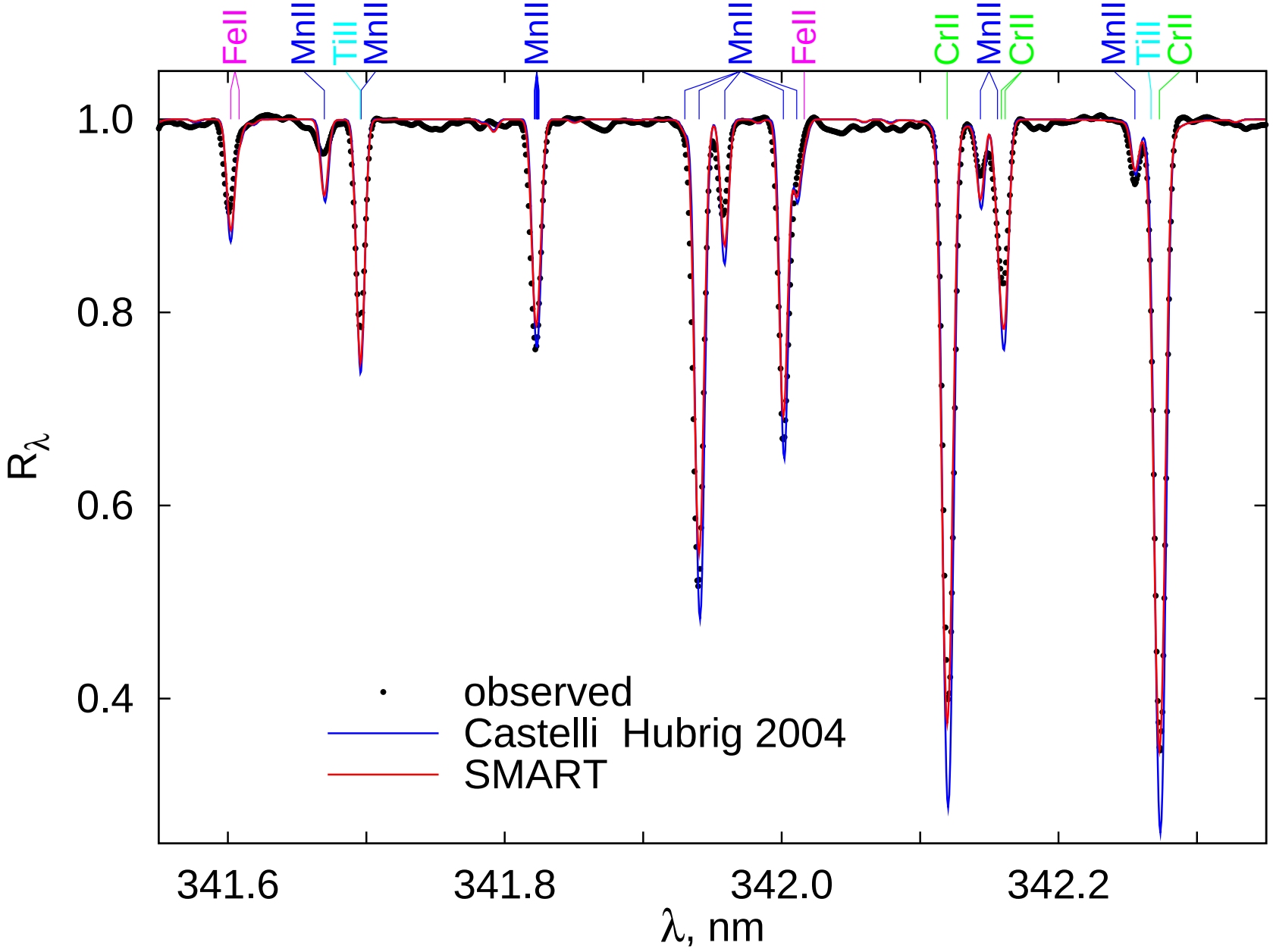
Appendix

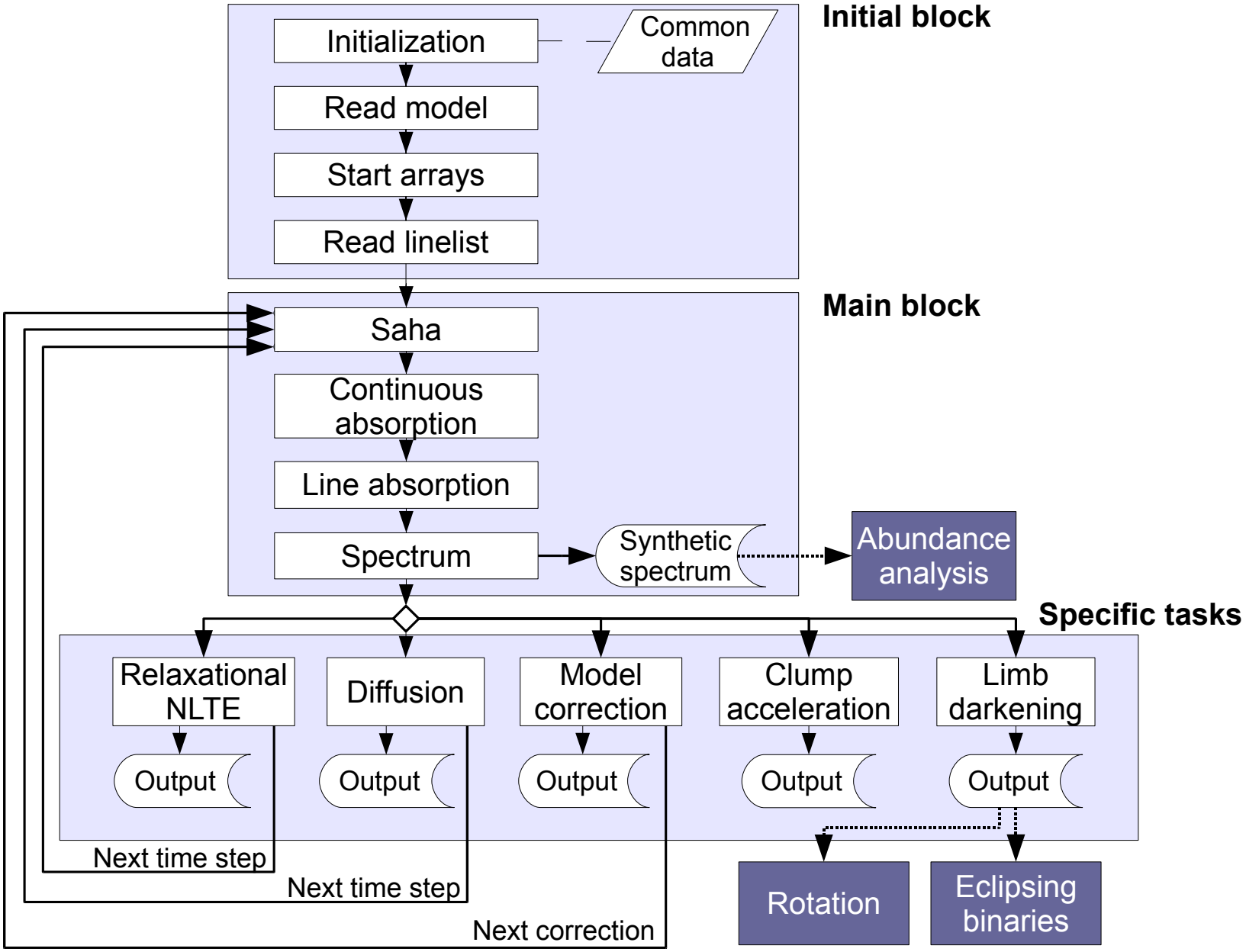
Spectrum of HgMn star HD 175640



Spectrum of HgMn star HD 175640



General structure of program SMART



Block "Saha"

Saha equation

$$\frac{X_i^{j+1}}{X_i^j} = a\frac{u_i^{j+1}}{u_i^j}\frac{T^{3/2}}{n_e}\exp(-E_i^j/kT)$$

X_i^j – fraction of ion j of element i

$u_i^j = \sum_k g_k W_k \exp(-E_k/kT)$ – partition function, where g_k – statistical weights,

W_k – survival probability of level k, E_k – excitation energy of level k

$a = \frac{2(2\pi k m_e)^{3/2}}{h^3}$ = 4.828 · 10^{15} $K^{-3/2}$ cm^{-3}

E_i^j – ionization energy of ion j, T – temperature, n_e – electron density

Diffusion coefficient of ion j

$$D_j = \frac{3k^2}{8e^4 Z_j^2}\sqrt{\frac{2k}{\pi m_p}}\sqrt{\frac{A+1}{A}}\frac{T^{5/2}}{n_e}\frac{1}{\ln\Lambda}$$

$$\Lambda = \frac{3k}{2e^3 Z_j}\sqrt{\frac{k}{\pi}}\frac{T^{3/2}}{\sqrt{n_e}}$$

Optical depth

The optical depth expresses the quantity of light removed from a beam by scattering or absorption during its path through a medium.

Definition of optical depth τ_ν

$$I_\nu / I_\nu^0 = e^{-\tau_\nu}$$

where I_ν^0 is the intensity of radiation at the source and I_ν is the observed intensity after a given path.

Rosseland mean optical depth

$$\tau = \int_{r_0}^{\infty} \kappa \, \rho \, dr$$

where Rosseland mean opacity

$$\frac{1}{\kappa} = \frac{\int_0^\infty \frac{1}{\kappa_\nu} \frac{dB_\nu}{dT} d\nu}{\int_0^\infty \frac{dB_\nu}{dT} d\nu}$$

Classification of CP stars (Preston 1974)

- **CP1**: Am stars (7 000 – 10 000 K, F5 – A4) – non-variable non-magnetic stars with Ca and/or Sc deficiency and enhanced heavy metals (1–2 dex). Most of them are binaries.
- **CP2**: Ap stars (8 000 – 15 000 K, F0 – B5) – variable magnetic stars with abundance spots. Si, Cr, Sr, Eu et al. enhanced by 3–6 dex.
- **CP3**: HgMn stars (10 000 – 15 000 K, A2 – B8) – non-variable non-magnetic stars with large overabundance of Hg (up to 6 dex) and Mn (up to 3 dex). Enhancement of heavy metals and deficiency of He, Al, Zn, Ni, Co. Isotopic anomalies. Very slow rotation.
- **CP4**: He stars
  - He-weak stars (14 000–21 000 K), He deficiency ∼1–2 dex;
    - He-weak stars with isotopic anomaly (overabundance of ^{3}He);
  - He-rich stars (21 000 – 30 000 K), $N_{\rm He}/N_{\rm H} \sim 0.5$ (norm ~ 0.1).

Isotopic anomalies in CP stars

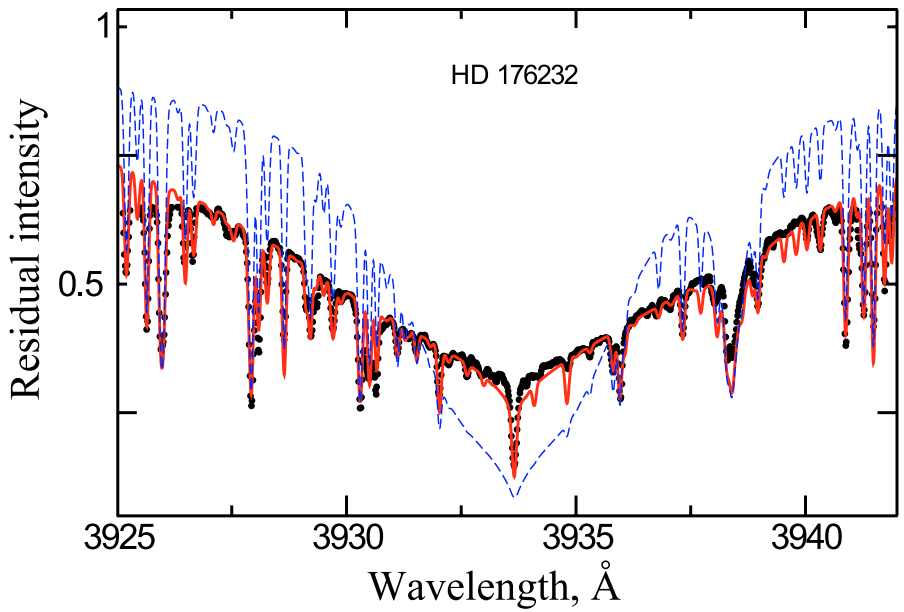
- **He**: 1961 Sargent & Jugaku (3 Cen A) – 1979 Hartoog & Cowley (8 stars) – 2005 Bohlender ...
- **Hg**: 1962 W.P. Bidelman – 1995–99 HST (HR 7775, χ Lupi) – 2003 Dolk et al. (31 HgMn stars) ...
- **Li**: 1964 Herbig – 2004–2007 Polosukhina & Shavrina ...
- **Pt**: 1973 Dworetsky & Vaughan – 1995–99 HST (HR 7775, χ Lupi) – 1999 Hubrig et al. (ESO VLT, 5 HgMn stars) ...
- **Tl**: 1996 Leckrone et al. (χ Lupi, HST)
- **Os**: 1998 Wahlgren et al. (χ Lupi, HST)
- **Ca**: 2004 Castelli & Hubrig (ESO VLT) – 2007 Cowley et al. (22 HgMn, 27 Ap, 18 other CP stars)...

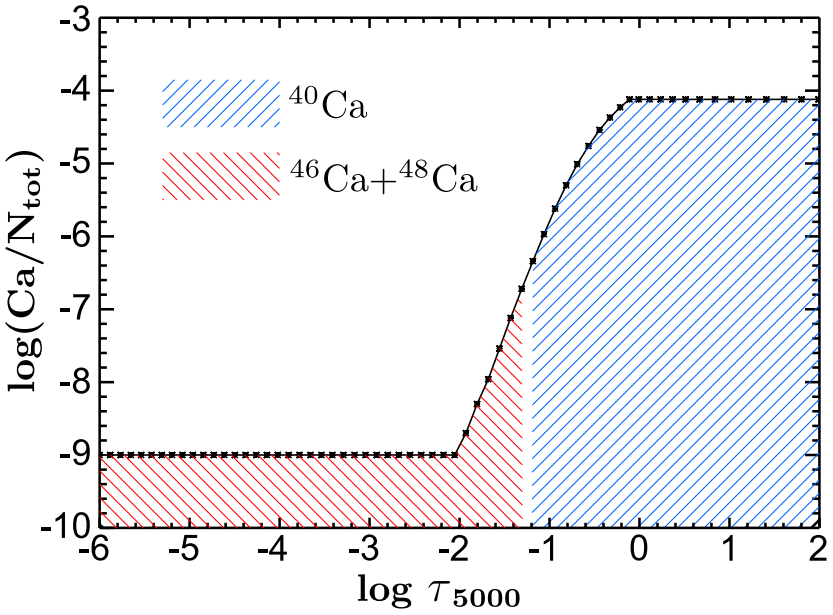
Although the overall picture of isotope variations is complex, there is a general trend:

- Heavy elements: heavier isotopes are overabundant
- Light elements: lighter isotopes are overabundant

Stratification and isotopic anomaly of calcium

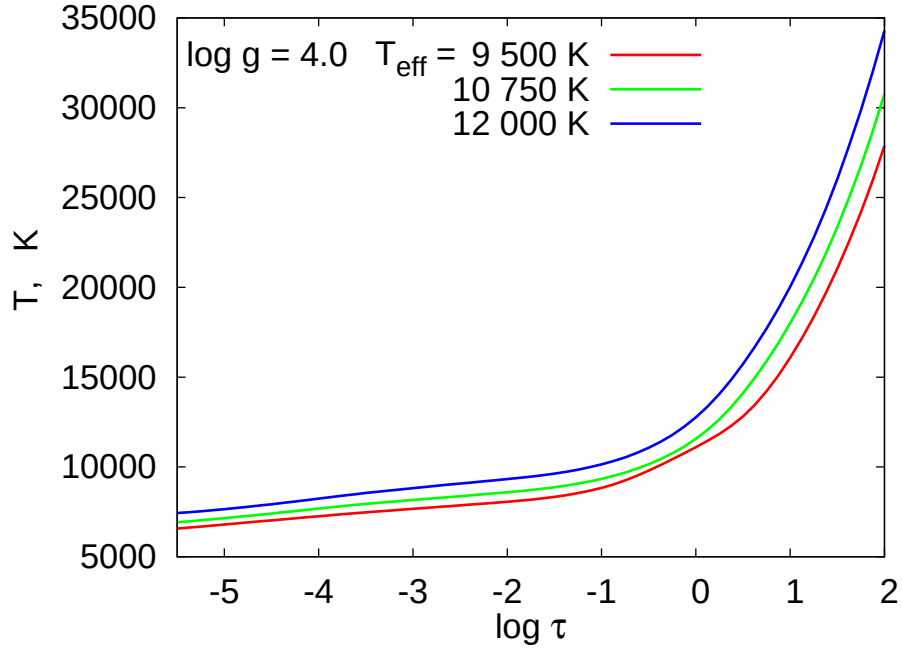
Deviation of observed in CP stars line profiles from those expected in homogeneous atmosphere provide strong observational evidence for an existence of abundance stratification.

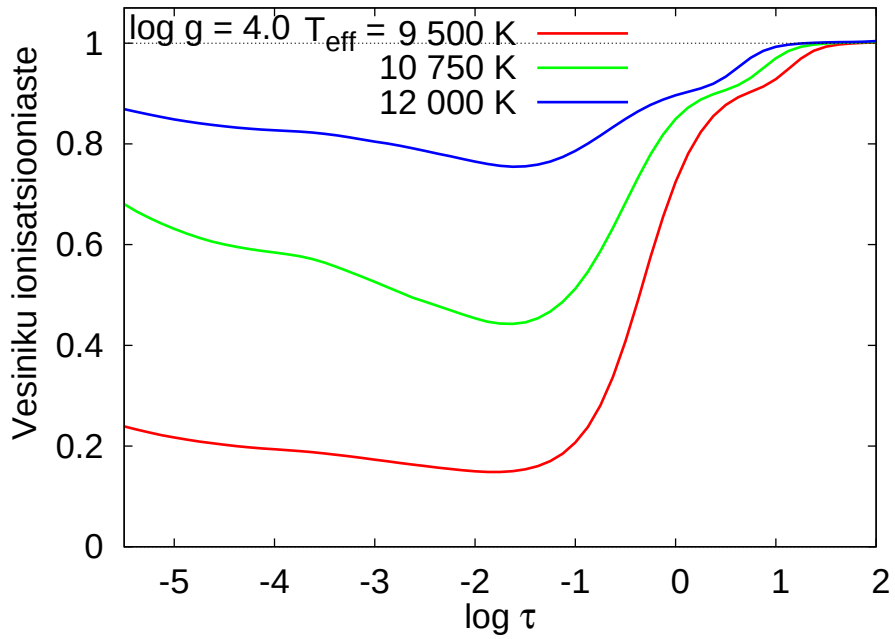


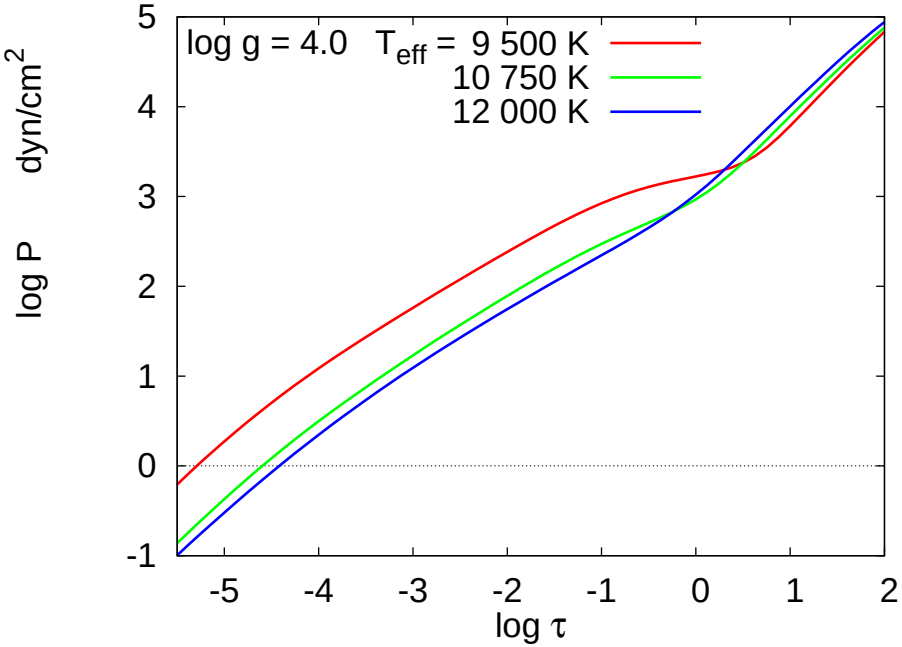


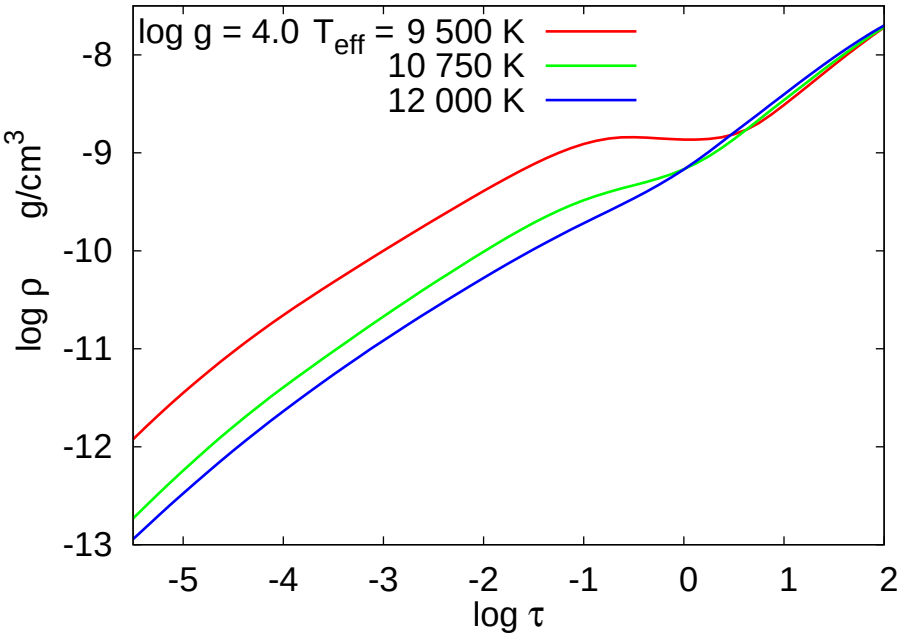
Comparison between the observed profiles (black) of the Ca II λ3933 Å line and calculations with the stratified (red) and homogeneous (blue) Ca distributions for Ap star HD 176232. Vertical stratification and isotopic separation of Ca derived for HD 176232 are shown on the right panel (Ryabchikova et al 2008, A&A 480, 811).

Physical conditions in atmospheres of CP stars

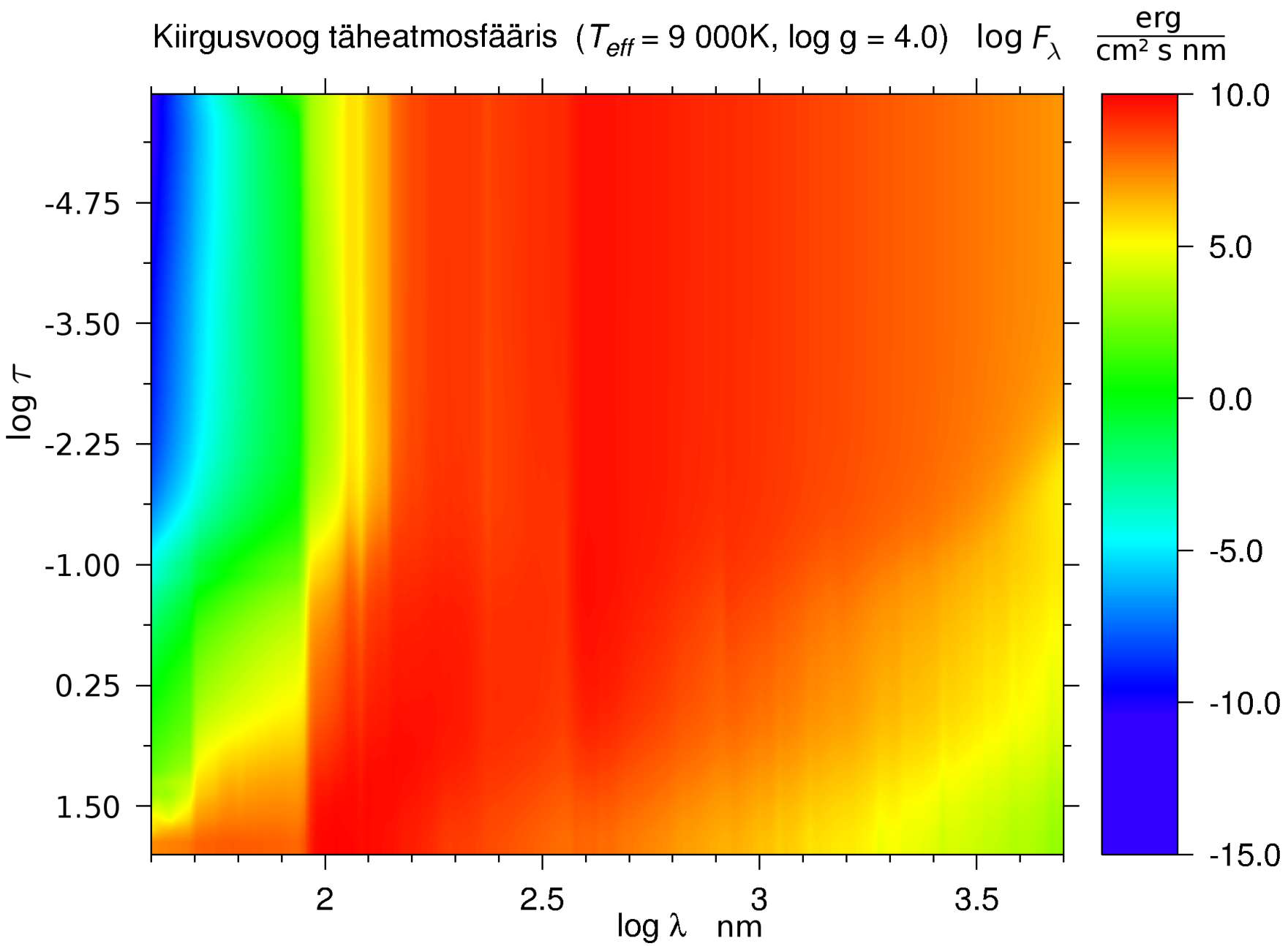








Radiative flux in stellar atmosphere



Diffusion in stellar plasma

Description of stellar plasma in this thesis is based on the following assumptions:

- Plasma can be considered as dilute gas for which the ideal gas equation of state applies ($P = NkT$)
- Maxwellian velocity distributions
- Same temperature for all ions and electrons
- Local thermodynamical equilibrium (LTE)
- Diffusion velocities are much smaller than thermal velocities
- Collisions are dominated by classical interactions between particles
- Collisions between ions of trace elements can be neglected and diffusion of every trace element can be considered separately
- Magnetic fields are lacking

Two commonly used formalisms

Descriptions of stellar plasma are all based on the Boltzmann equation

Boltzmann equation for species i

$$\frac{df_i}{dt} \equiv \frac{\partial f_i}{\partial t} + \mathbf{v_i} \cdot \frac{\partial f_i}{\partial \mathbf{r}} + \dot{\mathbf{v}}_\mathbf{i} \cdot \frac{\partial f_i}{\partial \mathbf{v_i}} = Coll(f_i)$$

where $f_i = f_i(\mathbf{r}, \mathbf{v}, t)$ distribution function of species i;
$Coll(f_i)$ collision term

Chapman-Enskog theory
Chapman, S. and Cowling, T. G.: The mathematical theory of non-uniform gases. Cambridge: University Press, 1970

Burgers' theory
Burgers, J. M.: Flow Equations for Composite Gases. New York: Academic Press, 1969

Comparison: Thoul, A., Montalbán, J., 2007, EAS Publ. Series 26, 25

Diffusion velocity

Diffusion velocity for mixture of two gases in presence of external forces (Chapman & Cowling, Ch. 14)

General equation of diffusion velocity

$$v_1 - v_2 = -\frac{N^2}{N_1 N_2} D_{12} \left\{ \underbrace{\nabla \ln \frac{N_1}{N}}_{\text{Concentration}} + \underbrace{\frac{N_1 N_2 (m_2 - m_1)}{N\rho} \nabla \ln P}_{\text{Pressure}} - \underbrace{\frac{\rho_1 \rho_2}{P\rho} (F_1 - F_2)}_{\text{Forces}} + \underbrace{\frac{D_T}{D_{12}} \nabla \ln T}_{\text{Temperature}} \right\}$$

where v_1, v_2 mean velocities of particles 1 and 2
N_1, N_2 number densities of particles 1 and 2, $N = N_1 + N_2$
m_1, m_2 masses of particles 1 and 2;
ρ_1, ρ_2 mass densities of particles 1 and 2, $\rho_i = m_i N_1$, $\rho = \rho_1 + \rho_2$;
D_{12} diffusion coefficient;
D_T thermal diffusion coefficient;
P gas pressure $P = P_1 + P_2$;
T temperature;
F_1, F_2 external forces on particles 1 and 2 per unit mass≡accelerations

Equation of diffusion velocity in stellar atmosphere

Following simplifications can be made:

- In case of hydrostatic equilibrium $\nabla P = \rho_1 F_1 + \rho_2 F_2$
- For trace element: $N_1 \ll N_2$
- In stellar atmospheres $\nabla \ln T \ll \nabla \ln P$ and thermal diffusion can be neglected.

Equation of diffusion velocity

$$v_1 = -D_{12}\left(\nabla \ln N_1 - \frac{m_1}{kT} F_1\right)$$

Radiative acceleration versus LID

Radiative acceleration of ion j in spectral line $l \rightarrow u$

$$a_j^{\mathrm{rad}} = \frac{\pi}{m_j c} \int_0^{\infty} X_{j,l}\, \sigma_{ul}^0 V(u_\nu, a) \mathcal{F}_\nu d\nu$$

Light-induced drift of ion j in spectral line $l \rightarrow u$

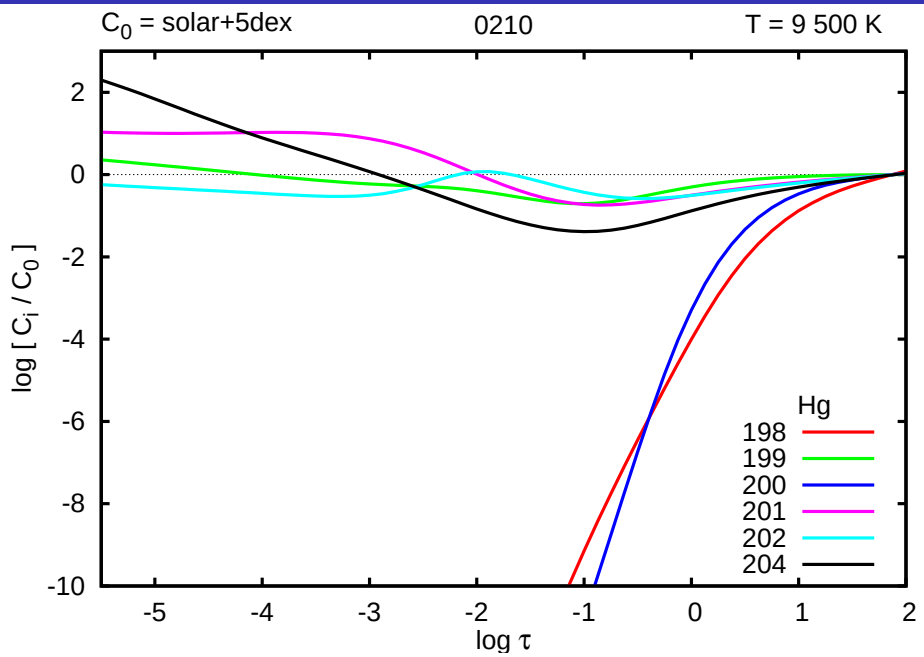
$$a_j^{\mathrm{LID}} = \varepsilon q \frac{\pi}{m_j c} \int\limits_0^{\infty} X_{j,l}\, \sigma_{ul}^0 \frac{\partial V(u_\nu, a)}{\partial u_\nu} \mathcal{F}_\nu\, d\nu$$

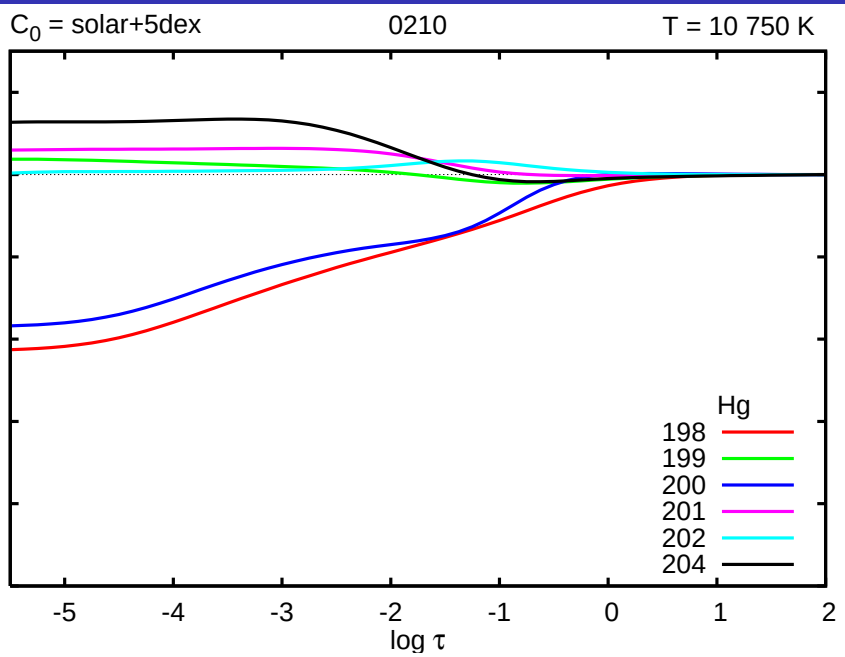
where $X_{j,l} = N_{j,l}/N_j$ is state l population fraction and σ_{ul}^0 is effective cross-section of photon absorption in transition $l \rightarrow u$. $\sigma_{ul}^0 = \frac{\pi\, e^2 f_{ul}}{m_e c \Delta\nu_D}$, where f_{ul} is oscillator strength and $\Delta\nu_D$ is Doppler line width.
Normalized Voigt function is defined by

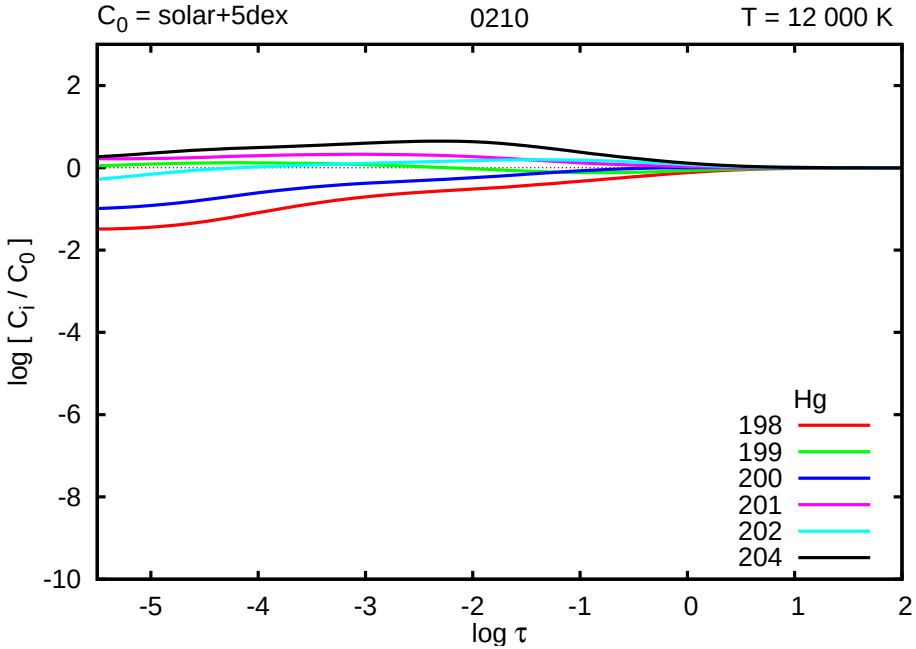
$$V(u_\nu, a) = \frac{a}{\pi^{3/2}} \int\limits_{-\infty}^{\infty} \frac{e^{-y^2}}{(u_\nu - y)^2 + a^2} dy\ ,$$

and its arguments are defined by $u_\nu = \Delta\nu/\Delta\nu_D$ and $a = \gamma/(4\pi\Delta\nu_D)$

Dependence on effective temperature





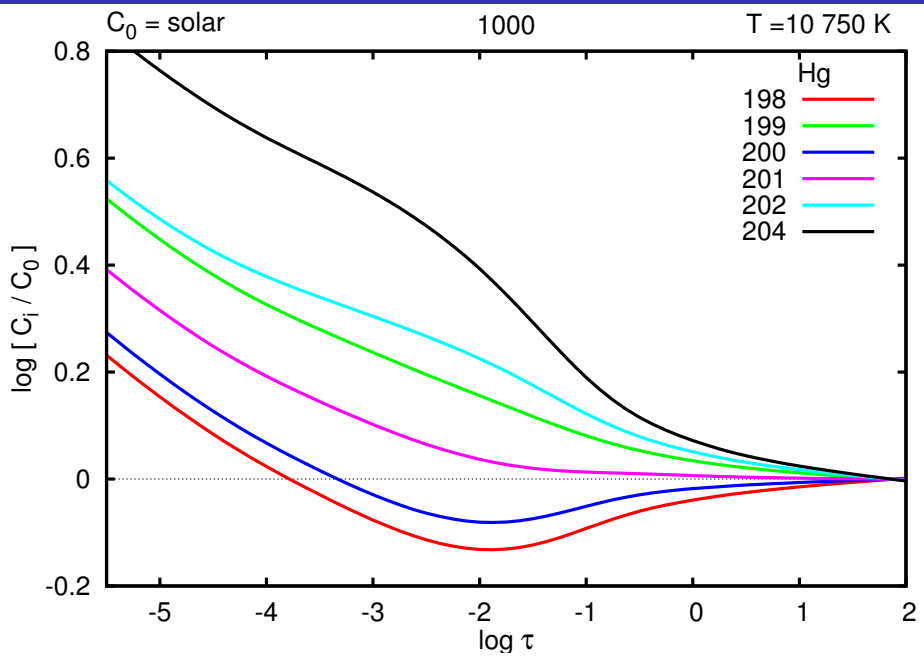


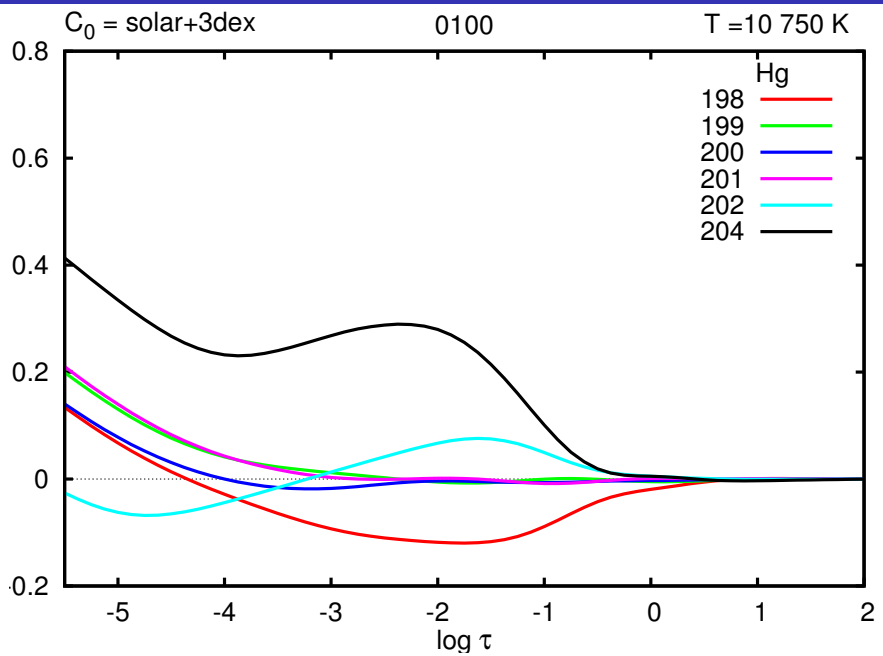
time = 210 years ($\Delta t = 1$ yr)

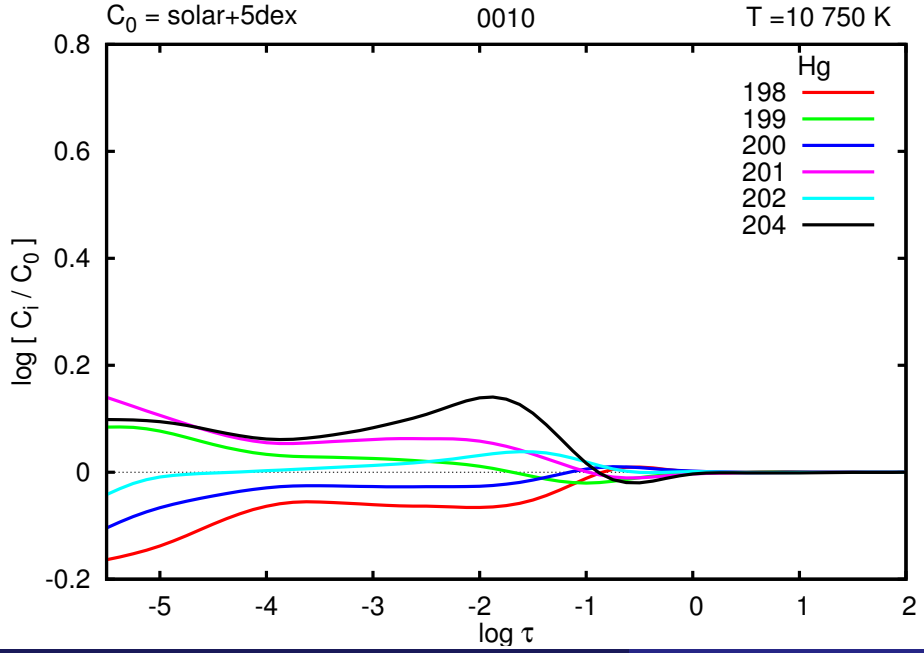
- $T_{\rm eff} = 9\ 500$ K – fastest
- $T_{\rm eff} = 10\ 750$ K
- $T_{\rm eff} = 12\ 000$ K – slowest

At higher temperatures free-flight time of plasma particles is smaller, leading thus to the smaller diffusion velocities.

Dependence on initial mercury abundance







Concentrations at time = 10 years

Model atmospheres:
$T_{\rm eff} = 10\,750\ K$, $\log g = 4$, $V \sin i = 0$

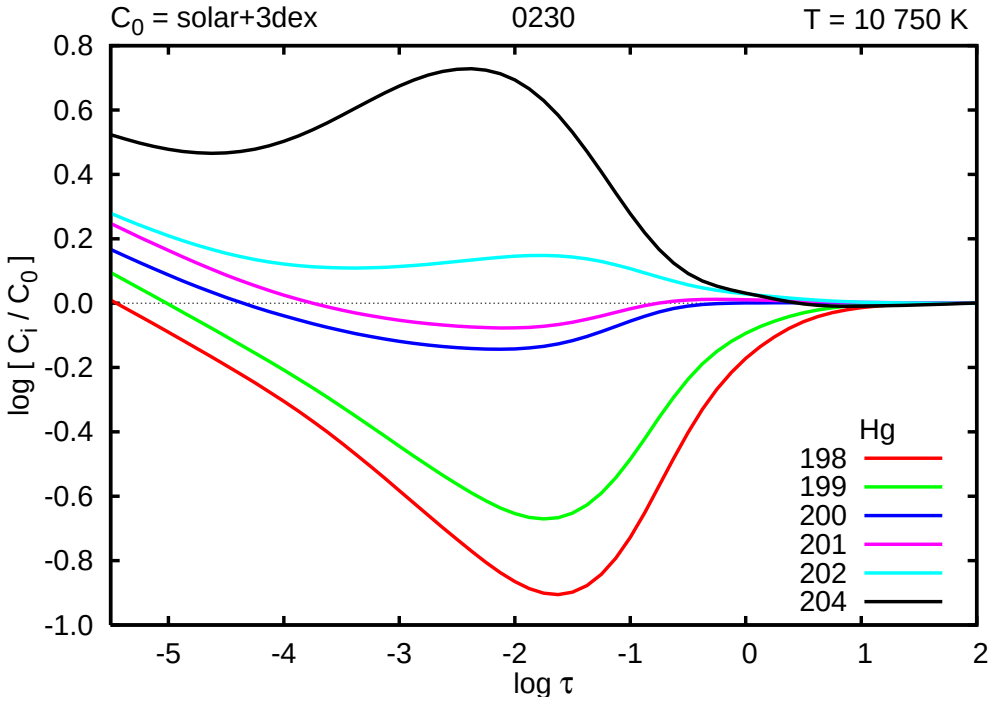
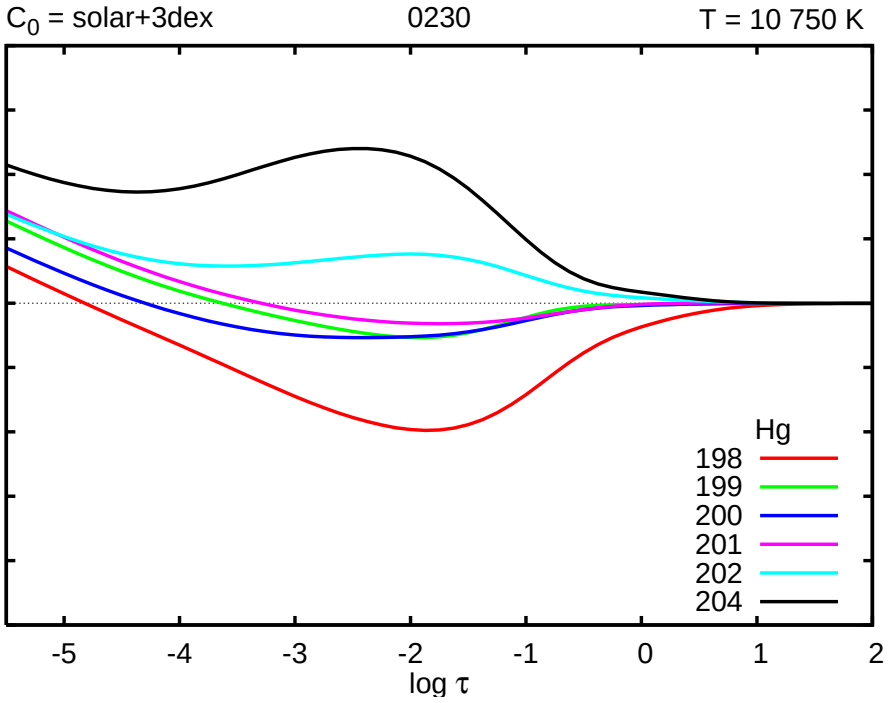
- C_0 = solar
- C_0 = solar + 3 dex
- C_0 = solar + 5 dex

Role of hyperfine splitting of Hg spectral lines

Concentration at time step 230

$T_{\rm eff} = 10\ 750$ K, $\log g = 4$, C_0 = solar + 3 dex

Without hyperfine splitting



With hyperfine splitting